TKNN

Quantization of the Hall conductivity

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1 Kubo formula

Starting from the Kubo formula, we want to obtain equation (5) of the seminal paper [1] by Thouless, Kohmoto, Nightingale, and den Nijs (TKNN). For zero temperature and $\omega \to 0$, the Kubo formula for the linear Hall conductivity of a two-dimensional periodic system gives

$$\begin{aligned}\sigma_H &= \frac{\sigma_{xy} - \sigma_{yx}}{2} \\ &= \frac{ie^2}{2\pi h} \sum_{\varepsilon_n < 0 < \varepsilon_m} \int_{\text{BZ}} d^2\boldsymbol{k} \, \frac{\langle n | \partial_1 H_{\boldsymbol{k}} | m \rangle \langle m | \partial_2 H_{\boldsymbol{k}} | n \rangle - \langle n | \partial_2 H_{\boldsymbol{k}} | m \rangle \langle m | \partial_1 H_{\boldsymbol{k}} | n \rangle}{[\varepsilon_n(\boldsymbol{k}) - \varepsilon_m(\boldsymbol{k})]^2},\end{aligned}$$

where we write $|n\rangle = |u_{n\boldsymbol{k}}\rangle$ for short[1]. Here we consider an insulator and the energy is defined with respect to the Fermi level. Thus n runs over filled bands and m runs over empty bands, and the integral runs over the entire Brillouin zone (BZ). The cell-periodic Bloch functions $|u_{n\boldsymbol{k}}\rangle$ are eigenstates of the Bloch Hamiltonian:

$$H_{\boldsymbol{k}} = e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} H e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \qquad H = \frac{p^2}{2m} + V(\boldsymbol{r}),$$

with $V(\boldsymbol{r})$ the crystal potential. Hence,

$$\langle n | \partial H_{\boldsymbol{k}} | m \rangle = (\varepsilon_m - \varepsilon_n) \langle n | \partial m \rangle,$$

where $|\partial m\rangle = \partial |m\rangle$. The Hall conductivity then becomes

$$\sigma_H = \frac{ie^2}{2\pi h} \sum_{\varepsilon_n < 0 < \varepsilon_m} \int_{\text{BZ}} d^2\boldsymbol{k} \left(\langle \partial_1 n | m \rangle \langle m | \partial_2 n \rangle - \langle \partial_2 n | m \rangle \langle m | \partial_1 n \rangle \right), \tag{1}$$

where we used

$$\partial \langle n | m \rangle = 0 \Rightarrow \langle n | \partial m \rangle = -\langle \partial n | m \rangle, \tag{2}$$

since the $|u_{n\boldsymbol{k}}\rangle$ for different band indices and fixed $\boldsymbol{k}$ are orthogonal. Note that the summand in Eq. (1) is asymmetric in n and m:

$$\langle \partial_1 n | m \rangle \langle m | \partial_2 n \rangle - \langle \partial_2 n | m \rangle \langle m | \partial_1 n \rangle = - \left(\langle \partial_1 m | n \rangle \langle n | \partial_2 m \rangle - \langle \partial_2 m | n \rangle \langle n | \partial_1 m \rangle \right),$$

making use of Eq. (2) and swapping the overlaps in each term. Thus, we can let m run over all eigenstates, because the extra terms, with n and m both running over occupied bands, cancel pairwise. Using the completeness relation,

$$\sum_m |u_{m\boldsymbol{k}}\rangle \langle u_{m\boldsymbol{k}}| = 1,$$

we find

$$\begin{aligned}\sigma_H &= \frac{ie^2}{2\pi h} \sum_{\varepsilon_n < 0} \int_{\text{BZ}} d^2\boldsymbol{k} \left(\langle \partial_1 n | \partial_2 n \rangle - \langle \partial_2 n | \partial_1 n \rangle \right) \\ &= \frac{ie^2}{2\pi h} \sum_{\varepsilon_n < 0} \int_{\text{BZ}} d^2\boldsymbol{k} \int_{\text{unit cell}} d^2\boldsymbol{r} \left(\frac{\partial u_n^*}{\partial k_1} \frac{\partial u_n}{\partial k_2} - \frac{\partial u_n^*}{\partial k_2} \frac{\partial u_n}{\partial k_1} \right),\end{aligned}$$

[1]Here, overlaps such as $\langle n | \partial H_{\boldsymbol{k}} | m \rangle$ correspond to a real-space integral over the unit cell for a continuum theory, and a sum over sublattices and orbitals in a lattice model: $\boldsymbol{r} \leftrightarrow$ sublattice index.

which recovers the result of the paper. Note that for a lattice model, the integral over the unit cell is replaced with a summation over sublattices and orbitals. This result can be written as

$$\sigma_H = \frac{e^2}{2\pi h}\int_{\mathrm{BZ}} d^2\boldsymbol{k}\, F_{12},$$

where F_{12} is the ground-state Berry curvature,

$$F_{12} = i\sum_{\varepsilon_n<0}\left(\langle \partial_1 n|\, \partial_2 n\rangle - \langle \partial_2 n|\, \partial_1 n\rangle\right).$$

2 Quantization of the Hall conductivity

In the original TKNN paper, it was not clearly demonstrated (in my opinion) why the Hall conductivity is quantized. It was only clarified in a follow-up paper by Kohmoto [2]. To show this, we consider a single isolated band. We first write

$$\frac{\partial u^*}{\partial k_1}\frac{\partial u}{\partial k_2} - \frac{\partial u^*}{\partial k_2}\frac{\partial u}{\partial k_1} = \nabla_{\boldsymbol{k}}\times u^*\nabla_{\boldsymbol{k}}u,$$

where we define the curl of a two-dimensional vector as a pseudoscalar, so that

$$\sigma_H = \frac{e^2}{2\pi h}\sum_{\varepsilon_n<0}\int_{\mathrm{BZ}} d^2\boldsymbol{k}\,\nabla_{\boldsymbol{k}}\times\boldsymbol{A}.$$

where

$$\boldsymbol{A}(\boldsymbol{k}) = i\,\langle u|\,\nabla_{\boldsymbol{k}}\,|u\rangle\,,$$

is the Berry connection of a single band. Since the BZ has no boundary, Stokes' theorem gives $\sigma_H = 0$, naively. Hence, we are led to conclude that a nonzero value of σ_H implies that $\boldsymbol{A}(\boldsymbol{k})$ is not smooth everywhere, so that Stokes' theorem does not apply to the whole BZ. In this case, there is no global smooth gauge for the Bloch state $|u_{\boldsymbol{k}}\rangle$. Thus, for an insulator with a finite value of σ_H, there always exist singularities somewhere in the BZ where the state vector is undefined. An explicit example for a two-band system can be found in many references. For example, see Section IV B of Ref. [3] for the Haldane model.

Now consider $N-1$ patches $D_n \in T^2$ $(n = 1,\ldots,N-1)$ of the BZ torus that do not overlap and their complement $D_N = T^2 - \cup_n D_n$. For each patch D_n, there exists a gauge that is smooth in D_n. These gauges are related by a gauge transformation:

$$|u_n\rangle = e^{-i\chi_n(\boldsymbol{k})}\,|u_N\rangle\,,$$

where the subscript now refers to different patches. Here, the phase factor $\chi_n(\boldsymbol{k})$ also has to contain singularities, which move singularities of the gauge $|u_N\rangle$ outside of D_n. The Berry connection transforms as

$$\boldsymbol{A}_n = i\,\langle u_n|\,\nabla_{\boldsymbol{k}}\,|u_n\rangle = \boldsymbol{A}_N + \nabla_{\boldsymbol{k}}\chi_n,$$

so that $\nabla_{\boldsymbol{k}}\chi_n$ acts as a transition function[2]. In each patch, the Berry connection (in the smooth gauge for that patch) is well behaved by definition, so we can use Stokes' theorem:

$$\begin{aligned}\int_{T^2} d^2\boldsymbol{k}\,\nabla_{\boldsymbol{k}}\times\boldsymbol{A} &= \sum_{n=1}^{N-1}\int_{D_n} d^2\boldsymbol{k}\,\nabla_{\boldsymbol{k}}\times\boldsymbol{A}_n + \int_{D_N} d^2\boldsymbol{k}\,\nabla_{\boldsymbol{k}}\times\boldsymbol{A}_N \\ &= \sum_{n=1}^{N-1}\oint_{\partial D_n} d\boldsymbol{k}\cdot\left(\boldsymbol{A}_n - \boldsymbol{A}_N\right),\end{aligned}$$

[2]For a more mathematical perspective accessible to physicists, see the discussion of the Wu-Yang monopole in Nakahara's Geometry, Topology and Physics: Section 1.9.2 [4].

where in the first step we used that the Berry curvature is gauge invariant, and where ∂D_n is the boundary of region D_n with $\partial D_N = - \cup_n \partial D_n$ where the sign indicates that the orientation of the boundary is opposite. Hence, the Hall conductivity (of an isolated band) can be expressed in terms of the winding number of the gauge transformation around the boundary:

$$\sigma_H = \frac{e^2}{2\pi h} \sum_n \oint_{\partial D_n} d\boldsymbol{k} \cdot \nabla_{\boldsymbol{k}} \chi_n = \frac{e^2}{h} \nu,$$

where ν is an integer. The last equality follows from the fact that the cell-periodic Bloch function in a given gauge is single valued. For example, for the topological phase of the Haldane model, the BZ can be divided in two patches for which there exist smooth gauges, where one patch contains the K point and the other one contains K'.

References

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[3] Christophe De Beule, Steven Gassner, Spenser Talkington, and E. J. Mele. *Floquet-Bloch theory for nonperturbative response to a static drive*, Phys. Rev. B **109** 235421 (2024). DOI: 10.1103/PhysRevB.109.235421.

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