Topology in condensed matter physics

0. Introduction

Some historical milestones

1931,	Dirac:	Dirac (magnetic) monopole
1961,	Skyrme	Topological solitons: skyrmions
1970-72,	Berezinskii Kosterlitz Thouless	BKT transition – driven by topological excitations (vertices). Nobel Prize 2016
1977	Leinaas Myrheim	anyons – particles in 2D that are neither fermions nor bosons
1980		Integer Quantum Hall Effect Nobel prize: von Klitzing, 1985
1982		Fractional QHE Nobel prize: Laughlin, Störmer, Tsui (1998)
1982	Haldane	Theory of antiferromagnetic Spin chains. Nobel Prize: 2016
1983	Thouless Kohmoto Nightingale Den Nijs	Topological band theory. Nobel Prize 2016 (Thouless)
1984		Berry phase
1988		Haldane model: QHE without Landau levels. Nobel prize: 2016

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2000-2001 Read, Green
Ivanov
Kitaev
Prediction of Majorana fermions in superconductors

2005-2006 Kane-Mele
Bernevig-Zhang
Quantum Spin Hall Effect (theory)

2007 Molenkamp
Experimental observation of QSHE

→ fast growth of the field of topological insulators and superconductors

2006-2009
Theoretical prediction and experimental discovery of magnetic skyrmions

2005 Geim
Novoselov
Graphene
Nobel prize 2010

Topology in condensed matter physics

1. Fundamental topological concepts

1.1. Guiding example I: Quantum particle on a ring (radius = 1 for simplicity)

Coordinate $\varphi \in [0, 2\pi]$

Φ - magnetic flux $\qquad \hbar = e = c = 1$

Hamiltonian: $\hat{H} = \frac{1}{2M}(-i\partial_\varphi - A)^2$

$A = \frac{\Phi}{\Phi_0}$ – vector potential

$\Phi_0 = \frac{hc}{e} \xrightarrow{\hbar=c=e=1} 2\pi$ flux quantum

Wave functions $\psi(\varphi)$; boundary condition $\psi(0) = \psi(2\pi)$

The stationary Schrödinger equation is, of course, trivially solved:

$\hat{H}\psi_n = \epsilon_n \psi_n$; $\psi_n(\varphi) = \frac{1}{\sqrt{2\pi}} e^{in\varphi}$; $\epsilon_n = \frac{1}{2M}(n - A)^2$

$n \in \mathbb{Z}$ (i.e. $n = 0, \pm 1, \pm 2, \ldots$)

Important: Observables, in particular energies ϵ_n, depend on A, even though the magnetic field is $= 0$ in the region accessible for the particle. This is Aharonov – Bohm effect

Feynman path integral (in imaginary time) $\tau = it$ for partition function

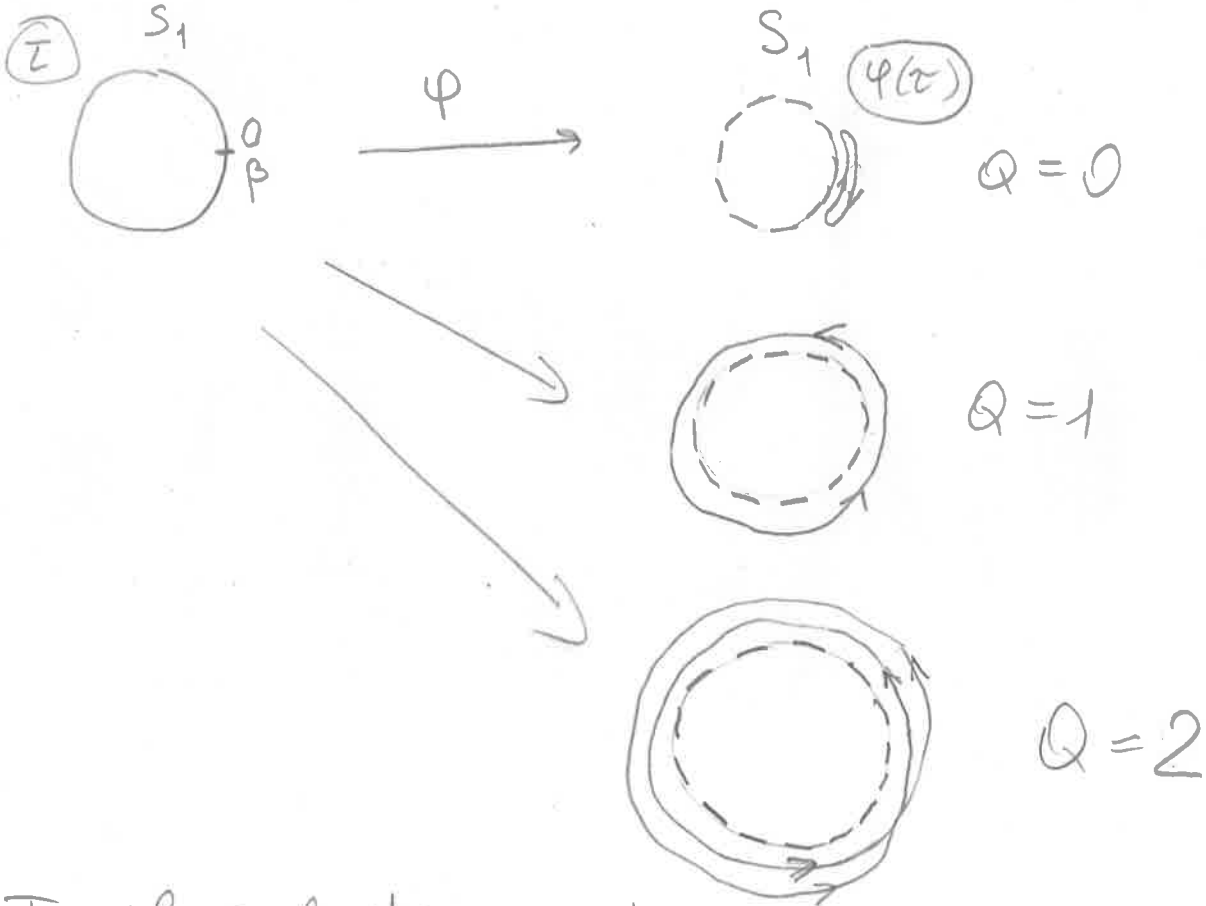
$$Z = \int_{\varphi(\beta)-\varphi(0) \in 2\pi\cdot\mathbb{Z}} D\varphi \, e^{-S[\varphi(\tau)]} \qquad \tau \in [0, \beta], \quad \beta = T^{-1}$$

$$S[\varphi] = \int d\tau \, L(\varphi, \dot{\varphi})$$

$$L(\varphi, \dot{\varphi}) = \frac{M}{2}\dot{\varphi}^2 - iA\dot{\varphi} \qquad \dot{\varphi} \equiv \frac{\partial \varphi}{\partial \tau}$$

$\varphi: S_1 \to S_1$ map $\tau \longmapsto \varphi(\tau)$

Q – winding number, $Q \in \mathbb{Z}$ $(Q = 0, \pm 1, \pm 2, \ldots)$



Topological term in the action:

$$S_{top} = \int_0^\beta d\tau \, (-iA\dot{\varphi}) = -iA[\varphi(\beta)-\varphi(0)] = -2\pi i \, Q A$$

$$Z = \sum_{Q\in\mathbb{Z}} e^{2\pi i Q A} \int_{\varphi(\beta)-\varphi(0)=2\pi Q} D\varphi\, e^{-\int d\tau \frac{M}{2}\dot{\varphi}^2}$$

Sum over distinct <u>topological sectors</u> characterized by the winding number $Q \in \mathbb{Z}$

* The top. term in the action, S_{top}, depends on $\varphi(\tau)$ only via the winding number Q; it cannot be changed by a continuous deformation of the trajectory $\varphi(\tau)$. This is why it is <u>topological</u>.
* As a related property, it does not affect eq. of motion:

$$\frac{\delta S[\varphi]}{\delta \varphi[\tau]} = 0 \iff M\ddot{\varphi} = 0$$

Euler-Lagrange equation

A does not enter!
(vector potential)

Nevertheless, the top. term does affect physical properties

* S_{top} is frequently called θ-term

$\theta = 2\pi A \rightarrow$ top. sectors have weights $e^{i\theta Q}$

Clearly, θ and $\theta + 2\pi n$ ($n \in \mathbb{Z}$) are equivalent.

$\rightarrow$ distinct physical situations are labeled by the <u>topological angle</u> $\theta \in [0, 2\pi]$

1.2. Guiding example II: Dirac monopole

Dirac 1931 Quantum-mechanical theory of a magnetic charge (monopole)

Maxwell eq. $\operatorname{div}\vec{B}=0$ $\longleftrightarrow$ no magnetic charge

But one can extend Maxwell equations by assuming existence of mag. charges:

$$\operatorname{div}\vec{B} = 4\pi\rho_m$$

Implications for quantum mechanics?

Imaging a monopole of strength (charge) g located at $\vec{r}=0$:

$$\operatorname{div}\vec{B} = 4\pi g\,\delta^3(\vec{r})$$

$\vec{\nabla}\left(\frac{1}{r}\right) = -\frac{\vec{r}}{r^3}$

$\Delta\left(\frac{1}{r}\right) = -4\pi\delta^3(\vec{r})$

$\rightarrow \vec{B} = g\frac{\vec{r}}{r^3}$ (in full analogy with electric field of a point charge)

$$\Phi = \oint_S \vec{B}\cdot d\vec{S} = 4\pi g$$ for a sphere or any other surface enclosing $\vec{r}=0$

Vector potential $\vec{A}$ for the monopole field?

$$\vec{A}^N(\vec{r}) = \frac{g}{r(r+z)}(-y\vec{e}_x + x\vec{e}_y) = \frac{g}{r}\frac{1-\cos\theta}{\sin\theta}\hat{e}_\varphi$$

$\vec{e}_\varphi = -\sin\varphi\,\vec{e}_x + \cos\varphi\,\vec{e}_y$

$\vec{e}_x, \vec{e}_y, \vec{e}_\varphi$ – unit vectors

(r, φ, θ) – polar coordinates

Calculate $\mathrm{rot}\,\vec{A}^N$

In polar coordinates the only non-zero component is $\propto \vec{e}_r$:

$$\mathrm{rot}\,\vec{A}^N = \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}\left(A^N_\varphi \sin\theta\right)\vec{e}_r = \frac{g}{r^2}\vec{e}_r ,$$

i.e. indeed the required monopole field.

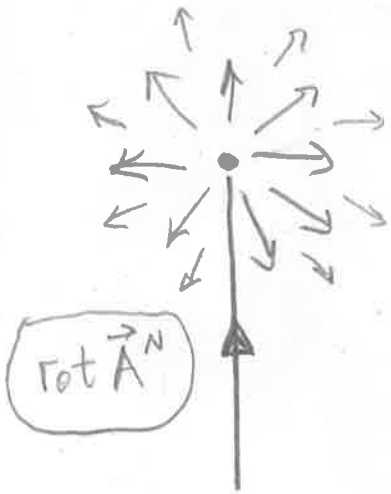
However, this is not fully correct since

$$\Phi = \oint_S \vec{B}\cdot d\vec{S} = \oint_S \mathrm{rot}\,\vec{A}\cdot d\vec{S} = \int_V \mathrm{div}\,(\mathrm{rot}\,\vec{A})\,d^3r = 0,$$

at variance with $\Phi = 4\pi g$ for $\vec{B} = \frac{g}{r^2}\vec{e}_r$.

The reason is the singularity at $\theta = \pi$ (i.e. at $r = -z$). In fact, a more accurate calculation yields (p. 5a)

$$\mathrm{rot}\,\vec{A}^N = \frac{g}{r^2}\vec{e}_r - \underbrace{4\pi g\,\delta(x)\delta(y)\theta(-z)\vec{e}_r}_{\text{"Dirac string"}}$$



The position of Dirac string is determined by our choice of $\vec{A}^N$. In particular, we can choose $\vec{A}$ in the form

$$\vec{A}^S(\vec{r}) = \frac{g}{r(r-z)}\left(y\vec{e}_x - x\vec{e}_y\right) =$$

$$= -\frac{g}{r}\,\frac{1+\cos\theta}{\sin\theta}\,\vec{e}_\varphi ,$$

with

$$\mathrm{rot}\,\vec{A}^S = \frac{g}{r^2}\vec{e}_r - 4\pi g\,\delta(x)\delta(y)\theta(z)\vec{e}_r$$

Addition to page 5 : derivation of $\mathrm{rot}\,\vec{A}^N$

$$A_x = -\frac{y}{r(r+z+\epsilon)} \quad ; \quad A_y = \frac{x}{r(r+z+\epsilon)}$$ included infinitesimal $\epsilon > 0$

$$\rightarrow B_z = \partial_x A_y - \partial_y A_x = \frac{2}{r(r+z+\epsilon)} - \frac{x^2+y^2}{r^3(r+z+\epsilon)} - \frac{x^2+y^2}{r^2(r+z+\epsilon)^2}$$

To get the δ-function term, focus on $r \simeq -|z|$.
The singularity comes from the first and the third term:

$$r+z = \sqrt{x^2+y^2+z^2}+z \simeq \frac{x^2+y^2}{2|z|}$$

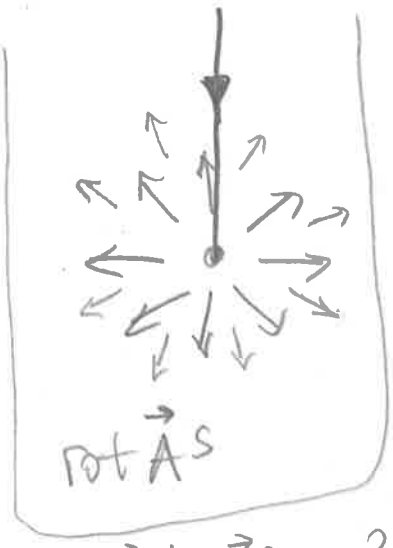
$$B_z = \frac{2}{|z|}\,\frac{1}{\frac{x^2+y^2}{2|z|}+\epsilon} - \frac{x^2+y^2}{|z|^2\left(\frac{x^2+y^2}{2|z|}+\epsilon\right)^2} =$$

$$= \frac{2}{|z|}\,\frac{\epsilon}{\left(\frac{x^2+y^2}{2|z|}+\epsilon\right)^2} \xrightarrow{\epsilon \to 0} 4\pi\,\delta(x)\delta(y),$$

since

$$\int dx\,dy\,\frac{2}{|z|}\,\frac{\epsilon}{\left(\frac{x^2+y^2}{2|z|}+\epsilon\right)^2} = 2\pi \int_0^\infty d\rho\,\rho\,\frac{2}{|z|}\,\frac{\epsilon}{\left(\frac{\rho^2}{2|z|}+\epsilon\right)^2} =$$

$$= 4\pi \int_0^\infty dw\,\frac{\epsilon}{(w+\epsilon)^2} = 4\pi \qquad \text{Q.E.D.}$$



To avoid singularities, we can use two vector potentials.

E.g. describe the northern hemisphere (U_N) with $\vec{A}^N$ and southern hemisphere (U_S) with $\vec{A}^S$

$$\vec{A}^N - \vec{A}^S = \frac{2g}{r\sin\theta}\vec{e}_\varphi = 2g\vec{\nabla}\varphi = \vec{\nabla}\Lambda\,; \quad \Lambda(\vec{r}) = 2g\varphi$$

gauge transformation

[we used $\vec{\nabla} f = \frac{\partial f}{\partial r}\vec{e}_r + \frac{1}{r}\frac{\partial f}{\partial\theta}\vec{e}_\theta + \frac{1}{r\sin\theta}\frac{\partial f}{\partial\varphi}\vec{e}_\varphi$]

Consider a particle with electric charge e and mass m moving in a field of magnetic monopole of charge g:

$$\frac{1}{2m}\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}\right)^2\psi(r) = E\psi(r)$$

Under a gauge transformation $\vec{A} \to \vec{A} + \vec{\nabla}\Lambda$, the wave function transforms as $\psi \to \exp\left(\frac{ie\Lambda}{\hbar c}\right)\psi$.

Thus, $\psi^S(\vec{r}) = \exp\left(\frac{-ie\Lambda(\vec{r})}{\hbar c}\right)\psi^N(\vec{r})\,; \quad \Lambda(\vec{r}) = 2g\varphi$

Let us take, e.g., $\theta = \frac{\pi}{2}$ (equator) and look at the behavior of $\psi^S(\vec{r})$ and $\psi^N(\vec{r})$ when $\vec{r}$ makes a circle from $\varphi = 0$ to $\varphi = 2\pi$. The wave functions $\psi^S(\vec{r})$ and $\psi^N(\vec{r})$ have to be single-valued

$\Rightarrow$ $\exp(-ie\Lambda(\vec{r})/\hbar c)$ should be single-valued on this circle (in fact, everywhere away from $\theta = 0, \pi$)

$$\Rightarrow \quad \frac{4\pi ge}{\hbar c} = 2\pi n \quad \Rightarrow \quad \frac{2eg}{\hbar c} = n \qquad n \in \mathbb{Z}$$

Dirac quantization condition

Thus, g is quantized: $g = \frac{\hbar c n}{2e}$, $n \in \mathbb{Z}$

Analogously, existense of mag. monopoles
(in fact, one monopole in the univese is sufficient)
implies quantization of electric charge
in units of $e = \frac{\hbar c n}{2g}$

[holds experimentally with an outstanding accuracy:

$$\left| \frac{q_p}{e} - 1 \right| < 10^{-21} \quad]$$

(q_p: proton, e: electron)

Comments: choice of $\vec{A}^N$ and $\vec{A}^S$ and of the path that we considered:
The argument is, however, entirely topological: one can take any two potentials with different positions of singulcerities (strings), and any path that winds around.

Indeed, the obtained quantization condition is

$$2\pi n = \delta_C\left(\frac{e\Lambda}{\hbar c}\right) = \oint_C \frac{e}{\hbar c} \vec{\nabla}\Lambda \cdot d\vec{r} = \frac{e}{\hbar c} \oint_C d\vec{r}\,(\vec{A}^N - \vec{A}^S)$$

change when one goes around a closed contour C (which was chosen to be the equator)

$$= \frac{e}{\hbar c}(\Phi_N + \Phi_S) = \frac{e}{\hbar c}\Phi = \frac{e}{\hbar c} \cdot 4\pi g$$

Quantization of magnetic flux through a closed surface $\Phi = n\Phi_0$ ($\Phi_0 = hc/e$)

1.3. Homotopy

Very generally, we are interested in classifying mappings $\Phi : M \longrightarrow T$

M - base manifold
T - target space

M: is usually compact or can be compactified to a sphere. So, we consider $M = S^k$ (k-dim. sphere)

T: usually a group $G = U(n), SU(n), SO(n), Sp(n)$ or a coset space G/H (including spheres $S^d \cong SO(d+1)/SO(d)$)

Two mappings Φ_1 and Φ_2, both $M \to T$ are <u>topologically equivalent</u> ($\equiv$ homotopic) if they can be continuosly deformed into each other. Such a deformation is termed <u>homotopy</u>.

All mappings topologically equivalent to a given one, Φ, form an <u>equivalence class</u> $[\Phi]$

The set of all equivalence classes $\{[\Phi]\}$ of mappings $\Phi : S^k \to T$ forms the <u>k-th homotopy group</u>, denoted as $\pi_k(T)$.

To show that this is indeed a group, we should define the group operation.
For this purpose, first deform the sphere S^k to a k-dimensional cube $[0;1]^k$ with all boundary points "glued together" (identified with a single point).

$\Phi_1(x_1, x_2, \dots, x_k)$
$\Phi_2(x_1, x_2, \dots, x_k)$ $\Big| \rightarrow$ define $\Phi_3 = \Phi_1 * \Phi_2$ according to

$$\Phi_3(x_1 x_2, \dots x_k) = \begin{cases} \Phi_1(2x_1, x_2, \dots x_k), & x_1 \in [0, \frac{1}{2}] \\ \Phi_2(2x_1 - 1, x_2, \dots x_k), & x_1 \in [\frac{1}{2}, 1] \end{cases}$$

This defines an operation on equivalence classes

$$[\Phi_1] * [\Phi_2] = [\Phi_3]$$

which satisfies all axioms of a group operation.

Examples of homotopy groups frequently encountered in physis:

Homotopy groups of spheres:

$\pi_n(S^n) = \mathbb{Z}$

$\pi_k(S^1) = 0$ for $k \geq 2$

$\pi_k(S^n) = 0$ for $k < n$

$\pi_k(S^n)$, $k > n$ — no general formula

Homotopy groups of Lie groups:

$\pi_1(SU(n)) = 0$; $\pi_1(U(n)) = \mathbb{Z}$ for all n

$$\pi_k(SU(n)) = \pi_k(U(n)) = \begin{cases} 0, & k \text{ even} \\ \mathbb{Z}, & k \text{ odd} \end{cases}$$

for $k > 1$, $n \geq (k+1)/2$

Bott periodicity

$$\pi_k(O(n)) = \begin{cases} 0, & k = 2,4,5,6 \pmod 8 \\ \mathbb{Z}_2, & k = 0,1 \pmod 8 \\ \mathbb{Z}, & k = 3,7 \pmod 8 \end{cases}$$

for $n \geq k+2$

$$\pi_k(Sp(n)) = \begin{cases} 0, & k = 0,1,2,6 \pmod 8 \\ \mathbb{Z}_2, & k = 4,5 \pmod 8 \\ \mathbb{Z}, & k = 3,7 \pmod 8 \end{cases}$$

for $n \geq (k-1)/4$

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2. Berry phase

2.1. General formalism: adiabatic evolution in Hilbert space

Consider a Hamiltonian that depends on a set of parameters $\vec{R} = (R_1, \ldots R_D)$ that change in time: $H(t) = H[\vec{R}(t)]$

For every $\vec{R}$: set of eigenstates of $H(\vec{R})$ $\quad H(\vec{R})\,|\psi_n[\vec{R}]\rangle = \epsilon_n(\vec{R})\,|\psi_n[\vec{R}]\rangle$

Assume that spectrum of $H(\vec{R})$ is <u>discrete</u> and <u>non-degenerate</u>. Let the state $|\psi(t)\rangle$ be the n-th eigenstate at $t=0$:

$$|\psi(t=0)\rangle = |\psi_n[\vec{R}(0)]\rangle$$

<u>Adiabatic theorem</u>: if the variation of H is very slow, the system remains in the n-th eigenstate of $H(t)$:

$$|\psi(t)\rangle = C_n(t)\,|\psi_n[\vec{R}(t)]\rangle \qquad C(t)\text{- phase factor}$$

For t-independent H: $C_n(t) = \exp\left(-\frac{i}{\hbar}\epsilon_n t\right)$ ← dynamical phase

→ write

$$C_n(t) = e^{i\gamma_n(t)} \exp\left[-\frac{i}{\hbar}\int_0^t dt'\,\epsilon_n[\vec{R}(t')]\right]$$

Substitute $|\psi(t)\rangle = C_n(t)\,|\psi_n[\vec{R}(t)]\rangle$ in Schrödinger eq:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H[\vec{R}(t)]\,|\psi(t)\rangle$$

Derivative of the dynamical phase cancels the r.h.s.

$$\rightarrow e^{-\frac{i}{\hbar}\int_0^t dt' \epsilon_n[\vec{R}(t')]} e^{i\gamma_n} \left[-i\hbar \frac{\partial \gamma_n}{\partial t} |\psi_n[\vec{R}(t)]\rangle + \right.$$

$$\left. + i\hbar \dot{\vec{R}} \frac{\partial}{\partial \vec{R}} |\psi_n(\vec{R}(t))\rangle \right] = 0$$

Multiply by $\langle \psi_n(\vec{R}(t))|$

$$\rightarrow \frac{\partial \gamma_n}{\partial t} = i \dot{\vec{R}} \langle \psi_n(\vec{R}(t)) | \frac{\partial}{\partial \vec{R}} | \psi_n(\vec{R}(t)) \rangle$$

$$\rightarrow \gamma_n(t) = i \int_0^t dt' \dot{\vec{R}} \langle \psi_n(\vec{R}(t)) | \frac{\partial}{\partial \vec{R}} | \psi_n(\vec{R}(t)) \rangle$$

$$= \int_C \vec{A}_n(\vec{R})\, d\vec{R}$$

C ← contour in parameter space

$$\vec{A}_n(\vec{R}) = i \langle \psi_n(\vec{R}) | \frac{\partial}{\partial \vec{R}} | \psi_n(\vec{R}) \rangle$$ Berry connection

The phase γ_n is purely geometric: depends only on the path C in $\vec{R}$-space but not on time dependence $\vec{R}(t)$ on this path.

The phase γ_n is in general gauge-invariant (depends on the choice of phase of $|\psi_n(\vec{R})\rangle$). However, consider a closed contour C in $\vec{R}$ space:

$$\gamma_n = \oint_C A_n(\vec{R})\, d\vec{R}$$ Berry phase, gauge-independent

↙ Observable

Verify gauge invariance of Berry phase

Gauge transformation: $|\psi_n(\vec{R})\rangle \longmapsto e^{i\beta(\vec{R})}|\psi_n(\vec{R})\rangle$

$$\vec{A}_n(\vec{R}) \longmapsto \vec{A}_n(\vec{R}) - \partial_{\vec{R}}\beta(\vec{R})$$

$$\gamma_n \longmapsto \gamma_n + \beta[\vec{R}(t=0)] - \beta[\vec{R}(t_{final})]$$

It is clear that γ_n is gauge-invariant for non-closed paths ($\vec{R}(t=0) \neq \vec{R}(t_{final})$) and becomes gauge-invariant for closed paths.

More accurately, $e^{i\gamma_n}$ is gauge-invariant for closed paths since $\beta[\vec{R}(t=0)] - \beta[\vec{R}(t_{final})]$ may be equal to $2\pi m$, $m \in \mathbb{Z}$, so that γ_n may be invariant up to $2\pi m$.

This subtle point is closely related to the discussion of Dirac monopole in Sec. 1.2, with two gauges $\vec{A}^N$ and $\vec{A}^S$. Furthermore, this will be important for topologically non-trivial situations below in this lecture course.

The Berry connection $\vec{A}_n(\vec{R})$ is analogous to vector potential of a magnetic field.

In this analogy, γ_n corresponds to magnetic flux.

What is an analog of magnetic field?

→ Berry curvature (analogous to $F_{\mu\nu}$ of el.-mag. field)

$$\Omega^n_{\mu\nu}(\vec{R}) = \partial_{R_\mu} A^n_\nu(\vec{R}) - \partial_{R_\nu} A^n_\mu(\vec{R})$$

antisymmetric tensor of rank 2

Stokes theorem for a closed path $C = \partial S$:

$$\gamma_n = \oint_{\partial S} \vec{A}_n(\vec{R})\, d\vec{R} = \frac{1}{2}\int_S dR_\mu \wedge dR_\nu\, \Omega^n_{\mu\nu}(\vec{R})$$

↖ exterior (wedge) product

$dR_\mu \wedge dR_\nu = - dR_\nu \wedge dR_\mu$ oriented element of the surface

($1/2$ is compensated by the fact that in the summation each pair $\mu\nu$ appears twice — as $\mu\nu$ and $\nu\mu$)

If the parameter space is 3-dimensional ($D=3$), this can be rewritten as

$$\gamma_n = \int_S \vec{b}_n \cdot d\vec{S},$$

where $\vec{b}_n = \nabla_{\vec{R}} \times \vec{A}_n = i \langle \vec{\nabla}_R \psi_n(\vec{R}) | \times | \nabla_{\vec{R}} \psi_n(\vec{R}) \rangle$ (analog of magnetic field)

$$\Rightarrow \quad \boxed{b_\mu = \frac{1}{2}\epsilon_{\mu\nu\lambda}\Omega_{\nu\lambda}}$$

Like magnetic field in electrodynamics, $\Omega^n_{\mu\nu}$ is gauge-invariant. It can be rewritten in an explicitly gauge-invariant form:

$$(*)\quad \Omega^n_{\mu\nu}(\vec{R}) = i \sum_{n' \neq n} \left[\frac{\langle \psi_n(\vec{R}) | \partial_{R_\mu} H | \psi_{n'}(\vec{R}) \rangle \langle \psi_{n'}(\vec{R}) | \partial_{R_\nu} H | \psi_n(\vec{R}) \rangle}{\left[\epsilon_n(\vec{R}) - \epsilon_{n'}(\vec{R})\right]^2} - \text{c.c.} \right]$$

Proof: $H(\vec{R})|\psi_n(\vec{R})\rangle = \epsilon_n(\vec{R})|\psi_n(\vec{R})\rangle$

Apply ∂_{R_ν} $\rightarrow$ $(\partial_{R_\nu} H)|\psi_n(\vec{R})\rangle = \partial_{R_\nu}\epsilon_n |\psi_n(\vec{R})\rangle + (\epsilon_n - H)|\partial_{R_\nu}\psi_n(\vec{R})\rangle$

$\rightarrow$

$$\langle \psi_{n'}(R)|\partial_{R_\nu} H|\psi_n(R)\rangle = (\epsilon_n - \epsilon_{n'})\langle \psi_{n'}(R)|\partial_{R_\nu}\psi_n(\vec{R})\rangle$$

Same with $\nu \to \mu$ and complex conjugation

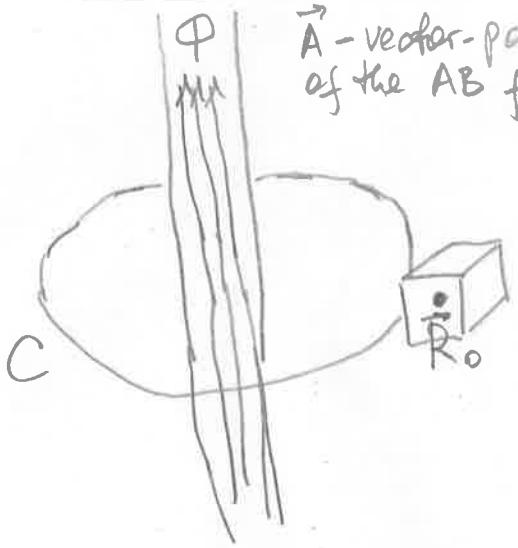
$\to$ Eq. (*) on p. 14 =

$$= i \sum_{n' \neq n} \left[\langle \partial_{R_\mu} \psi_n(\vec{R}) | \psi_{n'}(\vec{R}) \rangle \langle \psi_{n'}(\vec{R}) | \partial_{R_\nu} \psi_n(\vec{R}) \rangle - c.c. \right]$$

$$= i \left[\langle \partial_{R_\mu} \psi_n(\vec{R}) | \partial_{R_\nu} \psi_n(\vec{R}) \rangle - c.c. \right],$$

which is exactly $\Omega^n_{\mu\nu}$ Q.E.D.

2.2. Aharonov–Bohm effect as Berry phase



Consider a Hamiltonian of the type

$$H = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 + U(\vec{r} - \vec{R}_0)$$

$U(\vec{r} - \vec{R}_0)$ - potential ("box") that confines the particle to a vicinity of $\vec{R}_0$.

Now we adiabatically change $\vec{R}_0$ along a path C enclosing the AB flux Φ

(i.e. $\vec{R}_0$ plays a role of $\vec{R}$ in the above general discussion of the Berry phase)

Performing a calculation, one gets (exercise):

Berry connection (chosing a natural gauge):

$$\vec{A}_{Berry}(\vec{R}_0) = \frac{2\pi}{\Phi_0}\vec{A}(\vec{R}_0) \qquad \boxed{\Phi_0 = hc/e}$$

$$\gamma = \oint_C d\vec{R}_0 \, \vec{A}_{Berry}(\vec{R}_0) = 2\pi \frac{\Phi}{\Phi_0}$$

Berry phase = AB phase

2.3 Berry phase for spin $\frac{1}{2}$

$$H = \vec{h}\cdot\vec{\sigma} = \sum_{j=1}^{3} h_j \sigma_j \qquad \sigma_j - \text{Pauli matrices}$$

Parameter space (the space of $\vec{R}$ in the above general discussion)

is here: $\vec{h} \in \mathbb{R}^3 \setminus \{0\}$ The origin is removed because of level degeneracy there

Polar coordinates:

$\vec{h} = h(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$

Eigenstates (depend only on θ and φ, not on h):

$$|-\rangle_{\vec{h}} = \begin{pmatrix} \sin(\theta/2)\, e^{-i\varphi} \\ -\cos(\theta/2) \end{pmatrix} \qquad \epsilon_-(\vec{h}) = -h$$

$$|+\rangle_{\vec{h}} = \begin{pmatrix} \cos(\theta/2)\, e^{-i\varphi} \\ \sin(\theta/2) \end{pmatrix} \qquad \epsilon_+(\vec{h}) = +h$$

More generally, one can include arbitrary phase factors $e^{i\Theta_-(\theta,\varphi)}$ and $e^{i\Theta_+(\theta,\varphi)}$ in $|-\rangle_{\vec{h}}$ and $|+\rangle_{\vec{h}}$. This will correspond to another gauge choice for the Berry connection but will not affect the Berry curvature and the Berry phase.

Calculate the Berry connection for $|-\rangle$ (with $\Theta_-(\theta,\varphi) = 0$):

$$A_\theta^- = i\langle -|\partial_\theta|-\rangle = \frac{i}{2}\left(\cos\frac{\theta}{2}\sin\frac{\theta}{2} - \sin\frac{\theta}{2}\cos\frac{\theta}{2}\right) = 0$$

$$A^-_\varphi = i\langle -|\partial_\varphi|-\rangle = \sin^2\frac{\theta}{2}$$

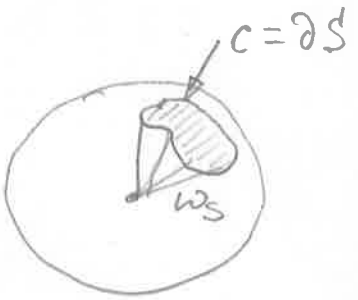
$$\Omega^-_{\theta\varphi} = \partial_\theta A^-_\varphi - \partial_\varphi A^-_\theta = \frac{1}{2}\sin\theta$$ Berry curvature

Berry flux through an element on S^2 with a solid angle $d\omega = \sin\theta\, d\theta\, d\varphi$:

$$\Omega^-_{\theta\varphi}\, d\theta\, d\varphi = \frac{1}{2}\sin\theta\, d\theta\, d\varphi = \frac{1}{2}\, d\omega$$

→ Berry phase for a loop $C = \partial S$ on S^2 is

$$\gamma_- = \frac{1}{2}\int_S d\omega = \frac{1}{2}\omega_S ,$$



where ω_S is the solid angle corresponding to S (area on a unit sphere)

The integral of Berry curvature over the entire S^2 is thus

$$\int \Omega^-_{\theta\varphi}\, d\theta\, d\varphi = \frac{1}{2}\int_{S^2} d\omega = \frac{1}{2}\cdot 4\pi = 2\pi$$

We can make a transformation from polar coordinates (h, θ, φ) to cartesian coordinates (h_1, h_2, h_3) in parametrization of $H(\vec{h})$. The Berry curvature will be

$$\Omega^-_{h_i h_j} = \Omega^-_{\theta\varphi}\frac{\partial(\theta,\varphi)}{\partial(h_i, h_j)} = \frac{\sin\theta}{2}\frac{\partial(\theta,\varphi)}{\partial(h_i,h_j)} .$$

The result for the "magnetic field" $b^-_i = \frac{1}{2}\epsilon_{ijk}\Omega^-_{h_j h_k}$ is:

$$b_i^- = \frac{1}{2}\frac{h_i}{|\vec{h}|^3} \quad , \text{i.e.,} \quad \vec{b}^- = \frac{1}{2}\frac{\vec{h}}{|\vec{h}|^3}$$

This can be immediately understood from the above result $\gamma_- = \frac{1}{2}\omega_S$, which should be independent of the choice of parametrization.

The following important and interrelated points should be empasized:

(i) From $\vec{b} = \mathrm{rot}\,\vec{A}$ one has, according to Stokes theorem

$$\oint_{\partial S} \vec{A}\, d\vec{h} = \int_S \vec{b}\, d\vec{S}$$

Applying this to a closed surface (whole S^2), one would get the total Berry flux (integral of Berry curvature) $= 0$, at variance with the value 2π found above.

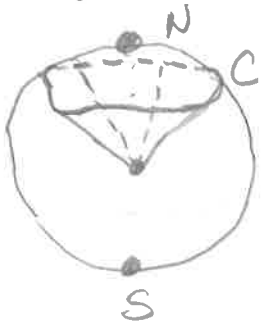
Explanation: $\vec{A}$ has a singularity on S^2, so that Stokes theorem cannot be applied to the whole S^2: <u>topological quantization</u> of total Berry flux (Chern number, see below) as an <u>obstruction to Stokes theorem.</u>

(ii) For our choice of gauge (see eigenstate choice on p. 16), the singular point for $|-\rangle$ is the south pole $\theta = \pi$ (since $e^{-i\varphi}$ is not defined there). Thus, in the above calculation of γ_- for a path C we should choose S (with $\partial S = C$) such that S does not contain south pole. We could choose a different gauge, e.g

$$|-\rangle_{\vec{h}} = \begin{pmatrix} \sin(\theta/2) \\ -\cos(\theta/2)\, e^{i\varphi} \end{pmatrix}$$

Now the singular point is the north pole, $\theta = 0$

Consider a contour C separating them:



First gauge: $\gamma_- = \frac{1}{2}\omega_s$

Second gauge:

$$\gamma_-' = -\frac{1}{2}(4\pi - \omega_s) = \frac{1}{2}\omega_s - 2\pi$$

(contour orientation changes if you look at it from the opposite side)

Thus, $\gamma_- \neq \gamma_-'$ but rather $\gamma_- = \gamma_-' \pmod{2\pi}$,

so that $e^{i\gamma_-} = e^{i\gamma_-'}$

(iii) The "magnetic field" $\vec{b} = \frac{1}{2}\frac{\vec{h}}{h^3}$ (i.e., the Berry curvature) is exactly that of a magnetic monopole with charge $g = \frac{1}{2}$ (see Sec. 1.2, p. 4)

The monopole is located at $\vec{h} = 0$, i.e. in the degeneracy point. (For $|+\rangle_{\vec{h}}$, the charge is $g = -1/2$.)

Thus, degeneracy points serve as sources / drains for the Berry curvature. The $\int$ of Berry curvature over a closed surface $= 2\pi$ times the net number of monopoles inside. (Each degeneracy point gives 2π or -2π.)

iv) It is not difficult to obtain the same result for the Berry curvature (and thus Berry phase) by starting from Eq. (*) on p. 14.
(Exercise. Hint: use cartesian coordinates for $\vec{h}$, consider first $\vec{h} \parallel z$ and then use rotational invariance.)

v) Extension to arbitrary spin S. (Exercise.)
Can be straightforwardly done by generalizing the calculation in (iv). The results for the state $|S, m\rangle$ (where $m = -S, \ldots, S$) reads

Hamiltonian:
$H(\vec{h}) = \vec{h} \cdot \vec{S}$
as before

$$\vec{b} = -m \frac{\vec{h}}{h^3}$$

vi) The Berry phase for the spin can be equivalently written as

$$\int d\theta d\varphi \, \Omega^{-}_{\theta\varphi} = \frac{1}{2} \int d\theta d\varphi \sin\theta = \frac{1}{2} \int d\theta d\varphi \, \vec{n} \cdot (\partial_\theta \vec{n} \times \partial_\varphi \vec{n})$$

$$= \frac{1}{2} \int dx dy \, \vec{n} \cdot (\partial_x \vec{n} \times \partial_y \vec{n}) \,,$$

where $\vec{n} \in S^2$ is a unit vector with polar coordinates (θ, φ), and in the last form $\vec{n}$ is considered as a function of two variables (parameters), $\vec{n} = \vec{n}(x, y)$

vii) Berry phase also emerges as a term in the action of a path for the spin; in that situation it is known as Wess-Zumino term. Wess-Zumino terms are closely related to topological θ-terms and will appear many times below in this lecture course.

3. Topological quantization of 2D Bloch bands and of 1D adiabatic pumping

3.1. Berry curvature and anomalous velocity in Bloch bands

Periodic potential and magnetic field.
Assume that magnetic flux through a unit cell of the lattice is $(P/q) \times \Phi_0$
→ enlarged (magnetic) lattice (more detailed, accurate analysis: Chapter 4)
→ usual Bloch theorem ; quasi-impuls $\vec{k}$

$$\psi_{n\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{r}} u_{n\vec{k}}(\vec{r})$$

(generalized) periodic boundary conditions for $u_{n\vec{k}}(\vec{r})$

Shrödinger eq:

$$h(\vec{k}) u_{n\vec{k}}(\vec{r}) = \epsilon_n(\vec{k}) u_{n\vec{k}}(\vec{r})$$

$$h(\vec{k}) = \frac{1}{2m}\left[\hat{\vec{p}} + \hbar\vec{k} + \frac{e}{c}\vec{A}(\vec{r})\right]^2 + V(\vec{r}).$$

$\vec{k}$ plays a role of a set of parameters.

→ define the corresponding Berry curvature
Eq. on p. (14), with $\vec{R} \to \vec{k}$:

$$\vec{b}_n(\vec{k}) = \nabla_{\vec{k}} \times \vec{A}_n = i \left\langle \vec{\nabla}_k u_{n\vec{k}} \middle| \times \middle| \vec{\nabla}_k u_{n\vec{k}} \right\rangle$$

We show now that the Berry curvature $\vec{b}_n(\vec{k})$ leads to a correction to the average velocity of Bloch states in the presence of a weak electric field $\vec{E}$ ("anomalous velocity")

$\vec{E}=0$: $\langle \psi_{n\vec{k}} | \hat{\vec{v}} | \psi_{n\vec{k}} \rangle = \langle u_{n\vec{k}} | \frac{1}{\hbar} \frac{\partial h(\vec{k})}{\partial \vec{k}} | u_{n\vec{k}} \rangle =$

$= \frac{1}{\hbar} \frac{\partial \epsilon_n(\vec{k})}{\partial \vec{k}}$

(electron charge: $-e$)

weak el. field $\vec{E}$ → $\delta H = e\vec{E}\cdot\vec{r}$ → first-order pert. theory

→ $|\delta\psi_{n\vec{k}}\rangle = e\vec{E} \sum'_{n',\vec{k}'} \frac{|\psi_{n'k'}\rangle\langle\psi_{n'k'}|\vec{r}|\psi_{nk}\rangle}{\epsilon_{nk}-\epsilon_{n'k'}}$

$= e\vec{E} \sum'_{n'k'} \frac{|\psi_{n'k'}\rangle\langle\psi_{n'k'}|[\vec{r},H]|\psi_{nk}\rangle}{(\epsilon_{nk}-\epsilon_{n'k'})^2}$

$= i\hbar e\vec{E} \sum'_{n'k'} \frac{|\psi_{n'k'}\rangle\langle\psi_{n'k'}|\hat{\vec{v}}|\psi_{nk}\rangle}{(\epsilon_{nk}-\epsilon_{n'k'})^2}$

$\langle |\vec{v}| \rangle$ with $k' \neq k$ vanish due to $\int d^d r\, e^{i(\vec{k}-\vec{k}')\vec{r}} \ldots$ where $\ldots$ is periodic with $\vec{r}$. We thus get

$$|\delta u_{n\vec{k}}\rangle = ie\vec{E} \sum_{n'\neq n} \frac{|u_{n'k}\rangle\langle u_{n'k}| \frac{\partial h(\vec{k})}{\partial \vec{k}} |u_{nk}\rangle}{(\epsilon_{nk}-\epsilon_{n'k})^2}$$

→ to the first order in $\vec{E}$ we have

$\langle \vec{v} \rangle = \langle u_{n\vec{k}} + \delta u_{n\vec{k}} | \frac{1}{\hbar} \frac{\partial h(\vec{k})}{\partial \vec{k}} | u_{n\vec{k}} + \delta u_{n\vec{k}} \rangle \simeq$

$\simeq \frac{1}{\hbar} \frac{\partial \epsilon_n(\vec{k})}{\partial \vec{k}} + \vec{v}_{a,n}(\vec{k})$, anomalous velocity

$$\vec{v}_{a,n}(\vec{k}) = \frac{ie}{\hbar} \sum_{n'\neq n} \frac{\langle u_{nk}| \frac{\partial h(\vec{k})}{\partial \vec{k}} |u_{n'k}\rangle \left[\vec{E}\cdot\langle u_{n'k}| \frac{\partial h(\vec{k})}{\partial \vec{k}} |u_{nk}\rangle\right] - c.c.}{(\epsilon_{nk}-\epsilon_{n'k})^2}$$

Use $\vec{a}\times(\vec{b}\times\vec{c}) = \vec{b}(\vec{a}\cdot\vec{c}) - \vec{c}(\vec{a}\cdot\vec{b})$

$$\rightarrow \vec{v}_{a,n}(\vec{k}) = \frac{ie}{\hbar}\vec{E}\times\left[\sum_{n'\neq n}\frac{\langle u_{nk}|\frac{\partial h(\vec{k})}{\partial \vec{k}}|u_{n'k}\rangle \times \langle u_{n'k}|\frac{\partial h(\vec{k})}{\partial \vec{k}}|u_{nk}\rangle}{(\epsilon_{nk}-\epsilon_{n'k})^2}\right]$$

$$= \frac{e}{\hbar}\vec{E}\times\vec{b}_n(\vec{k})$$

(used Eq. (*) on p. 14 for Berry curvature)

anomalous velocity

Comment: note that $\sum_n \vec{b}_n(\vec{k}) = 0$ (exchange $n \leftrightarrow n'$ in the sum)

Note that including the anomalous velocity makes semiclassical equations of motion highly symmetric:

$$\hbar\frac{d\vec{k}}{dt} = \nabla_{\vec{k}}\epsilon_n(\vec{k}) - \hbar\frac{d\vec{k}}{dt}\times\vec{b}_n(\vec{k})$$

$$\hbar\frac{d\vec{k}}{dt} = -\nabla_{\vec{k}}V(\vec{k}) - \frac{e}{c}\frac{d\vec{k}}{dt}\times\vec{B}(\vec{k})$$

Here we used $\vec{v}_a = \frac{d\vec{k}}{dt}\times\vec{b}_n(\vec{k})$, which extends the above formula by substituting $e\vec{E} \rightarrow \hbar\frac{d\vec{k}}{dt}$

Analyze symmetries of the Bloch-band Berry curvature $\vec{b}_n(\vec{k})$:

Time-reversal transformation:

$$\vec{v} \rightarrow -\vec{v}\ ;\quad \vec{k} \rightarrow -\vec{k}\ ;\quad \vec{E} \rightarrow \vec{E}$$

and thus $\vec{b}_n \rightarrow -\vec{b}_n$ (similar to mag. field)

Therefore, in system with time-reversal invariance

$$\vec{b}_n(\vec{k}) = -\vec{b}_n(-\vec{k})$$

Space-inversion transformation:

$\vec{v} \to -\vec{v}$; $\vec{k} \to -\vec{k}$; $\vec{E} \to -\vec{E}$

and thus $\vec{b}_n \to \vec{b}_n$ (again similar to magnetic field, which is a pseudovector)

Therefore, in a system with spatial inversion symmetry:

$$\vec{b}_n(\vec{k}) = \vec{b}_n(-\vec{k})$$

$\Rightarrow$ If both time-reversal and spatial inversion symmetries are present, $\vec{b}_n(\vec{k}) = 0$ for all $\vec{k}$

3.2. Topological quantization of Hall conductance of Bloch bands in 2D

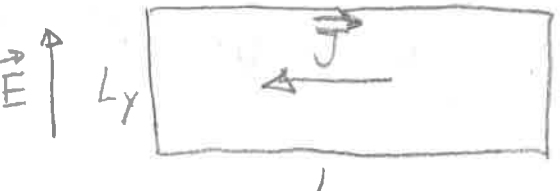
Consider a 2D system with a certain number of filled Bloch bands (i.e. a band insulator). Assume that the time-reversal symmetry is broken (by magnetic field or in a different way). Then $\vec{b}_n(\vec{k}) \neq 0$ (generically). Thus, a filled band n under in-plane electric field $\vec{E} \parallel \hat{i}$ yields a current $\parallel \hat{x}$ originating from anomalous velocity:

$$\vec{J}_n = -e \sum_{\vec{k} \in 1BZ} \vec{v}_{a,n}(\vec{k}) \frac{1}{L_x}$$

1BZ - first Brillouin zone

Current density

$$\vec{j}_n = \frac{\vec{J}_n}{L_y} = \frac{-e}{A} \sum_{\vec{k} \in 1BZ} \vec{v}_{a,n}(\vec{k})$$



$A = L_x L_y$ - area

Hall conductivity σ_{xy}^n : (≡ Hall conductance)

$$\vec{j}_n = \sigma_{xy}^n \vec{E} \times \hat{e}_z \; ; \qquad j_{n,x} = \sigma_{xy}^n E_y \; ; \quad \sigma_{xy}^n = -\sigma_{yx}^n$$

$$-\sigma_{xy}^n = \frac{e^2}{\hbar A} \sum_{\vec{k} \in 1BZ} b_n(\vec{k}) = \frac{e^2}{h} \int_{1BZ} \frac{dk_x\, dk_y}{2\pi}\, b_n(\vec{k})$$

Here we omitted the vector sign on $\vec{b}_n$ since it has only z component : $\vec{b}_n = b_n \hat{e}_z$. Also, one factor 2π is absorbed into $h = 2\pi\hbar$.

Thus, Hall conductance of a filled band is $= \frac{e^2}{2\pi h}$ × integral of Berry curvature over 1BZ.

If the band is not degenerate with any other band for any $\vec{E}$, this integral is quantized:

$$\frac{1}{2\pi} \int_{1BZ} dk_x\, dk_y\, b_n(\vec{k}) = C_n \in \mathbb{Z}$$

C_n - topological invariant — Chern number

→ quantization of Hall conductance:

$$-\sigma_{xy}^n = C_n \frac{e^2}{h}, \quad C_n \in \mathbb{Z}$$

Total Hall conductance is a sum of σ_{xy}^n over all filled bands.

2D band insulators with non-zero σ_{xy}^n are frequently called Chern insulators.

Proof of quantization of C_n (Chern number) (and thus of σ_{xy}^n)

$$\vec{b}_n(\vec{k}) = \nabla_{\vec{k}} \times \vec{A}_n(\vec{k}), \qquad \vec{A}_n(\vec{k}) = i\langle u_{n\vec{k}} | \vec{\nabla}_k u_{n\vec{k}} \rangle$$

If we could find a global smooth gauge, such that $\vec{A}_n(\vec{k})$ is well defined in the whole BZ, we would have $\int_{BZ} dk_x dk_y \, b(\vec{k}) = 0$ by virtue of Stokes theorem. Thus, $C_n \neq 0$ (i.e., $\sigma_{xy}^n = 0$) may only result from an obstruction to Stokes theorem, i.e. impossibility of finding such a smooth gauge.

To prove quantization of C_n, let us consider for simplicity a model on a lattice, in which case $|u_{n\vec{k}}\rangle$ is an N-component vector (N – number of sites per unit cell). We should have $N \geq 2$ to have a band insulator (Fermi energy between filled and empty band). Choose a gauge (i.e. the phase of $|u_{n\vec{k}}\rangle$) by requiring that the first component of $|u_{n\vec{k}}\rangle$ is real and positive. We can do it almost everywhere – except for points in BZ where this component vanishes. Consider a small vicinity of each such point – say, a circle of a small radius δ. Within this circle, choose another gauge – e.g. require that the second component is real and positive.

1 – gauge 1
2 – gauge 2

Relation between the two gauges at the boundary between 1 and 2:

$$|u_{n\vec{k}}\rangle_2 = e^{i\chi(\vec{k})} |u_{n\vec{k}}\rangle_1$$

→ relation of Berry connections:

$$\vec{A}_n^{(2)}(\vec{k}) = \vec{A}_n^{(1)}(\vec{k}) - \vec{\nabla}_k \chi(\vec{k})$$

Use Stokes theorem (for region 1 – with $\vec{A}^{(1)}$, and for region 2 with $\vec{A}^{(2)}$)

$$\rightarrow C_n = \frac{1}{2\pi} \int_{BZ} dk_x dk_y \, b_n(\vec{k}) = \frac{1}{2\pi} \oint_{\partial S_\delta} \left[\vec{A}_n^{(2)}(\vec{k}) - \vec{A}_n^{(1)}(\vec{k}) \right] d\vec{k}$$

$$= \frac{1}{2\pi} \oint_{\partial S_\delta} d\vec{k} \, \vec{\nabla}_k \chi(\vec{k}) = \underline{\text{total winding number}} \text{ of the phase } \chi \text{ (vorticity) around the singularity points}$$

Since wave functions $|u_{n\vec{k}}\rangle_1$ and $|u_{n\vec{k}}\rangle_2$ are single-valued on ∂S_δ, the winding number should be integer, which completes the proof.

Note that positions of singularities and individual contributions to C_n are gauge-dependent but the total C_n is gauge invariant.

Specific examples of models with non-trivial C_n of bands (TKNN, Haldane model) will be discussed later in the chapters on IQHE and on graphene.

3.3 Adiabatic pumping and its topological quantization

We consider now a Hamiltonian that depends on a single parameter λ, with periodic dependence

$$H(\lambda) = H(\lambda+1)$$

We will further consider λ slowly changing with time:

$$\lambda(t) = t/T$$

with large T, so that the evolution is adiabatic. We will focus on 1D filled-band situation. The quantity to be studied is a charge pumped in one cycle of evolution. We will show that this problem is closely related to that of σ_{xy} in a 2D filled band. The Brillouin zone in (k_x, k_y) was a torus; now we will have instead a torus (k, λ).

We begin by studying the adiabatic dynamics more accurately than in Sec. 2.1, where we were only interested in Berry phase.

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H(t) |\psi(t)\rangle ; \qquad H(t) = H\left[\vec{R}(t)\right]$$

$\vec{R}$ - set of parameters

Let $|\psi_n(t)\rangle \equiv |\psi_n[R(t)]\rangle$ be instantaneous eigenstates of $H(t)$ and $\epsilon_n(t) \equiv \epsilon_n[\vec{R}(t)]$ the corresponding energies

Expand

$$|\psi(t)\rangle = \sum_\ell \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} dt' \epsilon_\ell(t')\right) a_\ell(t) |\psi_\ell(t)\rangle$$

$$\Rightarrow \frac{\partial}{\partial t} a_n(t) = -\sum_\ell a_\ell(t) \langle \psi_n(t) | \frac{\partial}{\partial t} |\psi_\ell(t)\rangle \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} dt' \left[\epsilon_\ell(t') - \epsilon_n(t')\right]\right)$$

Choose the phase of $|\psi_n(t)\rangle$ by requiring

$$\langle \psi_n(t)| \frac{\partial}{\partial t} |\psi_n(t)\rangle = \dot{\vec{R}}(t) \langle \psi_n(t)| \nabla_{\vec{R}} |\psi_n(t)\rangle = 0.$$

This is <u>not</u> the single-valued choice that we adopted in Sec. 2.1. Rather, under a cyclic evolution, we will have

$$|\psi_n(t_{final})\rangle = e^{i\gamma_n} |\psi_n(t_0)\rangle,$$

where γ_n is the Berry phase.

$|\tilde{\psi}_n(t)\rangle = e^{i\gamma_n} |\psi_n(t)\rangle$ ← single-valued (Sec. 2.1)

We denote this choice of $|\psi_n(t)\rangle$ by $|\tilde{\psi}_n(t)\rangle$.

<u>Initially</u>, we have $a_m(0)=1$ and $a_{m'}(0)=0$ for $m' \neq m$.

In the adiabatic limit, the system remains in the state m. We calculate the first-order correction. (Set $a_\ell(t) = a_\ell(0) = \delta_{\ell m}$ in the r.h.s.)

We have $\frac{\partial}{\partial t} a_m = 0 \rightarrow a_m(t) = 1$;

$$\frac{\partial}{\partial t} a_{m'} = -\langle \tilde{\psi}_{m'}(t)| \frac{\partial}{\partial t} |\tilde{\psi}_m(t)\rangle \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' \left[\epsilon_m(t') - \epsilon_{m'}(t')\right]\right] \qquad (m' \neq m)$$

The factor $\langle \tilde{\psi}_{m'}(t)| \frac{\partial}{\partial t} |\tilde{\psi}_m(t)\rangle$ adiabatically slowly changes with t, while $\exp[\ ]$ quickly oscillates. We can thus integrate this equation by neglecting variation of $\langle\ |\ \rangle$, which yields $(m' \neq m)$

$$a_{m'}(t) = -i\hbar \frac{\langle \tilde{\psi}_{m'}(t)| \frac{\partial}{\partial t} |\tilde{\psi}_m(t)\rangle}{\epsilon_m(t) - \epsilon_{m'}(t)} \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' \left[\epsilon_m(t') - \epsilon_{m'}(t')\right]\right]$$

Substituting $a_m(t)$ and $a_{m'}(t)$ in the expansion of $|\psi(t)\rangle$ on page 28, we get

$$|\psi(t)\rangle = \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' \epsilon_m(t')\right] \left\{ |\tilde{\psi}_m(t)\rangle - i\hbar \sum_{m' \neq m} |\tilde{\psi}_{m'}(t)\rangle \frac{\langle \tilde{\psi}_{m'}(t)| \frac{\partial}{\partial t} |\tilde{\psi}_m(t)\rangle}{\epsilon_m(t) - \epsilon_{m'}(t)} \right\}$$

We can express the r.h.s. through the single-valued states $|\psi_m(t)\rangle$ by substituting $|\tilde{\psi}_m(t)\rangle = e^{i\gamma_m}|\psi_m(t)\rangle$; this will amount to replacing $|\tilde{\psi}_m\rangle \to |\psi_m\rangle$, $|\tilde{\psi}_{m'}\rangle \to |\psi_{m'}\rangle$ and including an overall factor $e^{i\gamma_m}$.

Now we calculate the anomalous velocity for 1D Bloch states under adiabatic evolution of the Hamiltonian, cf. Sec. 3.1.

$$v_n(k) = \langle u_{nk}+\delta u_{nk} | \frac{1}{\hbar}\frac{\partial h(k,t)}{\partial k} | u_{nk}+\delta u_{nk}\rangle =$$

$$= \frac{1}{\hbar}\frac{\partial \epsilon_n(k,t)}{\partial k} + v_{a,n}(k)$$

$$v_{a,n}(k,t) = \langle u_{nk}^{(t)} | \frac{1}{\hbar}\frac{\partial h(k,t)}{\partial k} | \delta u_{nk}^{(t)}\rangle + \text{c.c.}$$

For $|u_{nk}+\delta u_{nk}\rangle$ we use the formula for $|\psi(t)\rangle$ in the bottom of p. 29, with $|\tilde{\psi}_m(t)\rangle \to |u_{nk}(t)\rangle$. The phase factors (dynamical and Berry) drop out.

$$\to v_{a,n}(k,t) = -i\sum_{n'\neq n}\left\{\frac{\langle u_{nk}(t)|\frac{\partial h(k,t)}{\partial k}|u_{n'k}(t)\rangle\langle u_{n'k}(t)|\frac{\partial}{\partial t}|u_{nk}(t)\rangle}{\epsilon_n(k,t)-\epsilon_{n'}(k,t)} - \text{c.c.}\right\}$$

As in Sec. 2.1 (formula in the bottom of p. 14), we use

$$\langle u_{nk}(t)|\frac{\partial h(k,t)}{\partial k}|u_{nk'}(t)\rangle = [\epsilon_n(k,t)-\epsilon_{n'}(k,t)]\cdot \langle \frac{\partial}{\partial k}u_{nk}(t)|u_{nk'}(t)\rangle$$

→ Rewrite $v_{a,n}(k,t)$ as (using completeness)

$$v_{a,n}(k,t) = -i\sum_{n'\neq n}\left[\langle\frac{\partial}{\partial k}u_{nk}(t)|\frac{\partial}{\partial t}u_{nk}(t)\rangle - \langle\frac{\partial}{\partial t}u_{nk}(t)|\frac{\partial}{\partial k}u_{nk}(t)\rangle\right]$$

Thus, $v_{a,n}(k,t) = -\Omega^n_{kt}$ Berry curvature

This is fully analogous to the formula for anomalous velocity in a 2D band (under electric field), top of p 23, with $(k_1, k_2) \to (k, t)$ [or, equivalently (k, λ), where $\lambda = \lambda(t)$ is a parameter].

Total current carried by a filled band:

$$J_n(t) = (-e)\int_{BZ} \frac{dk}{2\pi} v_{a,n}(k,t) = e\int_{BZ} \frac{dk}{2\pi} \Omega^n_{kt}$$

Total charge pumped by a filled band in one cycle:

$$Q_n = \int_0^T dt\, J_n(t) = e\int_0^T dt \int_{BZ} \frac{dk}{2\pi} \Omega^n_{kt} = e\int_0^1 d\lambda \int_{BZ} \frac{dk}{2\pi} \Omega^n_{k\lambda} =$$

$$= e\,C_n$$

C_n – Chern number

→ quantization of pumped charge — Thouless 1983

("Thouless pumping")

If we have a set of control parameters $\vec{R}$ of H, and the cycle is

$$h(k,t) = h(k, \vec{R}(t)) \; ; \quad \vec{R}(t+T) = \vec{R}(t),$$

we can rewrite C_n as

$$C_n = \frac{1}{2\pi} \oint dR_\alpha \int \frac{dk}{2\pi} \Omega^n_{k R_\alpha}$$

The minimal version to have a non-trivial cycle is $\vec{R} = (R_1, R_2)$.

3.4. Chern number as winding number: Condition for a non-zero pumped charge

Consider the simplest case of a two-band Hamiltonian (2 lattice sites per unit cell). Also, let $\vec{R} = (R_1, R_2)$. We have $h(k, R_1, R_2)$ - 2×2 matrix, with eigenvalues $\epsilon_n(k, R_1, R_2)$, $n = 1, 2$; $\epsilon_2 \geq \epsilon_1$.

If $\epsilon_2(k, R_1, R_2) \neq \epsilon_1(k_1, R_1, R_2)$ for all (k, R_1, R_2), a contour in (R_1, R_2) plane can be continuously deformed to a point, and thus $C_n = 0$. Imagine that there is a point $(k^{(0)}, R_1^{(0)}, R_2^{(0)})$ at which $\epsilon_1 = \epsilon_2$ - band degeneracy. There may be also several such points.

Write h in terms of Pauli matrices:

$$h(k, R_1, R_2) = a_0 \cdot \mathbb{1} + a_1 \cdot \sigma_x + a_2 \cdot \sigma_y + a_3 \cdot \sigma_z$$

$$a_\mu \equiv a_\mu(k, R_1, R_2)$$

a_0 - does not play any role here; discard

Degeneracy $\leftrightarrow$ $a_1 = a_2 = a_3 = 0$

These are 3 conditions, and we have 3 variables (k, R_1, R_2) $\Rightarrow$ this will happen at isolated points.

Away from these points, define

$$\tilde{a}_i = \frac{a_i}{(a_1^2 + a_2^2 + a_3^2)^{1/2}}, \quad i = 1, 2, 3$$

Now $\{\tilde{a}_1, \tilde{a}_2, \tilde{a}_3\}$ belongs to a sphere S^2

We have thus a map : $T^1 \times \mathbb{R}^2 \to S^2$

torus (k) (R_1, R_2) $\{\tilde{a}_i\}$

For any cycle Γ_R in (R_1, R_2), we get a mapping

$$T^2 \longrightarrow S^2$$

two-dim. torus $\equiv T^1$ in k-space $\times T^1$ in R-space

Maps $T^2 \to S^2$ topologically maps $S^2 \to S^2$

$\pi_2(S^2) = \mathbb{Z}$: winding number $q \in \mathbb{Z}$

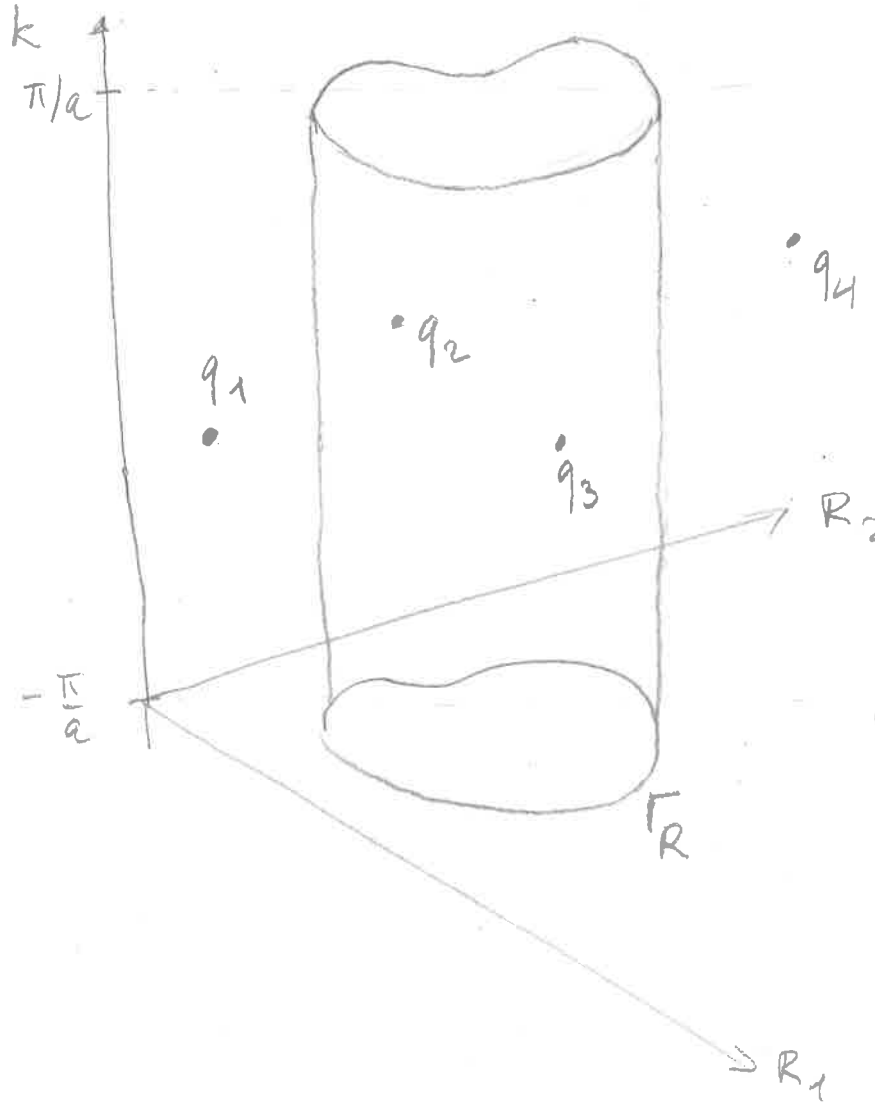
Chern numbers of two bands:

$$C_1 = -C_2 = q$$

Relation between Chern and winding numbers

Each of the degeneracy points serves as a monopole : the Hamiltonian h around it has the same form as for spin-$\frac{1}{2}$ system in Sec. 2.3 and gives a contribution $\pm 2\pi$ to the integral of Berry curvature, i.e. $+1$ or -1 to the Chern number.

The total Chern number thus counts the number of monopoles (degeneracy points), taking into account signs, inside the torus T^2, which is exactly the winding number of the map $T^2 \to S^2$ defined above.



$q_i = \pm 1$ monopole charges at degeneracy points

For a cycle Γ_R, the total q (and thus the Chern number $C_1 = -C_2$) is equal to

$$C_1 = -C_2 = q = \sum_i q_i$$

— over degeneracy points inside the torus $\Gamma_R \times T^1_k \sim T^2$

If there is more than 2 bands, we will have monopoles for each degeneracy of bands j and $j+1$
If the Fermi energy is between bands n and $n+1$, and we are interested in total pumped charge $Q_n^{tot} = \sum_{i \le n} Q_i$, we will have to count monopoles corresponding to $\epsilon_n = \epsilon_{n+1}$ within Γ_R.

This picture is directly translated to the Hall conductance of Bloch bands in 2D, Sec. 3.2. In that case, we can consider $h(k_1, k_2, s)$, where s is an additional parameter. The Brillouin zone (k_1, k_2) is a torus T^2, and we have a mapping $T^2 \to S^2$ as above. In the space (k_1, k_2, s) there are band degeneracy points that serve as monopoles. When we change (continuously) s, the monopoles will cross the torus, thus changing the winding number (and the Chern number) by ± 1.

3.5. Electric polarization of crystalline insulators

Change of electric polarization $P(x)$ is directly related to current. We consider 1D as above.

$\partial_x P(x,t) = -\rho(x,t)$ $\quad \rho(x,t)$ - charge density

$\partial_t \rho(x,t) = -\partial_x J(x,t)$ $\quad$ continuity

$\to \quad \partial_t P(x,t) = J(x,t)$

Using the result for $J_n(t)$ on p. 31, we get

$$\Delta P = e \sum_{n \leftarrow \text{filled bands}} \int_0^\lambda d\lambda' \int_{BZ} \frac{dk}{2\pi} \Omega^n_{k\lambda}$$

for the change of polarization as a result of an adiabatic process $\lambda = 0 \to \lambda$, which is in general not cyclic: $H(\lambda) \neq H(0)$.

The formula for ΔP can be simplified if one

choses the periodic gauge, in which A_λ is periodic in k. Then, upon substitution $\Omega^n_{k\lambda} = \partial_k A^n_\lambda - \partial_\lambda A^n_k$ into eq for ΔP, the first term yields zero after $\int dk$.

Berry connection

$$\rightarrow \quad \Delta P = e \sum_n \int_{BZ} \frac{dk}{2\pi} \int_0^\lambda d\lambda' \left(-\partial_\lambda A^n_k\right)$$

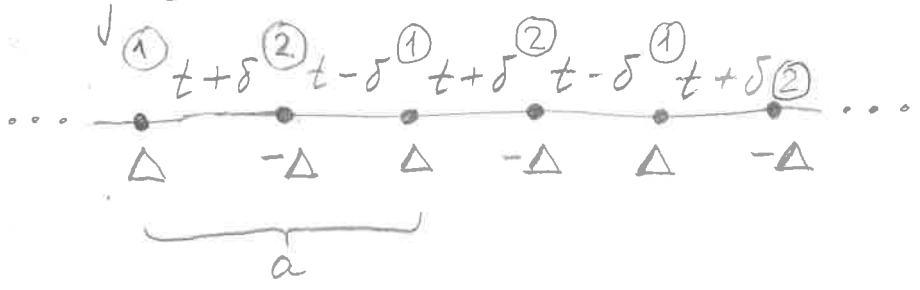
$$= -e \left[\sum_n \int_{BZ} \frac{dk}{2\pi} A^n_k \Big|_{\lambda=0}^{\lambda} + \text{integer} \right]$$

The integer uncertainty in the last formula is related to unknown (in this formula, where only the initial $\lambda = 0$ and final λ states are specified) number of cycles, each giving the integer pumped charge $Q_n = eC_n$ (and thus the same contribution to ΔP).

3.6. Example: Rice-Mele model

The Rice-Mele model is the simplest example of a two-band 1D model, in which one can realize the quantized (Thouless) pumping

$$H = \sum_j \left[\left(t + (-1)^{j-1}\delta\right)\left(c^+_{j+1} c_j + \text{h.c.}\right) + \Delta\,(-1)^{j-1} c^+_j c_j \right]$$



t – fixed
Δ, δ – varied
$t, \Delta, \delta \in \mathbb{R}$
$t > 0$

$$\hat{h}(k) = \begin{pmatrix} \Delta & t+\delta \\ t+\delta & -\Delta \end{pmatrix} + \begin{pmatrix} 0 & t-\delta \\ 0 & 0 \end{pmatrix} e^{-ika} + \begin{pmatrix} 0 & 0 \\ t-\delta & 0 \end{pmatrix} e^{ika}$$

$$= \begin{pmatrix} \Delta & t+\delta+(t-\delta)e^{-ika} \\ t+\delta+(t-\delta)e^{ika} & -\Delta \end{pmatrix}$$

$$= \vec{h}(k) \cdot \vec{\sigma} \qquad k \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right] \quad (1BZ)$$

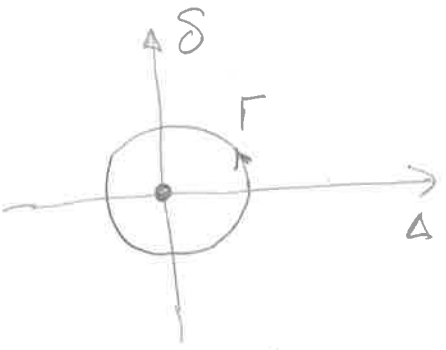
$$\vec{h}(k) = \left(t+\delta+(t-\delta)\cos ka,\ -(t-\delta)\sin ka,\ \Delta\right)$$

$$\epsilon(k) = \pm\left(4t^2\cos^2\frac{ka}{2} + 4\delta^2\sin^2\frac{ka}{2} + \Delta^2\right)^{1/2} = \pm|\vec{h}(k)|$$

There is a single degeneracy point:

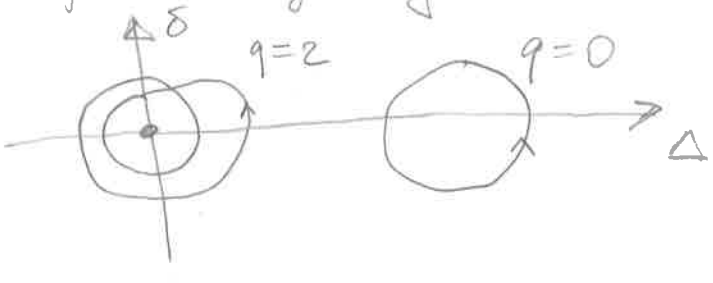
$$\Delta = 0, \quad \delta = 0, \quad k = \frac{\pi}{a} \quad \text{(which is the same as } -\frac{\pi}{a}\text{)}$$

For adiabatic pumping, the contour should not go through this point. The lower band is assumed to be filled, the upper band empty. Then, if the contour Γ goes once around the degeneracy point $(0,0)$, the pumped charge will be e:



In this case, the point $(\Delta=0,\ \delta=0,\ k=\frac{\pi}{a})$ will be inside the torus T^2, yielding a monopole inside S^2 in the mapping discussed above

More generally pumped charge is qe, where q is the number of windings of the contour Γ around $(0,0)$:



To obtain formally the pumped charge as a winding number, we use Sec. 2.3. The eigenstates of $\hat{h}(k)$ are parametrized by angular spherical coordinates θ, φ of $\vec{h}(k)$ (see p. 16)

The pumped charge (for the 1-> band, i.e. $n=1$)

$$Q_1 = eC_1 \; ; \quad C_1 = -C_2 = \int_0^1 d\lambda \int \frac{dk}{2\pi} \Omega^1_{k\lambda} \qquad \text{(see p. 31)}$$

$\leftarrow$ cycle in (Δ, δ) plane

In view of the invariance of the integral of Berry curvature with respect to reparametrization, we can make a change of variables $(k, \lambda) \to (\theta, \varphi)$.
As was found in Sec 2.3 (p. 17), $\Omega^1_{\theta\varphi} = \frac{1}{2}\sin\theta$

$$\Rightarrow \quad C_1 = -C_2 = \frac{1}{4\pi}\int \sin\theta \, d\theta \, d\varphi = \frac{1}{4\pi}\omega = q$$

where ω is the solid angle of the image of the torus T^2 in S^2. This is exactly the winding number q. If the degeneracy point $(0,0)$ is inside (outside) the cycle Γ, the image in S^2 will (will not) enclose the monopole, yielding $q=1$ (respectively, $q=0$).

4. Integer Quantum Hall Effect

This chapter is closely connected to Chapter 3 since 2D Chern insulators are realizations of IQHE.

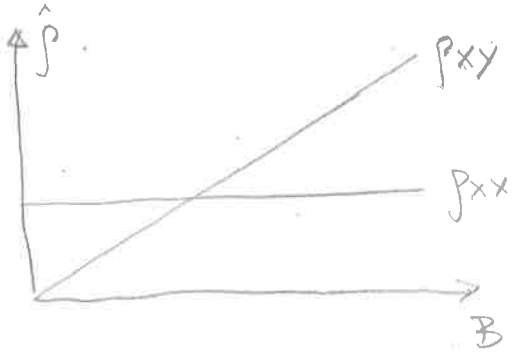
Classical Hall effect. Boltzmann equation for 2D gas in transverse magnetic field B, with impurity scattering (transport time τ)

→ resistivity tensor (n – density)

$$\hat{\rho} = \begin{pmatrix} \frac{m}{e^2 n \tau} & \frac{B}{nec} \\ -\frac{B}{nec} & \frac{m}{e^2 n \tau} \end{pmatrix}$$

Follows also from $\dot{\vec{p}} = -\frac{e}{mc}\vec{p}\times\vec{B} - e\vec{E} - \frac{\vec{p}}{\tau}$; $\vec{p} = m\vec{v}$,

$\vec{j} = -ne\vec{v}$; $\vec{j} = \hat{\sigma}\vec{E}$; $\hat{\rho} = \hat{\sigma}^{-1}$; $\vec{E} = \hat{\rho}\vec{j}$



Experiment 1980 von Klitzing, Dorda, Pepper
(1985 – Nobel prize von Klitzing)

IQH plateaus:

$$\begin{cases} \rho_{xx} = 0 \\ \rho_{xy} = \frac{h}{ne^2}, \quad n = 1, 2, \ldots \end{cases} \longleftrightarrow \begin{cases} \sigma_{xx} = 0 \\ \sigma_{yx} = n\frac{e^2}{h} \end{cases}$$

$R_H = \frac{h}{e^2} = 25812.807$ Ohm von Klitzing constant

Since 2019 serves in metrology for definition of Ohm (the value of R_H is fixed).

Experimental accuracy of quantization of IQHE plateaus: $\sim 10^{-10}$

⇔ Topology

4.1. Landau levels and IQHE

2D particle in magnetic field $\vec{B} \parallel z$

$\hat{H} = \frac{1}{2m}\left(\hat{\vec{p}} + \frac{e}{c}\vec{A}\right)^2$ $\quad \mathrm{rot}\,\vec{A} = \vec{B}$ $\quad$ (charge: $-e$)

Gauge freedom:

$\vec{A} = (0, Bx, 0)$ Landau gauge

$\vec{A} = \left(-\frac{B}{2}y, \frac{B}{2}x, 0\right)$ symmetric gauge

...

Landau gauge: $\hat{H} = \frac{1}{2m}\left[p_x^2 + \left(p_y + \frac{eB}{c}x\right)^2\right]$

$\psi(x,y) = e^{ik_y y}\chi(x)$

$-\frac{\hbar^2}{2m}\chi'' + \frac{m\omega_c^2}{2}(x-X)^2\chi(x) = E\chi(x)$

$\rightarrow$ harmonic oscillator

$\psi_{nX}(x,y) = e^{ik_y y} e^{-\frac{(x-X)^2}{2l_0^2}} H_n\left(\frac{x-X}{l_0}\right)$

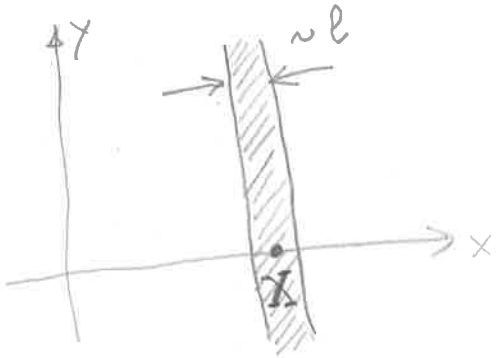
$E_n = \hbar\omega_c\left(n + \frac{1}{2}\right)$

$X = -k_y l_0^2$

$l_0 = \left(\frac{\hbar c}{eB}\right)^{1/2}$ magnetic length

$\omega_c = \frac{eB}{mc}$ cyclotron frequency

↖ Hermite polynomial $H_0(x) = 1$, $H_1(x) = x$ etc



E_n independent of X $\rightarrow$ degeneracy

$L_x \times L_y$ sample $\rightarrow$ $k_y = -\frac{2\pi n_y}{L_y}$, $n_y \in \mathbb{Z}$

$X = -k_y l_0^2$, $0 < X < L_x \rightarrow 0 < n_y < \frac{L_x L_y}{2\pi l_0^2}$

$\rightarrow$ number of states in one Landau level:

$N_S = \frac{L_x L_y}{2\pi l_0^2} = \frac{L_x L_y eB}{hc} = \frac{\Phi}{\Phi_0}$

Φ – flux through sample

$\Phi_0 = hc/e$ flux quantum

A filled Landau level $\leftrightarrow$ 1 electron per $2\pi l_0^2$ area

Filling factor $\nu = n \cdot 2\pi l_0^2 = \frac{hc}{e}\frac{n}{B} = \frac{N_e}{N_\Phi}$

(N_e – # of electrons, N_Φ – # of flux quanta)

Quantum-mechanical calculation of current:

$\hat{H} \to \hat{H} + e\mathcal{E}x$ $\quad$ $\mathcal{E}$ – electric field in x direction

→ still a harmonic oscillator

$$E_{nX} = \left(n+\frac{1}{2}\right)\hbar\omega_c + e\mathcal{E}X - \frac{1}{2}mv_D^2$$

$v_D = c\frac{\mathcal{E}}{B}$ drift velocity

$$\psi_{nX}(x,y) = e^{ik_y y}\chi\left(x - X + \frac{v_D}{\omega_c}\right)\cdot\frac{1}{\sqrt{L_y}}$$ ← normalization

Average velocity in each one-electron state

$$\langle v_y\rangle = \langle nX\left|\frac{\partial H}{\partial p_y}\right|nX\rangle = \frac{\partial E_{nX}}{\partial p_y} = e\mathcal{E}\frac{\partial X}{\partial p_y} = -\frac{e\mathcal{E}l_0^2}{\hbar} = -\frac{\mathcal{E}c}{B} = -v_D$$

$\langle v_x\rangle = 0$

Current density: $j_y = -e\langle v_y\rangle n = env_D = \frac{enc}{B}\cdot\mathcal{E}$

$$\to \begin{cases}\sigma_{yx} = nec/B \\ \sigma_{xx} = 0\end{cases}$$ classical result $\sigma_{yx} = \nu\frac{e^2}{h}$

This result follows also from Galilei invariance of the free-fermion (parabolic spectrum) system. In the coordinate frame that moves with $\vec{v}_d = c\frac{\vec{\mathcal{E}}\times\vec{B}}{B^2}$ one has $\vec{\mathcal{E}}' = 0$

$\Rightarrow$ no current $\Rightarrow$ $\vec{j} = -en\vec{v}_d$ in the original coordinate frame.

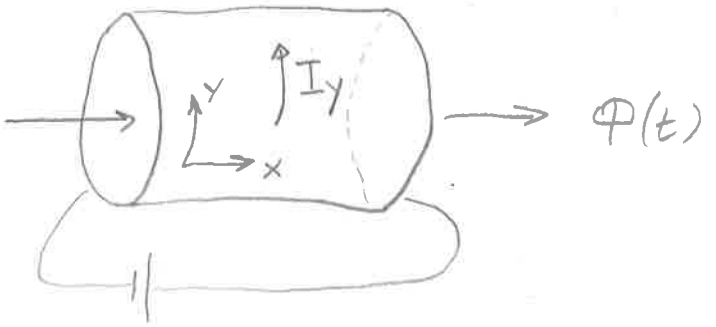
The Galilei invariance is broken by <u>disorder</u>, which leads to Anderson localization and is crucial for formation of QH plateaus in $\sigma_{xx}(n)$, $\sigma_{xy}(n)$.

The Galilei invariance is also broken by periodic potential. Note that one filled Landau level gives a contribution e^2/h to σ_{yx}. As we discuss below, a filled Landau level (for parabolic spectrum) can be viewed as a special case of a Chern band.

4.2. Laughlin gauge-invariance argument for Hall quantization. Bulk-boundary correspondence

Laughlin, 1981 ; Halperin, 1982 (there exist several modifications of the argument)

Wrap the 2D system to a cylinder



flux through the cylinder, adiabatically changed.
(This is NOT the flux of B that creates the QHE and is ⊥ to the surface of the cylinder)

V_x potential difference between the edges

Current in y direction

$$I_y = \langle \Psi | c \frac{\partial H}{\partial \Phi} | \Psi \rangle = c \frac{\partial E}{\partial \Phi}$$

Adiabatically slowly increase Φ by flux quantum Φ_0:

$$I_y \simeq c \frac{\Delta E}{\Phi_0}$$

The Hamiltonians $H(\Phi)$ and $H(\Phi + \Phi_0)$ [e.g. $H(0)$ and $H(\Phi_0)$] are equivalent → all eigenstates are the same.

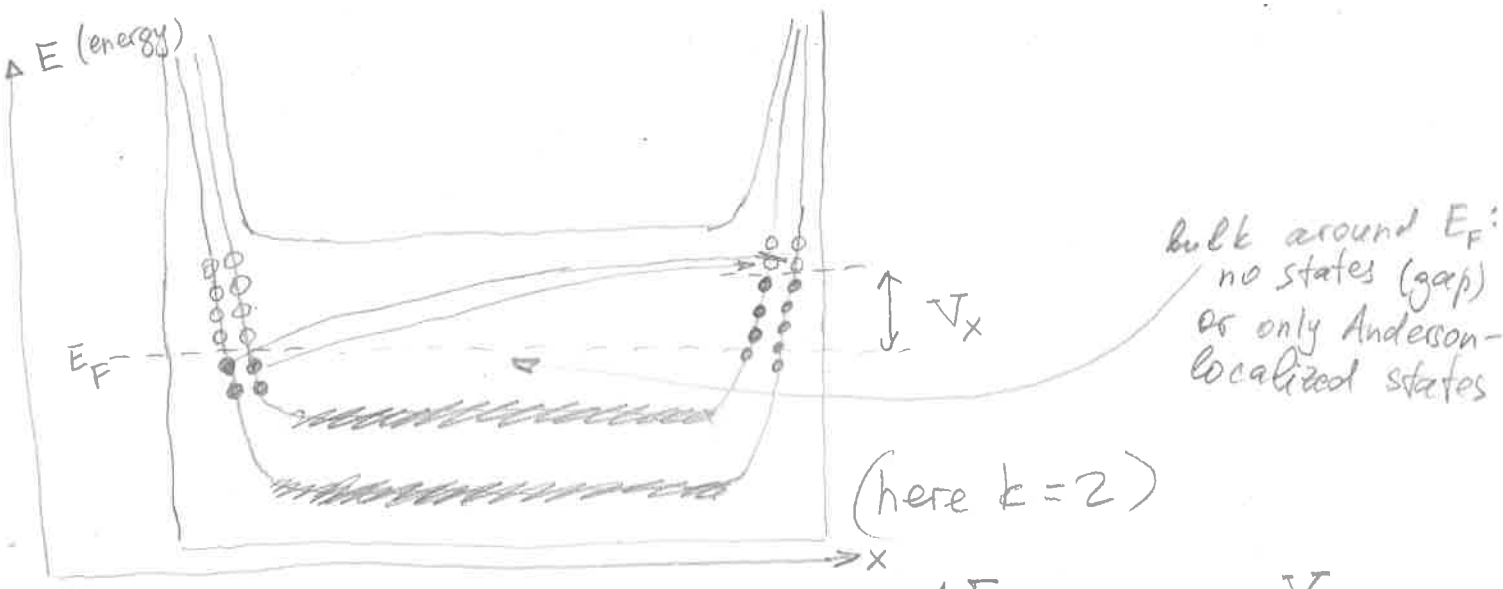
→ only occupation of states may have changed.

Only states near Fermi energy can be affected since the process is adiabatic.

Crucial assumption: Fermi energy is in the bulk gap.

Weaker version is sufficient: bulk states around E_F are Anderson-localized. Then bulk states are insensitive to the change of Φ → their occupation cannot change when $\Phi \to \Phi + \Phi_0$.

Thus, the only possibility is a transfer of $k \in \mathbb{Z}$ electrons from one edge to the other



$$\Delta E = k e V_x \quad \rightarrow \quad I_y = c \frac{\Delta E}{\Phi_0} = k \cdot \frac{e c V_x}{\Phi_0}$$

$$\Rightarrow \sigma_{yx} = \frac{I_y}{V_x} = k \cdot \frac{ec}{\Phi_0} = k \cdot \frac{e^2}{h} \qquad \boxed{k \in \mathbb{Z}}$$

Without disorder the evolution of states with changing Φ can be seen explicitly since Φ simply modifies k_y via $k_y \rightarrow k_y + 2\pi \frac{\Phi/\Phi_0}{L_y}$:

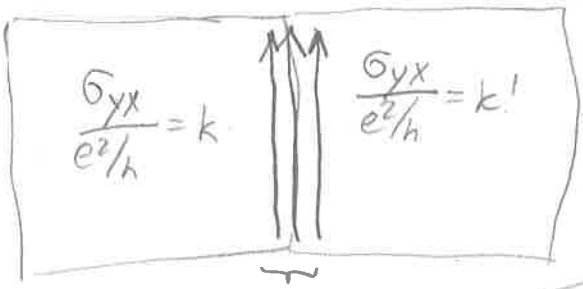
But the argument of Laughlin – Halperin holds also in the presence of disorder as long as bulk states near E_F are <u>Anderson – localized</u>

From Laughlin's argument, we clearly see <u>bulk-boundary correspondence</u>. Electrons can be transferred (i.e. boundary state population changed) $\longleftrightarrow$ there are delocalized edge modes.

For IQHE these are chiral modes.

$$\frac{\sigma_{yx}}{e^2/h} = k = \#\text{ of transfered electrons}$$
$$= \#\text{ of chiral edge modes.}$$

We will also see the bulk-boundary correspondance later in the field-theory formalism. More generally, edge modes should emerge at boundaries between topologically distinct phases:



$k-k'$ edge modes

4.3. Quantized Hall conductance as a topological invariant in the presence of interaction

(Niu, Thouless, Wu, 1985)

Consider now a system with both disorder and e-e interaction. Single-particle states are not defined any more, so that writing σ_{yx} as $\int$ over BZ does not work. However, it can be extended to the interacting case. Begin with Kubo formula

$$\sigma_{yx} = \frac{ie^2\hbar}{A} \sum_{n\neq 0} \frac{\langle \Psi_0 | \hat{v}_x | \Psi_n \rangle \langle \Psi_n | \hat{v}_y | \Psi_0 \rangle - \text{c.c.}}{(E_n - E_0)^2}$$

A - area of the system
Ψ_0 - many-body ground state
Ψ_n - many-body excited states

This is a generalization of the formula derived for band insulators without disorder and interaction in Sec. 3.1, 3.2

Sec. 3.1, 3.2: Hall conductivity of a band insulator (no disorder, no interaction)

$$\sigma_{yx} = \frac{e^2\hbar}{A} \sum_{n \in \{\text{filled bands}\}} \sum_{k \in 1BZ} \cdot$$

$$\cdot \; i \sum_{n' \neq n} \frac{\langle u_{nk} | v_x(k) | u_{n'k} \rangle \langle u_{n'k} | v_y(k) | u_{nk} \rangle - \text{c.c.}}{(\epsilon_{nk} - \epsilon_{n'k})^2}$$

$$\Omega^n_{k_x k_y} \equiv b_n$$

Here $v_i = \frac{1}{\hbar} \frac{\partial h(\vec{k})}{\partial k_i}$ – velocity $(i = x, y)$

Generalization to a system with interaction and disorder → Kubo formula as given on p. 45

Consider a system $L_x \times L_y$ wrapped into a torus, with fluxes Φ_x and Φ_y through the torus.

$\hat{I}_i = c \frac{\partial \hat{H}}{\partial \Phi_i}$ $i = x, y$ current $\qquad \hat{I}_i = -\frac{e}{L_i} \hat{V}_i$

$$\hat{V}_i = -\frac{L_i}{e} \hat{I}_i = -\frac{c}{e} L_i \frac{\partial \hat{H}}{\partial \Phi_i} = -\frac{\partial \hat{H}}{\partial (\hbar x_i)},$$

$$x_i = \frac{\Phi_i}{\hbar} \frac{e}{c L_i} = \frac{2\pi}{L_i} \frac{\Phi_i}{\Phi_0} \qquad \Phi_0 = hc/e$$

$$\sigma_{yx} = \frac{e^2}{\hbar A} i \sum_{n \neq 0} \frac{\langle \psi_0 | \frac{\partial \hat{H}}{\partial x_x} | \psi_n \rangle \langle \psi_n | \frac{\partial \hat{H}}{\partial x_y} | \psi_0 \rangle - c.c.}{(E_n - E_0)^2}$$

$\Omega^{(0)}_{x_x x_y}$ – Berry curvature of $|\psi_0\rangle$

Now, key assumptions:

(i) Fermi energy is in the gap.

Weaker version: Anderson localization of states around Fermi energy (i.e. low-lying bulk excitations)

(ii) Ground state is non-degenerate

Adiabatically change $\Phi_x : 0 \to \Phi_0$, $\Phi_y : 0 \to \Phi_0$

This corresponds to $\Delta x_i = \frac{2\pi}{L_i}$

Since bulk is gapped (or low-lying states are localized), σ_{yx} does not depend on x_i

$$\Rightarrow \quad \sigma_{yx} = \frac{e^2}{\hbar A} \frac{L_x L_y}{(2\pi)^2} \int_0^{2\pi/L_x} dx_x \int_0^{2\pi/L_y} dx_y \, \Omega^{(0)}_{x_x x_y} \qquad A = L_x L_y$$

$$= \frac{e^2}{h} \frac{1}{2\pi} \int_0^{2\pi/L_x} dx_x \int_0^{2\pi/L_y} dx_y \, \Omega^{(0)}_{x_x x_y} = \frac{e^2}{h} \cdot C, \qquad C \in \mathbb{Z}$$

Chern number

Comments:

* $(\varkappa_x, \varkappa_y)$ manifold is a torus T^2, fully analogous to (k_x, k_y) of clean non-interacting band insulator. In the latter case, adding fluxes simply shifts

$$k_x \to k_x + \varkappa_x, \quad k_y \to k_y + \varkappa_y$$

* The assumption of non-degenerate ground state is crucial. Otherwise, the ground state changes (within the degenerate subspace) upon inserting flux. This happens in FQHE.

4.4. Bloch bands in magnetic field and topological quantization of σ_{xy}

Harper 1955

Hofstadter 1976 "butterfly" fractality of spectrum

Thouless, Kohmoto, Nightingale, den Nijs 1982 (TKNN) topological quantization of σ_{xy} as Chern numbers of subbands

Hamiltonian $\hat{H}$ in periodic potential (no mag. field):

* $T_{\vec{a}} H T_{\vec{a}}^+ = H$ $\qquad T_{\vec{a}} = e^{\frac{i}{\hbar}\hat{\vec{p}}\vec{a}}$; $\vec{a} \in$ Bralais lattice
  ← translation operator
* all $T_{\vec{a}}$ commute

→ Bloch theorem: $T_{\vec{a}} \psi = e^{i\vec{k}\vec{a}} \psi$; $\vec{k}$ – Bloch wave vector

Now Hamiltonian in magnetic field:

$$H = \frac{1}{2m}\left[\vec{p} + \frac{e}{c}\vec{A}(r)\right]^2 \quad ; \quad \vec{\nabla} \times \vec{A}(\vec{r}) = \vec{B} \text{ (uniform field)}$$

$$H' \equiv T_{\vec{a}} H T_{\vec{a}}^+ = \frac{1}{2m}\left[\vec{p} + \frac{e}{c}A(\vec{r}+a)\right]^2 \neq H \to \text{no conventional Bloch theorem}$$

On the other hand, for uniform $\vec{B}$,

$$\vec{\nabla}\times\vec{A}(\vec{r}) = \vec{B} = \vec{\nabla}\times\vec{A}(\vec{r}+\vec{a})$$

$\rightarrow$ $\vec{A}(\vec{r})$ and $\vec{A}(\vec{r}+\vec{a})$ are related by gauge transformation

$$\vec{A}(\vec{r}+\vec{a}) = \vec{A}(\vec{r}) + \vec{\nabla} f_{\vec{a}}(\vec{r})$$

$$\rightarrow \quad H = e^{i\Phi_{\vec{a}}(\vec{r})} H' e^{-i\Phi_{\vec{a}}(\vec{r})} \qquad \boxed{\Phi_{\vec{a}}(\vec{r}) = \frac{e f_{\vec{a}}(\vec{r})}{\hbar c}}$$

$$\rightarrow \quad \tilde{T}_{\vec{a}} H \tilde{T}_{\vec{a}}^{+} = H, \qquad \tilde{T}_{\vec{a}} = e^{i\Phi_{\vec{a}}(\vec{r})} T_{\vec{a}}$$

magnetic translation operator

However, in general, $\left[\tilde{T}_{\vec{a}_1}, \tilde{T}_{\vec{a}_2}\right] \neq 0$

Check when this commutator is zero:

$$\tilde{T}_{\vec{a}_1}\tilde{T}_{\vec{a}_2}\tilde{T}_{\vec{a}_1}^{+} = e^{i\Phi_{\vec{a}_1}(\vec{r})} T_{\vec{a}_1} e^{i\Phi_{\vec{a}_2}(\vec{r})} T_{\vec{a}_2} T_{\vec{a}_1}^{+} e^{-i\Phi_{\vec{a}_1}(\vec{r})} =$$

$$= e^{i\Phi_{\vec{a}_1}(\vec{r}) + i\Phi_{\vec{a}_2}(\vec{r}+\vec{a}_1) - i\Phi_{\vec{a}_1}(\vec{r}+\vec{a}_2)} T_{\vec{a}_2} =$$

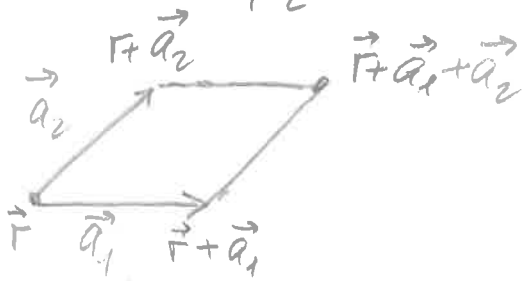
$$= e^{i\Phi_{\vec{a}_1}(\vec{r}) + i\Phi_{\vec{a}_2}(\vec{r}+\vec{a}_1) - i\Phi_{\vec{a}_1}(\vec{r}+\vec{a}_2) - i\Phi_{\vec{a}_2}(\vec{r})} \tilde{T}_{\vec{a}_2}$$

The total phase in exponential is

$$\left[\Phi_{\vec{a}_1}(\vec{r}) - \Phi_{\vec{a}_1}(\vec{r}+\vec{a}_2)\right] - \left[\Phi_{\vec{a}_2}(\vec{r}) - \Phi_{\vec{a}_2}(\vec{r}+\vec{a}_1)\right]$$

$$= \frac{e}{\hbar c}\oint_{P_{a_1a_2}} \vec{A}(\vec{r})\,d\vec{r} = \frac{e}{\hbar c}\Phi_{a_1a_2} = 2\pi\frac{\Phi_{a_1a_2}}{\Phi_0}$$

we use the definition of $\Phi_{\vec{a}_i}$ in the top of this page



$P_{a_1a_2}$ - parallelogram, $\Phi_{a_1a_2}$ - flux through it

$$\Rightarrow \boxed{\left[\tilde{T}_{\vec{a}_1}, \tilde{T}_{\vec{a}_2}\right] = 0 \quad \text{if} \quad \Phi_{\vec{a}_1\vec{a}_2}/\Phi_0 \in \mathbb{Z}}$$

Minimal choice: $\Phi_{\vec{a}_1 \vec{a}_2} = \Phi_0$,

i.e. exactly one flux quantum through the area of the Brillouin zone.

⇒ Landau levels can be viewed as a special case of Bloch bands. (Choice of $(\vec{a}_1, \vec{a}_2)$ is arbitrary, with the only condition that the unit cell area is Φ_0/B.)

Now consider $\hat{H}$ involving both: periodic potential and uniform magnetic field

$$H = \frac{1}{2m}\left[\vec{p} + \frac{e}{c}\vec{A}(\vec{r})\right]^2 + V(\vec{r})$$

Now, to have Bloch theorem, we need $\vec{a}_1, \vec{a}_2$ that are Bravais-lattice vectors (not necessarily primitive vectors) and that satisfy $\Phi_{\vec{a}_1 \vec{a}_2}/\Phi_0 \in \mathbb{Z}$.

This is possible if the flux through the unit cell of $V(\vec{r})$ is $(p/q)\Phi_0$; $p, q \in \mathbb{Z}$ (mutually prime). Then, there will be a <u>magnetic unit cell</u>, which includes q unit cells of $V(\vec{r})$, for which the flux is $p\Phi_0$ and thus the Bloch theorem holds.

→ <u>each band of the $B=0$ model splits into q subbands.</u>

Equivalently, each Landau level splits into p subbands.

Each subband n characterized by an integer Chern number $C^{(n)}$ and thus by $\sigma_{xy}^n = \frac{e^2}{h} C^{(n)}$, see Sec. 3.2.

The sum $\sum_n C^{(n)} = 0$.

Eigenfunction of $\hat{H}$ can be written in the Bloch form

$$\psi_{n\vec{k}}(\vec{r}) = e^{i\vec{k}\vec{r}}\, u_{nE}(\vec{r}),$$

Where $u_{n\vec{k}}(\vec{r})$ are invariant with respect to magnetic translations:

$\tilde{T}_{\vec{a}_j} u_{n\vec{k}}(\vec{r}) = u_{n\vec{k}}(\vec{r})$, which implies generalized periodic boundary conditions:

$$e^{i\phi_{\vec{a}_j}(\vec{r})}\, u_{n\vec{k}}(\vec{r}+\vec{a}_j) = u_{n\vec{k}}(\vec{r})$$

The simplest realization is a square-lattice tight-binding model, with magnetic field introduced as a phase factor of hopping matrix elements (Peierls' substitution)

$$t \to t e^{i\theta_\ell} \quad ; \quad \theta_\ell = \frac{e}{\hbar c}\int_\ell \vec{A}\cdot d\vec{r} \qquad \text{for each link } \ell$$

Choosing Landau gauge, one can reduce the Schrödinger equation to Harper equation (discrete 1D Schrödinger eq. in cosine potential). The spectrum of bands is the famous Hofstadter butterfly. For $p=1$ (i.e. $(1/q)\Phi_0$ flux through the lattice plaquette), almost all q subbands carry the Chern number $C^{(n)}=1$, except for one (for odd n) or two (for even n) subbands in the middle that "take care" of $\sum_n C^{(n)} = 0$. For large q (and $p=1$), subbands in the bottom (or top) of the band, where the tight-binding spectrum is parabolic, are usual Landau levels.