III.10a

HALL CONDUCTANCE AND CHERN NUMBERS

Tuesday lecture (3/12) I sketched the basics (or, some aspects of the basics ☺) of the IQHE, and I also reviewed how to set up a calculation of the HALL CONDUCTANCE from the KUBO FORMULA. So, today I'll try to show you how to carry through this calculation. (A caveat: I won't do the original version from TKNN (1982) which is quite tricky, but rather a "light version" which emphasizes the topological features of the problem ...)

So, for a starter, let's go back to Kubo ....

KUBO SLIDES
1-5

① Stress that Kubo ⇒ keep only leading terms in the expansion (eq. 6)

② $\vec{E}(t)$ is an applied macroscopic field (therefore treated as a classical field)

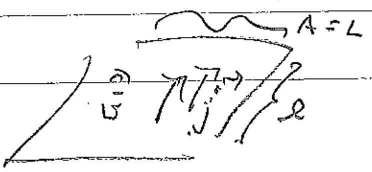
③ In (eq. 8), write $\langle J_i(t)\rangle = \langle J_i\rangle e^{-i\omega t}$ then divide by $E_j e^{-i\omega t}$. This gives the LHS $\sigma_{ij}(\omega) = \sigma_{xy}(\omega)$ with $i=x, j=y$

we need an $i\varepsilon$ prescription to make the integral ~~convergent and~~ to ensure CAUSALITY! → The ω-dependence comes from the integral!

An aside → ④ Note Hall conductance = Hall conductivity
resistance = resistivity

However longitudinal conductance G_{xx} ≠ longitudinal conductivity σ_{xx}

$G_{xx} = \sigma_{xx}\frac{A}{\ell}$



⑤ Binomial expansion in (12):

$$\overline{(1+x)^n} = 1 + nx + \mathcal{O}(x^2)$$

with $x = \frac{\hbar\omega}{E_n - E_0} \ll 1$ and $n = -1$

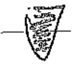
⑥ The leading term in the expansion of (11) vanishes due to rotational invariance $x \to y$, $y \to -x$ $\Rightarrow$ no divergence in the $\omega \to 0$ limit

* * *

Given Eq. (13) in the Kubo slides we shall now see how topology enters. We shall exploit a "figure of thought" which is quite common in the study of topological phases. It may appear somewhat artificial the first time you see it, but it's very powerful. (Alternatively, we could have broken down the many-particle states $|n\rangle$ and $|0\rangle$ to the cell-periodic Bloch states in the BZ (after Fourier transformation) and then using "Berryology" in the BZ to arrive at a Chern number. Perfectly doable, and closer to how TKNN (1982) did it, but technically cumbersome.) Here we opt for elegance!

GEDANKEN EXPERIMENT

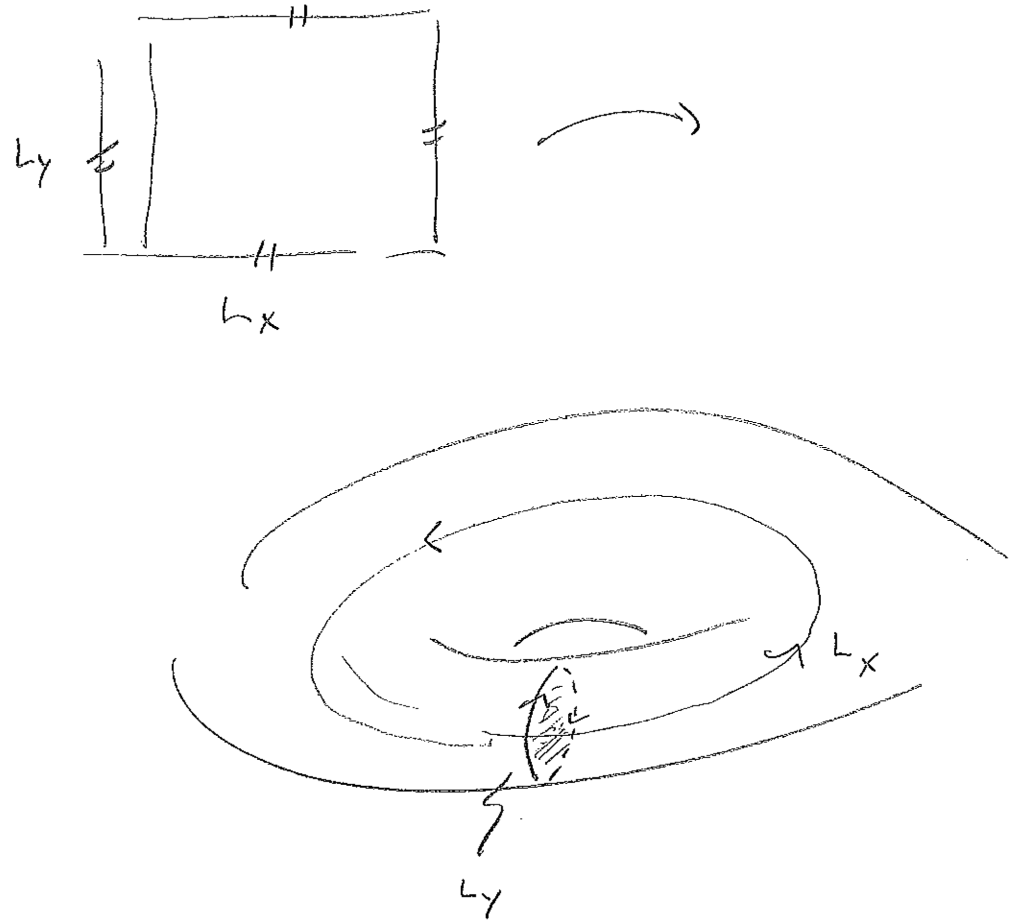
Thus, we wrap our quantum Hall sample around a (spatial) torus T^2 (not a BZ)!



We thread a uniform $\vec{B}$-field through the torus.

Choose a Landau gauge $A_x = 0$, $A_y = Bx$

(Note: before we had $A_x = -By$, $A_y = 0$.
The two choices are equivalent!)



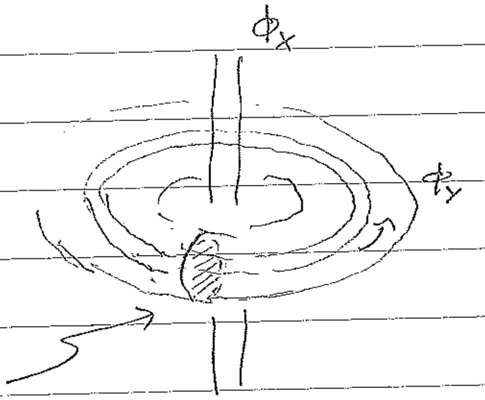
$$\tilde{\Phi}_y = \int \vec{B}\cdot d\vec{S} = \oint_{L_y} \vec{A}\cdot d\vec{l} = "\oint_{L_y} A_y dy" = \oint_{L_y} B_x dy$$

$$= B_x L_y \Rightarrow A_y = \frac{\tilde{\Phi}_y}{L_y}$$

$$\tilde{\Phi}_x = \int \vec{B}\cdot d\vec{S} = \oint_{L_x} \vec{A}\cdot d\vec{l} = "\oint_{L_x} A_x dx" = 0$$

Given this, we perturb the system by threading two fluxes,*/ Φ_x and Φ_y through the x- and y-cycles of the torus respectively

*/ x- and y- independent



$$\Phi_y = \int \vec{B}'\cdot d\vec{S} = \oint_{L_y} \vec{A}'\cdot d\vec{l} = A'_y L_y \Rightarrow A_y' = \frac{\Phi_y}{L_y}$$

Similarly : $A_x' = \frac{\Phi_x}{L_x}$

Thus, the new vector potential becomes

$$A_x = \underbrace{\frac{\Phi_x}{L_x}}_{A_x'} , \quad A_y = \underbrace{\frac{\Phi_y}{L_y}}_{A_y'} + Bx$$

The addition of the fluxes adds an extra term to the Hamiltonian (cf. eq. (1)* in the "Kubo slides")

$$\boxed{\text{from } {}^{*}\ \Delta H = -\vec{J}\cdot\vec{A}} \longrightarrow \Delta H = -\sum_{i=x,y} \frac{J_i \Phi_i}{L_i} \qquad (\text{III}.27)$$

Effect on the ground state from first-order perturbation theory

$$|\Psi_0'\rangle = \underbrace{|\Psi_0\rangle}_{"|0\rangle"} + \sum_{n\neq 0} \frac{\langle n|\Delta H|\Psi_0\rangle}{E_n - E_0} |n\rangle \qquad (\text{III}.28)$$

From (III,27), the perturbation from Φ_i yields

$$|\Psi_0'\rangle = |\Psi_0\rangle - \frac{1}{L_i}\sum_{n\neq 0} \frac{\langle n|J_i\Phi_i|\Psi_0\rangle}{E_n - E_0}|n\rangle \qquad (\text{III}.29)$$

$$\Rightarrow \underbrace{\frac{\partial}{\partial\Phi_i}|\Psi_0\rangle}_{\simeq\frac{(|\Psi_0'\rangle - |\Psi_0\rangle)}{\Phi_i}} = -\frac{1}{L_i}\sum_{n\neq 0} \frac{\langle n|J_i|\Psi_0\rangle}{E_n - E_0}|n\rangle \qquad (\text{III}.30)$$

. From now on, let's for simplicity choose $L_i = 1$ $(i=x,y)$

We can then use (III.30) to rewrite the Kubo formula for σ_{xy}:
(SEE KUBO FORMULA SLIDES WITH $|0\rangle \equiv |\Psi_0\rangle$)

$$\sigma_{xy} = i\hbar \sum_{n\neq 0} \frac{\langle\Psi_0|J_y|n\rangle\langle n|J_x|\Psi_0\rangle - \langle\Psi_0|J_x|n\rangle\langle n|J_y|\Psi_0\rangle}{(E_n - E_0)^2}$$

double sum $\sum_n \dots \sum_{n'} \dots \underbrace{\langle n|n'\rangle}_{\delta_{nn'}}$

$$\longrightarrow = i\hbar\left[\left\langle \frac{\partial\Psi_0}{\partial\Phi_y}\middle|\frac{\partial\Psi_0}{\partial\Phi_x}\right\rangle - \left\langle\frac{\partial\Psi_0}{\partial\Phi_x}\middle|\frac{\partial\Psi_0}{\partial\Phi_y}\right\rangle\right]$$

$$= i\hbar\left[\frac{\partial}{\partial\Phi_y}\left\langle\Psi_0\middle|\frac{\partial\Psi_0}{\partial\Phi_x}\right\rangle - \frac{\partial}{\partial\Phi_x}\left\langle\Psi_0\middle|\frac{\partial\Psi_0}{\partial\Phi_y}\right\rangle\right] \qquad (\text{III}.31)$$

SPECTRAL FLOW SLIDE

The spectrum of the Hamiltonian only depends on $\underbrace{\Phi_i}_{i=x,y}$ mod Φ_0

flux quantum

Hence, Φ_x and Φ_y also live on a torus, call it T^2_Φ, parameterized by $\theta_i = 2\pi\Phi_i/\Phi_0$, $\theta_i \in [0, 2\pi]$, $i=x,y$. *)

The Berry phase from changing θ_i is obtained by integrating the Berry connection.

$$\mathcal{A}_i = -i\langle\Psi_0|\frac{\partial}{\partial\theta_i}|\Psi_0\rangle, \quad i=x,y \qquad (\text{III}.32)$$

The corresponding Berry curvature is given by

$$F_{xy} = \frac{\partial\mathcal{A}_x}{\partial\theta_y} - \frac{\partial\mathcal{A}_y}{\partial\theta_x} \overset{(\text{III}.32)}{=} -i\left[\frac{\partial}{\partial\theta_y}\left\langle\Psi_0\middle|\frac{\partial\Psi_0}{\partial\theta_x}\right\rangle - \frac{\partial}{\partial\theta_x}\left\langle\Psi_0\middle|\frac{\partial\Psi_0}{\partial\theta_y}\right\rangle\right] \qquad (\text{III}.33)$$

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*) From SPECTRAL FLOW SLIDE: $E_n \sim \left(n + \frac{\Phi}{\Phi_0}\right)^2$

(III.12

$\Phi_0 = \frac{2\pi\hbar}{e}$

With $\frac{\partial}{\partial\phi_i} = \frac{e}{\hbar}\frac{\partial}{\partial\theta_i}$, $i = x, y$, it follows from (III.31) and (III.33) that

$$\sigma_{xy} = -\frac{e^2}{\hbar}\tilde{F}_{xy} \qquad \text{(III.34)}$$

N.B. (III.34) applies to a particular choice of θ_x, θ_y : $\tilde{F}_{xy} = \tilde{F}_{xy}(\theta_x, \theta_y)$.
The Hall conductivity obtained after averaging over all fluxes :

$$\sigma_{xy} = -\frac{e^2}{\hbar}\langle \hat{F}_{xy} \rangle = -\frac{e^2}{\hbar}\int_{T^2_\phi} \frac{d^2\theta}{(2\pi)^2}\hat{F}_{xy}(\theta_x, \theta_y)$$

$$= -\frac{e^2}{2\pi\hbar}\underbrace{\left(\frac{1}{2\pi}\int_{T^2_\phi} d^2\theta\, \hat{F}_{xy}(\theta_x, \theta_y)\right)}_{C_1 \text{ "first" Chern number!}}$$

$$= -\frac{e^2}{h}C_1 \qquad \text{(III.35)}$$

sometimes called TKNN invariant
after the authors of the 1982 paper :
Thouless, Kohmoto, Nightingale, den Nijs

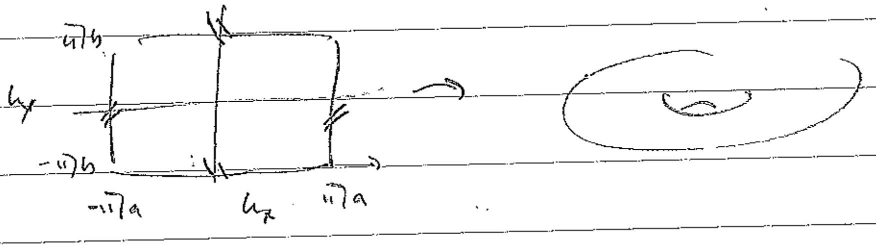
Barry Simon (the same year)
realized that the TKNN invariant
is a Chern number !

* * *

We can get one step closer to the original calculation by Thouless et al. by replacing T^2_ϕ with the Brillouin zone for particles on a <u>lattice</u>, which topologically is also a 2-torus in 2D. With this, we will obtain a stronger result, applying also to the CHERN INSULATOR (2D electrons subject to time-reversal breaking but with no net magnetic field... more about this later!)

We shall make three assumptions:

I. 2D single-particle spectrum decomposes into bands $n = 1, 2, \ldots$ parameterized by $\vec{k} \in T^2 = BZ$



II. Non interacting electrons

III. Gapped band structure : bands $< E_F$ completely filled
—"— $> E_F$ —"— empty

↙

"band insulator"

The topology originates from the way the phase of the cell-periodic Bloch states winds as we move around the BZ T^2, captured by the BERRY CONNECTION

$$\mathcal{A}_{\underset{\nwarrow \text{ band index}}{n,i}}(\vec{k}) = -i \langle u_{n\vec{k}} | \underset{\uparrow\, \frac{\partial}{\partial k^i}}{\partial_{k_i}} | u_{n\vec{k}} \rangle \quad , \; i = x, y \qquad \text{(III.36}$$

By integrating the Berry curvature

$$\hat{F}_{n,xy} = \frac{\partial \mathcal{A}_{n,x}}{\partial k_y} - \frac{\partial \mathcal{A}_{n,y}}{\partial k_x} \qquad (\overline{III}.37)$$

over T^2, one obtains the first Chern number for band n

$$C_n = \frac{1}{2\pi} \int_{T^2} d^2k \, \hat{F}_{n,xy} \qquad (\overline{III}.38)$$

Thouless et al. (1982) proved the famous TKNN formula in the presence of a magnetic field:

$$\sigma_{xy} = -\frac{e^2}{h} \sum_{\substack{n \in \text{filled} \\ \text{bands}}} C_n \qquad (\overline{III}.39)$$

We can actually do better, and prove $(\overline{III}.39)$ for any 2D lattice model that satisfies the assumptions $\overline{I}$ - $\overline{III}$. There is one caveat though! To obtain a nonzero Chern number, time-reversal symmetry must be broken (cf. my discussion of Berry fluxes in Lecture 14/11)

Kubo slides →

Writing the many-particle states $|0\rangle$ and $|n\rangle$ in (13) as tensor products of single-particle (cell-periodic) Bloch states $|u_{n,k}\rangle$ (anti-symmetrization is not important here), the Kubo formula for the Hall conductivity in (13) can be written as

SEE KUBO SLIDES p 7-8

$$\sigma_{xy} = i\hbar \overset{\swarrow \text{sum over filled bands}}{\sum_{E_n < E_F < E_m}} \int_{T^2} \frac{d^2k}{(2\pi)^2} \left(\frac{\langle u_{n,\vec{k}} | J_y | u_{m,\vec{k}} \rangle \langle u_{m,\vec{k}} | J_x | u_{n,\vec{k}} \rangle}{(E_n(\vec{k}) - E_m(\vec{k}))^2} - \frac{\langle u_{n,\vec{k}} | J_x | u_{m,\vec{k}} \rangle \langle u_{m,\vec{k}} | J_y | u_{n,\vec{k}} \rangle}{(E_n(\vec{k}) - E_m(\vec{k}))^2} \right)$$

E_n ↗ filled, E_m ↗ empty

$$(\overline{III}.40)$$

filled in the ground state

To understand the structure of the integrand in (III.40), let's look at a "toy system" with two bands α and β, and two particles with allowed momenta k_1 and k_2.

$$|0\rangle = |u_{\alpha,k_1}\rangle \otimes |u_{\alpha,k_2}\rangle \qquad \text{ground state}$$

$$|n\rangle = |u_{\alpha,k_1}\rangle \otimes |u_{\beta,k_2}\rangle \qquad \underline{\text{one}} \text{ possible excited state}$$

We then have that two-particle expectation values of the type that would enter into the Kubo formula in (13) take the form

$$\langle 0|J|n\rangle = \langle u_{\alpha,k_1}| \otimes \langle u_{\alpha,k_2}|\, J \left(|u_{\alpha,k_1}\rangle \otimes |u_{\beta,k_2}\rangle\right)$$

$$= \langle u_{\alpha,k_1}| \otimes \langle u_{\alpha,k_2}| \left(J |u_{\alpha,k_1}\rangle\right) \otimes |u_{\beta,k_2}\rangle$$

$$+ \langle u_{\alpha,k_1}| \otimes \langle u_{\alpha,k_2}| \left(|u_{\alpha,k_1}\rangle \otimes \left(J\, |u_{\beta,k_2}\rangle\right)\right).$$

$$= \langle u_{\alpha,k_1}| J |u_{\alpha,k_1}\rangle \underbrace{\langle u_{\alpha,k_2}|u_{\beta,k_2}\rangle}_{=0}$$

$$+ \underbrace{\langle u_{\alpha,k_1}|u_{\alpha,k_1}\rangle}_{=1} \langle u_{\alpha,k_2}| J |u_{\beta,k_2}\rangle$$

$$= \langle u_{\alpha,k_2}| J |u_{\beta,k_2}\rangle$$

We would also have terms of the form $\langle u_{\alpha,k_1}|J|u_{\beta,k_2}\rangle$ and hence the single integral over k in (III.40) should really be a double integral over k and k'. However, the final result will not be corrupted by our sloppiness here!

It will prove convenient to express the current operator in terms of the group velocity of the cell-periodic Bloch functions

$$\vec{J} = \frac{e}{\hbar} \nabla_{\vec{k}} \tilde{H}(k) \qquad (\text{III}.41)$$

where $\widehat{H}(\vec{k}) = e^{-i\vec{k}\cdot\vec{r}} H e^{i\vec{k}\cdot\vec{r}}$

$\uparrow \quad H\psi_{\vec{k}}(\vec{r}) = E_{\vec{k}}\psi_{\vec{k}}(\vec{r})$

Inserting (III.41) into (III.40), the rest is algebra.

Kubo
Slides

last two pages of

PREPARING FOR CALCULATING THE HALL CONDUCTIVITY : THE KUBO FORMULA

Simplest examples of lattice models with non-vanishing Chern numbers :

CHERN INSULATORS (a.k.a. "QUANTUM ANOMALOUS HALL INSULATORS")

Hall conductivity without a net magnetic field!

First construction of such a model (on a graphene lattice) in 1988 by Duncan Haldane, PRL 61, 2015 (1988).

Haldane
Slides

Let's look at a simpler case of a CHERN INSULATOR with two bands. The single-particle Hamiltonian acting on the cell-periodic Bloch states $|u_{n,k}\rangle$ has the general form

$$H(\vec{k}) = \vec{d}(\vec{k}) \cdot \underset{\swarrow}{\vec{\sigma}} + \varepsilon(k) \mathbb{1} \quad , \vec{k} \in T^2 \qquad (\text{III}.42)$$

$\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$

Energy eigenvalues for a given $\vec{k}$:

$$E(\vec{k}) = \varepsilon(\vec{k}) \pm |\vec{d}(\vec{k})| \qquad (\text{III}.43)$$

This describes an insulator if $\vec{d}(\vec{k}) \neq 0, \forall \vec{k}$ with band gap $\Delta(\vec{k}) = 2 \min |\vec{d}(\vec{k})|$.

To compute the Chern number C_1, ← for the lower filled band, and the corresponding Hall conductivity $\sigma_{xy} = -\frac{e^2}{h} C_1$, we can shortcut the long Kubo-formula calculation and use the fact * that C_1 coincides with the so called Pontryagin index which characterizes the mapping

$$\underset{\text{2-torus}}{\vec{k} \in T^2} \longrightarrow \underset{\text{unit sphere}}{S^2} \ni \vec{n}(\vec{k}) = \frac{\vec{d}(\vec{k})}{|\vec{d}(\vec{k})|}$$

Explicitly :

$$C_1 = \frac{1}{4\pi} \int_{T^2} d^2k \, \vec{n}(\vec{k}) \cdot \left(\frac{\partial \vec{n}}{\partial k_x} \times \frac{\partial \vec{n}}{\partial k_y} \right) \qquad (\text{III}.44)$$

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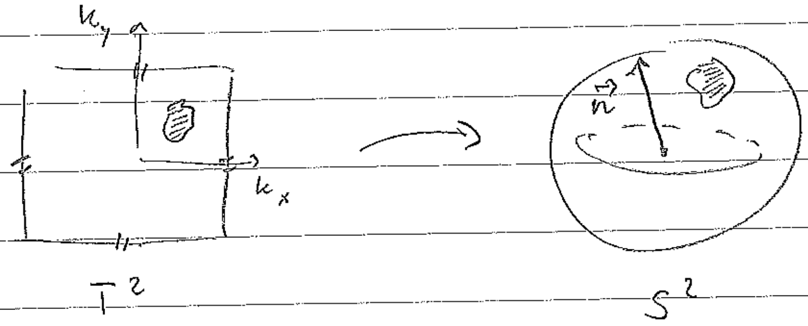
* E. Fradkin, "Field Theories of Condensed Matter Physics", p 685

In a picture



C counts how many times T^2 wraps around S^2.

A very simple example* of a lattice model with non-zero Chern number, defined on a square lattice:

$$\begin{cases} d_x(\vec{k}) = \sin k_x \\ d_y(\vec{k}) = \sin k_y \\ d_z(\vec{k}) = m + \cos k_x + \cos k_y \\ \varepsilon(\vec{k}) = 0 \end{cases} \qquad (\overline{\text{III}}.45)$$

Note that ($\overline{\text{III}}$.45) violates time reversal (a necessary condition for having a Chern insulator)

Feeding in ($\overline{\text{III}}$.45) into ($\overline{\text{III}}$.44) and doing the integral, one finds

HW PROBLEM

$$C = \begin{cases} -1 & -2 < m < 0 \\ 1 & 0 < m < 2 \\ 0 & |m| > 2 \end{cases}$$

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* cf. X.-L. Qi et al., Phys. Rev. B 74, 085308 (2006)