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Lecture 3 : The geometric structure of quantum states

Last lecture:

- quantum metric

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

- Relation to distance between states

$$\mathrm{tr}\left[P_n(k) P_n(k+q)\right] = 1 - \sum_{\alpha,\beta} q^\alpha q^\beta g^n_{\alpha\beta}(k) + \dots$$

- two-band model $\quad g^+_{\alpha\beta} = g^-_{\alpha\beta}$

$$g^\pm_{\alpha\beta}(k) = \tfrac{1}{4} \, \partial_\alpha n(k) \cdot \partial_\beta n(k)$$

with $\quad n = \frac{d}{|d|} \quad$ from $\quad H = d_0 + d \cdot \sigma$

- large quantum metric at band crossings

5. Real space interpretation of quantum metric

- a quick introduction to Wannier functions

i) $\sum_\beta H_{\alpha\beta}(k)\, v_n^\beta(k) = E_n(k) v_n^\alpha(k)$

slight change of notation to avoid confusions of notation

ii) lattice sites $|R, \alpha\rangle$ with

$$\langle r | R, \alpha\rangle = \delta(r - R - r_\alpha)$$

eigenstate of position operator

iii) Definition of Wannier function at R

$$|w_{R,n}\rangle = \underbrace{\sum_\alpha \sum_{R'} w_{R,R'}^{\alpha,n} |R'; \alpha\rangle}_{\text{expansion in lattice basis}}$$

with coefficients

$$w_{R,R'}^{\alpha,n} = \int_{BZ} e^{ik\cdot(R'-R)} v_n^\alpha(k)$$

Comments :

- Wannier functions are gauge-dependent due to $u_n^\alpha(k) \to e^{i\phi_n(k)} u_n^\alpha(k)$
- $\phi_n(k) = ck$ corresponds to positional shift
- Have to distinguish gauge-dependent and gauge-independent parts
- Minimize gauge-dependent part is part of Wannierization algorithms
- Gauge-independent spread of Wannier functions is given by momentum integral over quantum metric

  $\longrightarrow$ finite metric leads to so-called obstruction

  (cannot be perfectly localized spatially)

more details: RMP 84 1419 (2012)

- Connection to theory of electric polarization

i) Let us consider many-body position operator

$$\hat{X} = \sum_{i \in \text{sites}} \hat{x}_i$$

$\longrightarrow$ polarization operator $\hat{P} = -e\hat{X}$

ii) Generating functional of its moments with respect to Slater determinant from occupied bands:

$$C(q) = \langle \psi | e^{iq\cdot\hat{X}} | \psi \rangle$$

$$= 1 + i \sum_{\alpha} q_\alpha \langle \psi | \hat{X}_\alpha | \psi \rangle$$

$$- 1/2 \sum_{\alpha,\beta} q_\alpha q_\beta \langle \psi | \hat{X}_\alpha \hat{X}_\beta | \psi \rangle_c$$

$$+ 1/6 \sum_{\alpha,\beta,\gamma} q_\alpha q_\beta q_\gamma \langle \psi | \hat{X}_\alpha \hat{X}_\beta \hat{X}_\gamma | \psi \rangle_c$$

$$+ \dots$$

with cumulants

$$\langle \hat{X}_\alpha^2 \rangle = \langle (\hat{X}_\alpha - \langle \hat{X}_\alpha \rangle)^2 \rangle$$

$$\langle \hat{X}_\alpha^3 \rangle = \langle (\hat{X}_\alpha - \langle X_\alpha \rangle)^3 \rangle$$

PRB 107, 245136 (2023)

arxiv: 2409.16358

iii) Closed form for all orders

$$\frac{\log C(q)}{V} = \sum_\alpha q^\alpha \langle \psi | \hat{X}_\alpha | \psi \rangle + \sum_\alpha q^\alpha \left(\int_{BZ} \int_0^1 d\epsilon \, A_\alpha^k (k + q\epsilon) \right)$$

with volume of unit cell.

- First term is special as it is unique only up to $\mathbb{Z}$:

$$\langle \psi | \hat{X}_\alpha | \psi \rangle = \sum_{n \in occ} \int_{BZ} A_\alpha^n (k)$$

Berry connection

- Higher orders involve geometric quantity

$$A_\alpha^k (k') = \mathrm{tr}\Big[P_{occ}(k) \big(P_{occ}(k) P_{occ}(k') P_{occ}(k) \big)^{-1} \times P_{occ}(k) \, \partial_\alpha P_{occ}(k') \, P_{occ}(k') \Big]$$

which we can expand order by order in q.

$$\longrightarrow \quad \langle \hat{x}_\alpha \hat{x}_\beta \rangle_c = V \int_{BZ} \mathrm{Re}\ \underbrace{\mathrm{tr}\left[P_{occ}\, \partial_\alpha P_{occ}\, \partial_\beta P_{occ} \right]}_{\text{quantum metric}}$$

$$\langle \hat{x}_\alpha \hat{x}_\beta \hat{x}_\gamma \rangle_c = V \int_{BZ} \mathrm{Im}\ \underbrace{\mathrm{tr}\left[P_{occ}\, \partial_\alpha P_{occ}\, \partial_\beta \partial_\gamma P_{occ} \right]}_{\text{novel geometric quantity !}}$$

Ex: We exemplify the previous concepts for the SSH model setting $t' = 0$.

(1) Show that a Wannier function reads

$$| w_{j,\pm} \rangle = \frac{1}{\sqrt{2}} \left(\pm | j, A \rangle + | j+1, B \rangle \right).$$

(2) Calculate $\langle \hat{x} \rangle \equiv \langle w_{j,\pm} | \hat{x} | w_{j,\pm} \rangle$

and $\langle \hat{x}^2 \rangle \equiv \langle w_{j,\pm} | \hat{x}^2 | w_{j,\pm} \rangle$

using

$$\hat{x} = \sum_j j \left(| j, A \rangle\langle j, A | + | j, B \rangle\langle j, B | \right)$$

and show that the results agree with the gauge-invariant contributions obtained via the Berry connection and quantum metric.

E. Berry curvature and topology

We move on to the geometry arising from the phase of the Bloch states that we have seen in $\mathrm{tr}\left[P(k_1)\,P(k_2)\,P(k_3)\right]$.

For this, we consider

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

- this object is called quantum geometric tensor
- symmetric (real) part is quantum metric

  antisymmetric (imaginary) part is Berry curvature

$$\longrightarrow \quad \Omega^n_{\alpha\beta}(k) = i\,\mathrm{tr}\left[P_n(k)\,\partial_\alpha P_n(k)\,\partial_\beta P_n(k)\right] - (\alpha \leftrightarrow \beta)$$

The Berry curvature is the curl of the Berry connection

$$\Omega^n_{\alpha\beta}(k) = \partial_\alpha A^n_\beta - \partial_\beta A^n_\alpha$$

$\longrightarrow$ often defined $\Omega^n(k) = \left(\Omega^n_{yz}, \Omega^n_{zx}, \Omega^n_{xy}\right)$.

Ex: (1) Proof the relation between Berry curvature and connection by using $P_n = |u_n\rangle\langle u_n|$.

(2) Show that the curl of Berry connection is indeed gauge invariant.

(3) Show that the Berry curvature is additive in contrast to the quantum metric, e.g., $\Omega^{(12)}_{\alpha\beta} = \Omega^{1}_{\alpha\beta} + \Omega^{2}_{\alpha\beta}$ for $P_{(12)} = P_1 + P_2$.

(4) Show that $\Omega^{+}_{\alpha\beta} = -\Omega^{-}_{\alpha\beta}$ for a two-band model.

the Berry curvature for a two-band system reads

$$\Omega^{\mp}_{\alpha\beta}(k) = \mp \tfrac{1}{2}\, n(k)\cdot\left(\partial_\alpha n(k) \times \partial_\beta n(k)\right)$$

We can derive a useful different form via

$$\partial_\alpha n(k) = \frac{\partial_\alpha d(k)}{|d(k)|} - \underbrace{\frac{\partial_\alpha |d(k)|}{|d(k)|^2}\, d(k)}_{\text{is parallel to } n(k)}$$

$$\longrightarrow \boxed{\Omega^{\pm}_{\alpha\beta}(k) = \mp \frac{1}{2|d(k)|^3}\, d(k) \cdot \left(\partial_\alpha d(k) \times \partial_\beta d(k) \right)}$$

Let us construct a minimal model, so that $\Omega^{-}_{xy}(k)$ is nonzero:

$$d(k) = \begin{pmatrix} k_x \\ k_y \\ m \end{pmatrix}$$

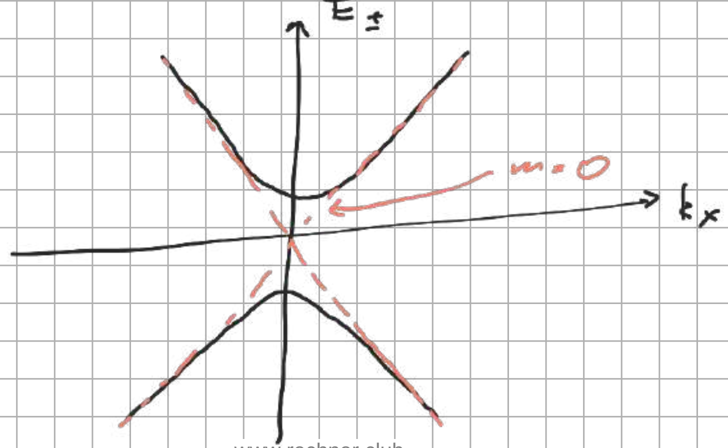
corresponds to $H(k_x, k_y) = \begin{pmatrix} m & k_x - i k_y \\ k_x + i k_y & -m \end{pmatrix}$

and is a gapped Dirac cone with energies

$$E_\pm(k_x, k_y) = \pm \sqrt{k_x^2 + k_y^2 + m^2}$$

Choose $k_x = r \cos\varphi$ and $k_y = r \sin\varphi$

$$\longrightarrow E_\pm = \pm\sqrt{r^2 + m^2}$$



The Berry curvature reads

$$\Omega_{xy}(k) = -\frac{m}{2\sqrt{(k_x^2 + k_y^2 + m^2)^3}}$$

which is strongly peaked at $\Gamma \equiv (0,0)$. We have

$$-\int_0^\infty dr \, \frac{mr}{2\sqrt{(r^2 + m^2)^3}} = -\tfrac{1}{2}\,\mathrm{sign}(m)$$

So the Berry curvature of a single Dirac cone is half-quantized with sign that depends on the sign of the gap (mass).
(sign in front of k_x and k_y also change sign)

We know that for a tight-binding model

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

is quantized to an integer, which is called the Chern number.

Step to tight-binding model

$$k_i \rightarrow \sin(k_i)$$

which is a typical procedure but of course not unique. The Berry curvature reads

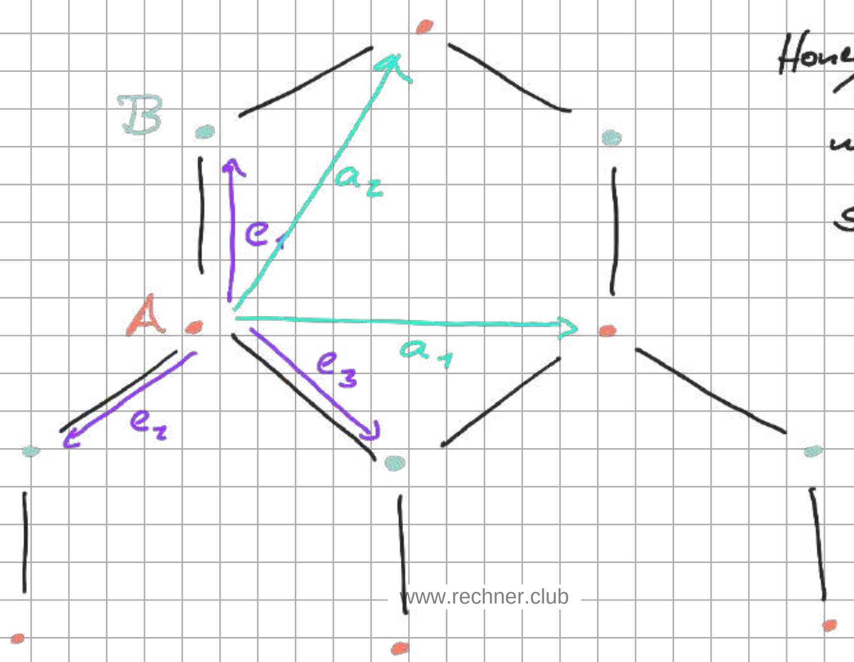
$$\Omega^{-}_{xy}(k) = - \frac{m \cos k_x \cos k_y}{2\sqrt{(m^2 + \cos^2 k_x + \cos^2 k_y)^3}}$$

$\longrightarrow$ we have multiple band crossings for $m=0$ at $(0,0)$, $(\pm\pi, \pm\pi)$, $(\pm\pi, 0)$, and $(0, \pm\pi)$.

$\longrightarrow$ Dirac cones with opposite charge so that Chern number is zero.

Example: Graphene and Haldane model

Goes back to Haldane PRL 61, 2015 (1988)



Honeycomb lattice with A and B sites

take $e_1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and construct e_2 and e_3 from $2\pi/3$ rotations.

$\rightarrow$ lattice vector

$$a_1 = e_3 - e_2$$

$$a_2 = e_1 - e_2$$

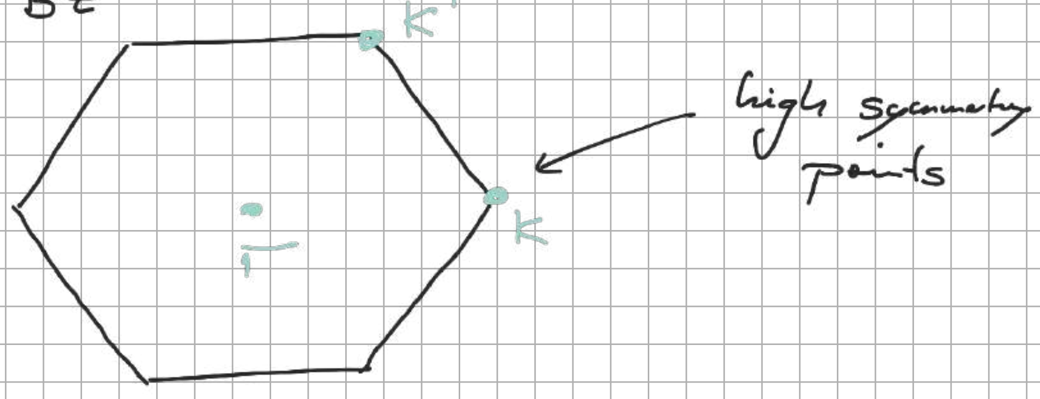
$$a_3 = (0, 0, 1) \quad \text{(for completeness)}$$

$\rightarrow$ reciprocal lattice vectors, e.g.,

$$b_1 = \frac{2\pi}{V_c} a_2 \times a_3$$

$$\text{with } V_c = a_1 \cdot (a_2 \times a_3) = \frac{3\sqrt{3}}{2}$$

BZ



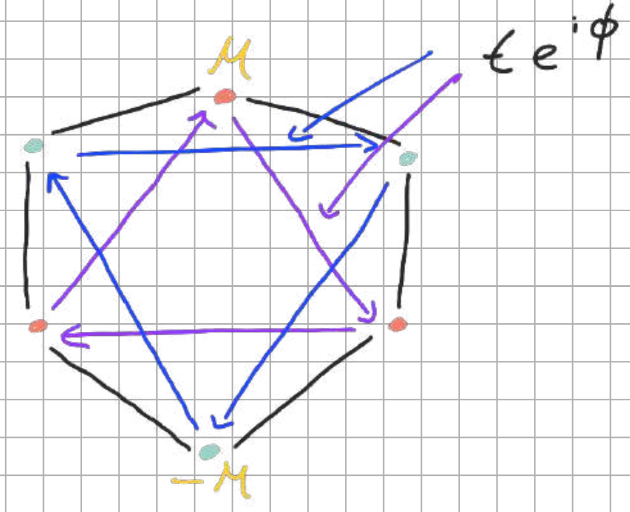
Ex: (1) Construct tight-binding Hamiltonian including equal hopping in e_i directions and show that linear band crossings occur at K and K'.

(2) Show that a energy shift between A and B sites, e.g., $M\left(c^{+}_{jA}c_{jA} - c^{+}_{jB}c_{jB}\right)$, gaps the band crossings.

(3) Show that the Chern number vanishes.

The Berry curvature has opposite sign at K and K'.

$\longrightarrow$ time reversal breaking with phase-dependent hopping can change that



Ex: Construct the corresponding tight-binding and Bloch Hamiltonian.

It turns out that for $\phi = \pi/2$

$$d_3(K) \approx 2M - 3\sqrt{3}\,t$$

$$d_3(K') \approx 2M + 3\sqrt{3}\,t$$

so that the mass of the Dirac cones can change their relative sign when $|M| = \frac{3\sqrt{3}}{2}|t|$.

Calculating the Chern number leads to the topological phase diagram