TKNN Invariant

Michael Geracie

9/30/13

Introduction

- plan: perform fully QM calculation of σ_{xy} that makes quantization manifest.
- Assume - noninteracting electrons
  - periodic potential
  - zero temperature

exact manipulations ~~$\Rightarrow \sigma_{xy} \propto$ topological invariant called chern~~

$\Rightarrow \sigma_{xy} \Rightarrow$ chern number

- first introduce background
  1. Berry Phase
  2. Magnetic Brillouin Zone / Chern Number
  3. Calculate Hall Conductance

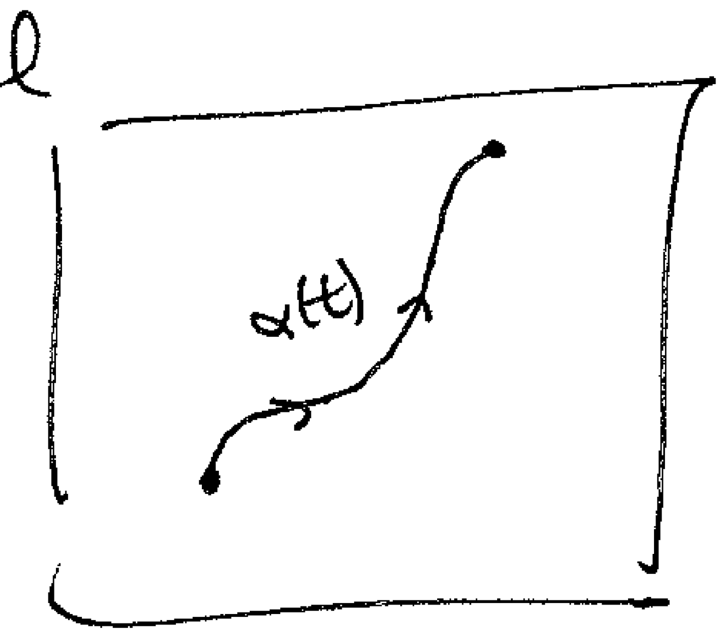
Berry Phase (following Nakahara)

- Problem: quantum particle $|\psi\rangle$ w/ hamiltonian $H(\alpha)$
  - α parameters that I vary.
- Usually α fixed & solution in terms of eigenstates $|n,\alpha\rangle$

$$H(\alpha)|n,\alpha\rangle = \varepsilon_n^\alpha |n,\alpha\rangle$$

~~Solution~~ of $i\frac{d}{dt}|\psi\rangle = H|\psi\rangle \Rightarrow |\psi\rangle = e^{-i\varepsilon_n^\alpha t}|n,\alpha\rangle$

- If slowly tuning $\alpha(t)$, anticipate $|\psi(t)\rangle \propto |n,\alpha(t)\rangle$



Naive guess: $|\psi(t)\rangle = \exp\left\{-i\int_0^t \varepsilon_n^{\alpha(t')}dt'\right\}|n,\alpha(t)\rangle$

$\Rightarrow$ does not solve SE

- try more general sol

$$|\psi(t)\rangle = \exp\left\{ i\gamma_n(t) - i\int_0^t E_n^{\alpha(t')}\,dt' \right\} |n,\alpha(t)\rangle$$

- Plug into TDSE

$$\Rightarrow \dot{\gamma}_n = i\langle n,\alpha(t)|\tfrac{d}{dt}|n,\alpha(t)\rangle$$

$$\Rightarrow \gamma_n(t) = i\int_0^t \langle n,\alpha(t')|\tfrac{d}{dt'}|n,\alpha(t')\rangle\,dt' = i\int_{\alpha(0)}^{\alpha(t)} \langle n,\alpha|\partial_{\alpha^i}|n,\alpha\rangle\,d\alpha^i$$

$$= \int_{\alpha(0)}^{\alpha(t)} A_i^n(\alpha)\,d\alpha^i$$

where $A_i^n = i\langle n,\alpha|\partial_i|n,\alpha\rangle$ is 1-form on parameter space $\mathcal{C}$

- Analogy w/ external gauge fields.

<u>In E&M</u> drag particle through field B in physical space $\vec{r}$, picks up phase

$$\gamma = \int_{\vec{r}(0)}^{\vec{r}(t)} A_i(x)\,dx^i \qquad \text{where} \qquad \vec{B} = \nabla\times A$$

Gauge freedom: $|\psi\rangle \to e^{\frac{ie\alpha(x)}{\hbar}}|\psi\rangle$

$$A_i \to A_i - \partial_i\alpha$$

<u>Berry</u> Drag system through $\mathcal{C}$, picks up phase

$$\gamma = \int_{\alpha(0)}^{\alpha(t)} A_i^n(\alpha)\,d\alpha^i$$

Under $|n,\alpha\rangle \to e^{i\beta(\alpha)}|n,\alpha\rangle$

$$A_i^n \to A_i^n - \partial_i\beta$$

- Think of A_i^n as gauge field on $\mathcal{C}$ associated to global phase symm of wavefunction at each point $\alpha\in\mathcal{C}$.

Note: Infinite number! One for each energy eigenstate.

Magnetic Brillouin Zone

Setup: • 2D sample w/ const $\vec{B} = +B\hat{z}$

(choose symmetric gauge $\vec{A} = \frac{1}{2}(\vec{B} \times \vec{r})$)

• lattice potential $U(x,y)$

$$U(x+a,y) = U(x,y+b) = U(x,y)$$

• Wish to determine band structure, but some complications

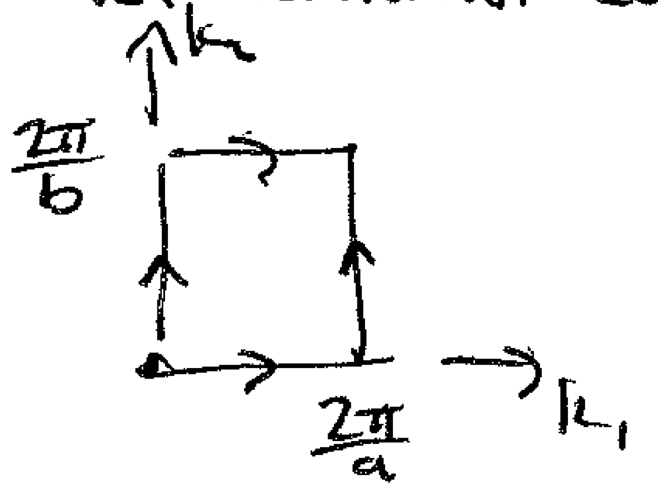
Recall usual story from Dung's talk:

• translationally invariant hamiltonian $\quad [T_{na}, H] = [T_{mb}, H] = 0$

$$[T_{na}, T_{mb}] = 0.$$

• choose wavefunctions diagonalizing them all

$$\psi(x,y) = e^{i\vec{k}\cdot\vec{r}}\, u_{\vec{k}}^{(\alpha)}(x,y), \quad \vec{k} \in \text{1st brillouin zone}$$



Vector Potential Complicates matters:

• $\vec{A}(\vec{r}) \neq \vec{A}(\vec{r}+\vec{R})$, so H not translationally invariant

• $T_{\vec{R}} = e^{i\vec{R}\cdot\vec{p}}$ not gauge invariant since $\vec{p} \to \vec{p} + e\nabla\alpha$

• Fix by covariantizing

$$\hat{T}_{\vec{R}} = e^{i\vec{R}\cdot(\vec{p}+e\vec{A})}$$

$\Rightarrow \hat{T}_{\vec{R}}$ invariant & commutes w/ $H = \frac{1}{2m}(p+eA)^2 + U$

• In our gauge, $\hat{T}_{\vec{R}} = T_{\vec{R}} e^{i\frac{e}{2}(\vec{B}\times\vec{R})\cdot\vec{r}}$, so this just regular translation + gauge transf

(makes sense since can use gauge transf to undo ⊛)

• Prob: $\hat{T}_{\vec{R}}$'s dont commute

$$\hat{T}_{na}\hat{T}_{mb} = e^{2\pi i nm\varphi}\hat{T}_{mb}\hat{T}_{na} \quad \text{where} \quad \varphi = \frac{e}{h}B(ab)$$

no. of flux quanta per unit cell

(just saying when travel in loop pick up phase $\propto$ flux contained in loop).

• can be fixed to if assume $\varphi = \frac{p}{q}$ since may choose multiple cells containing integer flux.

Ex.

$$\hat{T}_{qa}\hat{T}_{b} = \hat{T}_{b}\hat{T}_{qa}$$

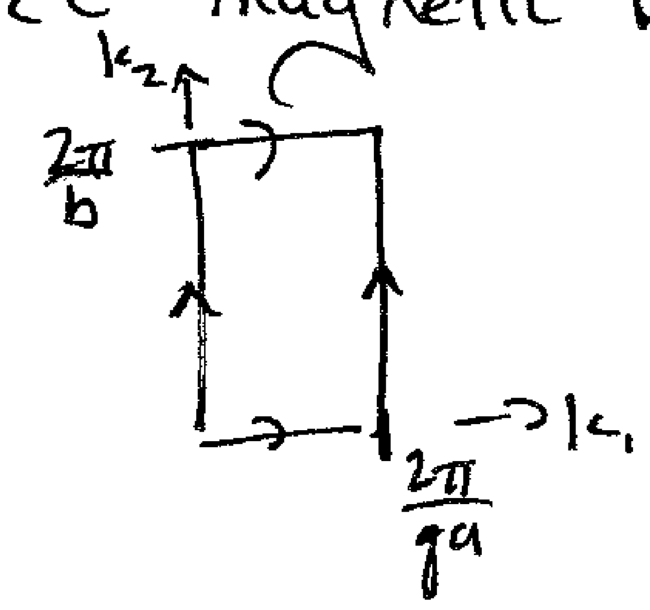
(in end will take limit for irrational φ)

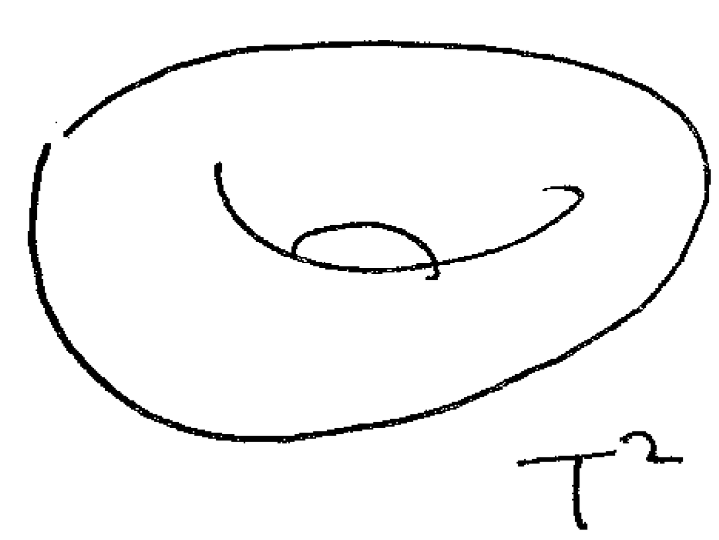
• call "magnetic unit cell"

• now have commuting operators & can choose eigenfunctions

$$\psi^{(\alpha)}_{\vec{k}}(x,y) = e^{i\vec{k}\cdot\vec{r}}\, u^{(\alpha)}_{\vec{k}}(x,y)$$

$\vec{k} \in$ "magnetic Brillouin zone"





remember magnetic Brillouin zone is torus!

Chern Number

- for each $\vec{k}$, $u_{\vec{k}}^{(\alpha)}$ are solutions to

(α) labels band

$$\left\{ \frac{\hbar^2}{2m}\left(-i\hbar\nabla + \hbar\vec{k} + e\vec{A}\right)^2 + U \right\} u_{\vec{k}}^{(\alpha)}(\vec{r}) = \varepsilon_{\vec{k}}^{(\alpha)} u_{\vec{k}}^{(\alpha)}$$

- H function of parameter $\vec{k} \in T^2$ so can define berry connection on T^2!

$$A_i^{(\alpha)}(\vec{k}) = i\langle u_{\vec{k}}^{(\alpha)} | \frac{\partial}{\partial k_i} | u_{\vec{k}}^{(\alpha)} \rangle$$

- under k-dep redef of global phase $u'_{\vec{k}} = e^{if(\vec{k})} u_{\vec{k}}$

$$A_i \to A_i - \partial_i f$$

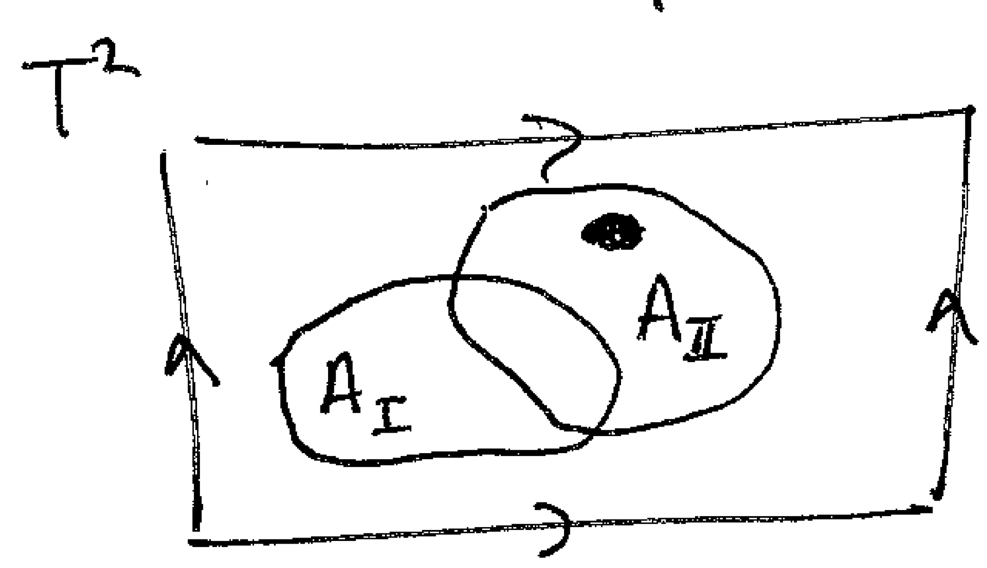
- Define chern no. to be "magnetic flux" through T^2

$$C_1^{(\alpha)} = \frac{1}{2\pi}\int_{T^2} (\nabla \times A^{(\alpha)})\, d^2k$$

- Theorem: C_1 is an integer

Nonrigorous argument:

- for $C_1 \neq 0$, $\vec{A}$ cannot be well defined on T^2 since $\int_T dA = \int_{\partial T} A = 0$
- most can ask: define A on diff open sets covering T^2, related by gauge transformations on overlap



$A_I = A_{II} + d\chi$ for some χ.

- Arises from inability to define phase on T^2

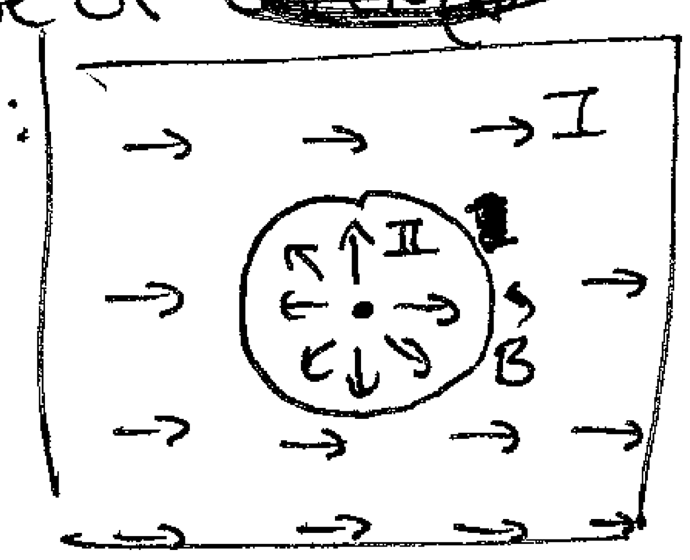
Try: • fix phase of u by declaring

$u_{\vec{k}}(x', y')$ real for some fixed (x', y').

• it may be $u_{\vec{k}'}(x', y') = 0$ for some $\vec{k}'$, does not work here.

• let II be small area containing $\vec{k}'$, I be everything else

Phase of $u_{\vec{k}}(x', y')$:



• define phase on II by fixing

$u_{\vec{k}}(x^2, y^2)$ real on II for some x^2, y^2

• defines new non const phase of $u_{\vec{k}}(x', y')$ on II.

• encircle $\vec{k}' \rightarrow$ phase wraps n times.

• I & II wavefunctions differ by gauge

$$|u^{II}_{\vec{k}}\rangle = e^{i\chi(\vec{k})}|u^{I}_{\vec{k}}\rangle \implies A_{II\,i} = A_{I\,i} - \partial_i \chi$$

A differs by gauge transf.

$$\therefore \frac{1}{2\pi}\int_{T^2}(\nabla \times A) = \frac{1}{2\pi}\int_{I}(\nabla \times A_I) + \frac{1}{2\pi}\int_{II}(\nabla \times A_{II}) = \frac{1}{2\pi}\int_B d\vec{k} \cdot (\vec{A}_I - \vec{A}_{II})$$

↑ I & II induce opp. orientations on B

$$= \frac{1}{2\pi}\int_B d\vec{k} \cdot \nabla \chi = \frac{1}{2\pi}(2\pi n) = n$$

General Case: • Chern no is total vorticity of phase on T^2.

• i.e. = no. of zeros of fixed component $u^{(\alpha)}_{\vec{k}}(x', y')$ viewed as func of $\vec{k}$

- ind. of (x', y')
- will not change under small def of $U(x,y)$
   - only when bands merge, & two A's become one does $\sum C_1^{(\alpha)}$ change.

Hall Conductance

- Will show $\sigma_{xy} = \frac{e^2}{h} \sum_{\alpha} C_1^{(\alpha)}$ sum over filled bands.

  - explicit quantization.

- Consider ε_F between bands, $T=0$, $\omega=0$. Kubo formula gives

$$\sigma_{xy} = \frac{e^2\hbar}{i} \sum_{\varepsilon^\alpha<\varepsilon^F<\varepsilon^\beta} \frac{\langle\alpha|v_y|\beta\rangle\langle\beta|v_x|\alpha\rangle - \langle\alpha|v_x|\beta\rangle\langle\beta|v_y|\alpha\rangle}{(\varepsilon^\alpha-\varepsilon^\beta)^2}$$

See: physics.stackexchange.com/questions/1906/kubo-formula-for-quantum-hall-effect

or Czycholl for proof.

- here $|\alpha\rangle$ eigenstate of H w/ eigenvalue ε^α
- $v_i = \frac{1}{m}(p_i + eA_i) = \frac{1}{\hbar}\frac{\partial H}{\partial k_i}$ velocity operator
- implicit $\vec{k}$ indices & $\int_{T^2} \frac{d^2k}{(2\pi)^2}$

- Now $\langle\alpha|\frac{\partial H}{\partial k_i}|\beta\rangle = \langle\alpha|\frac{\partial}{\partial k_i}(H|\beta\rangle) - \langle\alpha|H|\frac{\partial u^\beta}{\partial k_i}\rangle$

$$= (\varepsilon^\beta - \varepsilon^\alpha)\langle\alpha|\frac{\partial u^\beta}{\partial k_i}\rangle - \frac{\partial \varepsilon^\beta}{\partial k_i}\cancelto{0}{\langle\alpha|\beta\rangle} \text{ since } \varepsilon^\alpha<\varepsilon^F<\varepsilon^\beta$$

sim. $= -(\varepsilon^\beta - \varepsilon^\alpha)\langle\frac{\partial u^\alpha}{\partial k_i}|\beta\rangle$

Use it: $\sigma_{xy} = \frac{e^2}{i\hbar} \sum_{\varepsilon^\alpha<\varepsilon^F<\varepsilon^\beta} \left\{ \langle\frac{\partial u^\alpha}{\partial k_2}|\beta\rangle\langle\beta|\frac{\partial u^\alpha}{\partial k_1}\rangle - \langle\frac{\partial u^\alpha}{\partial k_1}|\beta\rangle\langle\beta|\frac{\partial u^\alpha}{\partial k_2}\rangle \right\}$

$$= \frac{e^2}{h}\frac{1}{2\pi i}\int_{T^2} d^2k \left(\langle\frac{\partial u^\alpha}{\partial k_2}|\frac{\partial u^\alpha}{\partial k_1}\rangle - \langle\frac{\partial u^\alpha}{\partial k_1}|\frac{\partial u^\alpha}{\partial k_2}\rangle \right)$$

using $\sum_{\varepsilon^\alpha<\varepsilon^F<\varepsilon^\beta} \left(|\alpha\rangle\langle\alpha| + |\beta\rangle\langle\beta|\right) = 1$ ✪

<u>proof:</u> Use $\circledast$ to show

$$\frac{\sigma_{xy}}{c} = \frac{e^2}{i\hbar} \sum_{\varepsilon^\alpha < \varepsilon_F} \Big\{ \Big\langle \frac{\partial u^\alpha}{\partial k_2} \Big| \frac{\partial u^\alpha}{\partial k_1} \Big\rangle - \Big\langle \frac{\partial u^\alpha}{\partial k_1} \Big| \frac{\partial u^\alpha}{\partial k_2} \Big\rangle$$

$$+ \sum_{\varepsilon^\gamma < \varepsilon_F} \Big(\Big\langle \frac{\partial u^\alpha}{\partial k_1} \Big| \gamma \Big\rangle \Big\langle \gamma \Big| \frac{\partial u^\alpha}{\partial k_2} \Big\rangle - \Big\langle \frac{\partial u^\alpha}{\partial k_2} \Big| \gamma \Big\rangle \Big\langle \gamma \Big| \frac{\partial u^\alpha}{\partial k_1} \Big\rangle \Big) \Big\}$$

move $\frac{\partial}{\partial k}$

$$\Big\langle \frac{\partial u^\alpha}{\partial k_2} \Big| \gamma \Big\rangle \Big\langle \gamma \Big| \frac{\partial u^\alpha}{\partial k_1} \Big\rangle = \Big\langle \frac{\partial u^\gamma}{\partial k_1} \Big| \alpha \Big\rangle \Big\langle \alpha \Big| \frac{\partial u^\gamma}{\partial k_2} \Big\rangle$$

cancel.

Thus $\dfrac{\sigma_{xy}}{c} = \dfrac{e^2}{h} \displaystyle\sum_{\varepsilon^\alpha < \varepsilon_F} \frac{1}{2\pi} \int d^2k \left(\nabla_k \times A^{(\alpha)} \right) = \frac{e^2}{h} \sum_{\varepsilon^\alpha < \varepsilon_F} C_1^{(\alpha)}$

where $A_i^{(\alpha)}(\vec{k}) = -i \langle u_{\vec{k}}^{(\alpha)} | \frac{\partial}{\partial k_i} | u_{\vec{k}}^{(\alpha)} \rangle$

- manifestly quantized
- stable to perturbations of $U(x,y)$
- can use to calculate $C_1^{(\alpha)}$ using simple potentials, see TKNN (1982)