Lattice Geometry Dependence and Independence: Important Applications of a Simple Law

Steven H. Simon and Mark S. Rudner, Phys. Rev. B **102**, 165148, 2020

EPSRC

UNIVERSITY OF OXFORD

Tight Binding Models

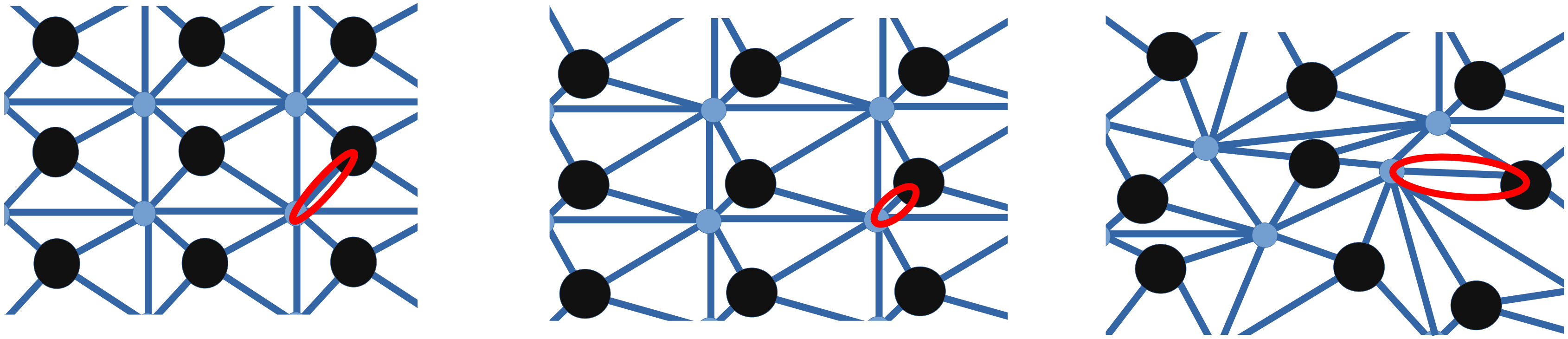
$$H = \sum_{i,j} t_{ij}\, c_i^\dagger c_j$$

Geometry Independent

Eigenenergies: ϵ_α

Eigenfunctions: $|\alpha\rangle = \sum_i \psi_i^{(\alpha)} |i\rangle$

We have still not specified any geometry! = “real space embedding”



Two ordered and one disordered geometry: Can all share the same *H*

Geometry Independent:

Eigenenergies, Eigenfunctions

Current along a bond i to j

$$j_{ij}^{(\alpha)} = \frac{-i}{2}\left(t_{ij}\psi_i^{(\alpha)*}\psi_j^{(\alpha)} - h.c.\right)$$

Geometry Dependent:

Charge distribution of an eigenstate

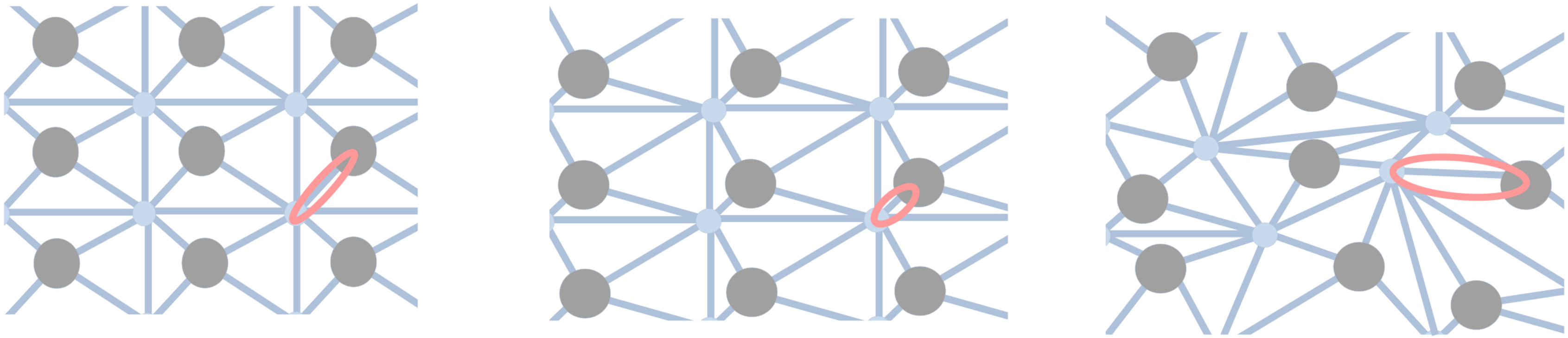
$$q_\alpha(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r_i}) |\psi_i^{(\alpha)}|^2$$

SUMMARY OF TALK

Crucial to keep track of which quantities are geometry independent and which are geometry dependent!

Analogous to gauge invariance, quantities which should be geometry indep must behave this way in any calculation.

Many “established” results in the literature fail this test!



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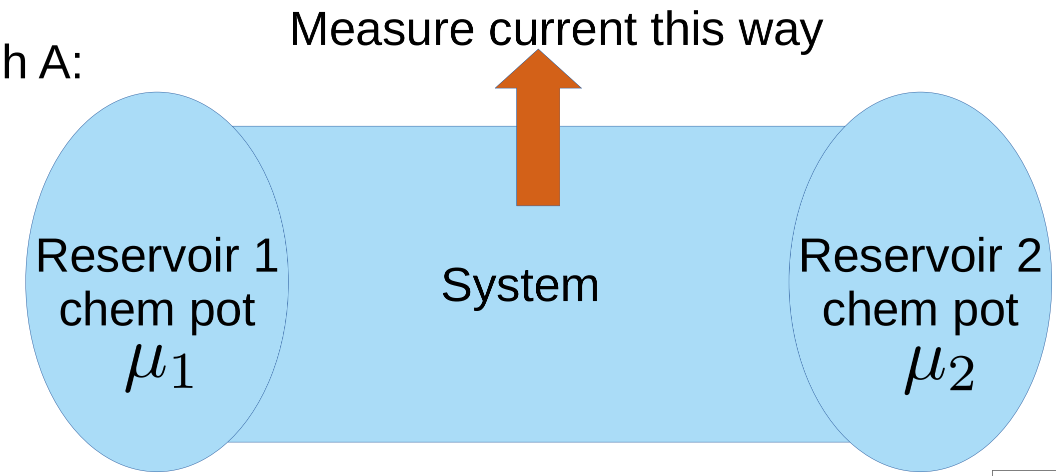
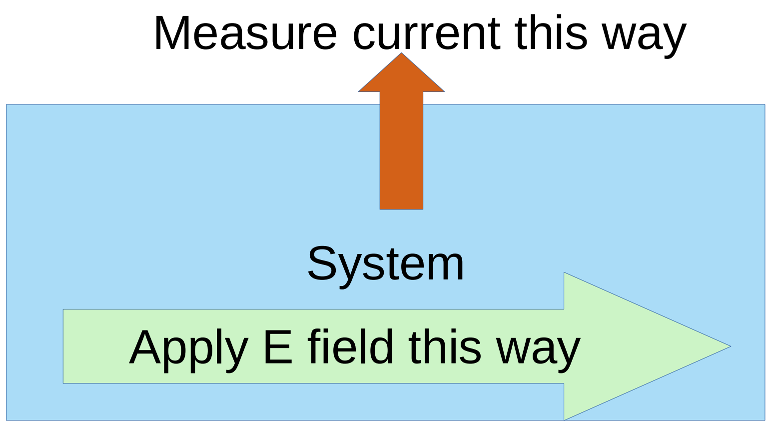
Example 1: Hall Response

Apply a bias in x-direction, measure current in y-direction

Approach A:



Approach B:



These look similar …. but
… are entirely different

A is geometry independent
B is geometry dependent

They cannot act the same!

Both can be measured
in cold atoms

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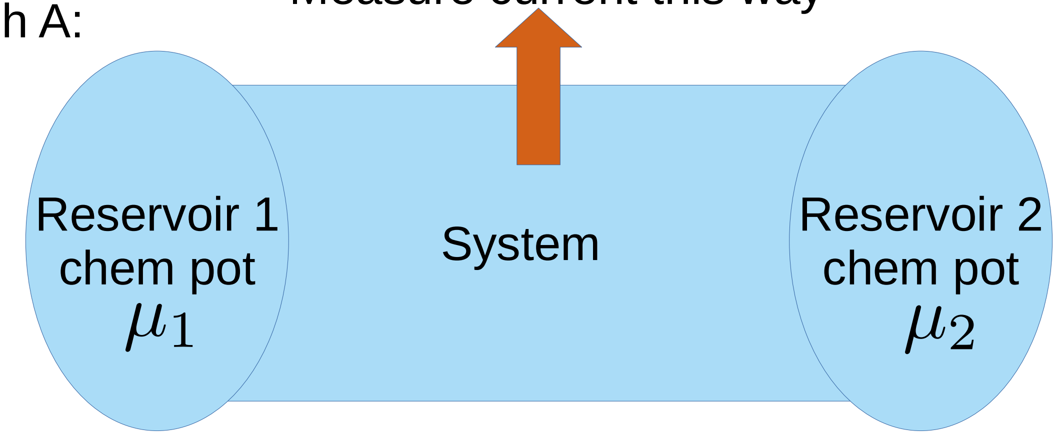

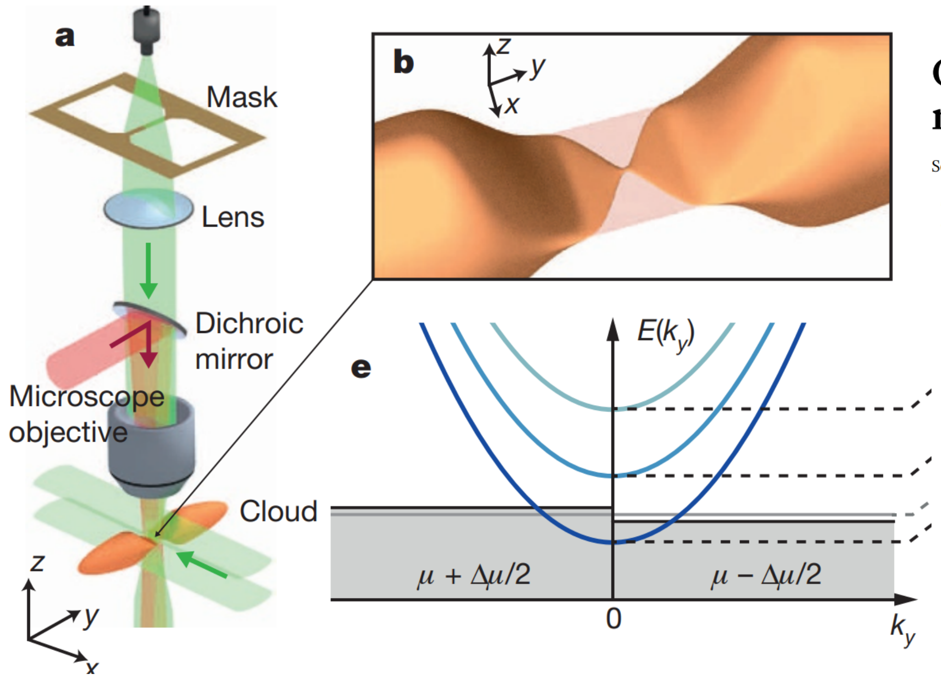

Observation of quantized conductance in neutral matter

Sebastian Krinner[1], David Stadler[1], Dominik Husmann[1], Jean-Philippe Brantut[1] & Tilman Esslinger[1]

NATURE | VOL 517 | 1 JANUARY 2015

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Example 1: Hall Response

Apply a bias in x-direction, measure current in y-direction

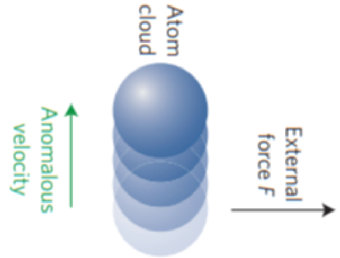
LETTERS

PUBLISHED ONLINE: 8 DECEMBER 2014 | DOI: 10.1038/NPHYS3171

nature physics

Measuring the Chern number of Hofstadter bands with ultracold bosonic atoms

M. Aidelsburger[1,2*], M. Lohse[1,2], C. Schweizer[1,2], M. Atala[1,2], J. T. Barreiro[1,2†], S. Nascimbène[3], N. R. Cooper[4], I. Bloch[1,2] and N. Goldman[3,5]



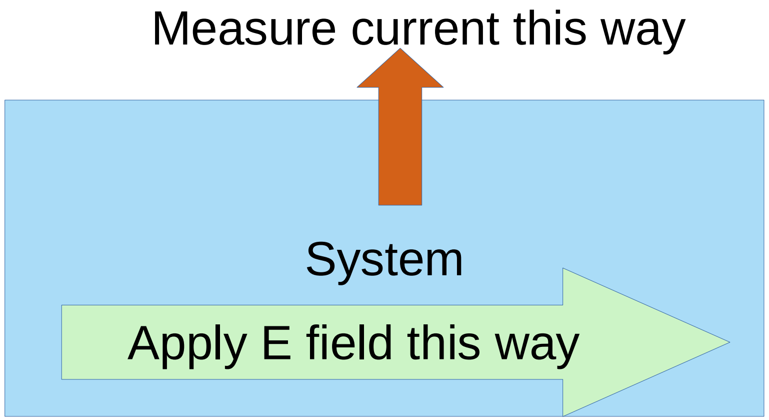
QUANTUM SIMULATION

Experimental reconstruction of the Berry curvature in a Floquet Bloch band

SCIENCE 27 MAY 2016 • VOL 352 ISSUE 6289 1091

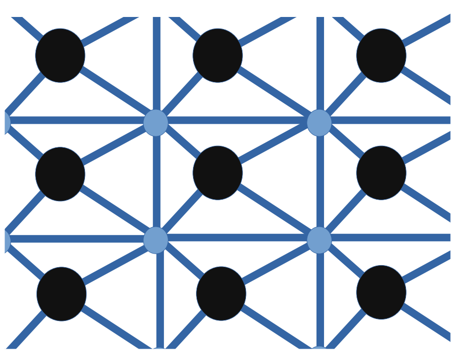
N. Fläschner,[1,2*] B. S. Rem,[1,2*] M. Tarnowski,[1] D. Vogel,[1] D.-S. Lühmann,[1] K. Sengstock,[1,2,3†] C. Weitenberg[1,2]

Approach B:

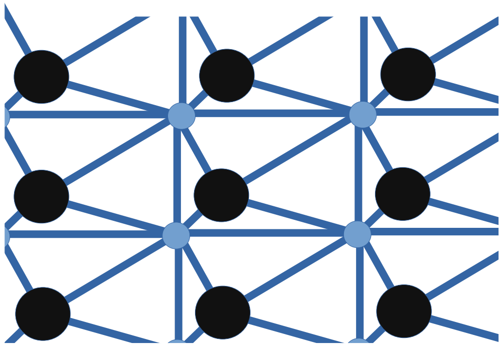


Both can be measured in cold atoms

Approach B:



vs



Apply E field this way

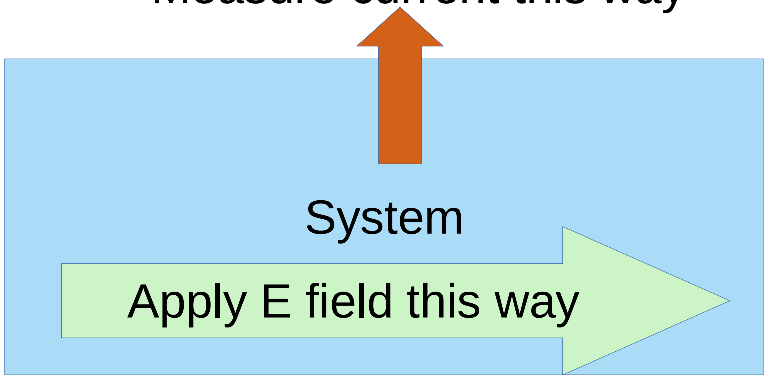
$$\mathbf{E}(\mathbf{r}) = \nabla\phi(\mathbf{r})$$

E may be uniform, but ϕ is not

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_i \phi(\mathbf{r}_i) c_i^\dagger c_i$$

Approach B:

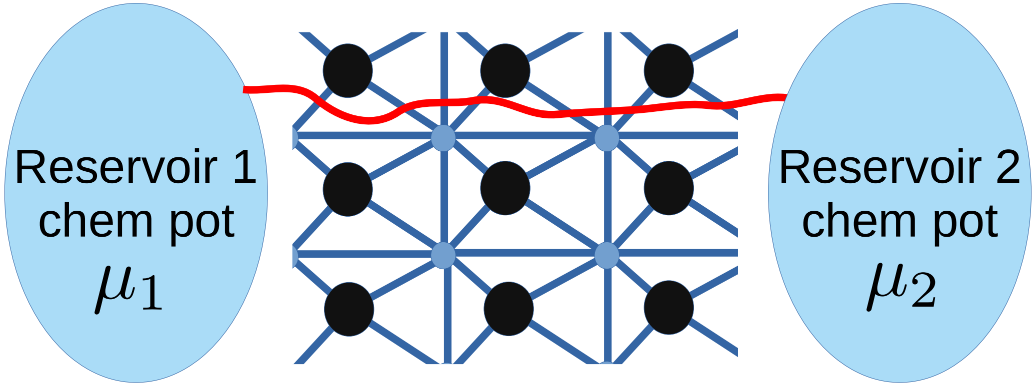
Measure current this way



Explicit geometry dependence

Approach A:

measure current crossing red line



$$H = \sum_{i,j} t_{ij}\, c_i^\dagger c_j \quad + \sum_i V_i c_i^\dagger c_i + \sum_i U_i n_i^2 + \ldots$$

Nowhere do we need to specify the position of any orbitals!

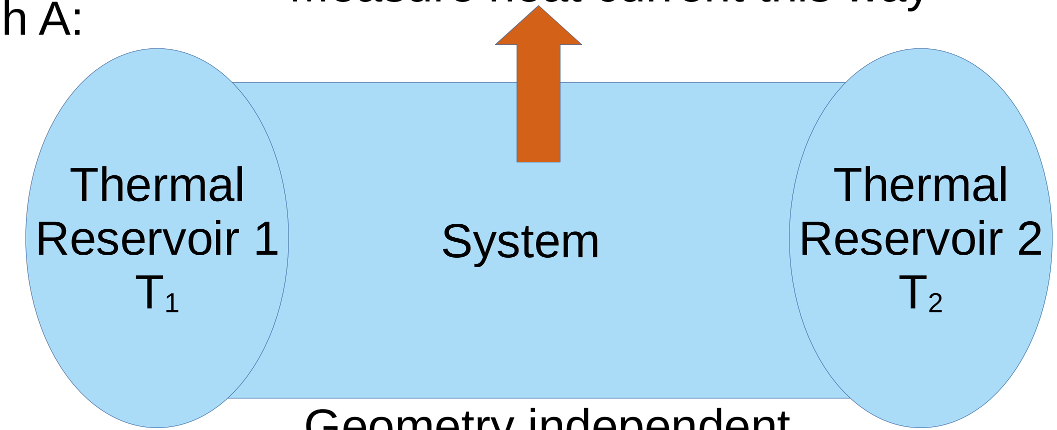
Hall current must be geometry indep!

Example 1a: Thermal Hall Response (Righi-Leduc Effect)

Apply thermal bias in x-direction, measure heat current in y-direction

Approach A:

Measure heat current this way



Geometry independent

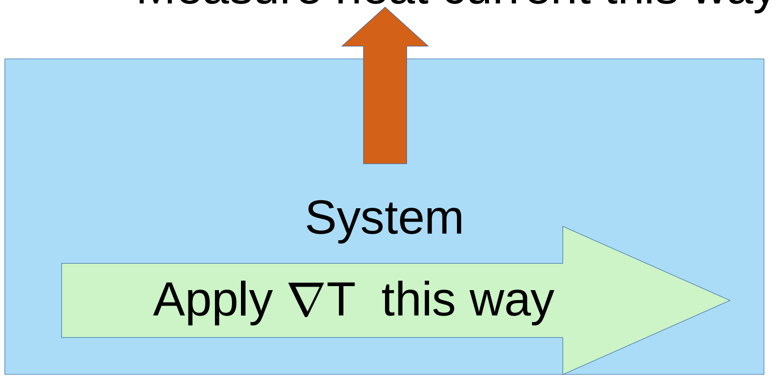
Isolated system
Heated only from ends

Similar story

… and also similar for other transport coefficients too

Approach B:

Measure heat current this way

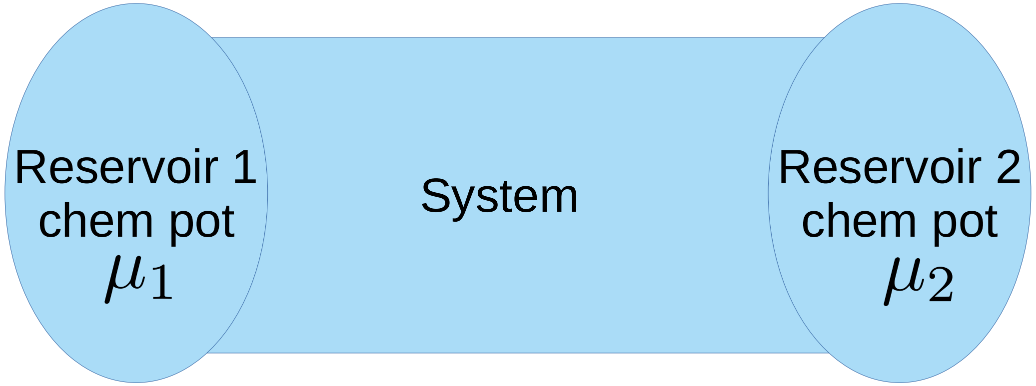


Geometry dependent

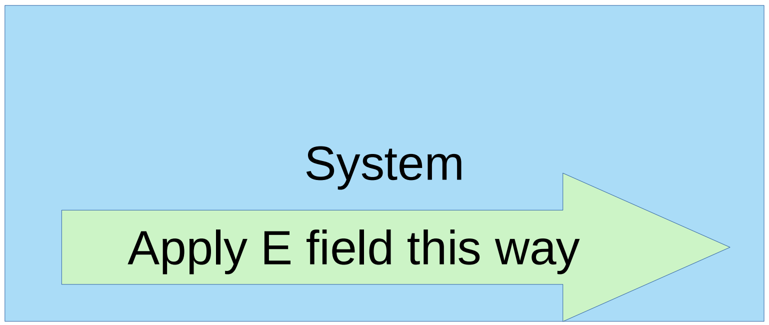
Coupling to (ex) Phonon Heat Bath everywhere

(Back to regular Hall)

Approach A: Geometry Independent



Approach B: Geometry Dependent



But could there be a conspiracy?… could (B) end up being unexpectedly geometry indep?

Q&A

You're Living in the Golden Age of Conspiracy Theories

How the coronavirus pandemic primed America for a new pandemic of misinformation.

Periodic crystal / no disorder / no interaction / 2D / Remove edges:

Calculations can be done exactly

Approach A: Geometry Independent

velocity

Fermi occupancy

$$\mathbf{j} = \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^2} \nabla_{\mathbf{k}}\epsilon(\mathbf{k})\, n(\mathbf{k})$$

$$n(\mathbf{k}) = \begin{cases} n_F(\varepsilon(\mathbf{k}) - \mu_1) & v_x(\mathbf{k}) > 0 \\ n_F(\varepsilon(\mathbf{k}) - \mu_2) & v_x(\mathbf{k}) < 0 \end{cases}$$

Right movers carry μ_1

Left movers carry μ_2

Approach B: Geometry Dependent (Kubo Formula [strictly ω to 0 limit])

$$\mathbf{j}_{Hall} = e\mathbf{E} \times \hat{z} \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^2} \Omega(\mathbf{k}) n(\mathbf{k})$$

Berry Curvature

But could there be a conspiracy?… could (B) end up being unexpectedly geometry indep?

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Detour: What is Berry Curvature?

Berry phase effects on electronic properties
Xiao, Chang, Niu
RMP 82, 1959, 2010

$$\dot{\mathbf{r}} = \nabla_{\mathbf{k}}\epsilon(\mathbf{k}) - \dot{\mathbf{k}} \times \boldsymbol{\Omega}(\mathbf{k})$$

$$\dot{\mathbf{k}} = -e\mathbf{E} - e\dot{\mathbf{r}} \times \mathbf{B}$$

Semiclassical dynamics
in Bloch Bands

$$H = \sum_{i,j} t_{ij} c_i^\dagger c_j$$

B, E must be small – large B put into band structure
WLOG we drop B

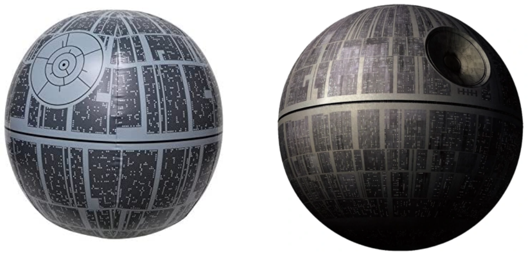
Filled Bloch band (2D):

$$\mathbf{j} = \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^2}\,\dot{\mathbf{r}}_{\mathbf{k}} = \underbrace{e\mathbf{E}}_{-\dot{\mathbf{k}}} \times \hat{z} \underbrace{\int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^2}\,\Omega(\mathbf{k})}$$

Chern Number (integer) = quantized Hall conduction
of filled band ("Chern-Insulator")

Gauss-Bonnet Theorem

$$\frac{1}{2\pi}\int_M K\,dA = \chi(M)$$



Quantized Hall Conductance in a Two-Dimensional Periodic Potential

D. J. Thouless, M. Kohmoto,[a] M. P. Nightingale, and M. den Nijs
Department of Physics, University of Washington, Seattle, Washington 98195
(Received 30 April 1982)

Landau Level:

$$\epsilon(\mathbf{k}) = \text{constant}$$

$$\Omega(\mathbf{k}) = \text{constant}$$

Calculating Berry Curvature?

Bloch function
Periodicity of unit cell

Bloch's theorem: Geometry indep

$$|\psi(\mathbf{k})\rangle = \sum_{\mathbf{R},\alpha} e^{i\mathbf{k}\cdot\mathbf{R}} \psi_\alpha(\mathbf{k})|\alpha, \mathbf{R}\rangle = e^{i\mathbf{k}\cdot\hat{\mathbf{r}}}|u(\mathbf{k})\rangle$$

Unit cell reference point
Orbital within unit cell

$$|u(\mathbf{k})\rangle = \sum_{\mathbf{R},\alpha} u_\alpha(\mathbf{k})|\alpha, \mathbf{R}\rangle$$

Only geom dep part

$$u_\alpha(\mathbf{k}) = \underbrace{e^{-i\mathbf{k}\cdot\mathbf{x}_\alpha}}\psi_\alpha(\mathbf{k})$$

$$\mathbf{A}(\mathbf{k}) = i\langle u(\mathbf{k})|\nabla_\mathbf{k}|u(\mathbf{k})\rangle$$ Berry Connection

$$\Omega(\mathbf{k}) = \nabla_\mathbf{k} \times \mathbf{A}(\mathbf{k})$$ Berry Curvature

$$\mathbf{x}_\alpha \rightarrow \mathbf{x}_\alpha + \delta\mathbf{x}_\alpha$$

$$\Omega(\mathbf{k}) \rightarrow \Omega(\mathbf{k}) + \nabla_\mathbf{k} \times \underbrace{(\delta\mathbf{x}_\alpha|u_\alpha(\mathbf{k})|^2)}_{\langle\delta\mathbf{x}\rangle_\mathbf{k}}$$

$$C = \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^2}\Omega(\mathbf{k})$$

unchanged

Periodic crystal / no disorder / 2D / Remove edges: Calculations can be done exactly

Approach A: Geometry Independent

Fermi occupancy

velocity

$$\mathbf{j} = \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^2} \nabla_{\mathbf{k}} \epsilon(\mathbf{k})\, n(\mathbf{k})$$

$$n(\mathbf{k}) = \begin{cases} n_F(\varepsilon(\mathbf{k}) - \mu_1) & v_x(\mathbf{k}) > 0 \\ n_F(\varepsilon(\mathbf{k}) - \mu_2) & v_x(\mathbf{k}) < 0 \end{cases}$$

With disorder both (A) and (B) become complicated. But (A) remains geometry indep

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$$\mathbf{j}_{Hall} = e\mathbf{E} \times \hat{z} \int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^2} \Omega(\mathbf{k}) n(\mathbf{k})$$

$$\mathbf{x}_\alpha \to \mathbf{x}_\alpha + \delta\mathbf{x}_\alpha$$

$$\Omega(\mathbf{k}) \to \Omega(\mathbf{k}) + \nabla_{\mathbf{k}} \times \langle \delta\mathbf{x} \rangle_{\mathbf{k}}$$

But could there be a conspiracy?… could (B) end up being unexpectedly geometry indep?

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No conspiracy

What about experiments in solid state?

(1) Electrons are charged, so *typically* one cannot apply chemical potential difference without electric field (although it is not impossible, at least in 2D)

Typically, one measures geometry dependent response.

(2) In spin systems with thermal transport, if the phonons decouple at low T, one *will* have geometry independent physics that violates Kubo!

Example 2: Fractional Chern Insulators and The Geometric Stability Conjecture

$$\mathbf{j} = e\mathbf{E} \times \hat{z} \underbrace{\int_{\mathrm{BZ}} \frac{d\mathbf{k}}{(2\pi)^2} \Omega(\mathbf{k})}$$

Chern Number (integer) = quantized Hall conduction of filled band ("Chern-Insulator")

Landau Level:

$$\epsilon(\mathbf{k}) = \text{constant}$$

$$\Omega(\mathbf{k}) = \text{constant}$$

More Generally

$\epsilon(\mathbf{k})$ Arbitrary

$\Omega(\mathbf{k})$ Arbitrary subject to integral being an integer

What happens with a partially filled band?

With no/weak interactions: Fermi sea fills lowest $\epsilon(\mathbf{k})$
With strong interactions: *might* form fractional quantum Hall state "Fractional Chern Insulator"

How do we design a hopping/interaction model to get FQHE

Example 2: Fractional Chern Insulators and The Geometric Stability Conjecture

FQHE is favored by band structures that "look" like Landau levels

⇒ $\Omega(\mathbf{k})$ should be constant in the Brillouin zone

Many authors (but in most detail by Jackson, Moller, Roy, Nat Comm 2015)

Observe correlation between size of FQH gaps and flatness of $\Omega(\mathbf{k})$

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Observe correlation between size of FQH gaps and flatness of $\Omega(\mathbf{k})$

This statement can’t be correct!

Every example studied used a particularly symmetric geometry of orbitals that happened to maximized flatness of Ω given the particular hopping/interaction model

Counter Example: Boson FQHE

$$H = \sum_{i,j} t_{ij} c_i^\dagger c_j + \sum_i U n_i^2$$

Geometry Independent Hamiltonian: FQH gaps indep of orbital positions

But $\Omega(\mathbf{k})$ changes with orbital positions!

Example 2: Fractional Chern Insulators and

The ***Modified*** Geometric Stability Conjecture

For each hopping/interaction model, one should first vary over geometry (ie., orbital positions) before measuring flatness of $\Omega(\mathbf{k})$

Conjecture: correlation between FQH gaps and this flatness of $\Omega(\mathbf{k})$
(given fixed [flat] dispersion)

Observe correlation between size of FQH gaps and flatness of $\Omega(\mathbf{k})$

Every example studied used a particularly symmetric geometry of orbitals that happened to maximized flatness of Ω given the particular hopping/interaction model

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Summary

Some quantities are geometry independent…
… others are geometry dependent

One cannot make geometry independent statements about geometry independent quantities and vice versa

Some objects (like Hall response) can be either geometry dependent or geometry independent depending on “details” of how they are probed.

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