II. Geometrical band theory

From Band theory (crystals, Bloch's theorem) + Berry phase (hidden geometry, fiber bundle) to the Anomalous quantum Hall effect (QHE).

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1) Band theory : review and notations

H is a single electron Hamiltonian that is invariant under translations of a Bravais lattice.

Let $H(\vec{k}) \equiv e^{-i\vec{k}\cdot\hat{\vec{r}}} H e^{i\vec{k}\cdot\hat{\vec{r}}}$ be the Bloch Hamiltonian that depends on a parameter $\vec{k}$ and involves H <u>and</u> the position operator $\hat{\vec{r}}$.

Bloch's theorem allows one to diagonalize H (and $H(\vec{k})$):

$$H|\psi_{n\vec{k}}\rangle = \mathcal{E}_n(\vec{k})|\psi_{n\vec{k}}\rangle \quad \text{with} \quad \mathcal{E}_n(\vec{k}+\underset{\uparrow \text{ in the reciprocal lattice}}{\vec{G}}) = \mathcal{E}_n(\vec{k})$$

n = band index $= 1, 2, 3, \ldots$

$\vec{k}$ = wavevector in the 1st Brillouin zone (BZ) which is a torus T^d

with $|\psi_{n\vec{k}}\rangle = e^{i\vec{k}\cdot\hat{\vec{r}}}|u_n(\vec{k})\rangle$ where $u_{n\vec{k}}(\vec{r}+\underset{\uparrow \text{ in the Bravais lattice}}{\vec{R}}) = u_{n\vec{k}}(\vec{r})$

$$\boxed{H(\vec{k})|u_n(\vec{k})\rangle = \mathcal{E}_n(\vec{k})|u_n(\vec{k})\rangle}$$

$\mathcal{E}_n(\vec{k})$ is the <u>energy spectrum</u>

$|u_n(\vec{k})\rangle$ are the <u>eigenstates</u> $\longrightarrow$ <u>geometry</u> of a fiber bundle, of an emergent gauge structure (Berry phases) [locally in $\vec{k}$]

$\longrightarrow$ <u>topology</u> of this fiber bundle [globally in $\vec{k}$ over the BZ]

base space = $\vec{k}$ in BZ

fiber = Hilbert space spanned by $|u_n(\vec{k})\rangle$

2) Berry phases in band theory (Berry 1984)

Main idea : dynamics of a Bloch electron shows a separation of time scales.

- slow degree of freedom, slow dynamics of $\vec{k}$, slow motion from unit cell to unit cell, "heavy system"

- fast degree of freedom, fast dynamics of n, fast motion within the unit cell, "light system"

Similar to an atom with internal levels: orbital motion and inner dynamics.

$$\Delta k = \frac{2\pi}{L} \rightarrow \Delta\varepsilon_k \sim \hbar v \Delta k \sim \underset{\substack{\uparrow \\ \text{hopping amplitude}}}{t}\, \Delta k\, a \sim t\,\frac{a}{L} \rightarrow \underbrace{\frac{\hbar}{\Delta\varepsilon_k} \sim \frac{\hbar}{t}\,\frac{L}{a}}_{\text{long time scale}} \gg \frac{\hbar}{t}$$

$$\Delta n = 1 \rightarrow \Delta\varepsilon_n \sim t \rightarrow \frac{\hbar}{\Delta\varepsilon_n} \sim \frac{\hbar}{t} \quad (\text{short time scale})$$

Reaction of the "light system" on the "heavy system" is through an emergent gauge field (see M. Berry, "The quantum phase, 5 years after" 1988; Born-Oppenheimer approximation).

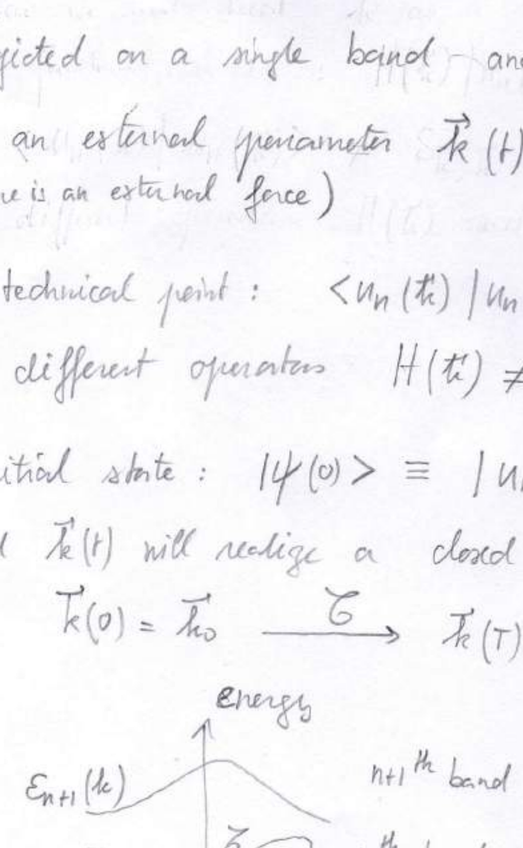
Here we will use the adiabatic theorem to follow the motion of an electron projected on a single band and whose dynamics is driven by the time evolution of an external parameter $\vec{k}(t)$: $\begin{cases} \vec{k} \text{ is now considered as a parameter (classical)} \\ n \text{ is still a quantum number} \end{cases}$
(there is an external force)

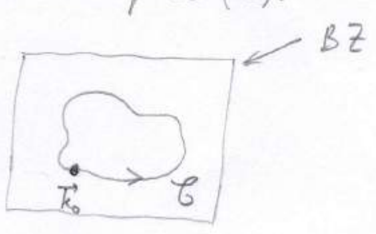
(A technical point: $\langle u_n(\vec{k}) | u_n(\vec{k}') \rangle \neq \delta_{\vec{k},\vec{k}'}$ as they are eigenvectors of different operators $H(\vec{k}) \neq H(\vec{k}')$.) to be discussed below

Initial state: $|\psi(0)\rangle \equiv |u_n(\vec{k}_0)\rangle$ $\qquad$ n is fixed (projection on a single band)

And $\vec{k}(t)$ will realize a closed path in parameter space (BZ).

$$\vec{k}(0) = \vec{k}_0 \xrightarrow{\ \mathcal{C}\ } \vec{k}(T) = \vec{k}_0$$





Remark: $\{|u_n(\vec{k})\rangle, \vec{k} \in BZ, \text{ fixed } n\}$ is called an adiabatic basis ⊛
it relies on a gauge choice (Berry gauge not em gauge). We could have taken $|\tilde{u}_n(\vec{k})\rangle = e^{i\phi_n(\vec{k})}|u_n(\vec{k})\rangle$ as another choice.

Adiabatic ansatz: $|\psi(t)\rangle \simeq \underbrace{e^{i\gamma(t)}}_{\text{to be found}}|u_n(\vec{k}(t))\rangle$ as the band n is non-degenerate

$$i\frac{d}{dt}|\psi(t)\rangle = H(\vec{k}(t))\,|\psi(t)\rangle \qquad H(t) \equiv H(\vec{k}(t)) = e^{-i\vec{k}(t)\cdot\hat{\vec{r}}}He^{i\vec{k}(t)\cdot\hat{\vec{r}}}$$

$$-\dot{\gamma}e^{i\gamma}|u_n\rangle + ie^{i\gamma}\dot{\vec{k}}\cdot|\nabla_{\vec{k}}u_n\rangle = e^{i\gamma}\varepsilon_n(\vec{k})|u_n\rangle$$

$\langle u_n|$

$$\dot{\gamma} = -\varepsilon_n(\vec{k}) + \dot{\vec{k}}\cdot\boxed{\underbrace{\langle u_n|i\vec{\nabla}_{\vec{k}}u_n\rangle}_{\equiv \vec{A}_n(\vec{k})}}$$

Berry connection (~ vector potential in $\vec{k}$-space)

Integrating on a full cycle: $$\gamma(T) - 0 = -\underbrace{\int_0^T dt\,\varepsilon_n(\vec{k}(t))}_{\text{dynamical phase (depends on } T)} + \underbrace{\oint_{\mathcal{C}} d\vec{k}\cdot\vec{A}_n(\vec{k})}_{\Gamma}$$

Γ Berry phase
geometrical phase
anholonomy
(does not depend on T but on the path $\mathcal{C}$ in parameter space)

One can show that the Berry phase is gauge-invariant for a closed path, but that the Berry connection depends on the gauge choice.

If the Berry connection is well defined on the whole patch of parameter space covered by $\mathcal{C}$ (the path) then we can use Stokes' theorem:

$$\boxed{\Gamma = \oint_{\mathcal{C}=\partial S} d\vec{k}\cdot\vec{A}_n(\vec{k})} = \int_S d^2\vec{S}\cdot\boxed{\vec{\Omega}_n(\vec{k}) = \vec{\nabla}_{\vec{k}}\times\vec{A}_n(\vec{k})} = \text{flux of Berry curvature}$$

Berry phase
(depends on $\underline{\mathcal{C}}$ and on $\underline{n}$)
(~ Aharonov-Bohm phase in $\vec{k}$-space)

Berry curvature
(~ magnetic field in $\vec{k}$-space)

The Berry curvature is gauge-independent (see below).

In 2D : $\vec{\Omega}_n(\vec{k}) = \Omega_n(\vec{k})\,\vec{u}_z$

$$\Omega_n(\vec{k}) = i\,\langle \partial_{k_x} u_n | \partial_{k_y} u_n \rangle + \text{c.c.}$$

Using first order perturbation theory, we can show that:

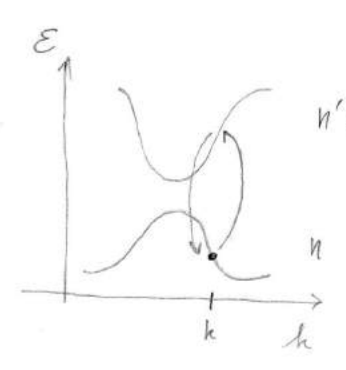
$$|\vec{\nabla}_{\vec{k}} u_n\rangle = \sum_{n'\neq n} |u_{n'}\rangle \frac{\langle u_{n'}|\vec{\nabla}_{\vec{k}} H(\vec{k})|u_n\rangle}{\varepsilon_{n'} - \varepsilon_n}$$

(Indeed $\quad H(\vec{k}+\delta\vec{k}) = \underbrace{H(\vec{k})}_{H_0} + \underbrace{\delta\vec{k}\cdot\vec{\nabla}_{\vec{k}} H(\vec{k})}_{V\ [\text{perturbation}]} + \dots$

$$\delta\vec{k}\cdot|\vec{\nabla}_{\vec{k}} u_n\rangle = |u_n(\vec{k}+\delta\vec{k})\rangle - |u_n(\vec{k})\rangle$$)

$$\Rightarrow \boxed{\Omega_n(\vec{k}) = i\sum_{n'\neq n}\frac{\langle u_n|\partial_{k_x} H(\vec{k})|u_{n'}\rangle\langle u_{n'}|\partial_{k_y} H(\vec{k})|u_n\rangle}{\left[\varepsilon_{n'}(\vec{k}) - \varepsilon_n(\vec{k})\right]^2} + \text{cc}}$$

obviously gauge-invariant, does not require a smooth gauge, involves all bands



Berry curvature is due to <u>inter-band effects</u>, ie to <u>virtual transition between bands</u> (<u>2nd order perturbation theory</u>)

The perturbation is due to the external force that drives the motion of $\vec{k}$. The coupling between bands comes from the velocity operator $\vec{\nabla}_{\vec{k}} H(\vec{k})$ which is not diagonal in $\{|u_n(\vec{k})\rangle\}$.

The Berry curvature exists only if there are several bands and if they are coupled. It is large when the band gap is small.

3) Emergent gauge structure: the Bloch (sub-)bundle

Where does the emergent geometrical structure come from?

- Separation of time scales between $\vec{k}$ and n $\Rightarrow$ adiabatic following of a single band (projection onto a single band). Back reaction of the fast dynamics ($n \rightleftarrows n'$) onto the slow dynamics ($\vec{k}$).

- $\underbrace{\langle u_n(\vec{k}) | u_n(\vec{k}') \rangle}$ $\neq \delta_{\vec{k},\vec{k}'}$ (*) whereas $\langle u_n(\vec{k}) | u_{n'}(\vec{k}) \rangle = \delta_{n,n'}$

  this overlap is a complex number

  the evolution of its phase with $\vec{k}$ $\rightarrow$ Berry connection, —— phase, —— curvature $\Big\}$ geometry of a fiber bundle

  $\langle u_n(\vec{k}+\delta\vec{k}) | u_n(\vec{k}) \rangle \simeq e^{i\,\delta\vec{k}\cdot\vec{A}_n(\vec{k})}$ at 1st order in $\delta\vec{k}$

  Chern number: topology of a fiber bundle

  the evolution of its modulus with $\vec{k}$ $\rightarrow$ quantum metric (distance between quantum states in the projective Hilbert space)

  $1 - |\langle u_n(\vec{k}+\delta\vec{k}) | u_n(\vec{k}) \rangle|^2 \simeq g_n^{ij}\,\delta k_i\,\delta k_j$ at 2nd order in $\delta\vec{k}$

- After projection on a single band, there is a $\Big\{$ fiber bundle / gauge structure

  B base space = parameter space = BZ torus T^d = projective Hilbert space (ie. Hilbert space after getting rid of the global gauge freedom $U(1)_{\text{Berry}}$)

  F fiber = Berry gauge freedom $U(1)$ = phase of $|u_n(\vec{k})\rangle$
  = 1-dim. complex vector space

  E fiber bundle = Hilbert space (after projection on a single band)

It is a complex one-dim. vector bundle also called a $U(1)$ principal bundle.

Is this bundle twisted or trivial? The answer is given by the first Chern number (also called TKNN number in the band theory context):

$$\boxed{C_n \equiv \frac{1}{2\pi}\int_{BZ=T^2} d^2\vec{k}\cdot\vec{\Omega}_n(\vec{k})} \sim \text{magnetic monopole charge}$$

It is an integer (via the same derivation as for the magnetic monopole).

4) Adiabatic pumping (Thouless 1983) ref: Xiao, Chang and Qian Niu, RMP 2010

a) A driven 1D crystal

We use a driven Hamiltonian $H(t)$ that is translation-invariant in space.

The Bloch Hamiltonian is $H(q,t) \equiv e^{-iq\hat{x}} H(t) e^{iq\hat{x}}$

$$H(q,t)\,|u_n(q,t)\rangle = \varepsilon_n(q,t)\,|u_n(q,t)\rangle$$

In the adiabatic limit, we have two parameters $q \in [-\frac{\pi}{a}, \frac{\pi}{a}[= T^1 = \text{1D BZ}$
$t \in [0, T[$

If the driving is periodic in time $H(t+T) = H(t) \Rightarrow (q,t) \in T^2$ torus

Let $|\psi(0)\rangle \equiv |u_n(q,0)\rangle$ be the initial state.

We want to find $|\psi(t)\rangle$ but go beyond the adiabatic limit considered by Berry. We use 1st order time-dependent perturbat° theory (see the Appendix in the above RMP 2010):

- $$|\psi(t)\rangle \simeq e^{i\gamma(t)} \left\{ |u_n(q,t)\rangle - i \sum_{n' \neq n} |u_{n'}\rangle \frac{\langle u_{n'}|\partial_t u_n\rangle}{\varepsilon_n - \varepsilon_{n'}} \right\}$$

$$\gamma(t) = \underbrace{-\int_0^t dt'\, \varepsilon_n(q,t')}_{\text{dyn. phase}} + \underbrace{\int_0^t dt' \langle u_n | i \dot{u}_n\rangle}_{\text{Berry phase}}$$ (this phase is not essential here)

- velocity operator $v_x(t) \equiv \dot{x} = \frac{1}{i}[x, H(t)]$

in the q-representation $v_x(q,t) \equiv e^{-iq\hat{x}}\, \hat{v}_x(t)\, e^{iq\hat{x}} = \frac{1}{i}[\hat{x}, H(q,t)] = \frac{\partial H(q,t)}{\partial q}$

- average velocity $= \langle \psi(t) | v_x(q,t) | \psi(t) \rangle$

$$= \cancel{e^{-i\gamma}} \left\{ \langle u_n| + i \sum_{n'\neq n} \frac{\langle \dot{u}_n|u_{n'}\rangle}{\varepsilon_n - \varepsilon_{n'}} \langle u_{n'}| \right\} \partial_q H(q,t) \cancel{e^{i\gamma}} \left\{ |u_n\rangle - i \sum_{n'\neq n} |u_{n'}\rangle \frac{\langle u_{n'}|\dot{u}_n\rangle}{\varepsilon_n - \varepsilon_{n'}} \right\}$$

$$= \underbrace{\langle u_n | \partial_q H | u_n \rangle}_{= \frac{\partial \varepsilon_n}{\partial q}(q,t)} + \underbrace{i \sum_{n' \neq n} \frac{\langle \dot{u}_n | u_{n'}\rangle \langle u_{n'} | \partial_q H | u_n\rangle}{\varepsilon_n - \varepsilon_{n'}} + \text{c.c.}}_{\text{anomalous velocity}}$$

= group velocity
[as $\partial_q(\langle u_n|u_n\rangle) = 0$]

anomalous velocity
(extra term due to virtual transitions to other bands)

but $\langle \dot{u}_n | u_{n'} \rangle = \dfrac{\langle u_n | \partial_t H(q,t) | u_{n'} \rangle}{\varepsilon_n - \varepsilon_{n'}}$

[This is again 1st order perturbat' theory as $|\dot{u}_n\rangle = \dfrac{|u_n(t+dt)\rangle - |u_n(t)\rangle}{dt}$

$$= \sum_{n' \neq n} |u_{n'}\rangle \frac{\langle u_{n'} | \partial_t H | u_n \rangle}{\varepsilon_{n'} - \varepsilon_n} \ ]$$

Therefore
$$\boxed{v_n(q,t) = \frac{\partial \varepsilon_n}{\partial q}(q,t) \underbrace{- i \sum_{n' \neq n} \frac{\langle u_n | \partial_q H | u_{n'} \rangle \langle u_{n'} | \partial_t H | u_n \rangle}{(\varepsilon_n - \varepsilon_{n'})^2} + c.c.}}$$

This is just the Berry curvature

$\Omega_n(q,t)$ — q is like q_x, t —— q_y

anomalous velocity induced by virtual transitions to other bands

b) <u>2D crystal in an electric field</u> (Karplus & Luttinger 1954)

Vectorial gauge (em) $\vec{A} = -\vec{\mathcal{E}}\, t$

$H_0 = \dfrac{\vec{p}^2}{2m} + V(\vec{r})$

$H_0(\vec{q}) \equiv e^{-i\vec{q}\cdot\hat{\vec{r}}} H_0\, e^{i\vec{q}\cdot\hat{\vec{r}}} = \dfrac{(\vec{p}+\vec{q})^2}{2m} + V(\vec{r})$

$H(t) = \dfrac{[\vec{p} + e\vec{A}(t)]^2}{2m} + V(\vec{r})$

$\Rightarrow H(\vec{q},t) = H_0(\vec{q} + e\vec{A}(t)) = H_0(\vec{k}(\vec{q},t))$ $\quad \vec{k}(\vec{q},t) \equiv \vec{q} + e\vec{A}(t) \equiv \vec{k}$

gauge-invariant momentum

$\dot{\vec{k}} = \dot{\vec{q}} + e\dot{\vec{A}} = \vec{0} - e\vec{\mathcal{E}}$ i.e. $\vec{k}(t) - \vec{k}(0) = -e\vec{\mathcal{E}}\, t$ This is indeed a pumping process

<u>ex:</u> $\vec{\mathcal{E}} = \mathcal{E}\, \vec{u}_y \rightarrow \vec{k}(t) = \left| \begin{array}{l} k_x(0) \\ k_y(0) - e\mathcal{E} t \end{array} \right.$

Bloch oscillation of period T_B such that $e\mathcal{E} T_B = 2\pi/a$

What is the current due to the electric field?

$\vec{v}_n(\vec{q},t) = \dfrac{\partial \varepsilon_n}{\partial \vec{q}}(\vec{q},t) - i \langle \partial_{\vec{q}} u_n | \partial_t u_n \rangle + c.c.$

but $\partial_{\vec{q}} = \partial_{\vec{k}}$ and $\partial_t = \dot{\vec{k}} \cdot \partial_{\vec{k}} = -e\vec{\mathcal{E}} \cdot \partial_{\vec{k}}$

$$\Rightarrow \boxed{\vec{v}_n(\vec{q},t) = \vec{v}_n(\vec{k}) = \vec{\nabla}_{\vec{k}}\, \varepsilon_n(\vec{k}) - e\vec{\mathcal{E}} \times \vec{\Omega}_n(\vec{k})}$$

anomalous velocity of Karplus and Luttinger; $\perp$ to $\vec{\mathcal{E}}$

<u>rk:</u> $v_n^{\alpha} = \partial_\alpha \varepsilon_n - i \langle \partial_{k_\alpha} u_n | (-e\mathcal{E}_\beta) | \partial_{k_\beta} u_n \rangle + c.c. = \partial_\alpha \varepsilon_n + e\mathcal{E}_\beta\, \Omega_n^{\alpha\beta}$

c) A parenthesis: The semiclassical equations of motion of a Bloch electron

Usually: $\begin{cases} \hbar\dot{\vec{k}} = -e\left(\vec{\mathcal{E}} + \dot{\vec{r}} \times \vec{B}\right) & \text{Lorentz force} \\ \dot{\vec{r}} = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}}\, \varepsilon_n(\vec{k}) & \text{group velocity} \end{cases}$ Peierls 30's

$\hbar\vec{k}$ is the gauge-invariant momentum $= \hbar\vec{q} + e\vec{A}$; $\hbar\vec{q}$ is the canonical momentum

Modified by Berry phases:

$$\begin{cases} \hbar\dot{\vec{k}} = -\vec{\nabla}_{\vec{\mathcal{R}}}\tilde{\varepsilon}_n - e\,\dot{\vec{\mathcal{R}}} \times \vec{B} = -e\left[\underbrace{\vec{\mathcal{E}}}_{-\vec{\nabla}_{\vec{\mathcal{R}}} A_0} + \dot{\vec{\mathcal{R}}} \times \vec{B}\right] \\ \dot{\vec{\mathcal{R}}} = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}}\tilde{\varepsilon}_n - \dot{\vec{k}} \times \vec{\Omega}_n(\vec{k}) \end{cases}$$

anomalous velocity
dual of the Lorentz force

$$\tilde{\varepsilon}_n(\vec{k}, \vec{\mathcal{R}}) \equiv \varepsilon_n(\vec{k}) - e A_0(\vec{\mathcal{R}}) - \vec{M}_n(\vec{k}) \cdot \vec{B} + \dots$$

orbital magnetic moment (emergent Zeeman effect)

$$\hbar\vec{k} = \hbar\vec{q} + \frac{e}{\hbar}\vec{A} = -i\hbar\vec{\nabla}_{\vec{r}} + \frac{e}{\hbar}\vec{A}$$ em gauge-invariant momentum

$$\vec{\mathcal{R}} = P_n\,\vec{r}\,P_n = \vec{r} + \vec{A}_n = i\vec{\nabla}_{\vec{q}} + \vec{A}_n$$ Berry gauge-invariant position

→ Zak phase, electric polarization

[cf. Xiao, Chang & Qian Niu, RMP 2010]

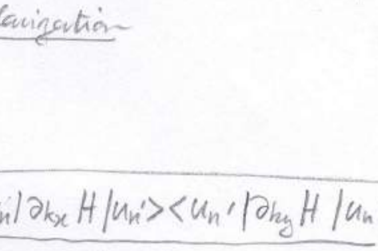
→ canonical position

$$\boxed{\vec{M}_n(\vec{k}) \equiv -\frac{e}{2}\left\langle\left(\hat{\vec{r}} - \langle\hat{\vec{r}}\rangle\right) \times \hat{\vec{v}}(\vec{k})\right\rangle} = +i\frac{e}{2\hbar}\sum_{n' \neq n} \frac{\langle u_n|\partial_{k_x}H|u_{n'}\rangle\langle u_{n'}|\partial_{k_y}H|u_n\rangle}{\varepsilon_n - \varepsilon_{n'}} + \text{c.c.}$$

This is analogous to the appearance of the Zeeman effect (with $g=2$) from the 3+1 Dirac equation upon projecting on the positive energy bands to obtain the Pauli equation.

5) The anomalous quantum Hall effect (AQHE)

Does a 2D band insulator conduct?
Electric field $\vec{\mathcal{E}}$, no magnetic field $\vec{B} = 0$.



current carried by a filled band:

$$\vec{j}_n = (-e)\,\frac{1}{A}\sum_{\vec{k}\in BZ} \underbrace{\vec{v}_n(\vec{k})}_{\frac{1}{\hbar}\vec{\nabla}_{\vec{k}}\mathcal{E}_n - \frac{e}{\hbar}\vec{\mathcal{E}}\times\vec{\Omega}_n(\vec{k})}$$

$$= -e \underbrace{\int_{BZ}\frac{d^2k}{(2\pi)^2}\,\vec{\nabla}_{\vec{k}}\,\mathcal{E}_n}_{\substack{=0 \text{ because} \\ \mathcal{E}_n(\vec{k}+\vec{G}) = \mathcal{E}_n(\vec{k})}} + \frac{e^2}{\hbar}\vec{\mathcal{E}}\times \underbrace{\int_{BZ}\frac{d^2k}{(2\pi)^2}\,\vec{\Omega}_n(\vec{k})}_{=\frac{1}{2\pi}\times C_n\,\vec{u}_z}$$

$$= \frac{e^2}{h}\,C_n\,\vec{\mathcal{E}}\times\vec{u}_z$$

If $\vec{\mathcal{E}} = \mathcal{E}_y\,\vec{u}_y$ then $j_x = \underbrace{\left(\frac{e^2}{h}\sum_{n<n_F} C_n\right)}_{\sigma_{xy}}\mathcal{E}_y$ (TKNN 1982)

There is a Hall current. It is quantized as $C_n \in \mathbb{Z} \Rightarrow \underbrace{\sum_{n<n_F} C_n}_{\text{Hall number}} \in \mathbb{Z}$

The Hall effect can only exist if time-reversal symmetry is broken.
But it does not require to break the translational symmetry of the lattice.
One does not need to apply a homogeneous magnetic field to get a QHE.
Here we did not show that $\sum_{n<n_F} C_n \neq 0$.

Next time, we will study a specific model for which $\sum_{n<n_F} C_n \neq 0$.