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

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

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

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

where we used

$$\partial \langle n | m \rangle = 0 \Rightarrow \langle n | \partial m \rangle = -\langle \partial n | m \rangle,$$

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. 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

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

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

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

[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.

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 $|u_{\boldsymbol{k}}\rangle$. Hence, for any gauge 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 Section IV B of my paper [3].

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 which there exist smooth gauges. 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 also has to contain singularities, which moves 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. In each patch, the Berry connection is well behaved by definition, so we can use Stokes' theorem:

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

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. 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.

References

[1] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs. *Quantized Hall Conductance in a Two-Dimensional Periodic Potential*, Phys. Rev. Lett. **49** 405–408 (1982). DOI: 10.1103/PhysRevLett.49.405.

[2] Mahito Kohmoto. *Topological invariant and the quantization of the Hall conductance*, Annals of Physics **160** (2) 343–354 (1985). DOI: https://doi.org/10.1016/0003-4916(85)90148-4.

[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.