mitscherling@pks.mpg.de

10.12.24

Introduction to Quantum Geometry

Overview:

1) Geometric structure of quantum states

a) Band dispersion, Bloch states, and projectors

b) Two-band systems: Bloch sphere

c) Berry phase

d) Quantum metric and Berry curvature

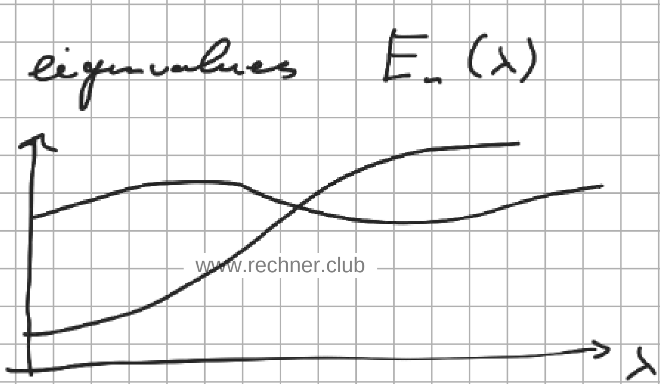
Basic setup

- continuous parameter $\lambda = (\lambda_1, \lambda_2, \ldots)$

  Ex: time, momentum, external fields, ...

- Hamiltonian $H(\lambda)$

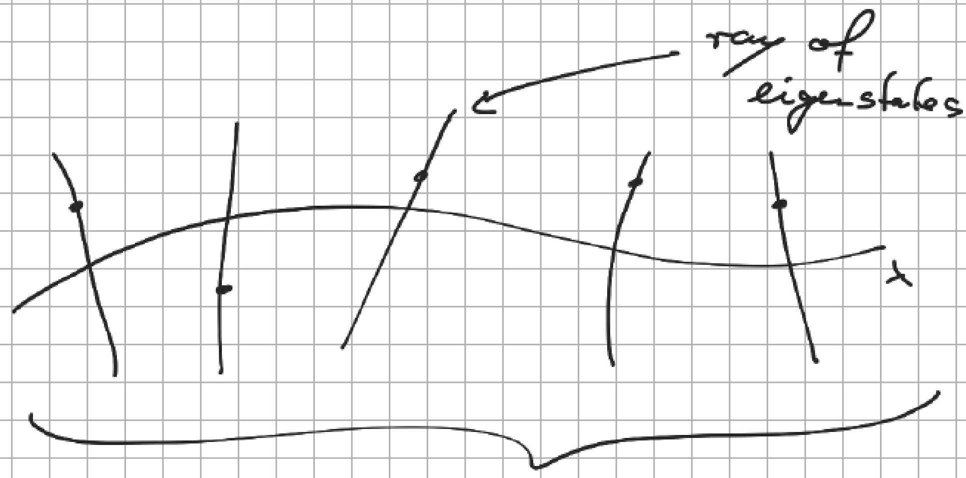
  $\longrightarrow$ eigenvalues $E_n(\lambda)$



$\longrightarrow$ eigenstates $|\psi_n(\lambda)\rangle$

(normalized up to $e^{i\phi_n(\lambda)}$)

complex projective bundle



states form complex projective bundle

$\longrightarrow$ this complicated structure leads to many physical phenomena (topology, quantum geometry, polarization, optical transitions, anomalous Hall effect, ...)

Q: How can we describe the physics in an efficient way avoiding a lot of technical issues?

$\longrightarrow$ better intuition

$\longrightarrow$ common principles

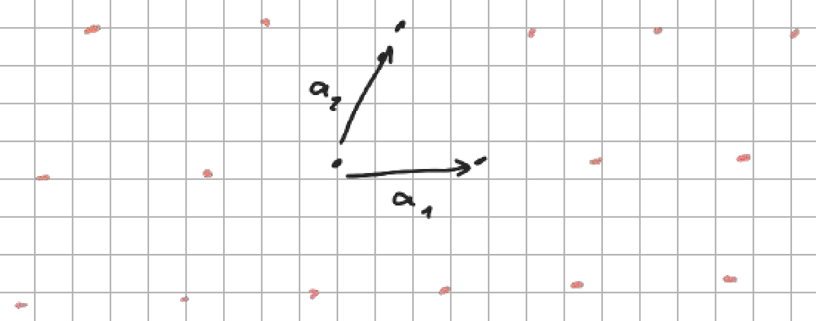
$\longrightarrow$ see connections

$\longrightarrow$ straightforward analytic and numerical results

A) Band dispersion, Bloch states, and projectors

- we consider a lattice characterized by a_i

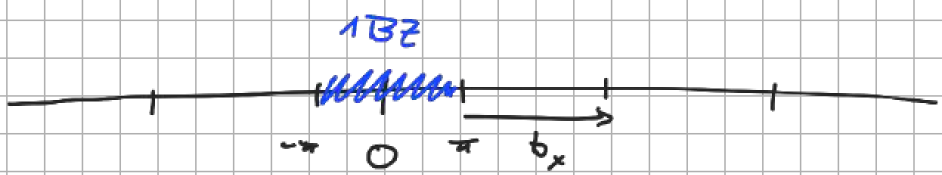
e.g. 2d



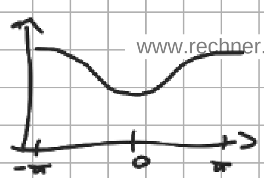
- Described by Bloch Hamiltonian $\hat{H}(k)$
- lattice momentum k
  - periodic in reciprocal lattice vectors b_i defined via $b_i \cdot a_j = 2\pi \delta_{ij}$
  - restricted to first Brillouin zone

$$k = \sum_i c_i b_i$$

with $c_i \in [0, 2\pi)$ or $[-\pi, \pi)$, e.g. 1d



- Diagonalizing of $H(k)$ gives
  - band dispersion $E_n(k)$, e.g.



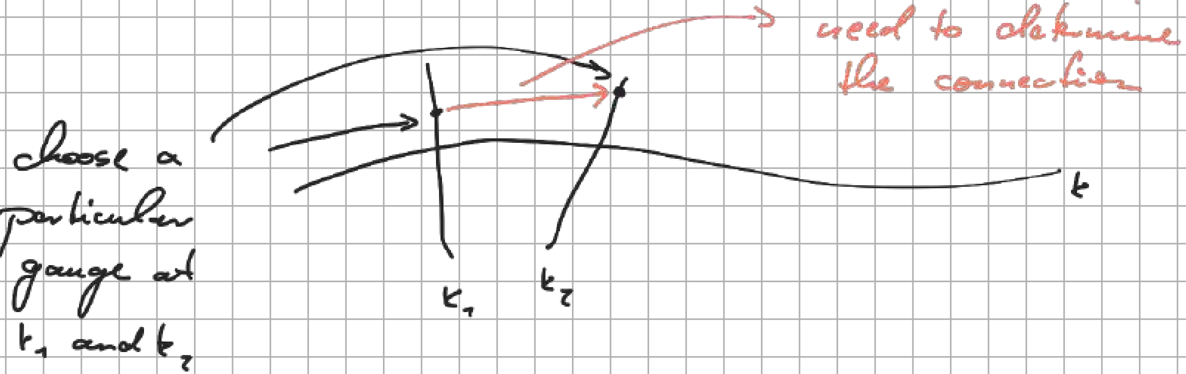
for

- Bloch states $|u_n(k)\rangle$

$\longrightarrow$ gauge redundancy

$$|u_n(k)\rangle \longrightarrow e^{i\phi_n(k)} |u_n(k)\rangle$$

Remark: this phase seems to be closely related to the global phase that is known to be physically irrelevant. The momentum dependence is crucial in this case. In other words,



$\longrightarrow$ this is done via the Berry connection

$$A_\alpha^{nm}(k) = i \langle u_n(k) | \partial_\alpha u_m(k)\rangle$$

with $\partial_\alpha \equiv \partial_{k_\alpha}$, which does depend on the phases chosen for the Bloch states:

$$A_\alpha^{nm}(k) \to e^{i(\phi_m(k) - \phi_n(k))} A_\alpha^{nm}(k) - \delta_{nm}\, \partial_\alpha \phi_n(k)$$

Summary:

(1) the change of the Bloch states under the shift in the momentum inherits a complex

internal structure from the Berry connection

(2) No observable can directly depend on the gauge freedom of the Bloch states because they are independent on the choice of basis.

1. Projectors

Goal: Reduce the gauge redundancy to a minimum

- We do this using projectors,

$$\hat{P}_n(k)\,\hat{P}_m(k) = \delta_{nm}\,\hat{P}_m(k) \qquad (1)$$

- For a non-degenerate band, we have

$$\hat{P}_n(k) = |u_n(k)\rangle\langle u_n(k)| \qquad (2)$$

$$\longrightarrow \cancel{e^{i\phi_n(k)}}\,|u_n(k)\rangle\langle u_n(k)|\,\cancel{e^{-i\phi_n(k)}} = \hat{P}_n(k)$$

For m-degenerate band, we have

$$\hat{P}_n(k) = \underbrace{\sum_{s=1}^{m}}_{\text{sum over subspace}} |u_{(ns)}(k)\rangle\langle u_{(ns)}(k)| \qquad (3)$$

Exercise:

(1) Show that the $\hat{P}_n$ defined in (2) and (3) satisfy (1).

(2) Show that $\hat{P}_n$ in (3) is $U(m)$-gauge invariant using

$$|u_{(ns)}(k)\rangle \longrightarrow \sum_{s'} U_{ss'}(k)\, |u_{(ns')}(k)\rangle .$$

- By construction,

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

- Completeness of basis

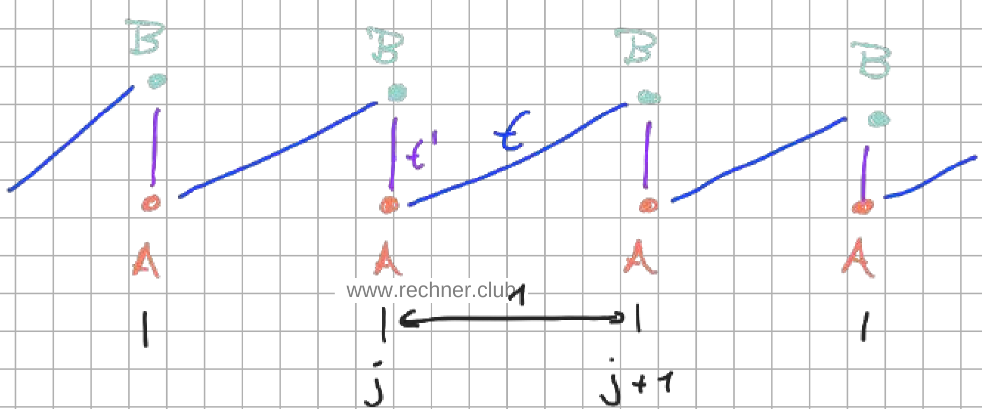
$$\sum_{n \in \text{bands}} \hat{P}_n(k) = \mathbb{1}_N$$

- Decomposition of Hamiltonian

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

2. Example: Su-Schrieffer-Heeger (SSH) model (part 1)

- "standard" model of topology introduction



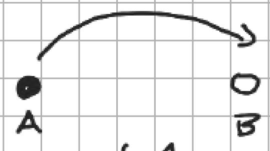
- Hamiltonian reads

assumed to be real

$$\hat{H} = \sum_j t\, \hat{c}^{+}_{j+1\,B}\, \hat{c}_{j\,A} + t'\, \hat{c}^{+}_{j\,A}\, \hat{c}_{j\,B} + h.c$$

creation operator

annihilation operator



$$c^{+}_{B}\, \hat{c}_{A}$$

- Use periodicity : Fourier transform

$$c^{+}_{j\sigma} = \frac{1}{\sqrt{2\pi}} \int_{BZ} e^{-ik\,(R_j + r_\sigma)}\, \hat{c}^{+}_{k\sigma}$$

$\int_{-\pi}^{\pi} dk$

a_j

here : $r_A = r_B = 0$ (position in unit cell)

$\longrightarrow$

$$\hat{H} = \int_{BZ} t\, e^{-ik}\, \hat{c}^{+}_{kB}\, c_{kA} + t'\, \hat{c}^{+}_{kA}\, \hat{c}_{kB} + h.c$$

$$\equiv \int_{BZ} \hat{\varphi}^{+}_{k}\, \hat{H}(k)\, \hat{\varphi}_{k}$$

with $\hat{\varphi}^{+}_{k} = \left(\hat{c}^{+}_{kA} \,,\, \hat{c}^{+}_{kB} \right)$

and $$\hat{H}(k) = \begin{pmatrix} 0 & t e^{ik} + t' \\ t e^{-ik} + t' & 0 \end{pmatrix}$$

- Diagonalization of matrix lead to

$$E_{\pm}(k) = \pm\sqrt{\epsilon^2 + t'^2 + 2\epsilon t' \cos k}$$

with Bloch states

$$|u_{\pm}(k)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm 1 \\ \frac{e^{-ik}\epsilon + t'}{\sqrt{\epsilon^2 + t'^2 + 2\epsilon t' \cos k}} \end{pmatrix}$$

satisfying $\langle u_n(k) | u_m(k)\rangle = \delta_{nm}$.

- The corresponding projectors are

$$P_{\pm}(k) = \frac{1}{2} \begin{bmatrix} 1 & \pm \frac{e^{ik}\epsilon + t'}{\sqrt{\epsilon^2 + t'^2 + 2\epsilon t' \cos k}} \\ \pm \frac{e^{-ik}\epsilon + t'}{\sqrt{\epsilon^2 + t'^2 + 2\epsilon t' \cos k}} & 1 \end{bmatrix}$$

Q: What are the three extreme limits of the SSH model? What are the underlying physical scenarios? How do the eigenstates behave in these cases?

B. Two-band systems: Bloch sphere

- momentum-dependent change of Bloch vector components crucial

- let's make a step back and consider a more general case using that $\hat{H}(k)$ is hermitian

$\longrightarrow$ expansion in $\mathbb{1}, \sigma_1, \sigma_2, \sigma_3$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- We have

$$\hat{H}(k) = d_0(k) \overset{\mathbb{1}}{} + d(k) \cdot \sigma \qquad (4)$$

with $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ and

$d(k) = (d_1(k), d_2(k), d_3(k))$.

$\longrightarrow$ determine coefficients via

$$d_0(k) = 1/2 \ \mathrm{tr}\, \hat{H}(k)$$

$$d_i(k) = 1/2 \ \mathrm{tr}\left[\hat{H}(k)\, \sigma_i\right]$$

- Band dispersions are

$$E_\pm(k) = d_0(k) \pm |d(k)|$$

- Bloch states are characterized by $n(k) = \frac{d(k)}{|d(k)|}$

$\longrightarrow$ projector reads

$$\hat{P}_\pm(k) = \tfrac{1}{2}\left(\mathbb{1}_2 \pm n(k)\cdot\sigma\right) \quad (5)$$

- to perform manipulations use identity

$$(n(k_1)\cdot\sigma)(n(k_2)\cdot\sigma) = n(k_1)\cdot n(k_2)\,\mathbb{1} + i\left(n(k_1)\times n(k_2)\right)\cdot\sigma$$

Exercise: Prove that (5) is an orthonormal projector and eigenfunction of (4).

1. Distance and phase between Bloch states

- typical quantity of interest

$$\langle u(k_1)|u(k_2)\rangle ,$$

which is gauge dependent : $e^{-i(\phi(k_1)-\phi(k_2))}$

$\longrightarrow$ let's consider its absolute value

"fidelity of pure state"

$$|\langle u(k_1)|u(k_2)\rangle|^2 = \mathrm{tr}\left[\hat{P}(k_1)\,\hat{P}(k_2)\right]$$

$$= 1/4\ \mathrm{tr}\left[(1 \pm n(k_1)\cdot\sigma)(1 \pm n(k_2)\cdot\sigma)\right]$$

$$= 1/4\ \left(2 + \mathrm{tr}\left[(n(k_1)\cdot\sigma)(n(k_2)\cdot\sigma)\right]\right)$$

$\mathrm{tr}[\sigma] = 0$

$\mathrm{tr}[1_2] = 2$

$$= 1/2\ \left(1 + n(k_1)\cdot n(k_2)\right)$$

- $k_1 = k_2$: parallel vectors $\longrightarrow 1$

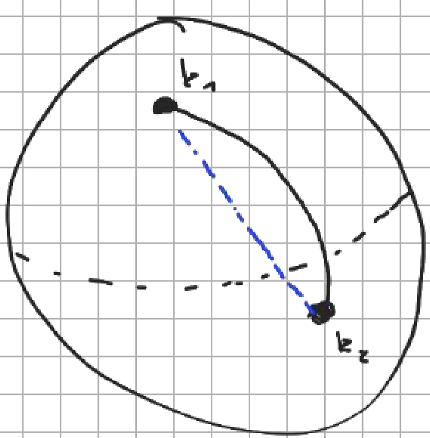
orthogonal : $n(k_1)\cdot n(k_2) = -1$

$\leftrightarrow \ |\langle u(k_1)|u(k_2)\rangle|^2 = 0$

- distance on Bloch sphere

$\hat{=}$ arc length $s = \Theta = \arccos\left(n(k_1)\cdot n(k_2)\right)$

$\hat{=}$ angle between unit vectors



$\longrightarrow$ distance function for quantum states

$$D\left(|u(k_1)\rangle, |u(k_2)\rangle\right) = 1 - |\langle u(k_1)|u(k_2)\rangle|^2$$

("naive" definition $\| |u(k_1)\rangle - |u(k_2)\rangle \|^2$ would not work)

- phase information of Bloch states

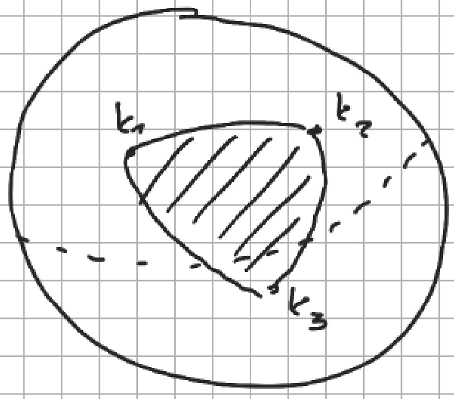
  - two-point function not sufficient

    $\longrightarrow$ three-point function

$$\langle u(k_1) | u(k_2) \rangle \langle u(k_2) | u(k_3) \rangle \langle u(k_3) | u(k_1) \rangle$$

$$= \mathrm{tr} \left[P(k_1) \, P(k_2) \, P(k_3) \right]$$

- for two-band case



$$\tfrac{1}{8} \, \mathrm{tr} \left[(1 \pm n_1 \cdot \sigma)(1 \pm n_2 \cdot \sigma)(1 \pm n_3 \cdot \sigma) \right]$$

$$= \tfrac{1}{8} \Big(2 + \mathrm{tr}\left[(n_1 \cdot \sigma)(n_2 \cdot \sigma) \right] + \ldots$$

$$\pm \mathrm{tr} \left[(n_1 \cdot \sigma)(n_2 \cdot \sigma)(n_3 \cdot \sigma) \right] \Big)$$

$$= \tfrac{1}{4} \Big(1 + n_1 \cdot n_2 + n_2 \cdot n_3 + n_3 \cdot n_1$$

$$\pm i \, (n_1 \times n_2) \cdot n_3 \Big)$$

Excercise: Show that the two- and three-point functions are sufficient to capture all n-point functions constructed from projectors of non-degenerate bands. For this, first show

$$\mathrm{tr}\left[P_1 P_2 P_3 P_4\right] \mathrm{tr}\left[P_3 P_1\right] = \mathrm{tr}\left[P_1 P_2 P_3\right] \mathrm{tr}\left[P_3 P_4 P_1\right]$$

for $P_i = |u(k_i)\rangle\langle u(k_i)|$.