TKNN Invariant

Michael Gerace
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Introduction

- plan: perform fully QM calculation of $\gamma_y$ that makes quantization manifest.
- Assume: non-interacting electrons
  - periodic potential
  - zero temperature
- exact manipulations $
\Rightarrow \gamma_y \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 $H(\alpha)$
  - $\alpha$ parameters that I vary.
  - Usually $\alpha$ fixed & solution in terms of eigenstates $|n,\alpha\rangle$
  
  $H(\alpha)|n,\alpha\rangle = E_n^\alpha|n,\alpha\rangle$

- Equation of $i\hbar \frac{d}{dt}|\Psi\rangle = H|\Psi\rangle$ $\Rightarrow |\Psi(t)\rangle = e^{-iE_n^\alpha t}|n,\alpha\rangle$

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

  Naive guess: $|\Psi(t)\rangle = \exp \left\{ -i \int_0^t E_n^{\alpha(t)} dt \right\} n,\alpha(t)\rangle$

  $\Rightarrow$ does not solve SE
\[ |\Psi(t)\rangle = \exp \left( i \int_0^t \sum n_i \alpha_i(t) \right) \int \langle n, \alpha(t) | \rangle \]

* Plug into TDS
e
\[ \Rightarrow \gamma_n = \int \langle n, \alpha(t) | \frac{\partial}{\partial t} | n, \alpha(t) \rangle \]
\[ \Rightarrow \gamma_n(t) = i \int_0^t \langle n, \alpha(t') | \frac{\partial}{\partial t} | n, \alpha(t) \rangle dt' = i \int_{\alpha(t')}^{\alpha(t)} \langle n, \alpha(t') | \partial_\alpha | n, \alpha \rangle d\alpha \]
\[ = \int_{\alpha(t')}^{\alpha(t)} A^n_{\alpha(i)} d\alpha \]

where \( A^n_i = i \langle n, \alpha | \partial_\alpha | n, \alpha \rangle \) is 1-form on parameter space \( C \)

* Analogy w/ external gauge fields.

In \( E+M \) drag particle through field, picks up phase

\[ \gamma = \int_{\alpha(t')}^{\alpha(t)} A^n_i(x) d\alpha \]

where \( B = \nabla \times A \)

Gauge freedom: \( |\psi\rangle \rightarrow e^{i A_{\alpha}} |\psi\rangle \)

\[ A_{\alpha} \rightarrow A_{\alpha} - \partial_\alpha \]

Berry Drag system through \( C \), \( \beta \) picks up phase

\[ \gamma = \int_{\alpha(t')}^{\alpha(t)} A^n_{\alpha(i)} d\alpha \]

Under \( \langle n, \alpha | \rightarrow e^{i A_{\alpha}} \langle n, \alpha | \)

\[ A^n_{\alpha} \rightarrow A^n_{\alpha} - \partial_\alpha \]

* Think of \( A^n_i \) as gauge field on \( C \) associated to global phase symm of wavefunction at each point \( \alpha \in \Omega \).

**Note:** Infinite number! One for each energy eigenstate.
Magnetic Brillouin Zone

Setup:

- 2D sample w/ const \( \mathbf{B} = B \mathbf{r} \)

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

- lattice potential \( U(x, y) \)
  
  \[ U(x+\mathbf{a}, y) = U(x, y+\mathbf{b}) = U(x, y) \]

- wish to determine bond structure, but some complications

Recall usual story from Dung's talk:

- translationally invariant Hamiltonian
  
  \[ [T_{\alpha}, H] = [T_{\beta}, H] = 0 \]
  \[ [T_{\alpha}, T_{\beta}] = 0. \]

- choose wavefunctions diagonalizing them all
  
  \[ \Psi(x, y) = e^{i \mathbf{k} \cdot \mathbf{r}} \Phi_{\mathbf{k}}(x, y), \quad \mathbf{k} \in 1st \ brillouin \ zone \]

Vector Potential Complicates matters:

- \( \mathbf{A}(\mathbf{r}) \neq \mathbf{A}(\mathbf{r} + \mathbf{\ell}) \), so \( H \) not translationally invariant \( \mathbb{\bigstar} \)

- \( T_{\mathbf{\ell}} = e^{i \mathbf{k} \cdot \mathbf{\ell}} \) not gauge invariant since \( \mathbf{\ell} \rightarrow \mathbf{\ell} + e \mathbf{\ell} \)

- Fix by covariantizing
  
  \[ \hat{T}_{\mathbf{\ell}} = e^{i \mathbf{k} \cdot (\mathbf{\ell} + e \mathbf{a})} \]

\( \Rightarrow \hat{T}_{\mathbf{\ell}} \) invariant \& commutes w/ \( H = \frac{1}{2m} (p + eA)^2 + U \)
In our gauge, \( \hat{T}^a = T^a e^{i \frac{2\pi}{\hbar} (\mathbf{R} \cdot \mathbf{A})} \), so this just regular translation + gauge transf

(makes sense since can use gauge transf to undo \( \hat{Q} \))

- Prob: \( \hat{T}^a \)'s don't commute

\[
\hat{T}^a \hat{T}^b = e^{i \gamma_{ab}} \hat{T}^b \hat{T}^a \quad \text{where} \quad \gamma = \frac{e}{\hbar} \mathbf{B} \text{per unit cell}
\]

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

- Can be fixed to if assume \( \Phi = \frac{\pi}{4} \) since may choose multiple cells containing \( \frac{1}{2} \) integer flux.

Ex.

\[
\hat{T}_a \hat{T}_b = \hat{T}_b \hat{T}_a
\]

(in end will take limit for irrational \( \Phi \))

- Call "magnetic unit cell"

- Now have commuting operators + can choose eigenfunctions

\[
\chi^\text{m}(x,y) = e^{i k \cdot F} \psi^\text{m}(x,y)
\]

\( \Gamma \in \text{"magnetic Brillouin zone"} \)

Remember magnetic Brillouin zone is torus!
Chern Number

- for each \( k \), \( u_k^{(l)} \) are solutions to
  \[
  \frac{\hbar^2}{2m} \left( -i \hbar \nabla + ik + eA \right)^2 + U(r) u_{k}^{(l)}(r) = \varepsilon_{k}^{(l)} u_{k}^{(l)}
  \]
  (\( \varepsilon \)) labels band

- \( H \) function of parameter \( k \in T^2 \) so can define berry correction on \( T^2 \):
  \[
  A_{i}^{(l)}(k) = i \langle u_k^{(l)} | \frac{\partial}{\partial k_i} | u_k^{(l)} \rangle
  \]

- under \( k \)-dep redef of \( \lambda \) local phase \( u_k^{(l)} = e^{i\lambda(k)} u_k^{(l)} \)
  \[ A_i \rightarrow A_i - \partial_i \lambda \]

- Define chern no. to be "magnetic flux" through \( T^2 \)
  \[
  C_{\gamma} = \frac{1}{2\pi i} \int_{T^2} (\nabla \times A^{(l)}) \, d^2k
  \]

- Theorem: \( C_{\gamma} \) is an integer

Nonrigorous argument:

- for \( C_{\gamma} \neq 0 \), \( \lambda \) 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

\[
A_\alpha = A_\beta + d\chi \text{ for some } \chi.
\]
- Arises from inability to define phase on $T^2$

Try:
- fix phase of $u$ by declaring
  
  $U_k(x',y')$ real for some fixed $(x',y')$.

- it may be $U_k(x',y') = 0$ for some $k'$, does not work here.

- let $II$ be small area containing $I'$, $I$ be everything else

  \[ \text{Phase of } U_k(x,y) \]

  \[ \rightarrow \rightarrow \rightarrow I \]

  \[ \rightarrow \rightarrow \rightarrow - \]

  \[ \rightarrow \rightarrow \rightarrow - \]

  \[ \rightarrow \rightarrow \rightarrow - \]

- define phase on $II$ by fixing
  
  $U_k(x'^2,y'^2)$ real on $II$ for some $x'^2,y'^2$

- defines new non-constant phase of $U_k(x',y')$ on $II$.

- encircle $I'$: phase wraps $n$ times.

- $I + II$ wavefunctions differ by gauge

  \[ |U_k^{II} \rangle = e^{i\chi(x)} |U_k^I \rangle \quad \Rightarrow \quad A_{II} = A_I \quad \partial_x \]

  \[ A \text{ differs by gauge trans.} \]

- \[ \frac{1}{2\pi} \int_{T^2} (\nabla \chi) = \frac{1}{2\pi} \int_{I} (\nabla \chi_I) + \frac{1}{2\pi} \int_{II} (\nabla \chi_{II}) = \frac{1}{2\pi} \int_{\partial B} \hat{e}_\mu (A_{II}^{\mu} - A_{I}^{\mu}) \]

  \[ \text{I + II induce app. orientations on B} \]

  \[ \text{General Case:} \quad \text{Chern no is vorticity of phase on } T^2. \]

  \[ \text{i.e. no. of zeros of fixed component } u_k^{\infty}(x',y') \text{ viewed as func of } I' \]

  \[ \text{ind. of } (x',y') \]

  \[ \text{will not change under small def of } U_k(x,y) \]

  \[ \text{only when bands merge, } 2 \text{ As become one does } \]

  \[ \text{C \text{ change}.} \]
Hall Conductance

- Will show \( \sigma_{xy} = \frac{e^2}{h} \varepsilon C_i \) sum over filled bands.
  - explicit quantization.

- Consider \( E_F \) between bonds, \( T=0, \omega=0 \). Kubo formula gives

\[
\sigma_{xy} = \frac{e^2}{c} \sum \frac{\langle \alpha | \nu_i \rangle \langle \nu_i | \beta \rangle - \langle \alpha | \nu_i \beta \rangle \langle \nu_i | \alpha \rangle}{(E_\alpha - E_\beta)^2}
\]

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

or Caycholl for proof.

- here \( |\alpha\rangle \) eigenstate of \( H \) w/ eigenvalue \( E_\alpha \)

- \( \nu_i = \frac{1}{m} (p_i + eA_i) = \frac{\hbar}{m} \partial / \partial k_i \) velocity operator

- implicit \( k_i \) indices \( \partial / \partial k_i \)

- Now \( \langle \alpha | \partial / \partial k_i | \beta \rangle = \langle \alpha | \frac{1}{m} (i\hbar \partial / \partial k_i) (H | \beta \rangle - \langle \alpha | H | \partial / \partial k_i \nu_i \rangle \)

\[
= (E_\beta - E_\alpha) \langle \alpha | \partial / \partial k_i | \nu_i \rangle - \frac{\hbar^2}{m} \partial / \partial k_i \langle \nu_i | \alpha \rangle
\]

\( \therefore \)

\[ \lim_{E_\beta \rightarrow E_\alpha} = -(E_\alpha - E_\beta) \langle \partial / \partial k_i | \nu_i \rangle \beta \]

Use it:

\[
\sigma_{xy} = \frac{e^2}{h} \sum \sum \left\{ \langle \alpha | \nu_i \rangle \langle \nu_i | \beta \rangle - \langle \alpha | \nu_i \beta \rangle \langle \nu_i | \alpha \rangle \right\}
\]

\[
= \frac{e^2}{h} \sum \sum \left\{ \langle \alpha | \langle \nu_i | \beta \rangle - \langle \alpha | \nu_i \beta \rangle \langle \nu_i | \alpha \rangle \rangle \right\}
\]

\( \sum \sum \langle \alpha | \langle \nu_i | \beta \rangle - \langle \alpha | \nu_i \beta \rangle \langle \nu_i | \alpha \rangle \rangle = 1 \)
proof: use \( \Phi \) to show

\[
\frac{\mathcal{E}_{xy}}{\mathcal{C}} = \frac{e^2}{\hbar} \sum_{\varepsilon > \varepsilon_F} \left( \langle \psi_{\varepsilon} | \psi_{\varepsilon} \rangle \right) - \langle \psi_{\varepsilon} | \psi_{\varepsilon} \rangle
\]

\[
+ \sum_{\varepsilon > \varepsilon_F} \langle \psi_{\varepsilon} | \langle \phi_{\varepsilon_i} \phi_{\varepsilon_j} \rangle \rangle \sum_{\varepsilon > \varepsilon_F} \langle \psi_{\varepsilon} | \langle \phi_{\varepsilon_i} \phi_{\varepsilon_j} \rangle \rangle
\]

\[
\text{cancel} \Rightarrow \langle \psi_{\varepsilon} | \alpha \rangle \langle \alpha | \psi_{\varepsilon} \rangle
\]

Thus \( \mathcal{E}_{xy} = \frac{e^2}{\hbar} \sum_{\varepsilon > \varepsilon_F} \frac{1}{2 \pi} \int d^2 k \langle \psi_{\varepsilon} | \hat{A}^{(1)} \rangle = \frac{e^2}{\hbar} \sum_{\varepsilon > \varepsilon_F} C^{(1)} \)

where \( \hat{A}^{(1)}(k) = -i \langle \psi_{\varepsilon} | \frac{\partial}{\partial k} | \psi_{\varepsilon} \rangle \)

- manifestly quantized

- stable to perturbations of \( U(x, y) \)

- can use to calculate \( C^{(1)} \) using simple potentials, see TKNN (1982)