Lecture 4

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Last lectures

- projectors $\hat{P}_n \hat{P}_m = \delta_{nm} \hat{P}_n$
- for both non-degenerate bands

$$\hat{P}_n(k) = |u_n(k)\rangle\langle u_n(k)|$$

and degenerate bands

$$\hat{P}_n(k) = \sum_s |u_{(ns)}(k)\rangle\langle u_{(ns)}(k)|$$

$\longrightarrow$ gauge-invariant

- easy evaluation of derivatives
- identity for derivative

$$\partial_\alpha \hat{P} = \partial_\alpha \hat{P} \hat{P} + \hat{P} \partial_\alpha \hat{P}$$

with $\partial_\alpha = \partial / \partial k_\alpha$

- decomposition of Bloch Hamiltonian

$$\hat{H}(k) = \sum_n E_n(k) \hat{P}_n(k)$$

- quantum geometric tensor

$$Q_{\alpha\beta} = \mathrm{tr}\,[\hat{P}\partial_\alpha \hat{P}\partial_\beta \hat{P}]$$

$$= g_{\alpha\beta} - 1/2\,\Omega_{\alpha\beta}$$

with quantum metric

$$g_{\alpha\beta} = g_{(\alpha\beta)} = \mathrm{Re}\,Q_{\alpha\beta}$$

$$= 1/2\,\mathrm{tr}\,[\partial_\alpha \hat{P}\partial_\beta \hat{P}]$$

and Berry curvature

$$\Omega_{\alpha\beta} = \Omega_{[\alpha\beta]} = -2\,\mathrm{Im}\,Q_{\alpha\beta}$$

$$= i\,\mathrm{tr}\,[\hat{P}\partial_\alpha \hat{P}\partial_\beta \hat{P}] - (\alpha \leftrightarrow \beta)$$

- Chern number

$$C_n = -2\pi \int_{BZ} \frac{d^2k}{(2\pi)^2}\,\Omega^n_{xy}(k) \quad \in \mathbb{Z}$$

II. Quantum geometry of linear conductivity

A. Coupling to electric field

- we restrict ourselves to a spatially

uniform electric field $E(t)$

$\longrightarrow$ different electromagnetic gauge choices are possible

1) length gauge with $E \cdot \hat{r}$

2) velocity gauge (or incomplete Weyl gauge)

- set scalar potential $\phi = 0$

- $E(t) = -\frac{\partial}{\partial t} A(t)$

$\longrightarrow E(\omega) = i\omega A(\omega)$

We are using the velocity gauge in the following.

- Concept of minimal coupling for non-relativistic charged particle in an electromagnetic field in continuous space with position $\hat{x}$ and momentum $\hat{p}$ operators

$$\hat{p} \longrightarrow \hat{p} - qA$$

with charge $q = -e$. ($\phi = 0$ here)

We identify the transformation of $\hat{p}$ that produces such a shift using

$$[\hat{x}_j, \hat{p}_{j'}] = i\delta_{jj'} \qquad (*)$$

($\hbar = 1$ for simplicity) and the identity

$$e^{\hat{O}}\hat{B}e^{-\hat{O}} = \hat{B} + [\hat{O}, \hat{B}] + \tfrac{1}{2}[\hat{O}, [\hat{O}, B]] + \ldots$$

$\longrightarrow$

$$e^{iqA\cdot\hat{x}}\,\hat{p}_j\,e^{-iqA\cdot\hat{x}}$$

$$= e^{iq\sum_{j'} A_{j'}\hat{x}_{j'}}\,\hat{p}_j\,e^{-iq\sum_{j'} A_{j'}\hat{x}_{j'}}$$

$$= e^{\underbrace{iq\sum_{j'\neq j} A_{j'}\hat{x}_j}_{=\hat{O}}}\,\underbrace{e^{iqA_j\hat{x}_j}\,\hat{p}_j\,e^{-iqA_j\hat{x}_j}}_{=\hat{B}}\,e^{\underbrace{-iq\sum_{j'\neq j} A_{j'}\hat{x}_j}_{=-\hat{O}}}$$

$$\xrightarrow{(*)} [\hat{O}, \hat{B}] = 0$$

$$= e^{\underbrace{iqA_j\hat{x}_j}_{=\hat{O}}}\,\underbrace{\hat{p}_j}_{=\hat{B}}\,e^{\underbrace{-iqA_jx_j}_{=-\hat{O}}}$$

$$= \hat{p}_j + [iqA_j\hat{x}_j, \hat{p}_j] + \ldots$$

$$\overset{(*)}{=} \hat{p}_j - qA_j$$

- We transform the same idea from continuous space to a lattice introducing

$$\hat{H}[A(t)] = e^{-ie A(t) \cdot \hat{r}} \hat{H} e^{ie A(t) \cdot \hat{r}}$$

with

$$\hat{r} = \sum_{R,\alpha} (R + r_\alpha) \hat{n}_{R,\alpha} ,$$

where $\hat{n}_{R,\alpha} = \hat{c}^+_{R,\alpha} \hat{c}_{R,\alpha}$ with fermionic creation and annihilation operators satisfying

$$\{ \hat{c}_j , \hat{c}^+_{j'} \} = \delta_{jj'}$$

$$\{ \hat{c}_j , \hat{c}_{j'} \} = \{ \hat{c}^+_j , \hat{c}^+_{j'} \} = 0$$

with anticommutator

$$\{ \hat{A} , \hat{B} \} = \hat{A}\hat{B} + \hat{B}\hat{A}$$

Ex: (1) Show that the particle number operator commutes, i.e., $[\hat{n}_j , \hat{n}_{j'}] = 0$.

(2) Show that $\hat{c}^+_j \hat{c}^+_j = 0$ and $\hat{c}_j \hat{c}_j = 0$.

(3) Show that $\hat{n}_j^s = \hat{n}_j$ for all $s \in \mathbb{N}$.

(4) Show that $\hat{n}_j \hat{c}^+_j = \hat{c}^+_j$.

(5) Show the identity

$$e^{i\alpha \hat{n}_j} = 1 - (1 - e^{i\alpha}) \hat{n}_j$$

for $\alpha \in \mathbb{R}$ using the Taylor series of the exponential function.

(6) Show that $\hat{c}_j^+ e^{i\alpha \hat{n}_j} = \hat{c}_j^+$.

(7) Show that $e^{i\alpha \hat{n}_j} \hat{c}_{j'}^+ = \hat{c}_{j'}^+ e^{i\alpha \hat{n}_j}$ for $j \neq j'$.

- Minimal coupling for a tight-binding Hamiltonian

$$\hat{H}_0 = \sum_{R,R'} \sum_{\alpha,\alpha'} t_{\alpha\alpha'}(R - R')\, \hat{c}^+_{R,\alpha} \hat{c}_{R',\alpha'}$$

$$= \sum_k \sum_{\alpha,\alpha'} H_{\alpha\alpha'}(k)\, \hat{c}^+_{k,\alpha} \hat{c}_{k,\alpha'}$$

for which we calculate

$$\hat{H}[A(t)] = e^{-ieA(t)\cdot\hat{r}}\, \hat{H}_0\, e^{ieA(t)\cdot\hat{r}}.$$

(1) We notice that $(A \equiv A(t))$

$$e^{-ieA\cdot\hat{r}} = e^{-ieA\cdot\left(\sum_{R',\alpha'} (R' + r_{\alpha'})\hat{n}_{R'\alpha'}\right)}$$

$$= \prod_{R',\alpha'} e^{-ieA\cdot(R' + r_{\alpha'})\hat{n}_{R'\alpha'}}$$

(2) We identify the transformation of $\hat{c}^{+}_{R,\alpha}$

($\hat{c}_{R,\alpha}$ then calculated by

complex transposition)

$$e^{-ieA\cdot\hat{r}}\,\hat{c}^{+}_{R,\alpha}\,e^{ieA\cdot\hat{r}}$$

$$= e^{-ieA\cdot(R+r_\alpha)\hat{n}_{R\alpha}}\,\hat{c}^{+}_{R,\alpha}\,e^{ieA\cdot(R+r_\alpha)\hat{n}_{R\alpha}}$$

$$= \left(1-\left(1-e^{-ieA\cdot(R+r_\alpha)}\right)\hat{n}_{R\alpha}\right)\hat{c}^{+}_{R,\alpha}$$

$$= e^{-ieA\cdot(R+r_\alpha)}\,\hat{c}^{+}_{R,\alpha}$$

$\longrightarrow$ this phase is called <u>Peierls phase factor</u>

Thus, the tight-binding Hamiltonian coupled to a vector potential reads

$$\hat{H}[A(t)] = \sum_{R,R'}\sum_{\alpha,\alpha'} t_{\alpha\alpha'}(R-R')\underbrace{e^{-ieA(t)\cdot(R-R'+r_\alpha-r_{\alpha'})}}_{\text{particles get a phase when hopping spatially}}\,\hat{c}^{+}_{R\alpha}\,\hat{c}_{R'\alpha'}$$

Comment: spatially local effects of the external field are not included

(3) We calculate the effect of the minimal coupling in the momentum basis using the Fourier transform

$$\hat{c}^{\dagger}_{k,\alpha} = \frac{1}{\sqrt{N_c}} \sum_{R} e^{ik\cdot(R+r_\alpha)} \hat{c}^{\dagger}_{R,\alpha}$$

normalization N_c number of unit cells

$$\longrightarrow \quad e^{-ieA\cdot\hat{r}} \hat{c}^{\dagger}_{k,\alpha} e^{ieA\cdot\hat{r}}$$

$$= \frac{1}{\sqrt{N_c}} \sum_{R,\alpha} e^{ik\cdot(R+r_\alpha)} e^{-ieA\cdot\hat{r}} \hat{c}^{\dagger}_{R,\alpha} e^{ieA\cdot\hat{r}}$$

$$= \frac{1}{\sqrt{N_c}} \sum_{R,\alpha} e^{i(k-eA)\cdot(R+r_\alpha)} \hat{c}^{\dagger}_{R,\alpha}$$

$$= \hat{c}^{\dagger}_{k-eA(t),\alpha}$$

We find

$$\hat{H}[A(t)] = \sum_{k}\sum_{\alpha,\alpha'} H_{\alpha\alpha'}(k)\, \hat{c}^{\dagger}_{k-eA(t),\alpha}\, \hat{c}_{k-eA(t),\alpha'}$$

$$= \sum_{k}\sum_{\alpha,\alpha'} \underbrace{H_{\alpha\alpha'}(k+eA(t))}\, \hat{c}^{\dagger}_{k,\alpha}\, \hat{c}_{k,\alpha'}$$

the vector potential leads to a shift in lattice momentum

→ expansion in $A(t)$ leads to momentum derivatives of the

B. Multi-state geometry

We have a closer look at the momentum derivatives of the Hamiltonian using the expansion

$$\hat{H}(k) = \sum_n E_n(k)\,\hat{P}_n(k) \quad .$$

- Let us calculate $\left(\hat{H} = \hat{H}(k) \text{ and } E_n = E_n(k)\right)$

$$\hat{P}_n\,\partial_\alpha \hat{H}\,\hat{P}_m$$

$$= \sum_l \hat{P}_n\,\partial_\alpha\left(E_l\,\hat{P}_l\right)\hat{P}_m$$

$$= \sum_l \partial_\alpha E_l\ \underbrace{\hat{P}_n\,\hat{P}_l\,\hat{P}_m}_{=\,\delta_{nl}\,\delta_{nm}\,\hat{P}_n}$$

$$+ \sum_l E_l\ \underbrace{\hat{P}_n\,\partial_\alpha\hat{P}_l\,\hat{P}_m}_{\text{more detailed calculation required}}$$

- $\hat{P}_n\,\partial_\alpha\hat{P}_l\,\hat{P}_m$

$$= \hat{P}_n\left(\hat{P}_l\,\partial_\alpha\hat{P}_l + \partial_\alpha\hat{P}_l\,\hat{P}_l\right)\hat{P}_m$$

$$= \underbrace{\hat{P}_n \hat{P}_\ell}_{= \delta_{n\ell} \hat{P}_n} \partial_\alpha \hat{P}_\ell \hat{P}_m + \hat{P}_n \partial_\alpha \hat{P}_\ell \underbrace{\hat{P}_\ell \hat{P}_m}_{= \delta_{m\ell} \hat{P}_m}$$

$$= \delta_{n\ell} \underbrace{\hat{P}_n \partial_\alpha \hat{P}_n \hat{P}_m}_{} + \delta_{m\ell} \hat{P}_n \partial_\alpha \hat{P}_m \hat{P}_m$$

$$= \hat{P}_n \partial_\alpha \hat{P}_n \hat{P}_m \hat{P}_m$$

$$= \delta_{nm} \underbrace{\hat{P}_n \partial_\alpha \hat{P}_n \hat{P}_n}_{=0} - \hat{P}_n \hat{P}_n \partial_\alpha \hat{P}_m \hat{P}_m$$

$$= - \hat{P}_n \partial_\alpha \hat{P}_m \hat{P}_m$$

$$= - (\delta_{n\ell} - \delta_{m\ell}) \hat{P}_n \partial_\alpha \hat{P}_m \hat{P}_m$$

$$= i (\delta_{n\ell} - \delta_{m\ell}) \hat{e}_\alpha^{nm}$$

with $\hat{e}_\alpha^{nm} = i \hat{P}_n \partial_\alpha \hat{P}_m \hat{P}_m$

- Let's combine the result

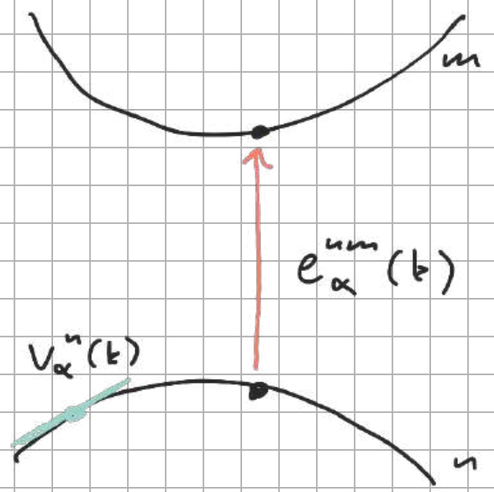
$$\boxed{\hat{P}_n \partial_\alpha H \hat{P}_m = \delta_{nm} v_n^\alpha P_n + i \varepsilon_{nm} \hat{e}_\alpha^{nm}}$$

with $v_n^\alpha = \partial_\alpha E_n$ and $\varepsilon_{nm} = E_n - E_m$.

Comment :

1) Intraband contributions $(n = m)$ involve the quasiparticle velocity v_n^α

2) Interband contributions ($n \neq m$) involve the quantity $\hat{e}_\alpha^{nm}$, which takes the role of a transition matrix element



3) We will find transitions $n \to m \to n$, which corresponds to

$$\mathrm{tr}\left[\hat{e}_\alpha^{nm}\, \hat{e}_\beta^{mn}\right]$$

Let us introduce the quantity

$$Q_{\alpha\beta}^{mn} = \mathrm{tr}\left[\hat{P}_n\, \partial_\alpha \hat{P}_m\, \partial_\beta \hat{P}_n\right]$$

multi-state quantity

in analogy to the quantum geometric tensor $Q_{\alpha\beta}^{n} = \mathrm{tr}\left[\hat{P}_n\, \partial_\alpha \hat{P}_n\, \partial_\beta \hat{P}_n\right]$. We have

$$Q_{\alpha\beta}^{mn} = \mathrm{tr}\left[\hat{P}_n\, \partial_\alpha \hat{P}_m\, \partial_\beta \hat{P}_n\right]$$

$$= \mathrm{tr}\left[P_n \left(P_m \partial_\alpha P_m + \partial_\alpha P_m P_m \right) \partial_\beta P_n \right]$$

$$= \delta_{nm} \, Q^n_{\alpha\beta}$$

$$- \mathrm{tr}\left[e^{nm}_\alpha e^{mn}_\beta \right]$$

so that we have $Q^{mn}_{\alpha\beta} = - \mathrm{tr}\left[e^{nm}_\alpha e^{mn}_\beta \right]$

for $m \neq n$.

4) In analogy we can introduce the two-state quantum metric and Berry curvature

$$Q^{mn}_{\alpha\beta} = g^{mn}_{\alpha\beta} - \tfrac{i}{2} \Omega^{mn}_{\alpha\beta}$$

with $g^{mn}_{\alpha\beta} = \mathrm{Re}\, Q^{mn}_{\alpha\beta}$ and

$\Omega^{mn}_{\alpha\beta} = -2\, \mathrm{Im}\, Q^{mn}_{\alpha\beta}$.

5) The two-state and single-state quantum geometric tensors are related via

$$\sum_{m\neq n} Q^{mn}_{\alpha\beta} = \sum_{m \neq n} \mathrm{tr}\left[\hat{P}_n \partial_\alpha \hat{P}_m \partial_\beta \hat{P}_n \right]$$

$$= \mathrm{tr}\left[\hat{P}_n \partial_\alpha (1 - \hat{P}_n) \partial_\beta \hat{P}_n \right]$$

$$= - Q^n_{\alpha\beta}$$

6) Let us consider $n \neq m$ only. Then,

$$\hat{e}_\alpha^{nm} = \frac{\hat{P}_n \partial_\alpha \hat{H} \hat{P}_m}{i \, \varepsilon_{nm}}$$

$$\longrightarrow Q_{\alpha\beta}^{mn} = - \frac{(\partial_\alpha H)_{nm} (\partial_\beta H)_{mn}}{(\varepsilon_{nm})^2}$$

with $(\partial_\alpha H)_{nm} = \langle u_n | \partial_\alpha H | u_m \rangle$

for non-degenerate bands

$\longrightarrow \Omega_{\alpha\beta}^{n} = -2 \sum_{m \neq n} \operatorname{Im} Q_{\alpha\beta}^{mn}$ leads to a commonly used formula for the Berry curvature.

Ex: We focus on the case with $n \neq m$.

(1) Show that $Q_{\alpha\beta}^{nm} = Q_{\beta\alpha}^{mn}$.

(2) Show that $\overline{Q_{\alpha\beta}^{mn}} = Q_{\beta\alpha}^{mn}$, where the overline denotes complex conjugation.

(3) Show that $g_{\alpha\beta}^{mn} = g_{(\alpha\beta)}^{(mn)}$ and $\Omega_{\alpha\beta}^{mn} = \Omega_{[\alpha\beta]}^{[mn]}$ with $O_{(ab)} = 1/2 \, (O_{ab} + O_{ba})$ and $O_{[ab]} = 1/2 \, (O_{ab} - O_{ba})$.