OU Physics REU

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Quantum Geometry and Thermal Transport

Overview

1. Solid State Basics
2. The Quantum Integer Hall Effect
3. Quantum Geometry; Topological Invariants
4. Kubo Formulas; Correlation Functions
5. Thermal Conductivity
6. Flat Bands and Further Work

Chapter 1:
Solid State Basics

Solid State Basics

Part 1: Second Quantization

- Undergraduate quantum mechanics: single-particle systems, simple potentials.
- Condensed matter: many-body physics, complex periodic systems.
- How do we go from single-particle states to many-particle states?

$$\Psi(x,t) \rightarrow \Psi(x_1 \ldots x_N, t)$$

Solid State Basics

Part 1: Second Quantization

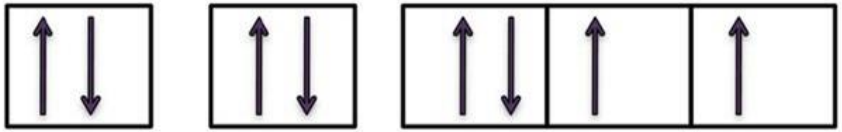
- Each individual particle in a many-body state can be expressed in a single particle basis.
- So naively, any (tensor) product of N single particle basis vectors is a suitable N-body state.
- A general N-body state can be written as a linear combination of these products.

$$\Psi(x_1 \ldots x_N, t) = \sum_{k_1 \ldots k_N} C(k,t) \psi_{k_1}(x_1) \ldots \psi_{k_N}(x_N)$$

Solid State Basics

Part 1: Second Quantization

- Not quite!
- The many-body state represents **identical** particles.
- This enforces an interchange symmetry, which constrains the form of the Hilbert space and can be quite complicated.
- New tool: **Second Quantization.**
- All states are expressed using creation and annihilation operators, $c_\alpha^\dagger$ and c_α.
- Counting states instead of tracking particles.



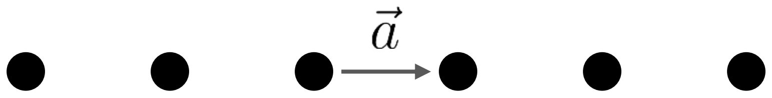
Chapter 1 Part 2

Transition Slide! Yippee!

WELCOME TO THE BOUILLON ZONE

Solid State Basics

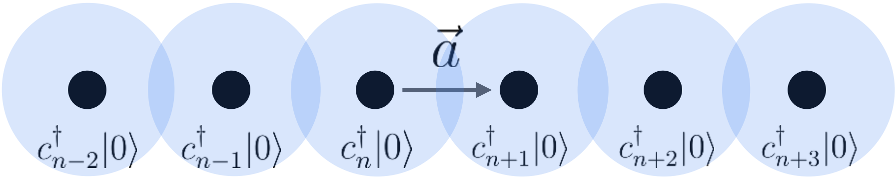
Part 2: Lattices and Reciprocal Space



- In solid state physics, we are interested in systems with **periodic potentials**.
- For example, consider a single electron in a 1D lattice of hydrogen nuclei, as shown above.
- The electron will feel a periodic sum of coulomb potentials. We ask, what are the energy eigenstates?

Solid State Basics

Part 2: Lattices and Reciprocal Space

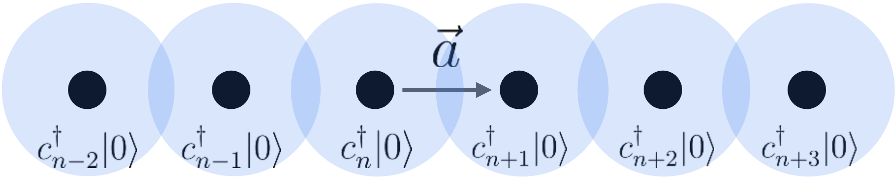


- The Schrodinger equation for this system is very difficult to solve directly.
- Instead, we use the tools of linear algebra and second quantization.
- We define an orthogonal single-particle basis localized at each nuclus.
- Each basis state is denoted by a creation operator $c_n^\dagger|0\rangle$.

$$H = \sum_{nm} c_n^\dagger \langle n|T+U|m\rangle c_m$$

Solid State Basics

Part 2: Lattices and Reciprocal Space



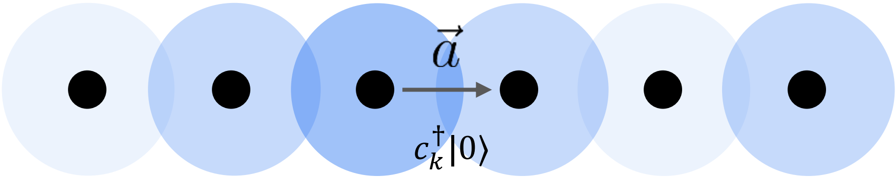
- Finding the eigenstates is reduced to diagonalizing H.
- We recall **Bloch's Theorem.**

> Eigenstates of a periodic Hamiltonian will have the same periodicity, up to a phase defined by a plane wave.

- So, instead of considering the individual atomic sites as our basis, it will be more useful to use their Fourier Transform.

Solid State Basics

Part 2: Lattices and Reciprocal Space



- New basis, indexed by a wavevector k.

$$c_k = \frac{1}{\sqrt{N}}\sum_n e^{-ik\cdot n} c_n\,; \quad c_k^\dagger = \frac{1}{\sqrt{N}}\sum_n e^{ik\cdot n} c_n^\dagger$$

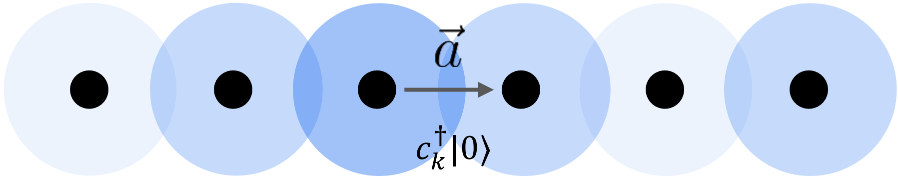
- In this new basis, it can be shown the Hamiltonian becomes

$$H = \sum_k c_k^\dagger h_k c_k$$

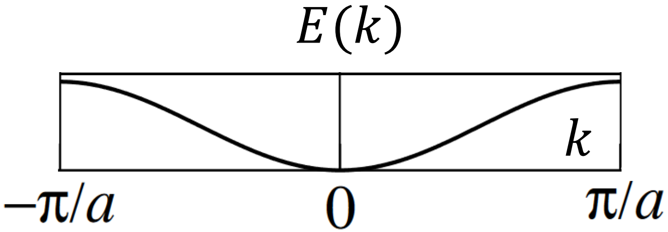
- Notice this is diagonal in k!
- That is, k is a good quantum number.

Solid State Basics

Part 2: Lattices and Reciprocal Space



- The space of all possible k is called the **Reciprocal Space.**
- This space is also a periodic lattice. The basic unit cell is called the **Brillouin Zone.**
- h_k gives us the energy of the eigenstate at each point in the Brillouin zone. This is called the **Band Structure.**



Solid State Basics

Part 3: General Systems

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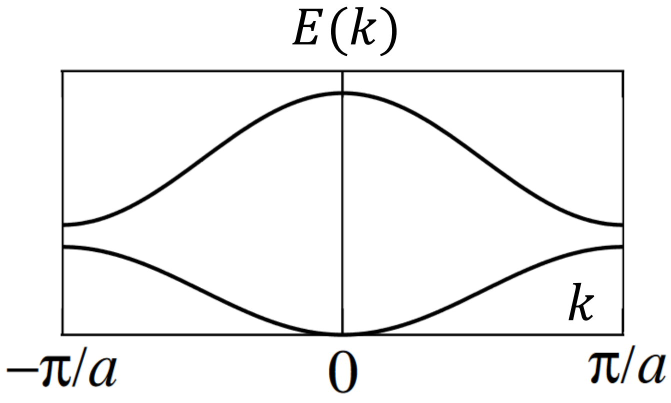
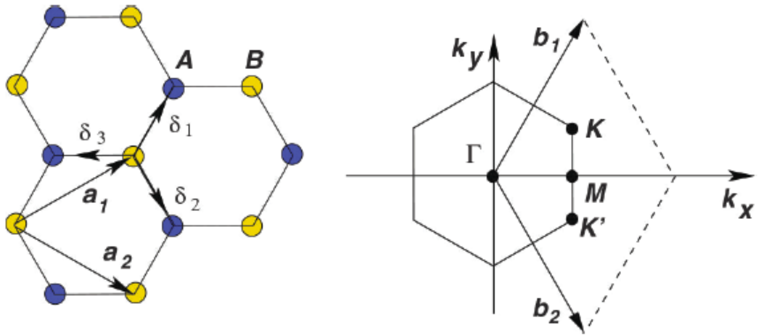


- In general, systems can have multiple localized states per lattice point
- This results in multiple bands in the Brillouin zone (h_k becomes a matrix).
- In many-electron systems, the single particle states are distributed thermally according to the Fermi distribution $f(k)$.

Solid State Basics

Part 3: General Systems

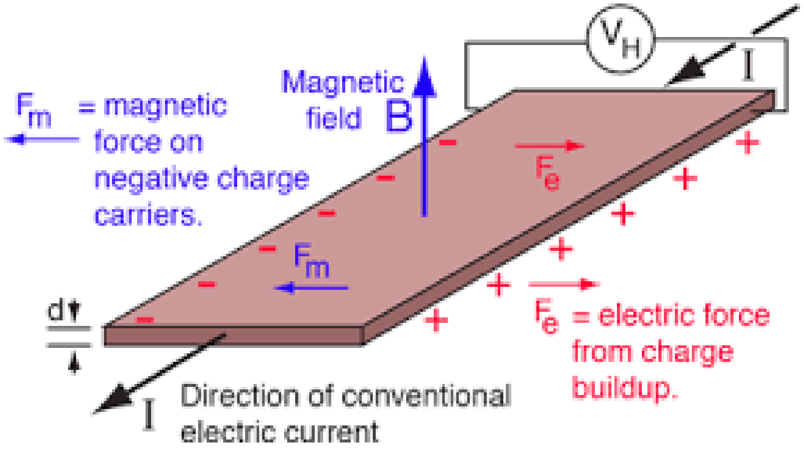


- In higher dimensional systems, the dimension of the Brillouin zone always matches the dimension of the lattice.
- We will focus on 2D systems, starting with possibly the first topological property observed in condensed matter.

Chapter 2:
The Quantum Integer Hall Effect

The Quantum Integer Hall Effect

- Recall the classical Hall effect



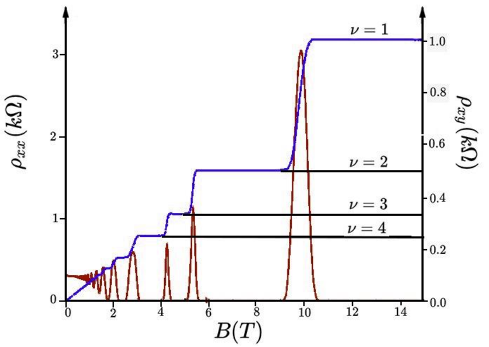
- We have a current J_x perpendicular to the electric field E_y.

The Quantum Integer Hall Effect

- The proportionality constant between the Hall current and the electric field is called the **Hall Conductance** σ_{xy}.

$$J_x = \sigma_{xy} E_y$$

- Turns out, when the magnetic field is sufficiently strong, the Hall conductance becomes quantized in integer multiples of $e^2/\hbar$.

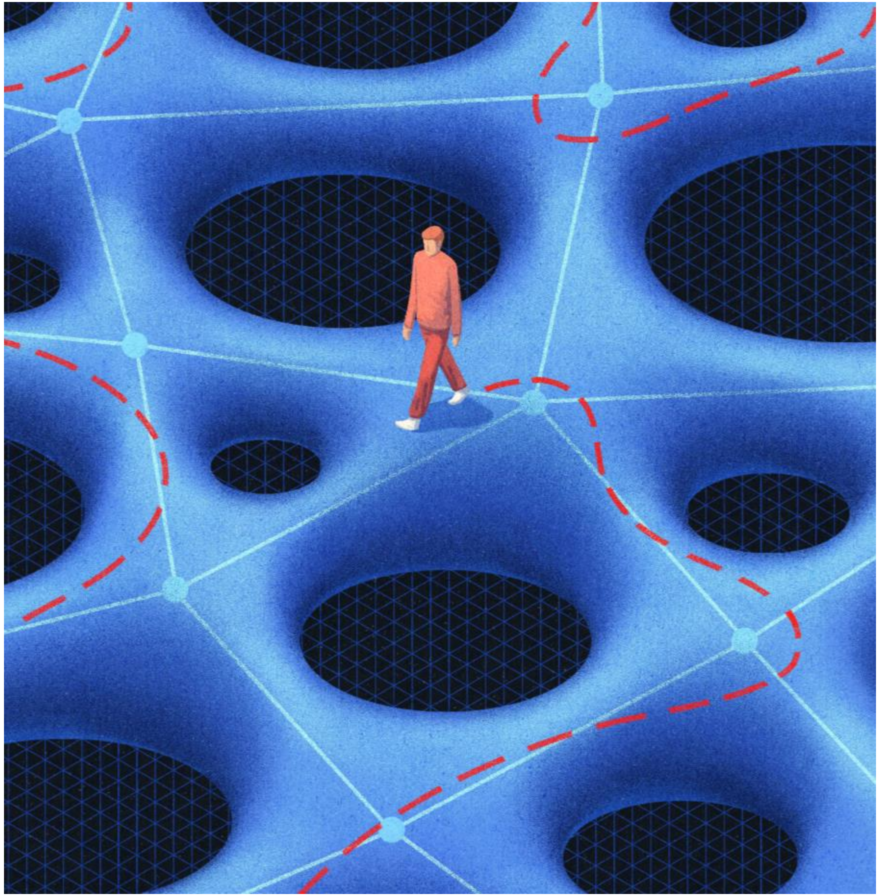


This is the Quantum Integer Hall Effect

The Quantum Integer Hall Effect

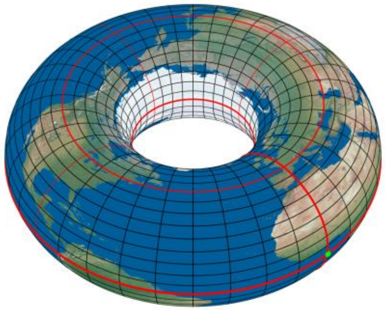
- This is often explained using the quantized motion of charged particles in a magnetic field (Landau levels).
- The Hall conductance can be more generally expressed in terms of the **Quantum Geometry.**
- This can have a nonzero effect even in the absence of a magnetic field, so it can be thought of as the more fundamental source of the Hall conductance.

Chapter 3:
Quantum Geometry;
Topological Invariants



Quantum Geometry

- Recall, every band in the Brillouin zone is a **Manifold**. For 2D systems, this manifold is (a priori) a torus.
- Every point k on this manifold represents an energy eigenstate $|nk\rangle$.
- This allows us to define a natural geometry – distance and curvature – on this manifold.



Quantum Geometry

- Two points k_1, k_2 are "closer" if their states $|nk_1\rangle, |nk_2\rangle$ are more similar.
- This motivates the definition of the **Quantum Metric**, which measures distance in the Brillouin zone.

$$g_n^{\mu\nu} = \frac{1}{2}(\langle\partial^\mu nk|\partial^\nu nk\rangle + \langle\partial^\nu nk|\partial^\mu nk\rangle)$$

- A curvature can also be defined on this manifold using parallel transport. The **Berry Curvature** is given by

$$\Omega_n^{\mu\nu} = i(\langle\partial^\mu nk|\partial^\nu nk\rangle - \langle\partial^\nu nk|\partial^\mu nk\rangle)$$

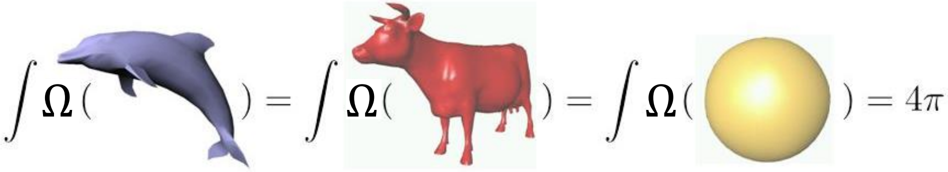
Quantum Geometry

- Together these form the **Quantum Geometric Tensor**.
- By itself, this tensor is not a topological invariant. Stretching/bending the Brillouin zone will change its value.
- However, as we know by the Chern-Gauss-Bonnet theorem, the integral of the Berry Curvature over the whole manifold is a topological invariant related to the Euler Characteristic.

Quantum Geometry

- This is the source of the quantization of the Hall conductance.
- If we can relate the Hall conductance to the integral of the Berry curvature (the **Chern Number**), we can demonstrate its quantization.

$$\int_{\mathcal{M}} \Omega \, dA = 2\pi \, \chi(\mathcal{M})$$



Chapter 4:

Kubo Formulas; Correlation Functions

Kubo Formulas

- So, how do we relate the Hall conductance to the Berry curvature?
- We start with the Kubo formula, which relates the **linear response** of an observable A to the time dependent perturbation H'.

$$\delta\langle A(t)\rangle = -i\int_{t_0}^{\infty} dt'\theta(t-t')\langle[A(t), H'(t')]\rangle_0 e^{-\eta(t-t')}$$

- For the Hall conductance, the observable we use is the current operator j, and the perturbation we use is $j \cdot A_{\text{ext}}$.

Kubo Formulas

- By comparing the result to the definition of electrical conductivity, we find

$$\sigma^{\mu\nu}(\omega) = \frac{1}{\hbar\omega_+ A}\int_0^\infty dt\, e^{i\omega_+ t}\langle[j^\mu(t), j^\nu(0)]\rangle$$

- These are called **Correlation Functions.**
- Evaluating the integral and skipping a bunch of steps, we get

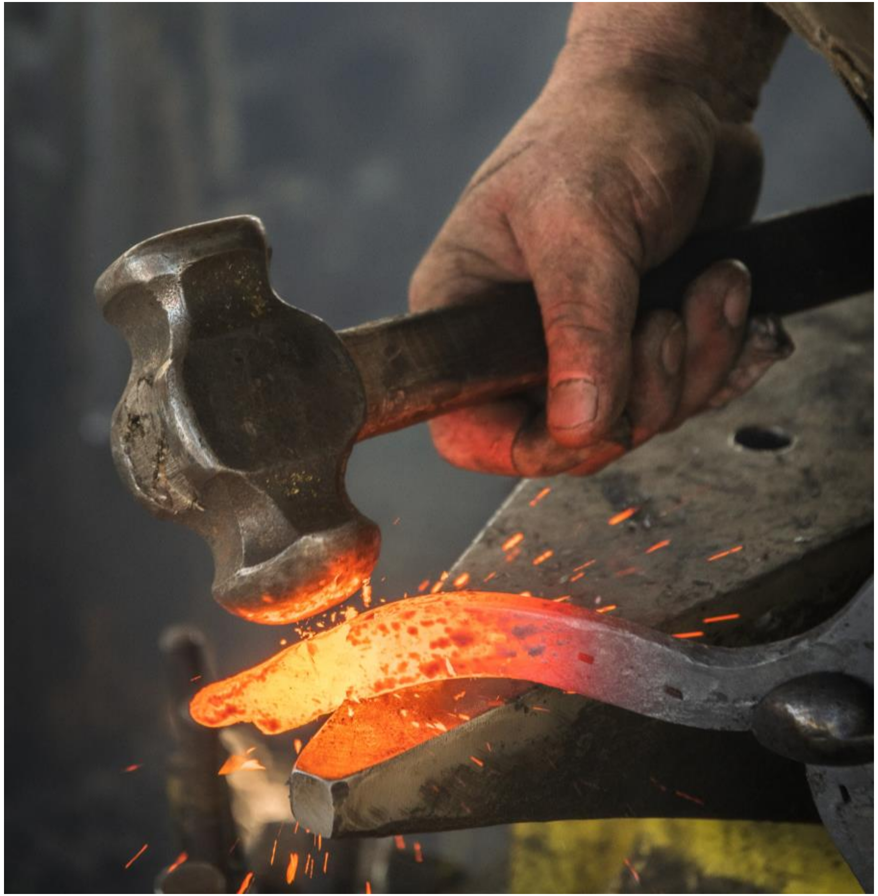
$$\sigma^{\mu\nu}(0) = -\frac{e^2}{\hbar}\sum_n \int_{\mathrm{BZ}} f_n(k)\Omega_n^{\mu\nu}$$

which is what we have stated before.

Kubo Formulas

- We now ask if we can do the same process for different currents.
- Can we relate the thermal conductivity to the quantum geometry?
- If the Hall conductance is related to the Berry phase, can we relate the longitudinal conductance to the quantum metric?
- These are the research questions I tackled this summer.

Chapter 5:
Thermal Conductivity



Thermal Conductivity

- I first derived the energy current operator $\boldsymbol{j}_q^E$ from the continuity equation

$$\frac{\partial K(x)}{\partial t} + \nabla \cdot \boldsymbol{j}^E(x) = 0$$

- Here K is the energy density operator. After Fourier transforming and a bunch of operator algebra, we have

$$\boldsymbol{j}_q^E = \frac{1}{\hbar} \sum_k c_k^\dagger h_k (\partial_k h_k) c_{k+q}$$

Thermal Conductivity

- To get the thermal conductivity, we analyze the heat current $\boldsymbol{J}^Q = \boldsymbol{J}^E - \mu \boldsymbol{J}^P$ up to linear response.
- Here, there are two “forces” that drive the corresponding currents.
- One relates to the temperature gradient, while the other relates to the potential and concentration gradient.
- The coefficients relating the currents to the forces are the **correlation functions** between the currents.

Thermal Conductivity

- I will sketch the derivation of the energy-energy current correlation function used to calculate the Hall conductivity ($\mu \neq \nu$).

$$L_{\mu\nu}^{(QQ)}(i\omega) = \frac{1}{\omega\beta\hbar}\int_0^{\beta\hbar} d\tau\, e^{i\omega\tau}\langle T_\tau[j_\mu^Q(\tau)j_\nu^Q(0)]\rangle$$

- This involves matrix elements in the form

$$\langle m|j_\mu^Q|n\rangle = \langle m|H_k(\partial_\mu H_k)|n\rangle$$

Thermal Conductivity

- Here m, n are energy eigenstates, so we can write
$$\langle m|H_k(\partial_\mu H_k)|n\rangle = E_m\langle m|(\partial_\mu H_k)|n\rangle$$
$$= E_m(E_n - E_m)\langle m|\partial_\mu|n\rangle$$
- Which is very close to the form of the Berry curvature!
- I will now state the result.

$$L_{\mu\nu}^{(QQ)} = -\frac{1}{\beta\hbar}\left(\sum_{mn}\int_{\mathrm{BZ}}\frac{A\,d^2\mathbf{k}}{(2\pi)^2}E_m E_n f_m(\mathbf{k})\Omega_{mn}^{\mu\nu}\right)$$

- Here

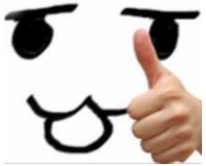
$$\Omega_{mn}^{\mu\nu} = i(\langle m|\partial_\mu|n\rangle\langle n|\partial_\nu|m\rangle - \langle m|\partial_\nu|n\rangle\langle n|\partial_\mu|m\rangle)$$

is not quite the Berry Curvature.

Thermal Conductivity

Other results:

1. I derived the conventional current-current conductivity using this method, which matched the TKNN formula.
2. I derived $L_{\mu\nu}^{(PQ)}$, which is the same as $L_{\mu\nu}^{(QQ)}$ except the energy factor is $(E_n + E_m)/2$.
3. I derived the longitudinal correlators, which are also close to but not quite the quantum metric.



$$K_{\alpha\beta} = \frac{1}{k_B T^2 A}\left[L_{\alpha\beta}^{(QQ)} - \frac{L_{\alpha\beta}^{(PQ)}\left[\epsilon_{\alpha\gamma} L_{2\gamma}^{(PP)} L_{1\beta}^{(PQ)} - \epsilon_{\alpha\gamma} L_{1\gamma}^{(PP)} L_{2\beta}^{(PQ)}\right]}{(L_{11}^{(PP)})^2 + (L_{12}^{(PP)})^2}\right]$$

Full thermal conductivity assuming $J^P = 0$. Second term is related to the thermoelectric effect.

$$L_{\mu\nu}^{(PP)} = -\frac{1}{\beta\hbar}\left(\sum_m \int_{\mathrm{BZ}} \frac{A\, d^2\mathbf{k}}{(2\pi)^2} f_m(\mathbf{k}) \Omega_m^{\mu\nu}\right)$$

$$L_{\mu\nu}^{(PQ)} = -\frac{1}{2\beta\hbar}\left(\sum_{mn} \int_{\mathrm{BZ}} \frac{A\, d^2\mathbf{k}}{(2\pi)^2} (E_m + E_n) f_m(\mathbf{k}) \Omega_{mn}^{\mu\nu}\right)$$

$$L_{\mu\nu}^{(QQ)} = -\frac{1}{\beta\hbar}\left(\sum_{mn} \int_{\mathrm{BZ}} \frac{A\, d^2\mathbf{k}}{(2\pi)^2} E_m E_n f_m(\mathbf{k}) \Omega_{mn}^{\mu\nu}\right)$$

$$L_{\mu\mu}^{(PP)}(\omega) = \frac{2i}{\beta\hbar\omega}\left(\sum_{mn} \int_{\mathrm{BZ}} \frac{A\, d^2\mathbf{k}}{(2\pi)^2} \omega_{mn} f_m(\mathbf{k}) g_{mn}^{\mu\mu}\right)$$

$$L_{\mu\mu}^{(PQ)}(\omega) = \frac{i}{\beta\hbar\omega}\left(\sum_{mn} \int_{\mathrm{BZ}} \frac{A\, d^2\mathbf{k}}{(2\pi)^2} \omega_{mn} (E_m + E_n) f_m(\mathbf{k}) g_{mn}^{\mu\mu}\right)$$

$$L_{\mu\mu}^{(QQ)}(\omega) = \frac{2i}{\beta\hbar\omega}\left(\sum_{mn} \int_{\mathrm{BZ}} \frac{A\, d^2\mathbf{k}}{(2\pi)^2} \omega_{mn} E_m E_n f_m(\mathbf{k}) g_{mn}^{\mu\mu}\right)$$

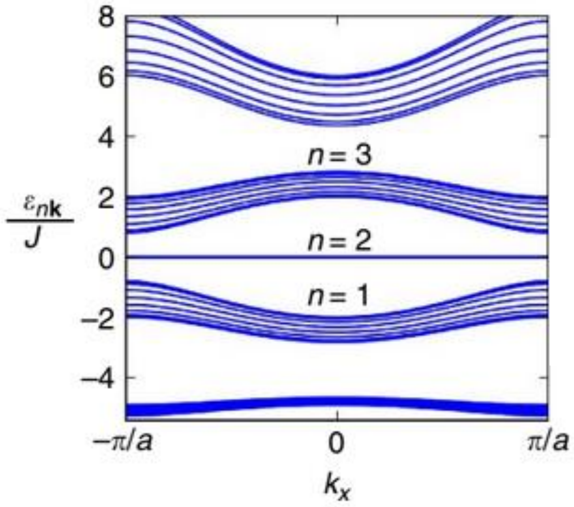
All transverse and longitudinal correlation functions.

Chapter 6:

Flat Bands and Further Work

Flat Bands and Further Work

- Recall, a **flat band** is a band in the Brillouin zone whose energy is constant.
- Condensed matter physicists like flat band systems because with no dispersion, the quantum geometry becomes more evident.



Flat Bands and Further Work

- Looking at the equation,

$$L_{\mu\nu}^{(QQ)} = -\frac{1}{\beta\hbar}\left(\sum_{mn}\int_{\mathrm{BZ}}\frac{A\,d^2\mathbf{k}}{(2\pi)^2}E_m E_n f_m(\mathbf{k})\Omega_{mn}^{\mu\nu}\right)$$

  we see the energy levels E_m and E_n obscure the quantum geometry.
- If we had flat bands, we could take E_m, E_n out of the k integral.
- The next step is to calculate the electrical and thermal conductivity using a generic **flat band** Hamiltonian and see if we get any topological invariants out.

Wait What?

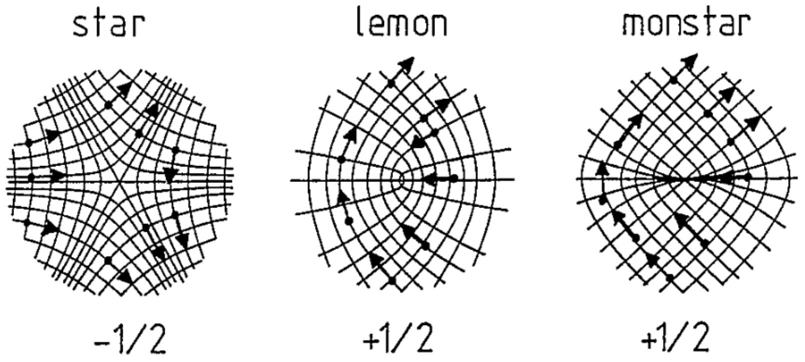
Wait What?

- How can a flat band conduct?
- Isn't the slope of $E(k)$ the velocity of the state?
- If we have a constant energy, how could we have any current at all?
- How could we have any conductivity?
- Aren't these states stationary?

- Well, the fact we have any conductivity at all is interesting, as we are dealing with **insulators.**
- Typically, filled bands cannot conduct.
- There must be something more going on!

Flat Bands and Further Work

- The answer is in the topology.
- In multi-band systems, h_k is not just a number but a matrix. $\partial_k h_k \neq 0$.
- It contains information on both the energy of the states and the **Vorticity.**
- This can create singularities in the Berry curvature and thus influence the topology of the Brillouin zone.



Flat Bands and Further Work

- Look back at

$$\sigma^{\mu\nu}(0) = -\frac{e^2}{\hbar}\sum_n \int_{\mathrm{BZ}} f_n(k)\Omega_n^{\mu\nu}$$

- The topology influences the calculation of this integral because different topological spaces must be parameterized indifferent ways.
- We say a torus has trivial topology because we can define a smooth single-valued gauge on it.
- So, the integral becomes trivial by Stokes' Theorem.

Questions?

References

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