目　录

Research diary

Quan Sheng Wu

February 7, 2015

第一章

Some Research Notes

1.1 Calculation Chern number

There are a few ways to calculate Chern number. We can classified into two classes. One is reciprocal space system, like Kubo formula in reciprocal space form [1--3]. The other is in real space system, like Streda method[4], Prodan′ method [5], C*−algebras method [6], Kubo formula in lattice model form [7]. All the real space Chern number calculation can be deduced from reciprocal space calculation.

1.1.1 TKNN number

The relation between Chern number and physical quantity was introduced by TKNN [1]. In their paper, they gives the formula to calculate Chern number in reciprocal space.

$$C = \frac{i}{A} \sum_{\varepsilon_\alpha < E_F} \sum_{\varepsilon_\beta > E_F} \frac{(\partial \hat{H}/\partial k_1)_{\alpha\beta}(\partial \hat{H}/\partial k_2)_{\beta\alpha} - (\partial \hat{H}/\partial k_2)_{\alpha\beta}(\partial \hat{H}/\partial k_1)_{\beta\alpha}}{(\varepsilon_\alpha - \varepsilon_\beta)^2}$$

$\hat{H}$is the Hamiltonian in k space.

1.1.2 Kubo formula in real space lattice form

The main idea for real space Chern number calculation is to calculate Chern number on a finite lattice model. the normal way to calculate it is with Kubo formula.

$$\sigma_{xy} = \frac{ie^2\hbar}{N_x N_y} \sum_n \sum_{m \neq n} (f(E_n) - f(E_m)) \frac{\langle n|v_x|m\rangle\langle m|v_y|n\rangle}{(\epsilon_n - \epsilon_m)^2} \tag{1.1}$$

$f(E_n)$is fermi distribution, after simplification,

$$\sigma_{xy} = \frac{ie^2\hbar}{N_x N_y} \sum_{\epsilon_n < E_F} \sum_{\epsilon_m > E_F} \frac{\langle n|v_x|m\rangle\langle m|v_y|n\rangle - \langle n|v_y|m\rangle\langle m|v_x|n\rangle}{(\epsilon_n - \epsilon_m)^2} \tag{1.2}$$

v_x, v_y are velocity operator,

$$v_x = \frac{1}{i\hbar}[x, H] \tag{1.3}$$

x is position operator, $x = \sum_n c_n^\dagger n c_n$, if the one dimensional Hamiltonian H is

$$H = \sum_n \epsilon_n c_n^\dagger c_n + t \sum_n c_{n+1}^\dagger c_n + t \sum_n c_n^\dagger c_{n+1} \tag{1.4}$$

then

$$v_x = \frac{t}{i\hbar}\sum_n \left(c^\dagger_{n+1}c_n - c^\dagger_n c_{n+1}\right) \tag{1.5}$$

In two dimension

$$H = \sum_{m,n}\epsilon_{m,n}c^\dagger_{m,n}c_{m,n} + t\sum_{m,n}\left(c^\dagger_{m,n+1}c_{m,n} + c^\dagger_{m,n}c_{m,n+1}\right) + t\sum_{m,n}\left(c^\dagger_{m+1,n}c_{m,n} + c^\dagger_{m,n}c_{m+1,n}\right) \tag{1.6}$$

$$v_x = \frac{t}{i\hbar}\sum_{m,n}\left(c^\dagger_{m+1,n}c_{m,n} - c^\dagger_{m,n}c_{m+1,n}\right) \tag{1.7}$$

$$v_y = \frac{t}{i\hbar}\sum_{m,n}\left(c^\dagger_{m,n+1}c_{m,n} - c^\dagger_{m,n}c_{m,n+1}\right) \tag{1.8}$$

after using twist boundary

$$H = \sum_{m,n}\epsilon_{m,n}c^\dagger_{m,n}c_{m,n} + t\sum_{m,n}\left(c^\dagger_{m,n+1}c_{m,n} + c^\dagger_{m,n}c_{m,n+1}\right) + t\sum_{m,n}\left(c^\dagger_{m+1,n}c_{m,n} + c^\dagger_{m,n}c_{m+1,n}\right) \tag{1.9}$$

$$+t\sum_n\left(c^\dagger_{N_x,n}c_{1,n}e^{i\theta} + c^\dagger_{1,n}c_{N_x,n}e^{-i\theta}\right) + t\sum_m\left(c^\dagger_{m,N_y}c_{m,1}e^{i\varphi} + c^\dagger_{m,1}c_{m,N_y}e^{-i\varphi}\right) \tag{1.10}$$

$$v_x = \frac{t}{i\hbar}\sum_{m,n}\left(c^\dagger_{m+1,n}c_{m,n} - c^\dagger_{m,n}c_{m+1,n}\right) + \frac{t}{i\hbar}\sum_n\left(c^\dagger_{N_x,n}c_{1,n}e^{i\theta} - c^\dagger_{1,n}c_{N_x,n}e^{-i\theta}\right) \tag{1.11}$$

$$v_y = \frac{t}{i\hbar}\sum_{m,n}\left(c^\dagger_{m,n+1}c_{m,n} - c^\dagger_{m,n}c_{m,n+1}\right) + \frac{t}{i\hbar}\sum_m\left(c^\dagger_{m,N_y}c_{m,1}e^{i\varphi} - c^\dagger_{m,1}c_{m,N_y}e^{-i\varphi}\right) \tag{1.12}$$

It is suggested by Niu et.al[8] that Chern number can be get by averaged the hall conductance with different twist boundary.

$$C = \frac{h}{e^2}\frac{1}{4\pi^2}\int d\theta d\phi \sigma_{xy}(\theta,\phi) \tag{1.13}$$

1.1.3 Streda formula

The original Streda formula[9] is

$$\sigma_{\mu\nu} = -\frac{1}{4\pi A}\int dE f(E)\left\langle Tr\left[J_\mu \frac{dG_+(E)}{dE}J_\nu G_\delta + h.c.\right]\right\rangle_{imp} \tag{1.14}$$

J_μ is the current operator in μ direction, $G_\pm(E) = \left[E - H - H_{imp} \pm i\eta\right]^{-1}$, $G_\delta = G_+ - G_-$, H_{imp} is the interaction with the impurities. $\langle ...\rangle_{imp}$ represents the average over different disorder configurations.

In M. Onoda's paper, they only focus on the metallic states, so they just replace $G_{\pm}(E)$ by $\left[E - H \pm i(2\tau)^{-1}\right]^{-1}$ to consider the disorder effect. They reduce Streda's formula into

$$\sigma_H = -\frac{i}{A}\sum_{\alpha\alpha'} \mathrm{e}_z \cdot [\langle\psi_\alpha|\mathrm{J}|\psi_{\alpha'}\rangle\langle\psi_{\alpha'}|\mathrm{J}|\psi_\alpha\rangle\times] \times \frac{\tau^2[f^\tau(E_\alpha) - f^\tau(E_{\alpha'})]}{1 + [(E_\alpha - E_{\alpha'})\tau]^2} \tag{1.15}$$

$f^\tau(E)$ is $f(E)$ with inverse temperature replaced by $64\tau/(3\pi)$

1.1.4 Prodan's way

Emil Prodan gives an elegant way to calculate Chern number for disordered system.

$$C = -\frac{2\pi i}{N^2}\sum_{n,\alpha}\langle n,\alpha|P[-i[\hat{x}_1,P],-i[\hat{x}_2,P]]|n,\alpha\rangle \tag{1.16}$$

where

$$[x,P] = i\sum_{m=1}^{Q} c_m(e^{-im\hat{x}\Delta_i}Pe^{im\hat{x}\Delta_i} - e^{im\hat{x}\Delta_i}Pe^{-im\hat{x}\Delta_i}) \tag{1.17}$$

where $\Delta = 2\pi/N$, and P is the projector onto the occupied spectrum

$$P = \sum_{\alpha\in occupied} |\nu_\alpha\rangle\langle\nu_\alpha| \tag{1.18}$$

$c_m, m = 1,2,..,Q$ can be deduced by solve a linear equation

$$\hat{A}C^T = \frac{1}{2\Delta}(1,0,0,...,0)^T \tag{1.19}$$

$$A_{ij} = j^{2i-1} \tag{1.20}$$

$$i,j \in \{1,...,Q\} \tag{1.21}$$

1.1.5 C*−algebra method

In the paper of T. A. Loring and M. B. Hastings, they gave another method to calculate topological index, which called Bott index. It can be calculated by the following procedure.

$$P = \sum_{\alpha\in occupied} |\nu_\alpha\rangle\langle\nu_\alpha| V = Pe^{i2\pi\hat{x}}PU = Pe^{i2\pi\hat{y}}Pm = \frac{1}{2\pi}Im[tr(log(VUV^\dagger U^\dagger))] \tag{1.22}$$

□

参考文献

[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, Aug 1982.

[2] Takahiro Fukui, Yasuhiro Hatsugai, and Hiroshi Suzuki. Chern numbers in discretized brillouin zone: Efficient method of computing (spin) hall conductances. Journal of the Physical Society of Japan, 74(6):1674--1677, 2005.

[3] Mahito Kohmoto. Topological invariant and the quantization of the hall conductance. Annals of Physics, 160(2):343 -- 354, 1985.

[4] Masaru Onoda, Gen Tatara, and Naoto Nagaosa. Anomalous hall effect and skyrmion number in real and momentum spaces. Journal of the Physical Society of Japan, 73(10):2624--2627, 2004.

[5] Emil Prodan. Disordered topological insulators: a non-commutative geometry perspective. Journal of Physics A: Mathematical and Theoretical, 44(11):113001, 2011.

[6] T. A. Loring and M. B. Hastings. Disordered topological insulators via c * -algebras. EPL (Europhysics Letters), 92(6):67004, 2010.

[7] Paramita Dutta, Santanu K. Maiti, and S. N. Karmakar. Integer quantum hall effect in a lattice model revisited: Kubo formalism. Journal of Applied Physics, 112(4):--, 2012.

[8] Qian Niu, D. J. Thouless, and Yong-Shi Wu. Quantized hall conductance as a topological invariant. Phys. Rev. B, 31:3372--3377, Mar 1985.

[9] L Smrcka and P Streda. Transport coefficients in strong magnetic fields. Journal of Physics C: Solid State Physics, 10(12):2153, 1977.