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Lecture 5

Last lecture

- we couple the tight-binding model to a spatially uniform electric field $E(t)$
- velocity gauge: $E(\omega) = i\omega A(\omega)$

  with vector potential $A(\omega)$
- the external field leads to a phase under hopping: Peierls phase factor
- In momentum basis,

$$H[A(t)] = \sum_k \sum_{\alpha,\alpha'} \underbrace{H_{\alpha\alpha'}(k + eA(t))}_{\text{Bloch Hamiltonian}} \hat{c}^+_{k\alpha} \hat{c}_{k\alpha'}$$

- Derivative of Hamiltonian

$$\hat{P}_n \partial_\alpha \hat{H} \hat{P}_m = \delta_{nm} v^\alpha_n \hat{P}_n + i \varepsilon_{nm} \hat{e}^{nm}_\alpha$$

with quasiparticle velocity

$$v^\alpha_n = \partial_\alpha E_n$$

and interband transition rates

$$\hat{e}^{nm}_{\alpha} = i \, \hat{P}_n \, \partial_\alpha \hat{P}_m \, \hat{P}_m$$

- two-state quantum geometric tensor

$$Q^{mn}_{\alpha\beta} = \delta_{nm} Q^{n}_{\alpha\beta} - \mathrm{tr}\left[\hat{e}^{nm}_{\alpha} \hat{e}^{mn}_{\beta}\right]$$
$$= g^{mn}_{\alpha\beta} - {}^{i}\!/_{2}\, \Omega^{mn}_{\alpha\beta}$$

- tracing out of remote bands leads to

$$\sum_{m \neq n} Q^{mn}_{\alpha\beta} = - Q^{n}_{\alpha\beta}$$

C. Linear conductivity tensor

- A sketch how to carefully derive the conductivity formula:

 1) Change from time to imaginary time to Matsubara frequencies $i q_0$
 (allows perturbation theory at finite temperature)
 Step back via analytic continuation

of the functions, i.e.,

$$iq_0 \to \omega + i\eta$$

with $\eta > 0$ small (or 0^+).

2) Electrical current is calculated via

$$j^{\alpha}_{iq_0}[A] = -\frac{1}{V}\frac{\delta\,\Omega(A)}{\delta A^{\alpha}_{-iq_0}}$$

spatial component

bosonic Matsubara frequency

system volume

functional derivative

using the grand canonical potential $\Omega(A)$ as a function of the vector potential A. It is obtained by

Feynman path integral

$$Z[A] = \int D[\bar{\psi}\psi]\, e^{-S[\bar{\psi},\psi,A]}$$

euclidean action

$$\equiv e^{-\beta\Omega(A)}$$

and $\beta = 1/k_BT$ with T temperature.

3) We focus on the leading order in A (or E) defining the linear conductivity tensor

$$J^{\alpha}(\omega) = \sum_{\beta} \sigma^{\alpha\beta}(\omega)\, E^{\beta}(\omega) \,,$$

which is given by

$$\sigma^{\alpha\beta}(\omega) = -\frac{1}{i(\omega+i\eta)} \frac{e^2}{\hbar} \frac{k_B T}{V} \sum_{ik_0, k}$$

fermionic Matsubara frequencies

$$\times \operatorname{tr}\Big[\hat{G}(ik_0 + iq_0, k)\, \partial_\beta \hat{H}(k)$$
$$\times \hat{G}(ik_0, k)\, \partial_\alpha \hat{H}(k) - (iq_0 = 0)\Big]\Big|_{iq_0 \to \omega + i\eta}$$

Matsubara Green's functions

subtract the $iq_0 = 0$ part

- We use the expansion of the Hamiltonian for the Green's function

$$\hat{G}(ik_0, k) \equiv \left[ik_0 + \mu - \hat{H}(k)\right]^{-1}$$
$$= \sum_{n} \frac{\hat{P}_n(k)}{ik_0 - E_n(k)}$$

and obtain

$$\sigma^{\alpha\beta}(\omega) = \frac{e^2}{\hbar}\frac{1}{V}\sum_k \sum_{n,m} \tilde{\omega}_{nm}(k,\omega) \times \mathrm{tr}\left[\hat{P}_n(k)\,\partial_\beta \hat{H}(k)\,\hat{P}_m(k)\,\partial_\alpha \hat{H}(k)\right]$$

- We use all our previous knowledge and obtain

$$\mathrm{tr}\left[\hat{P}_n(k)\,\partial_\beta \hat{H}(k)\,\hat{P}_m(k)\,\partial_\alpha \hat{H}(k)\right]$$

$$= \mathrm{tr}\left[\left(\delta_{nm}\, v_n^\beta \hat{P}_n + i\,\varepsilon_{nm}\, \hat{e}_\beta^{nm}\right) \times \left(\delta_{nm}\, v_n^\alpha P_n + i\,\varepsilon_{mn}\, \hat{e}_\alpha^{mn}\right)\right]$$

$$= \delta_{nm}\, v_n^\alpha v_n^\beta\, \mathrm{tr}\left[\hat{P}_n\right] - (\varepsilon_{nm})^2\, Q_{\beta\alpha}^{mn}$$

- Matsubara summation

$$\tilde{\omega}_{nm}(k,\omega) = -\frac{1}{i(\omega+i\eta)}\left[S^{(2)}(E_n(k)-iq_0, E_m(k)) - S^{(2)}(E_n(k), E_m(k))\right]\Bigg|_{iq_0 \to \omega+i\eta}$$

with

$$S^{(2)}(E_n(k) - iq_0, E_m(k))$$

$$= k_B T \sum_{ik_0} \frac{1}{ik_0 + iq_0 - E_n(k)} \, \frac{1}{ik_0 - E_m(k)}$$

$$= \begin{cases} \dfrac{f_n(k) - f_m(k)}{-iq_0 + E_n(k) - E_m(k)} & n \neq m \\[2ex] f_n'(k) \, \delta_{iq_0, 0} & n = m \end{cases},$$

where $f_n(k) \equiv f(E_n(k))$ and $f_n'(k) \equiv f'(E_n(k))$.

Ex: Prove this result via the residue theorem. The fermionic Matsubara frequencies are defined as $ik_0 = \frac{(2n+1)i\pi}{\beta}$ and the bosonic Matsubara frequencies are defined as $iq_0 = \frac{2ni\pi}{\beta}$. The Fermi function on the complex plane $f(z) = \frac{1}{e^{\beta z}+1}$ has poles at the fermionic Matsubara frequencies with residue $-1/\beta$ for $\beta = 1/k_B T$.

We obtain

$$\tilde{w}_{nm}(k,\omega) = \begin{cases} \dfrac{1}{E_n(k)-E_m(k)} \dfrac{f_n(k) - f_m(k)}{i(\omega + i\eta - E_n(k) + E_m(k))} & n \neq m \\ \dfrac{f_n'(k)}{i(\omega + i\eta)} & n = m \end{cases}$$

- We separate the summation over band indices in the formula of $\sigma^{\alpha\beta}(\omega)$ into those involving single bands ("intraband") and multiple bands ("interband"):

$$\sigma^{\alpha\beta}(\omega) = \sigma^{\alpha\beta}_{intra}(\omega) + \sigma^{\alpha\beta}_{inter}(\omega)$$

$\longrightarrow$

a) $$\sigma^{\alpha\beta}_{intra}(\omega) = \frac{e^2}{\hbar} \int_{BZ} \frac{d^d k}{(2\pi)^d} \sum_n \underbrace{\frac{f_n'(k)\, v_n^{\alpha}(k)\, v_n^{\beta}(k)}{i(\omega + i\eta)}}_{\text{"spectral"}} \underbrace{tr[\hat{P}_n(k)]}_{\text{"geometric"}}$$

$$\equiv \frac{e^2}{\hbar} \int_{BZ} \frac{d^d k}{(2\pi)^d} \sum_n w_n^{intra}(k,\omega)\, tr[\hat{P}_n(k)]$$

b)

$$\sigma^{\alpha\beta}_{\text{inter}}(\omega) = -\frac{e^2}{\hbar}\int_{BZ}\frac{d^dk}{(2\pi)^d}\sum_{\substack{n,m\\n\neq m}}\frac{\left(E_n(k)-E_m(k)\right)\left(f_n(k)-f_m(k)\right)}{i\left(\omega+i\eta-E_n(k)+E_m(k)\right)}Q^{mn}_{\beta\alpha}(k)$$

$$\equiv -\frac{e^2}{\hbar}\int_{BZ}\frac{d^dk}{(2\pi)^d}\sum_{\substack{n,m\\n\neq m}} w^{\text{inter}}_{nm}(k,\omega)\,Q^{mn}_{\beta\alpha}(k)$$

- We use the symmetry of the conductivity tensor $\sigma^{\alpha\beta}(\omega)$ in indices α and β to identify a second structure within the equations, with a straightforward physical interpretation, since

$$j^{\alpha}(\omega) = \sum_{\beta}\sigma^{\alpha\beta}(\omega)E^{\beta}(\omega).$$

We define

$$\sigma^{(\alpha\beta)}(\omega) \equiv 1/2\left(\sigma^{\alpha\beta}(\omega)+\sigma^{\beta\alpha}(\omega)\right),$$

$$\sigma^{[\alpha\beta]}(\omega) \equiv 1/2\left(\sigma^{\alpha\beta}(\omega)-\sigma^{\beta\alpha}(\omega)\right),$$

which is a unique decomposition of $\sigma^{\alpha\beta}(\omega)$.

$\longrightarrow$

a) From the formula, we see that

$$\sigma^{\alpha\beta}_{\text{intra}}(\omega) = \sigma^{\beta\alpha}_{\text{intra}}(\omega)$$

b) The interband term is not yet symmetric or antisymmetric. For this, we calculate

$$\sum_{\substack{n,m \\ n\neq m}} w_{nm}^{inter} Q_{\beta\alpha}^{mn}$$

$$= \sum_{\substack{n,m \\ n\neq m}} \left(w_{nm}^{inter} g_{\beta\alpha}^{mn} - \tfrac{i}{2} w_{nm}^{inter} \Omega_{\beta\alpha}^{mn} \right)$$

$$= \sum_{\substack{n,m \\ n\neq m}} \left(w_{(nm)}^{inter} g_{\alpha\beta}^{mn} + \tfrac{i}{2} w_{[nm]}^{inter} \Omega_{\alpha\beta}^{mn} \right)$$

$$= \left(\sum_{\substack{n,m \\ n<m}} + \sum_{\substack{n,m \\ m<n}} \right) \left(w_{(nm)}^{inter} g_{\alpha\beta}^{mn} + \tfrac{i}{2} w_{[nm]}^{inter} \Omega_{\alpha\beta}^{mn} \right)$$

$$= 2 \sum_{\substack{n,m \\ n<m}} \left(w_{(nm)}^{inter} g_{\alpha\beta}^{mn} + \tfrac{i}{2} w_{[nm]}^{inter} \Omega_{\alpha\beta}^{mn} \right)$$

Thus, we obtain <u>two</u> interband contributions

$$\sigma_{inter}^{(\alpha\beta)}(\omega) = -\frac{2e^2}{\hbar} \int_{BZ} \frac{d^d k}{(2\pi)^d} \sum_{\substack{n,m \\ n<m}} w_{(nm)}^{inter}(k,\omega)\, g_{\alpha\beta}^{mn}(k)$$

and

$$\sigma_{inter}^{[\alpha\beta]}(\omega) = -\frac{ie^2}{\hbar} \int_{BZ} \frac{d^d k}{(2\pi)^d} \sum_{\substack{n,m \\ n<m}} w_{[nm]}^{inter}(k,\omega)\, \Omega_{\alpha\beta}^{mn}(k)$$

involving the two-state quantum metric $g_{\alpha\beta}^{mn}$ and Berry curvature $\Omega_{\alpha\beta}^{mn}$ with

$$w^{\text{inter}}_{(nm)}(k,\omega) = \frac{\varepsilon_{nm} f_{nm}}{2i}\left[\frac{1}{\omega + i\eta - \varepsilon_{nm}} + \frac{1}{\omega + i\eta + \varepsilon_{nm}}\right]$$

$$w^{\text{inter}}_{[nm]}(k,\omega) = \frac{\varepsilon_{nm} f_{nm}}{2i}\left[\frac{1}{\omega + i\eta - \varepsilon_{nm}} - \frac{1}{\omega + i\eta + \varepsilon_{nm}}\right].$$

with short notation $\varepsilon_{nm} \equiv E_n - E_m$ and

$f_{nm} \equiv f_n - f_m$.

D. Ordinary conductivity

Let us assume nondegenerate bands, $\mathrm{tr}[\hat{P}_n] = 1$.

Then, the intraband conductivity reads

$$\sigma^{\alpha\beta}_{\text{intra}}(\omega) = \frac{e^2}{\hbar}\int_{BZ}\frac{d^dk}{(2\pi)^d}\sum_n \frac{f_n'(k)\, v_n^\alpha(k)\, v_n^\beta(k)}{i(\omega + i\eta)}$$

determined by the respective quasiparticle velocities v_n.

Using

$$\lim_{\eta \to 0^+} \frac{1}{x + i\eta} = \text{p.v.}\,\frac{1}{x} - i\pi\,\delta(x)$$

we identify the Drude weight $D_{\alpha\beta}$

$$\mathrm{Re}\,\sigma^{\alpha\beta}_{\text{intra}}(\omega) = D_{\alpha\beta}\,\delta(\omega)$$

in the clean limit $\eta \to 0^+$.

For finite $\eta \equiv \hbar/\tau$ in the dc limit ($\omega = 0$), we have

$$\sigma^{\alpha\beta}_{\text{intra}}(0) = \tau e^2 \int_{BZ} \frac{d^d k}{(2\pi)^d} \sum_n \frac{f_n(k)}{m_n^{\alpha\beta}(k)} \qquad (1)$$

with effective mass $m_n^{\alpha\beta}(k) \equiv \dfrac{\hbar^2}{\partial_\alpha \partial_\beta E_n(k)}$. This result reduces to the Drude formula $\dfrac{\tau e^2 n}{m}$ for parabolic bands $E_n \approx \dfrac{k^2}{2m}$.

Ex: Show (1) by first showing that

$$f_n'(k)\, v_n^\alpha(k) = \partial_\alpha f_n(k).$$

E. Intrinsic anomalous Hall effect

We have a closer look at the interband contributions in the dc ($\omega = 0$) and clean ($\eta \to 0^+$) limit. The antisymmetric part involves

$$w^{\text{inter}}_{[nm]}(k,0) = \frac{\varepsilon_{nm}(k) f_{nm}(k)}{2i}\left[-\frac{1}{\varepsilon_{nm}(k)} - \frac{1}{\varepsilon_{nm}(k)}\right] = i f_{nm}(k)$$

In this case, we can perform one band summation

$$\sum_{\substack{n,m\\n<m}} w^{inter}_{[nm]}(k,0)\,\Omega^{mn}_{\alpha\beta}(k)$$

$$= i/_2 \sum_{\substack{n,m\\n\neq m}} \left(f_n(k) - f_m(k)\right)\Omega^{mn}_{\alpha\beta}(k)$$

$$= -i \sum_{n} f_n(k)\,\Omega^{n}_{\alpha\beta}(k)$$

with (single-state) Berry curvature. We have found a Hall response without magnetic field in a clean system: intrinsic anomalous Hall effect.

$$\sigma^{xy}_{AHE} \equiv \sigma^{[xy]}_{inter}(0) = -\frac{e^2}{\hbar}\int_{BZ}\frac{d^dk}{(2\pi)^d}\sum_n f_n(k)\,\Omega^n_{xy}(k)$$

(so-called TKNN formula by Thouless et. al. PRL 49, 405 (1982))

For an insulator with occupied bands with finite Chern number (Chern insulator) in two dimensions, we have quantized transport

$$\sigma^{xy}_{AHE} = \frac{e^2}{h}\sum_{n\in occ} C_n$$

proportional to von Klitzing constant h/e^2.

F. Optical conductivity and metric sum rule

We continue by considering a finite frequency ω and note that for $\eta \to 0^+$

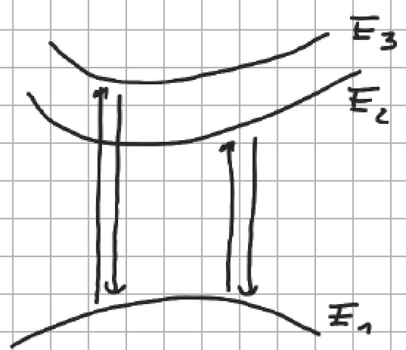
$$\mathrm{Re}\, w^{\mathrm{inter}}_{(nm)}(k,\omega) = \mathrm{Re}\left(\frac{\varepsilon_{nm} f_{nm}}{2i} \left[\frac{1}{\omega + i\eta - \varepsilon_{nm}} + \frac{1}{\omega + i\eta + \varepsilon_{nm}} \right] \right)$$

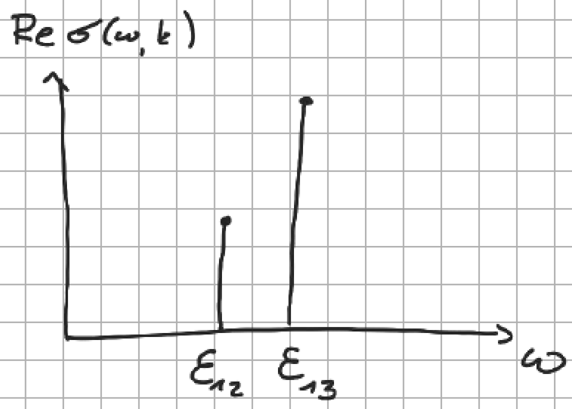
$$= -\tfrac{\pi}{2}\, \varepsilon_{nm} f_{nm} \left(\delta(\omega - \varepsilon_{nm}) + \delta(\omega + \varepsilon_{nm}) \right)$$

Assuming that $\omega > 0$, we obtain

$$\mathrm{Re}\, \sigma^{(\alpha\beta)}_{\mathrm{inter}}(\omega) = \frac{\pi e^2}{\hbar} \int_{BZ} \frac{d^d k}{(2\pi)^d} \sum_{\substack{n,m \\ n<m}} f_{nm}(k)\, g^{mn}_{\alpha\beta}(k)\, \varepsilon_{nm}(k)\, \delta(\omega - \varepsilon_{nm})$$

describing the resonant transitions between bands





Ex: (1) Show that $g^{mn}_{\alpha\beta} \equiv Q^{mn}_{(\alpha\beta)} = \tfrac{1}{2}\, \mathrm{tr}\left[\partial_\alpha \hat{P}_m \partial_\beta \hat{P}_n\right]$.

(2) Show that

$$\sum_{n \in \mathrm{occ}} \sum_{m \in \mathrm{unocc}} g^{mn}_{\alpha\beta} = -g^{\mathrm{occ}}_{\alpha\beta},$$

which is the quantum metric of the occupied states with projectors $\hat{P}_{occ} = \sum_{n \in occ} \hat{P}_n$.

For an insulator, we have $f_{nm} = 1$ for $n \in occ$ and $m \in unocc$. Thus, we have the sum rule

$$\boxed{\int_0^\infty d\omega \, \frac{\mathrm{Re}\, \sigma_{inter}^{(\alpha\beta)}(\omega)}{\omega} = \frac{\pi e^2}{\hbar} \int_{BZ} \frac{d^d k}{(2\pi)^d} \, g_{\alpha\beta}^{occ}(k)}$$

(Souza - Wilkens - Martin sum rule

PRB 62, 1666 (2000))

relating the linear optical conductivity to the Wannier function spread of the occupied bands.