Quantization of the Hall conductivity in a periodic system

Linear Hall response of a band insulator

Christophe De Beule (christophe.debeule@gmail.com)

---

1 Anomalous velocity and the Hall conductivity

In order to calculate the Hall conductivity for a crystalline solid, we need to consider the response of the electrons in the crystal to a constant electric field. We can account for the electric field in a translational-invariant way with a homogeneous time-dependent vector potential $\boldsymbol{A}$, so that (in Gaussian units)

$$\boldsymbol{E} = -\frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t}.$$

The Hamiltonian becomes

$$H = \frac{1}{2m}\left[\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}(t)\right]^2 + V(\boldsymbol{r}),$$

where $V(\boldsymbol{r})$ is the crystal potential. The wave function can be written as (Bloch's theorem)

$$\psi(\boldsymbol{r}, t) = e^{i\boldsymbol{q}\cdot\boldsymbol{r}} u_{\boldsymbol{q}}(\boldsymbol{r}, t),$$

where $u_{\boldsymbol{q}}(\boldsymbol{r}, t)$ is a cell-periodic time-dependent Bloch function. Its time dependence is governed by the Bloch Hamiltonian:

$$\mathcal{H}(\boldsymbol{q}, t) = e^{-i\boldsymbol{q}\cdot\boldsymbol{r}} H(t) e^{i\boldsymbol{q}\cdot\boldsymbol{r}} \equiv \mathcal{H}(\boldsymbol{k}),$$

where $\boldsymbol{k} = \boldsymbol{k}(t)$ is the gauge-invariant crystal momentum

$$\boldsymbol{k} = \boldsymbol{q} + \frac{e}{\hbar c}\boldsymbol{A}. \tag{1}$$

Explicitly, one finds

$$\mathcal{H}(\boldsymbol{k}) = \frac{(\boldsymbol{p} + \hbar\boldsymbol{k})^2}{2m} + V(\boldsymbol{r}).$$

Under a gauge transformation,

$$\begin{aligned}
&\psi(\boldsymbol{r}, t) \to e^{-\frac{ie}{\hbar c}\chi(\boldsymbol{r})}\psi(\boldsymbol{r}, t) \\
&\boldsymbol{A}(\boldsymbol{r}, t) \to \boldsymbol{A} + \nabla\chi \\
&\mathcal{H}(\boldsymbol{q}, t) \to e^{-i\boldsymbol{q}\cdot\boldsymbol{r} + \frac{ie}{\hbar c}\chi(\boldsymbol{r})} H e^{i\boldsymbol{q}\cdot\boldsymbol{r} - \frac{ie}{\hbar c}\chi(\boldsymbol{r})},
\end{aligned}$$

so that $\boldsymbol{k}$ remains invariant. The velocity operator is given by

$$\boldsymbol{v}(\boldsymbol{k}) = e^{-i\boldsymbol{q}\cdot\boldsymbol{r}}\left[H, \boldsymbol{r}\right] e^{i\boldsymbol{q}\cdot\boldsymbol{r}} = \frac{1}{\hbar}\nabla_{\boldsymbol{k}} H(\boldsymbol{k}).$$

In order to find the response of the system to an applied electric field, we consider the time dependence of the Bloch functions,

$$i\hbar\frac{d}{dt}\left|u(t)\right\rangle = \mathcal{H}(\boldsymbol{k}(t))\left|u(t)\right\rangle, \tag{2}$$

The general solution is expressed in terms of the instantaneous eigenstates

$$|u(t)\rangle = \sum_n c_n(t) e^{i\theta_n(t)}|n(t)\rangle, \qquad \theta_n(t) = -\frac{1}{\hbar}\int_{t_0}^{t} dt' \varepsilon_n(t'),$$

where

$$\mathcal{H}(t)|n(t)\rangle = \varepsilon_n(t)|n(t)\rangle, \qquad \langle n(t)|m(t)\rangle = \delta_{nm}. \tag{3}$$

Furthermore, we assume that the spectrum is nondegenerate (no band crossings). Substituting this expression into the time-dependent Schrödinger [Eq. (2)] gives a system of differential equations that determine $c_m(t)$,

$$\dot{c}_m(t) = -\sum_n c_n e^{i(\theta_n-\theta_m)}\langle m|\dot{n}\rangle. \tag{4}$$

Taking the time derivative of Eq. (3) gives

$$\dot{c}_m(t) = -c_m\langle m|\dot{m}\rangle - \sum_{n\neq m} c_n e^{i(\theta_n-\theta_m)}\frac{\langle m|\dot{\mathcal{H}}|n\rangle}{\varepsilon_n-\varepsilon_m}.$$

Up to this point, all results are exact. In the *adiabatic approximation*, we assume that

$$\left|\frac{\langle m|\dot{\mathcal{H}}|n\rangle}{\varepsilon_n-\varepsilon_m}\right| \ll 1,$$

which means that H changes slowly compared to the level spacing. We obtain

$$\dot{c}_m(t) = -c_m\langle m|\dot{m}\rangle.$$

In our case, the time dependence of the Bloch Hamiltonian is implicit,

$$\dot{\mathcal{H}} = \dot{\boldsymbol{k}}\cdot\nabla_{\boldsymbol{k}}\mathcal{H} = -e\boldsymbol{E}\cdot\boldsymbol{v},$$

and the adiabatic approximation corresponds to an electric field that is small compared to the level spacing. The solution is given by

$$c_m(t) = c_m(0)\exp\left(-\int_0^t dt'\langle m|\dot{m}\rangle\right).$$

So if the system is initially in an eigenstate $|n\rangle$ at $t=0$, we have $c_m(0)=\delta_{nm}$ and it will remain the same apart from a phase. If the adiabatic evolution is cyclic, this phase becomes gauge-invariant (Berry phase).

For a constant electric field, the adiabatic evolution is not cyclic and so we can safely neglect this phase. To obtain a better approximation, we substitute this result in Eq. (4) for $m\neq n$,

$$\dot{c}_m(t) = -e^{i(\theta_n-\theta_m)}\langle m|\dot{n}\rangle,$$

with the approximate solution,

$$c_m(t) = -i\hbar e^{i(\theta_n-\theta_m)}\frac{\langle m|\dot{n}\rangle}{\varepsilon_n-\varepsilon_m}.$$

where we neglected all terms with more than one time derivative. In lowest order the eigenstate becomes

$$|n\rangle \to |n\rangle - i\hbar\sum_{m\neq n}|m\rangle\frac{\langle m|\dot{n}\rangle}{\varepsilon_n-\varepsilon_m}.$$

The expectation value of the velocity operator in the perturbed state is given by

$$\boldsymbol{v}_n(\boldsymbol{k}) = \frac{1}{\hbar}\nabla_{\boldsymbol{k}}\varepsilon_n(\boldsymbol{k}) + 2\,\mathrm{Im}\sum_{m\neq n}\frac{\langle n(\boldsymbol{k})|\nabla_{\boldsymbol{k}}\mathcal{H}|m(\boldsymbol{k})\rangle\langle m(\boldsymbol{k})|\dot{n}(\boldsymbol{k})\rangle}{\varepsilon_n(\boldsymbol{k})-\varepsilon_m(\boldsymbol{k})}.$$

Again by taking a derivative of equation (3), the second term in the expression for $\boldsymbol{v}_n$ becomes

$$2\,\mathrm{Im}\sum_m \langle\nabla_{\boldsymbol{k}} n|m\rangle\,\langle m|\,\dot{n}\rangle = 2\,\mathrm{Im}\langle\nabla_{\boldsymbol{k}} n|\dot{n}\rangle. \tag{5}$$

Here we included n in the summation because this term is real so it does not contribute to the sum. Furthermore from (1),

$$\frac{d}{dt} = \dot{\boldsymbol{k}}\cdot\nabla_{\boldsymbol{k}} = -\frac{e}{\hbar}\boldsymbol{E}\cdot\nabla_{\boldsymbol{k}},$$

and (5) becomes (component wise)

$$v_{n,i} = \frac{1}{\hbar}\partial_{k_i}\varepsilon_n - \frac{ie}{\hbar}\left(\langle\partial_{k_i}n|\,\partial_{k_j}n\rangle - \langle\partial_{k_j}n|\,\partial_{k_i}n\rangle\right)E^j = \frac{1}{\hbar}\partial_{k_i}\varepsilon_n - \frac{e}{\hbar}F_{n,ij}E^j, \tag{6}$$

where F_{ij} are the components of the Berry curvature. This equation can be rewritten in terms of the Berry field strength which is defined as

$$\Omega^k = \frac{1}{2}\varepsilon^{knm}F_{nm}.$$

Contraction with a permutation symbol yields

$$\varepsilon_{ijk}\Omega^k = \frac{1}{2}\varepsilon_{kij}\varepsilon^{knm}F_{nm} = \frac{1}{2}\left(\delta_i^n\delta_j^m - \delta_i^m\delta_j^n\right)F_{nm} = F_{ij},$$

because $F_{ji} = -F_{ij}$. Substituting in (6) gives,

$$\boxed{\boldsymbol{v}_n = \frac{1}{\hbar}\nabla_{\boldsymbol{k}}\varepsilon_n - \frac{e}{\hbar}\left(\boldsymbol{E}\times\boldsymbol{\Omega}_n\right).}$$

This is an important result. We find that the electric field produces a transverse velocity in the adiabatic limit. If the Fermi level is in the band gap, the ground-state current density at zero temperature is given by

$$\begin{aligned} J_i &= -e\sum_n\int\frac{d^2\boldsymbol{k}}{(2\pi)^2}\,v_{n,i} \\ &= \left(\frac{e^2}{2\pi h}\sum_n\int d^2\boldsymbol{k}\,F_{n,ij}\right)E^j, \end{aligned}$$

where the summation runs over all occupied bands, and the integral is over the entire Brillouin zone, because we consider an insulator. Hence, the longitudinal part vanishes and the Hall conductivity is given by

$$\boxed{\sigma_{xy} = \frac{e^2}{h}\sum_n\mathcal{C}_n, \qquad \mathcal{C}_n = \frac{1}{2\pi}\int d^2\boldsymbol{k}\,F_{n,xy},}$$

where $\mathcal{C}_n$ is the Chern number of the n-th band.

2 Chern number for a square lattice

The Berry curvature can be written in terms of the Berry connection (this can be seen as a gauge field in momentum space),

$$\begin{aligned} A_i &= i\,\langle n|\,\partial_{k_i}\,|n\rangle \\ F_{ij} &= \partial_{k_i}A_j - \partial_{k_j}A_i. \end{aligned}$$

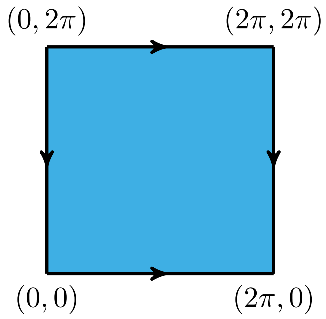

Figure 1: The Brillouin zone (BZ) of a square lattice. The BZ has the topology of a torus such that the four corners represent the same state.

For a *square lattice* with unit lattice constant, the Chern number can be written as

$$\mathcal{C}_n = \frac{1}{2\pi}\int_0^{2\pi} dk_x \int_0^{2\pi} dk_y \,\left(\partial_{k_x} A_y - \partial_{k_y} A_x\right).$$

The integral becomes

$$\int_0^{2\pi} dk_y \,\left[A_y(2\pi, k_y) - A_y(0, k_y)\right] - \int_0^{2\pi} dk_x \,\left[A_x(k_x, 2\pi) - A_x(k_x, 0)\right].$$

States at $(k_x, 0)$ and $(k_x, 2\pi)$, and states at $(0, k_y)$ and $(2\pi, k_y)$ represent the same state up to a momentum-dependent phase factor,

$$\begin{aligned} |n(k_x, 2\pi)\rangle &= e^{i\theta_x(k_x)}\,|n(k_x, 0)\rangle\,, \\ |n(2\pi, k_y)\rangle &= e^{i\theta_y(k_y)}\,|n(0, k_y)\rangle\,, \end{aligned} \tag{7}$$

which implies

$$\begin{aligned} A_x(k_x, 2\pi) &= i\,\langle n(k_x, 2\pi)|\,\partial_{k_x}\,|n(k_x, 2\pi)\rangle = -\partial_{k_x}\theta_x(k_x) + A_x(k_x, 0), \\ A_y(2\pi, k_y) &= i\,\langle n(2\pi, k_y)|\,\partial_{k_y}\,|n(2\pi, k_y)\rangle = -\partial_{k_y}\theta_y(k_y) + A_y(0, k_y). \end{aligned}$$

The Chern number becomes

$$\mathcal{C}_n = \frac{1}{2\pi}\left[\theta_y(0) - \theta_y(2\pi) + \theta_x(2\pi) - \theta_x(0)\right].$$

In the four corners of the Brillouin zone, equation (7) gives

$$\begin{aligned} e^{i\theta_x(0)}\,|n(0,0)\rangle &= |n(0, 2\pi)\rangle\,, \\ e^{i\theta_x(2\pi)}\,|n(2\pi,0)\rangle &= |n(2\pi, 2\pi)\rangle\,, \\ e^{i\theta_y(0)}\,|n(0,0)\rangle &= |n(2\pi, 0)\rangle\,, \\ e^{i\theta_y(2\pi)}\,|n(0,2\pi)\rangle &= |n(2\pi, 2\pi)\rangle\,, \end{aligned}$$

which implies that

$$|n(2\pi, 2\pi)\rangle = e^{i(\theta_x(0)+\theta_y(2\pi))}\,|n(0,0)\rangle = e^{i(\theta_y(0)+\theta_x(2\pi))}\,|n(0,0)\rangle\,.$$

This can only be true if

$$\theta_y(0) - \theta_y(2\pi) + \theta_x(2\pi) - \theta_x(0) = 2\pi\nu,$$

so that the Chern number is given by an integer $\mathcal{C}_n = \nu$. The Hall conductivity of a single fully-occupied band is quantized:

$$\sigma_{xy} = \nu e^2/h.$$