Computing the Berry Phase on a Fermi Loop by a Lattice Approximation

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Consider a two-dimensional free-fermion system with translation symmetry, and write its Hamiltonian as $H(\boldsymbol{k})$ with $\boldsymbol{k} = (k_x, k_y)$. By linear-response theory, the Hall coefficient in a system with a Fermi surface is given by the integral of the Berry curvature over the negative-energy states:

$$\sigma_{\mathrm{H}} = \frac{i}{2\pi} \sum_n \int_{E_n(\boldsymbol{k})<0} F_n(\boldsymbol{k}). \tag{1}$$

Here n labels the bands. By Stokes' theorem, the fractional part can be written as the Berry phase on the Fermi loop [1]:

$$\sigma_{\mathrm{H}} = \frac{i}{2\pi} \sum_n \oint_{E_n(\boldsymbol{k})=0} A_n(\boldsymbol{k}) \mod 1. \tag{2}$$

For an efficient way to compute the fractional part, see for instance Ref. [2].

For an insulator, the method of Ref. [3] is well known for numerical computations of the quantized Hall coefficient. With a mild extension, one can also treat the case where Fermi loops are present.

Approximate the Brillouin zone by a lattice. At a momentum point $\boldsymbol{k}$, write a frame of negative-energy states as

$$U_{\boldsymbol{k}} = (u_{1\boldsymbol{k}}, \dots, u_{m_{\boldsymbol{k}}\boldsymbol{k}}) \in \mathrm{Mat}_{m_{\boldsymbol{k}} \times N}(\mathbb{C}), \quad U_{\boldsymbol{k}}^\dagger U_{\boldsymbol{k}} = 1_{m_{\boldsymbol{k}}}. \tag{3}$$

Here one should note that the number $m_{\boldsymbol{k}}$ of bands with $E_n(\boldsymbol{k}) < 0$ depends on the momentum point $\boldsymbol{k}$. For a triangle 012 in the Brillouin zone (a quadrilateral would also work), the following matrix is well defined even when the numbers of bands m_0, m_1, m_2 are different:

$$W_{012} = U_0^\dagger U_2 U_2^\dagger U_1 U_1^\dagger U_0 \in \mathrm{Mat}_{m_0 \times m_0}, \quad \mathrm{rank}(W_{012}) = \min(m_0, m_1, m_2) =: m_{012}. \tag{4}$$

Thus the eigenvalues of W_{012} take the form

$$\mathrm{Spec}(W_{012}) = (z_1, \dots, z_{m_{012}}, 0, \dots). \tag{5}$$

Define the generalized Berry flux by

$$F_{012} = \mathrm{Arg}(z_1 \cdots z_{m_{012}}). \tag{6}$$

Equivalently, if $P_{\boldsymbol{k}} = U_{\boldsymbol{k}} U_{\boldsymbol{k}}^\dagger$ denotes the orthogonal projection at $\boldsymbol{k}$, then F_{012} can also be computed as the argument of the product of the nonzero eigenvalues of $P_2 P_1 P_0$.

The Hall coefficient, including its integer part, is given by the sum of these generalized Berry fluxes:

$$\sigma_{\mathrm{H}} = \frac{i}{2\pi} \sum_{\Delta^2} F_{\Delta^2}. \tag{7}$$

It is clear that this formula agrees with Ref. [3] in the insulating case. In the metallic case, since only the Berry flux of the occupied bands contributes, it gives the Berry phase on the Fermi loop modulo 1.

References

[1] F. D. M. Haldane, *Berry Curvature on the Fermi Surface: Anomalous Hall Effect as a Topological Fermi-Liquid Property*, arXiv:cond-mat/0408417.

[2] Xinjie Wang, David Vanderbilt, Jonathan R. Yates, Ivo Souza, *Fermi-surface calculation of the anomalous Hall conductivity*, arXiv:0708.0858.

[3] T. Fukui, Y. Hatsugai, H. Suzuki, *Chern Numbers in Discretized Brillouin Zone: Efficient Method of Computing (Spin) Hall Conductances*, arXiv:cond-mat/0503172.