

TKKN formula

(Thouless, Kohmoto, Nightingale, den Nijs, 1982)

Starting from the Kubo formula of conductivity based on the linear response theory. We consider a Hamiltonian $H = H_0 \left(k + \frac{e}{\hbar} A \right) \sim H_0(k) + j \cdot A = H_0(k) + H_1$, where $H_0(k)$ is the unperturbed Hamiltonian and H_1 is the perturbation from external field. In the dc limit, the conductivity tensor is given by

$$\begin{aligned} \sigma_{\alpha\beta} &= i\hbar \sum_{nm} (n_F(\epsilon_n) - n_F(\epsilon_m)) \frac{(j_\alpha)_{nm}(j_\alpha)_{mn}}{(\epsilon_n - \epsilon_m)^2} \\ &= i\hbar \sum_{nm} n_F(\epsilon_n) \frac{(j_\alpha)_{nm}(j_\alpha)_{mn} - (j_\beta)_{nm}(j_\alpha)_{mn}}{(\epsilon_n - \epsilon_m)^2} \end{aligned}$$

where n_F is the Fermi distribution function, j is the current operator $j_\alpha = \frac{e}{\hbar} \frac{\partial H_0}{\partial k_\alpha}$ and $(j_\alpha)_{nm} = \langle u_n | j_\alpha | u_m \rangle$. Here ϵ_n and $|u_n\rangle$ are the eigen-energy and eigen wavefunction of unperturbed Hamiltonian H_0 .

Since $(j_\alpha)_{nm} = \langle u_n | j_\alpha | u_m \rangle = \frac{e}{\hbar} \langle u_n | \frac{\partial H_0}{\partial k_\alpha} | u_m \rangle = \frac{e}{\hbar} (\epsilon_n - \epsilon_m) \langle \frac{\partial u_n}{\partial k_\alpha} | u_m \rangle$, the formula for Hall conductivity can be simplified as

$$\sigma_{xy} = \frac{ie^2}{\hbar} \sum_n n_F(\epsilon_n) \left(\langle \frac{\partial u_n}{\partial k_x} | \frac{\partial u_n}{\partial k_y} \rangle - \langle \frac{\partial u_n}{\partial k_y} | \frac{\partial u_n}{\partial k_x} \rangle \right)$$

Here the summation over n include the integral over the momentum k . Consider only on zero temperature, the formula is rewritten as

$$\sigma_{xy} = \frac{ie^2}{\hbar} \int \frac{d^2k}{(2\pi)^2} \sum_{n \text{ occ}} \left(\langle \frac{\partial u_n}{\partial k_x} | \frac{\partial u_n}{\partial k_y} \rangle - \langle \frac{\partial u_n}{\partial k_y} | \frac{\partial u_n}{\partial k_x} \rangle \right)$$

In which the summation over n is just for all the occupied band.

In terms of the Berry curvature $\mathcal{F}_n^{ij}(\vec{k})$

$$\sigma_{xy} = \frac{e^2}{\hbar} \int \frac{d^2k}{(2\pi)^2} \sum_{n \text{ occ}} \mathcal{F}_n^{xy}(\vec{k})$$