Geometrical nonlinear phenomena in solids ①

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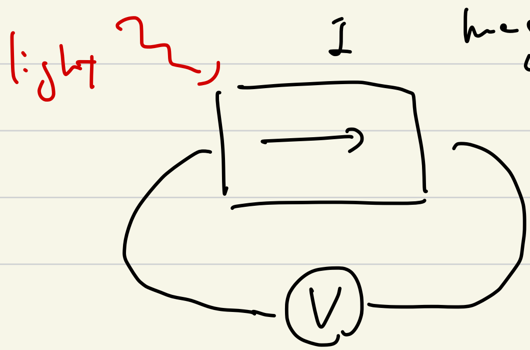
1. Introduction

- Geometry / topology in solids
  ⇐ QHE, topological insulators

- Response phenomena:
  electric transport, optical, thermal, magnetic } nonlinear response



1. Geometry in solids

semiclassics

Berry connection / curvature

2. Geometric nonlinear optical response

Shift current ← diagrams

3. Shift current in correlated electron systems.

· excitons, magnons, phonons

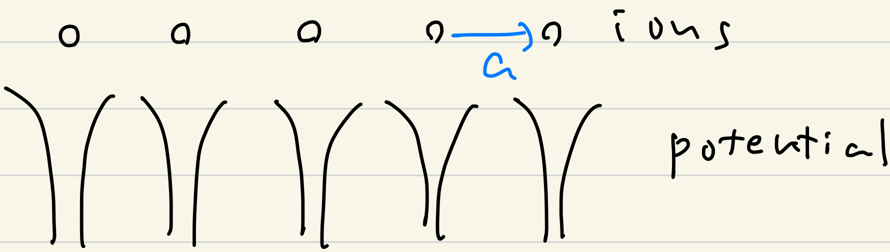
(Quantized circular photogalvanic effect in Weyl semimetals)

半古典近似

2. Geometry in solids

Band theory and Berry connection

$e^- \longrightarrow$ electron



- Schrödinger eq.

$$\underbrace{\Big[-\frac{\hbar^2}{2m}\nabla^2 + \underbrace{V(r)}_{\text{periodic}}\Big]}_{H(r)}\psi(r) = E\,\psi(r)$$

$$V(r+\underbrace{a}_{\text{lattice constant}}) = V(r)$$

$$H(r+a) = H(r)$$

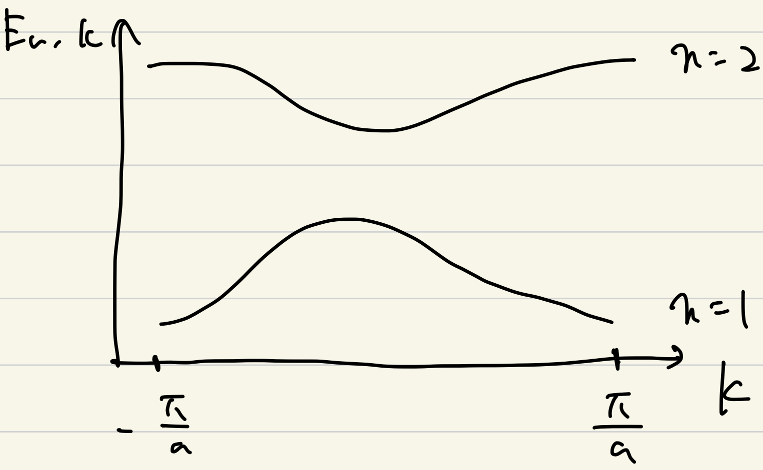
Bloch's theorem:

$$\psi_{n,k}(r) = \frac{1}{\underbrace{\sqrt{N}}_{\#\text{ unit cells}}} \underbrace{u_{nk}(r)}_{\text{periodic}} e^{ikr}$$

$$u_{n,k}(r+a) = u_{n,k}(r)$$

momentum $k \in$ Brillouin zone

square lattice $\left(-\frac{\pi}{a}, \frac{\pi}{a}\right)^d$



- position operator (redundancy due to the periodic structure)

Maybe : $r = i\partial_k$

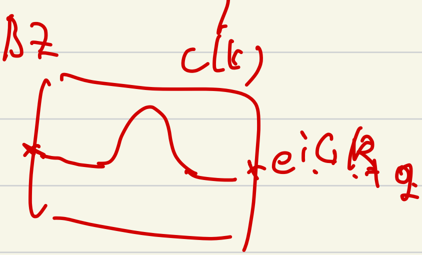
$\longleftrightarrow \left(\underbrace{p}_{\hbar k} = \frac{\hbar}{i}\partial_r \right)$ canonical conjugate

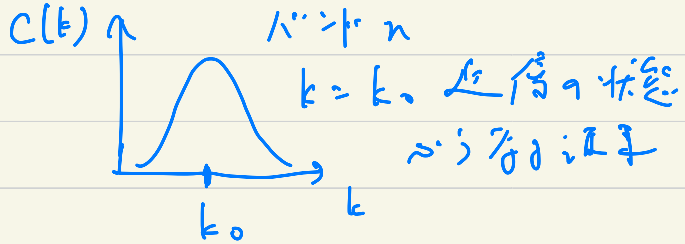
To check this, consider $\langle r \rangle$ for

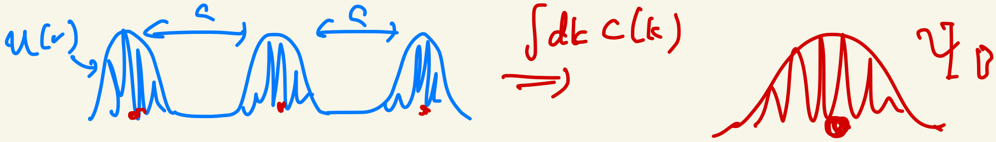
a Bloch wave packet Ψ_B :

$$\Psi_B = \frac{1}{\sqrt{N}} \int \frac{dk}{(2\pi)^d} \underbrace{c(k)}_{\text{weight factor}} \underbrace{e^{ikr} u_{nk}(r)}_{\text{Bloch wave function}}$$

BZは周期的







Bloch state : extended in r, fixed k

Bloch wave packet : localized in r & k
with finite widths

$\Leftarrow$ $\langle r \rangle$ is well defined

$$\langle r \rangle = \int dr\, \Psi_B^*(r)\, r\, \Psi_B(r)$$

$$= \frac{1}{N} \int \underbrace{\frac{dk}{(2\pi)^d}}_{[dk]} \underbrace{\frac{dk'}{(2\pi)^d}}_{[dk']} dr\, c^*(k')\, u^*_{nk'}(r)\, e^{-ik'r} \times r \times c(k)\, u_{nk}(r)\, e^{ikr}$$

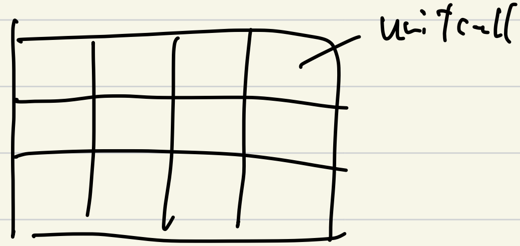
$$= \frac{1}{N} \int [dk][dk']\, dr\, c^*(k')\, u^*_{nk'}\, u_{nk}\, c(k) \times \underbrace{r\, e^{i(k-k')r}}_{-i\partial_k e^{i(k-k')r}}$$

kについて部分積分。表面項はおとす。

$$= \frac{1}{N}\int [dk][dk']\, \underline{\underline{dr}}\; c^*(k')\, i\partial_k \Big[\underset{(r)}{u^*_{nk'}}\; \underset{(r)}{u_{nk}}\; c(k) \Big]$$

$$\times\, e^{i(k-k')r}$$

$$\int dr \to \underbrace{\sum_{R}}_{\text{lattice vector}} \int_{\text{unit cell}} dr$$



$$\sum_R e^{i(k-k')r} = \underbrace{N}_{\#\text{ unit cells}} (2\pi)^d\, \delta(k-k')$$

$$= \int [dk][dk']\, c^*(k') \int_{\text{unit cell}} dr\;\; i\partial_k \Big[u^*_{nk'}\, u_{nk}\, c(k) \Big]$$

$$\times (2\pi)^d\, \delta(k-k')$$

$$= \int [dk)\, \underbrace{dk'}\; c^*(\underset{\substack{\downarrow \\ k}}{k'}) \int_{\text{unit cell}} dr \Big[u^*_{n\underset{\searrow k}{k'}}\, i(\partial_k u_{nk})\, c(k)$$

$$+\, u^*_{n\underset{\downarrow k}{k'}}\, u_{nk}\, i\partial_k c(k) \Big]$$

$$\times\, \underbrace{\delta(k-k')}$$

$\langle r \rangle$

$$= \int [dk]\, c^*(k) \Big[i \langle u_{nk} | \partial_k u_{nk} \rangle\, c(k) + i \underbrace{\langle u_{nk} | u_{nk} \rangle}_{\to 1}\, \partial_k c(k) \Big]$$

$$= \int [dk]\, c^*(k) \Big[i\partial_k + \underbrace{i \langle u_{nk} | \partial_k u_{nk} \rangle}_{\text{Berry connection } a_n(k)} \Big] c(k)$$

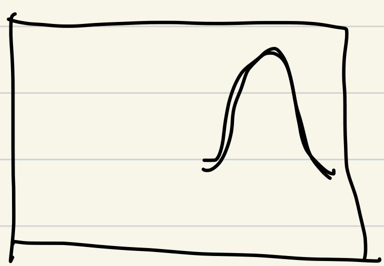
position operator

$$r = i\partial_k + a_n(k) \qquad \text{covariant derivative}$$

$$a_n(k) = i \langle u_{nk} | \partial_k u_{nk} \rangle$$

← dimension of length

unitcell



position of the wave packet within the unit cell

intracell cordinate

e^{-ikR} ← specifies the unit cell

- $C(k) = 1$ in Ψ_0 gives a Wannier function (localized wave packet at some unit cell for a given band)

$$W(r) = \frac{1}{\sqrt{N}} \int [dk]\, u_{nk} e^{ikr}$$

Define the polarization P as

$$P = q \int dr\, r\, |W(r)|^2$$

$$= q \int [dk]\, c^*(k) \left(i\partial_k + a(k) \right) C(k)$$

$\downarrow$ $C(k) = 1$

$$= q \underbrace{\int [dk]\, a(k)}_{\text{Berry phase}}$$

⇒ Berry phase formula for P

2.2 Berry curvature & anomalous velocity

Berry curvature: $F_n(k) = \nabla \times a_n(k)$

Consider

$$v = \frac{dr}{dt} = -\frac{i}{\hbar}[r, H]$$

for Ψ_0 with semiclassics:

$$\langle v \rangle = -\frac{i}{\hbar}\langle [i\partial_k + a_n(k), H'] \rangle$$

$$H' = H \underbrace{- qEx}_{\text{static potential in } E}$$

$(q = -|e|)$

$e^-_0 \Rightarrow$

$E (\propto x)$

$$\langle v_y \rangle = -\frac{i}{\hbar}\langle [y, H(k) - qEx] \rangle$$

$$= -\frac{i}{\hbar}\langle [y, H(k)] \rangle + \frac{iq}{\hbar} E \langle [y, x] \rangle$$

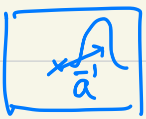
$$= \frac{1}{\hbar}\partial_{k_y} E_n(k) - \frac{iq}{\hbar} E \langle [x, y] \rangle$$

ψ_0 で期待値

・半古典 ⇒ 位置演算子は共変微分

局在化させた ψ_0 についての結果で近似

$$[x, y] = [i\partial_{k_x} + a_{x,n},\ i\partial_{k_y} + a_{y,n}]$$



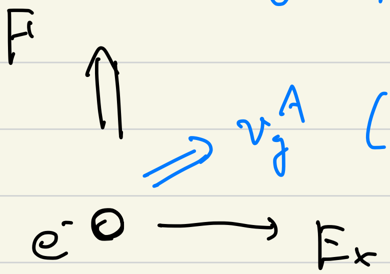
$$= i\partial_{k_x} a_{y,n} - i\partial_{k_y} a_{x,n}$$

$$= i[\nabla \times a]_z$$

$$= i F_n(k)$$

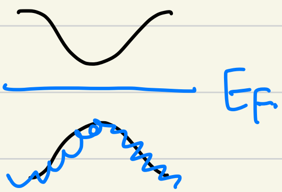
Berry curvature : noncommutativity of x & y in solids

$$\langle v_y \rangle = \underbrace{\frac{1}{\hbar}\partial_{k_y} E_n(k)}_{\text{group velocity}} + \underbrace{\frac{q}{\hbar} E F_n(k)}_{\text{anomalous velocity}}$$



$(\sim$ Hall current$)$

· For an insulator (a filled band):



$$\Rightarrow J_y = q\int \frac{dk}{(2\pi)^d} \langle v_y \rangle$$

$$= q\int \underbrace{[dk]}_{dk_y}\left[\cancel{\frac{1}{\hbar}\underbrace{\partial_{k_y}}_{}\underbrace{E_n(k)}_{0}} + \frac{q}{\hbar} E F_n(k)\right]$$

バンドの周期性

$$J_y = \frac{q^2}{\hbar} E_x \int [dk]\, F(k)$$

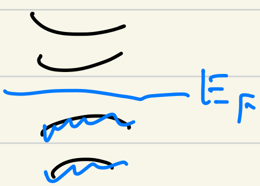
Hall conductivity $J_y = \sigma_{yx} E_x$

$$\sigma_{xy} = -\sigma_{yx} \Rightarrow$$

$$\underset{\text{ホール伝導度}}{\sigma_{xy}} = -\frac{q^2}{\hbar} \int \underset{\frac{dk}{(2\pi)^d}}{[dk]}\, F(k)$$

In 2D:

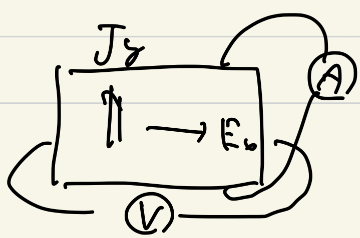
$$\sigma_{xy} = -\frac{q^2}{h} \underbrace{\int \frac{d^2k}{2\pi} F(k)}_{\text{Chern \# } C \in \mathbb{Z}} = -\frac{q^2}{h} C$$



multiband case:

$$\sigma_{xy} = -\frac{q^2}{h} \sum_n C_n$$

Quantum Hall effect



(Quantized anomalous Hall effect)