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Lecture 7: The geometric structure of quantum states

Last lecture: Gauge-invariant description of quantum state properties of $H(k)$

- $P_n P_m = \delta_{nm} P_n$
- two-band: $P_\pm = \frac{1}{2}(\mathbb{1} \pm n \cdot \sigma)$

  with $n = \frac{d}{|d|}$ and $\hat{H} = d_0 + d \cdot \sigma$
- two-point function:

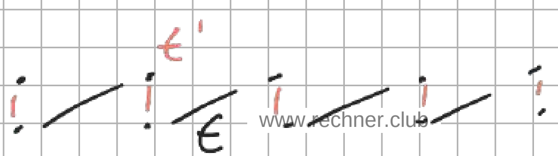
  $$\mathrm{tr}\left[P_n(k_1)\, P_n(k_2) \right]$$

  $\longrightarrow$ distance between states
- three-point function:

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

  $\longrightarrow$ phase information

Example of Bloch sphere for SSH model

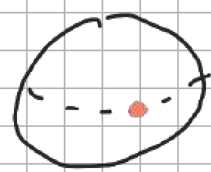


$$n(k) = \frac{1}{\sqrt{\epsilon^2 + \epsilon'^2 + 2\epsilon\epsilon' \cos k}} \begin{pmatrix} \epsilon \cos k + \epsilon' \\ -\epsilon \sin k \\ 0 \end{pmatrix}$$

- Restricted to equator due to chiral symmetry, $\sigma_z H(k) \sigma_z = -H(k)$

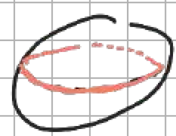
- For $|\epsilon| \ll |\epsilon'|$:

$$n(k) = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$



- For $|\epsilon'| \ll |\epsilon|$:

$$n(k) = \begin{pmatrix} \cos k \\ -\sin k \\ 0 \end{pmatrix}$$



C. Berry phase

$$A_\alpha(k) = i \langle u(k) | \partial_\alpha u(k) \rangle$$

is gauge dependent $A_\alpha(k) \to A_\alpha(k) - \partial_\alpha \phi(k)$

- a gauge invariant quantity is the

geometric / Berry phase

$$e^{i\gamma(C)} = e^{i\int_{-\pi}^{\pi} dk\, A(k)}$$

(closed loop)

$$\longrightarrow e^{i\int_{-\pi}^{\pi} dk\,(A(k) - \partial_\alpha \phi(k))} = e^{i\gamma(C)}$$

$\rightarrow$ discontinuities of size $2\pi\mathbb{Z}$

for closed loop C

$\longrightarrow \int_{-\pi}^{\pi} dk\, A(k)$ is unique up to $2\pi\mathbb{Z}$

- Gauge-invariant operator for any path

$$A^k_\alpha(k) = i/2 \sum_n [P_n(k), \partial_\alpha P_n(k)]$$

Kato potential ($\rightarrow$ Marin's lectures)

- For two-band model using $P_+ + P_- = 1$

$$\rightarrow \quad A^k_\alpha(k) = i\,[P_\pm, \partial_\alpha P_\pm]$$

$$= i/4\,[1 \pm n\cdot\sigma, \partial_\alpha(1 \pm n\cdot\sigma)]$$

$$= i/4\,[n\cdot\sigma, \partial_\alpha n\cdot\sigma]$$

$$= i/4\,(n\cdot\partial_\alpha n\, 1 + i(n\times\partial_\alpha n)\cdot\sigma - \partial_\alpha n\cdot n\, 1 - i(\partial_\alpha n\times n)\cdot\sigma)$$

$$= -1/2\,(n\times\partial_\alpha n)\cdot\sigma$$

$$\longrightarrow \frac{1}{2\pi}\int_{-\pi}^{\pi} dk\, A^k(k) = \begin{cases} 1/2\,\sigma_z & |t'|<|t| \\ 0 & \text{else} \end{cases}$$

Ex: In anticipation of the discussion of optical responses, we define

$$e_\alpha^{mn}(k) = i P_m(k)\, \partial_\alpha P_n(k) P_m(k)$$

with band indices n, m.

(1) Show that $e^{nn}(k) = 0$.

(2) Show that $(e_\alpha^{mn})^\dagger = e_\alpha^{nm}$.

(3) Show that

$$A_\alpha^k(k) = -\tfrac{1}{2} \sum_{n,m} \left(e_\alpha^{mn}(k) + e_\alpha^{nm}(k) \right)$$

D. Quantum metric

Let us expand

$$\mathrm{tr}\left[P_n(k)\, P_n(k+q) \right]$$

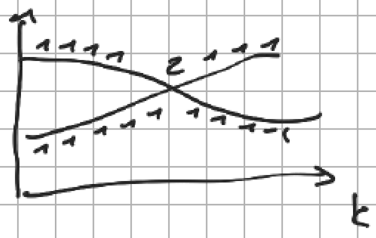
for small q using

$$P_n(k+q) = P_n(k) + \sum_\alpha q_\alpha \partial_\alpha P_n(k) + \tfrac{1}{2} \sum_{\alpha,\beta} q_\alpha q_\beta\, \partial_\alpha \partial_\beta P_n(k) + \dots$$

- zeroth order: $\mathrm{tr}[PP] = \mathrm{tr}[P]$

is the rank of the projector

Assume that it is constant for all k, no band crossings



- first order :

$$\mathrm{tr}\,[P\,\partial_\alpha P]$$

$$= 1/2\,(\mathrm{tr}\,[P\,\partial_\alpha P] + \mathrm{tr}\,[\partial_\alpha P\,P])$$

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

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

$$= 1/2\;\partial_\alpha\,\underbrace{\mathrm{tr}\,[P]}_{\text{const in } k} = 0$$

Important identity

$$\boxed{\partial P = \partial P\,P + P\,\partial P}$$

$$\longrightarrow\quad \mathrm{tr}\,[P_n(k)\,P_n(k+q)]$$

$$= 1 + 1/2\sum_{\alpha,\beta} q_\alpha q_\beta\;\mathrm{tr}\,[P_n(k)\,\partial_\alpha\partial_\beta P_n(k)]$$

Ex : Show that

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

via the projector identity for $\partial_\alpha\partial_\beta P$.

We define the quantum (or Fubini-Study) metric

$$g^n_{\alpha\beta}(k) = 1/2 \; tr\left[\partial_\alpha P_n(k) \, \partial_\beta P_n(k) \right]$$

1. Certain properties of the quantum metric

- metric is real and symmetric in $\alpha \leftrightarrow \beta$
- it is a pseudo-metric (can have more zeros than a metric)
- metric depends on choice of projector P

$$g_{\alpha\beta} = 1/2 \; tr\left[\partial_\alpha P \, \partial_\beta P \right]$$

$\longrightarrow$ different metrics

- metric arising from all states

$$P_{all} = \sum_n P_n = 1$$

vanishes. $\longrightarrow$ standard property in geometry and topology

- Different metrics can be related, e.g.

$$P_{(12)} = P_1 + P_2$$

with corresponding metrics $g^1_{\alpha\beta}$ and $g^2_{\alpha\beta}$ has metric

$$g^{(12)}_{\alpha\beta} = 1/2 \; \mathrm{tr}\left[\partial_\alpha (P_1 + P_2)\, \partial_\beta (P_1 + P_2)\right]$$

$$= g^1_{\alpha\beta} + g^2_{\alpha\beta}$$

$$+ 1/2 \left(\underbrace{\mathrm{tr}\left[\partial_\alpha P_1\, \partial_\beta P_2\right]}_{\text{can be negative}} + (\alpha \leftrightarrow \beta) \right)$$

- One can construct the matrix

$$g = (g_{\alpha\beta})$$

  - can be diagonalized by new coordinate system of momentum
  - $g_{\alpha\beta}$ for $\alpha \neq \beta$ often nonzero / negative.

- Only quantity with trace, single-band, two derivatives, symmetric, local, e.g.

$$\mathrm{tr}\left[A^k_\alpha(k)\, A^k_\beta(k)\right] = 2 g^{+}_{\alpha\beta}(k)$$

for two-band system.

Ex: (1) Show that by explicit construction.

(2) Show that $\mathrm{tr}\left[A^k_\alpha(k)\, A^k_\beta(k)\right] = \sum_n g^n_{\alpha\beta}(k)$

for arbitrary number of bands. For this, first show

$$\sum_m \mathrm{tr}\left[e_\alpha^{mn}\, e_\beta^{mn}\right] = \mathrm{tr}\left[P_n\, \partial_\alpha P_n\, \partial_\beta P_n\right].$$

2. Quantum metric of a two-band system

- Strong constraint : $P_+ + P_- = 1$

$$\longrightarrow \partial_\alpha P_+ = -\,\partial_\alpha P_-$$

leads to

$$\boxed{g^+_{\alpha\beta}} = 1/2\ \mathrm{tr}\left[\partial_\alpha P_+\, \partial_\beta P_+\right]$$
$$= 1/2\ \mathrm{tr}\left[(-\partial_\alpha P_-)(-\partial_\beta P_-)\right]$$
$$= \boxed{g^-_{\alpha\beta}}$$

- using projector form

$$\boxed{g^\pm_{\alpha\beta}} = 1/8\ \mathrm{tr}\left[\partial_\alpha(1 \pm n\cdot\sigma)\,\partial_\beta(1 \pm n\cdot\sigma)\right]$$
$$\boxed{= 1/4\ \partial_\alpha n \cdot \partial_\beta n}$$

- Let's consider spherical coordinates

$$n(k) = \begin{pmatrix} \sin\Theta(k)\cos\varphi(k) \\ \sin\Theta(k)\sin\varphi(k) \\ \cos\Theta(k) \end{pmatrix}$$

$$\longrightarrow g^\pm_{\alpha\beta}(k) = 1/4\Big(\partial_\alpha\Theta(k)\,\partial_\beta\Theta(k)$$
$$+ \sin^2\Theta(k)\,\partial_\alpha\varphi(k)\,\partial_\beta\varphi(k)\Big)$$

with metric of sphere

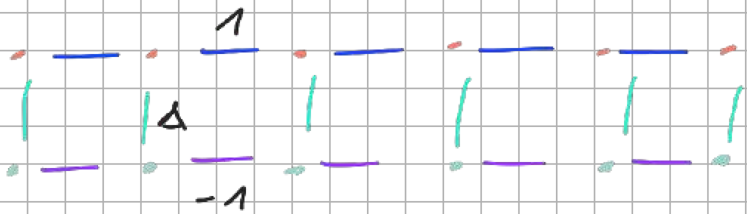
$$ds^2 = d\Theta^2 + \sin^2\Theta \, d\varphi^2$$

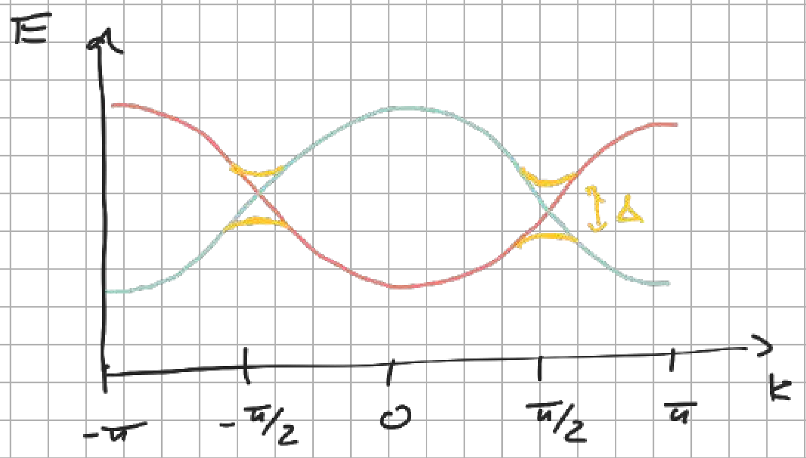
$\longrightarrow$ $g(k)$ is pullback of metric of the sphere onto the BZ, e.g. $\Theta \to \Theta(k)$

3. Sources of quantum metric

Let us consider the model

$$\hat{H} = \sum_j c^\dagger_{j+1,A} c_{jA} - c^\dagger_{j+1,B} c_{jB} + \Delta \, c^\dagger_{jA} c_{jB} + h.c.$$





"band inversion"

→ Bloch Hamiltonian

$$H(k) = \begin{pmatrix} \cos k & \Delta \\ \Delta & -\cos k \end{pmatrix}$$

$$\longrightarrow \quad d(k) = (\Delta, 0, \cos k)$$

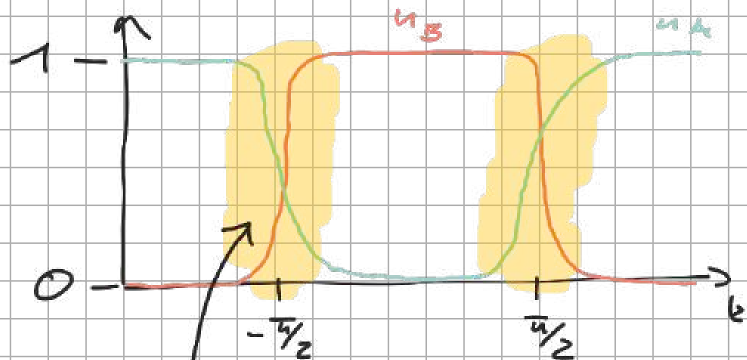
- The sub-lattice character change with k:

$$\langle n_A(k) \rangle \equiv \mathrm{tr}\left[P_-(k) P_A \right]$$

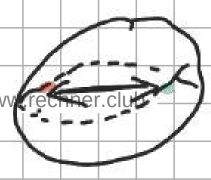
$$= 1/2 \left(1 - \frac{\cos k}{\sqrt{\Delta^2 + \cos^2 k}} \right)$$

$$\langle n_B(k) \rangle = 1/2 \left(1 + \frac{\cos k}{\sqrt{\Delta^2 + \cos^2 k}} \right)$$

with $P_A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ $\quad P_B = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$



expect large metric here

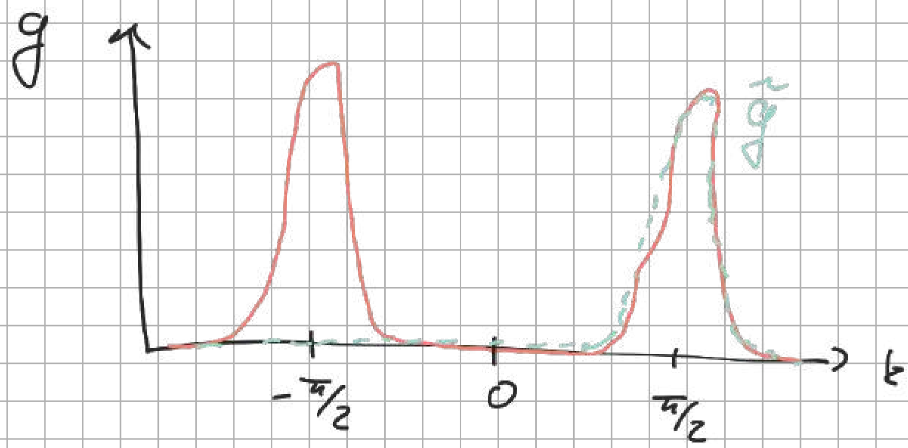


large change on Bloch sphere

- calculate quantum metric

$$g(k) = 1/4 \, \partial_k u(k) \cdot \partial_k u(k)$$

$$= \frac{\Delta^2 \sin^2 k}{(1 + \cos 2k + 2\Delta^2)^2}$$



- can construct low-energy model for localized metric:

$$\hat{H} = \begin{pmatrix} -(k - \pi/2) & \Delta \\ \Delta & k - \pi/2 \end{pmatrix}$$

$$\longrightarrow \quad \tilde{g}(k) = \frac{\Delta^2}{((k - \pi/2)^2 + \Delta^2)^2}$$

- for $\Delta \to 0$ we have

$$\tilde{g}(k) = \frac{\pi}{8\Delta} \, \delta(k - \pi/2)$$

4. Tunable quantum metric

- find toy models with specific quantum metric properties needed in the study of flat band physics.

- a simple example:

$$d(k) = \left(\cos(\varkappa k), \sin(\varkappa k), 0 \right)$$

$$\longrightarrow \quad g(k) = \varkappa^2/4$$

Ex: (1) Construct the corresponding tight-binding Hamiltonian.

(2) How can we physically interpret the corresponding quantum metric?

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A non-trivial generalization is

$$d(k) = \begin{pmatrix} \cos\left[\varkappa \cos k\right] \\ \sin\left[\varkappa \sin k\right] \\ 0 \end{pmatrix}$$

$$\longrightarrow \quad g(k) = \frac{\varkappa^2}{4} \sin^2 k$$