Assignment - 10

Kubo formula to TKNN formula

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Kubo formula:

$$\sigma_{\alpha\beta}(\omega) = \frac{i e^2 \hbar}{a} \sum_{\substack{l,m \\ l \neq m}} \frac{f(E_l) - f(E_m)}{E_l - E_m} \frac{\langle l | v_\alpha | m \rangle \langle m | v_\beta | l \rangle}{\hbar\omega + E_l - E_m}, \quad (1)$$

where, (i) ω is the frequency of the applied electric field

(ii) a is the area of the system

(iii) $f(E_n)$ is the fermi-dirac distribution at the n^{th} level.

(iv) $\langle l | \hat{v}_\alpha | m \rangle$ is the $(l,m)^{th}$ matrix element of the α^{th} component of velocity operator

(v) $\hat{v}_\alpha$ is the projected operator ($P \hat{v} |_{\text{position}} P$), where P is the projection operator onto eigenstate space $|l\rangle$.

$$\hat{v}_\alpha = \frac{[\hat{R}_\alpha, \hat{H}]}{i\hbar} = \frac{d\hat{R}_\alpha}{dt},$$ where $\hat{H}$ is the Hamiltonian.

$$\Rightarrow \langle m|\hat{v}_\alpha|l\rangle = \frac{1}{i\hbar}\left[\langle m|\hat{R}_\alpha\hat{H}|l\rangle - \langle m|\hat{H}\hat{R}_\alpha|l\rangle\right] = \frac{E_l - E_m}{i\hbar}\langle m|\hat{R}_\alpha|l\rangle$$

Consider D.C. electric field $(\omega \to 0)$ and $0K$
$0K$ temperature.

The hall conductivity σ_{xy} becomes:

$$\sigma_{xy} = \frac{-ie\hbar^2}{a}\sum_{\substack{l,m\\ l\neq m}}\left[\Theta(\mu - E_l) - \Theta(\mu - E_m)\right]\frac{\langle l|\hat{v}_x|m\rangle\langle m|\hat{v}_y|l\rangle}{(E_l - E_m)^2}$$

where $f(E)\big|_{T=0K} = \Theta(\mu - E)$ $\quad\mu$ is the chemical potential.

$\Rightarrow \sigma_{xy}$ is non-zero only when $E_m > \mu > E_l$ or $E_l > \mu > E_m$.

$$\Rightarrow \sigma_{xy} = \frac{-ie^2\hbar}{a}\left[\sum_{E_m>\mu>E_l} \frac{\langle l|v_x|m\rangle\langle m|v_y|l\rangle}{(E_l-E_m)^2} - \sum_{E_l>\mu>E_m} \frac{\langle m|v_x|l\rangle\langle l|v_y|m\rangle}{(E_l-E_m)^2}\right]$$

changing the dummy index in the second term from $m \to l$ & $l \to m$,

$$\sigma_{xy} = \frac{-ie^2\hbar}{a}\left[\sum_{E_m>\mu>E_l} \frac{\langle l|v_x|m\rangle\langle m|v_y|l\rangle}{(E_l-E_m)^2} - \sum_{E_m>\mu>E_l} \frac{\langle l|v_x|m\rangle\langle m|v_y|l\rangle}{(E_m-E_l)^2}\right]$$

$$= ie^2\hbar \sum_{E_m>\mu>E_l} \frac{\left[\left(\frac{E_m-E_l}{i\hbar}\right)\langle l|\hat{x}|m\rangle\left(\frac{E_l-E_m}{i\hbar}\right)\langle m|\hat{y}|l\rangle - \left(\frac{E_m-E_l}{i\hbar}\right)\langle l|\hat{y}|m\rangle\left(\frac{E_l-E_m}{i\hbar}\right)\langle m|\hat{x}|l\rangle\right]}{(E_l-E_m)^2}$$

$$\sigma_{xy} = \frac{-i e^2}{\hbar a} \sum_{\mu > E_l} \sum_{E_m > \mu} \left[\langle l | \hat{X} | m \rangle \langle m | \hat{Y} | l \rangle - \langle l | \hat{Y} | m \rangle \langle m | \hat{X} | l \rangle \right]$$

$$= \frac{-i e^2}{\hbar a} \sum_{\mu > E_l} \left[\langle l | \hat{X} \underbrace{\Big(\sum_{E_m > \mu} | m \rangle \langle m | \Big)}_{1 - \sum_{E_m < \mu} |m\rangle\langle m|} \hat{Y} | l \rangle - \langle l | \hat{Y} \underbrace{\Big(\sum_{E_m > \mu} | m \rangle \langle m | \Big)}_{1 - \sum_{E_m < \mu} |m\rangle\langle m|} \hat{X} | l \rangle \right]$$

$$\sigma_{xy} = \frac{-i e^2}{\hbar a} \sum_{\mu > E_l} \left[\langle l | \hat{X}\hat{Y} - \hat{Y}\hat{X} | l \rangle + \Big(\sum_{E_m < \mu} \cancel{\langle l | \hat{Y} | m \rangle \langle m | \hat{X} | l \rangle} - \cancel{\langle l | \hat{X} | m \rangle \langle m | \hat{Y} | l \rangle} \Big) \right]$$

$$\Rightarrow \sigma_{xy} = \frac{-i e^2}{\hbar a} \sum_{\mu > E_l} \langle l | \underbrace{\hat{X}\hat{Y} - \hat{Y}\hat{X}} | l \rangle = \frac{-i e^2}{\hbar a} \sum_l \langle l | [\hat{X}, Y] | l \rangle$$

Projected operators onto $|l\rangle \rightarrow$ energy eigenstates subspace (not whole space) so don't commute.

~ Also implies Berry phase over all energy states (whole space) $= 0$ since $[\hat{X}, \hat{Y}] = 0$ in whole space.

we now find the momentum representation of $\hat{x}$ by finding $\hat{x}$ in momentum space.

$$[\hat{x}, \hat{p}_x] = i\hbar$$

Suppose $\hat{x} \to i\hbar\, \partial_{p_x}$

$$[\hat{x}, \hat{p}_x]\tilde{\psi}(p_x) \to (i\hbar\, \partial_{p_x}\, p_x - p_x \cdot i\hbar\, \partial_{p_x})\, \tilde{\psi}(p_x)$$

$$= i\hbar\left(\tilde{\psi}(p_x) + \cancel{p_x \frac{\partial \tilde{\psi}}{\partial p_x}} - \cancel{p_x \frac{\partial}{\partial p_x}\tilde{\psi}(p_x)}\right)$$

$$= i\hbar\, \tilde{\psi}(p_x)$$

which satisfies the commutation relation.

We can choose $|e\rangle$ to be the Bloch states, indexed by canonical momentum k_x & k_y

$$\hat{k}_x = \frac{\hat{p}_x}{\hbar}, \quad \hat{k}_y = \frac{\hat{p}_y}{\hbar} \Rightarrow \hat{x} \xrightarrow[\text{momentum}]{\text{canonical}} i\,\partial_{k_x}$$

The expectation value is the sum over all Bloch states with energy indexed by l (or l^{th} band index).

$$\Rightarrow \langle l | \hat{x}\,\hat{y} | l \rangle = \frac{a}{(2\pi)^2} \int_{BZ} \psi^*_{\vec{k},l} \left[i\partial_{k_x} \cdot i\partial_{k_y} \left(\psi_{\vec{k},l} \right) \right] dk_x\, dk_y$$

$$= -a \int_{BZ} \frac{dk_x\, dk_y}{(2\pi)^2} \langle \underbrace{\psi_{\vec{k},l} | \partial_{k_x} \partial_{k_y} | \psi_{\vec{k},l}}_{\partial_{k_x} \langle \psi_{\vec{k},l} | \partial_{k_y} | \psi_{\vec{k},l} \rangle - \langle \partial_{k_x} \psi_{\vec{k},l} | \partial_{k_y} \psi_{\vec{k},l} \rangle} \rangle$$

$$\mathrm{I} \qquad\qquad \mathrm{II}$$

The integral over I is 0 as integral over k_x is trivial & due to periodicity of BZ, the values of the integrand at the upper & lower indices are the same.

$$\Rightarrow \langle l | \hat{x}\,\hat{y} \rangle = \alpha \int \frac{dk_x\, dk_y}{(2\pi)^2} \langle \partial_{k_x} \psi_{\vec{k},l} | \partial_{k_y} \psi_{\vec{k},l} \rangle$$

Substituting into $\sigma_{x,y}$,

$$\sigma_{xy} = \frac{-ie^2}{\frac{h}{\cancel{2\pi}}\,\cancel{\alpha}} \left[\alpha \int_{BZ} \frac{dk_x dk_y}{(2\pi)^{\cancel{2}}} \sum_{E_l<\mu} \left(\langle \partial_{k_x} \psi_{\vec{k},l} | \partial_{k_y} \psi_{\vec{k},l} \rangle - \langle \partial_{k_y} \psi_{\vec{k},l} | \partial_{k_x} \psi_{\vec{k},l} \rangle \right) \right]$$

Since $A_{k_x,l} = -i \sum_{F<\mu} \langle \psi_{\vec{k},l} | \partial_{k_x} | \psi_{\vec{k},l} \rangle$, X component Berry connection for all occupied bands,

$$\Rightarrow \left(\vec{\nabla}_{\vec{k}} \times \vec{A}_{\vec{k},l} \right)_z = -i \sum_{E_l<\mu}^{-l} \left(\langle \partial_{k_x} \psi_{\vec{k},l} | \partial_{k_y} \psi_{\vec{k},l} \rangle - \langle \partial_{k_y} \psi_{\vec{k},l} | \partial_{k_x} \psi_{\vec{k},l} \rangle \right),$$

which is the Berry curvature for all the occupied bands.

$$\Rightarrow \sigma_{xy} = \frac{e^2}{h} \int_{BZ} \frac{dk_x\, dk_y}{2\pi} \left(\vec{\nabla}_{\vec{k}} \times \vec{A}_{\vec{k},l} \right) = \frac{e^2}{h} \times C ,$$

where C is the chern no: defined by:

$$C := \int_{BZ} \frac{dk_x\, dk_y}{2\pi} \left(\vec{\nabla}_{\vec{k}} \times \vec{A}_{\vec{k},l} \right)$$