ASYMMETRY

Unveiling, Design, and Development of
Asymmetric Quantum Matters

科研費
KAKENHI

Quantum-geometric effects in superconductors

Akito Daido

Kyoto University

Outline

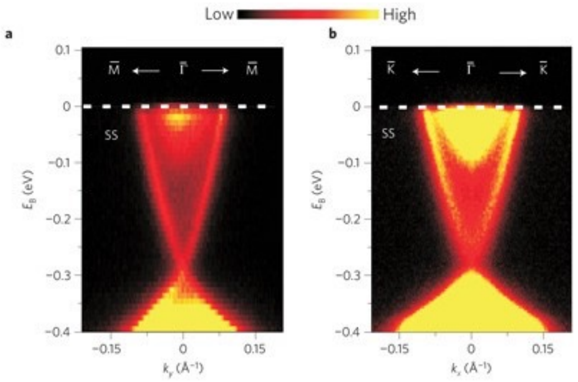
- Introduction
  - Background: Topological materials, Quantum geometry
  - Recent research: Quantum-geometric effects
- Our motivation
- Brief introduction of our previous works
- Today's main topic:

  Quantum-geometric effects in thermodynamic responses of SCs

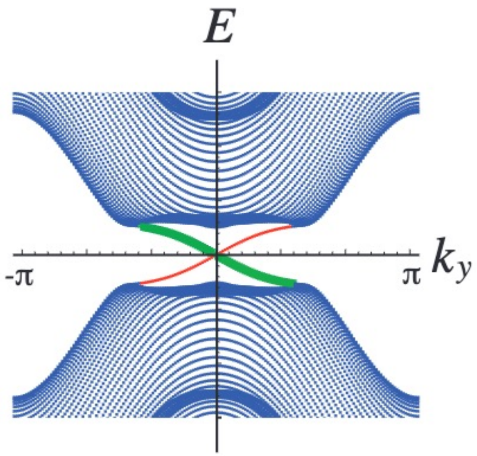
- Summary

Topological materials

Topological insulators & superconductors



Xia *et al*. Nat. Phys. (2009)



Sato *et al*. PRL (2009)

	Symmetry			Dimension							
AZ	T	C	S	1	2	3	4	5	6	7	8
A	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$
AIII	0	0	1	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0
AI	1	0	0	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$
BDI	1	1	1	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$
D	0	1	0	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$
DIII	-1	1	1	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$	0
AII	-1	0	0	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$\mathbb{Z}$
CII	-1	-1	1	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0
C	0	-1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0
CI	1	-1	1	0	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0

Schnyder *et al*. (2009)

and those with crystalline symmetries., interactions,
and/or in non-Hermitian/open-quantum systems, etc.

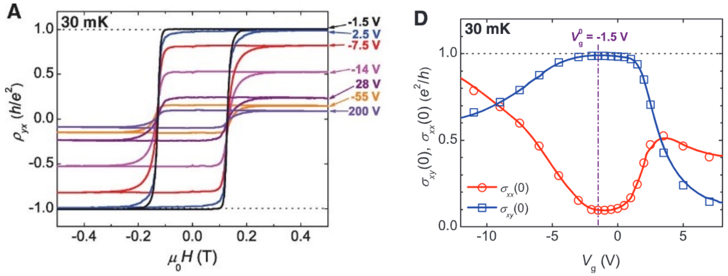
Widely accepted as (possible) material phases
not only by theorists and but also by experimentalists

Topological materials

Why topological and related materials are important?

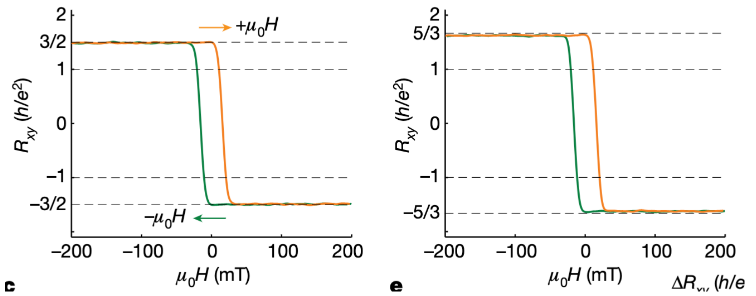
- Topological boundary states
- Proposed/observed Unconventional material properties   e.g., various Hall effects

Quantized anomalous HE



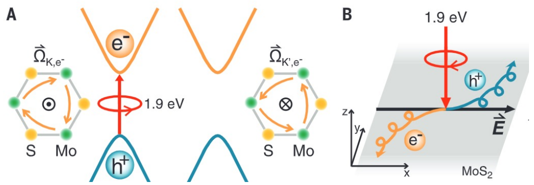
C.-Z. Chang *et al*., Science **340,** 167 (2013).

Fractionally QAHE in twisted $MoTe_2$



H. Park *et al*., Nature **622**, 74 (2023).

+ **Non-quantized AHE, Spin HE, Valley HE, and so on.**



K. F. Mak *et al*., Science **344**, 1489 (2014).

Search for topological and related materials:

Guiding principle to discover interesting physics

Quantum geometry

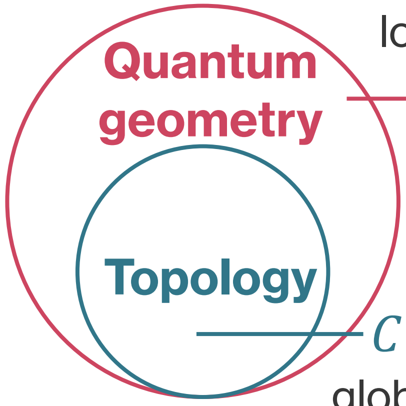
Why is the guiding principle so successful?

■ Topological materials have *quantum geometry*

- ≡ Nontrivial $\boldsymbol{k}$-dependence of Bloch states
- e.g., Berry curvature

$$H_{\mathrm{N}}(\boldsymbol{k})|u_n(\boldsymbol{k})\rangle = \epsilon_n(\boldsymbol{k})|u_n(\boldsymbol{k})\rangle$$

$$\Omega_n(\boldsymbol{k}) = i\,\langle\partial_{k_x}u_n(\boldsymbol{k})|\partial_{k_y}u_n(\boldsymbol{k})\rangle - (x \leftrightarrow y)$$



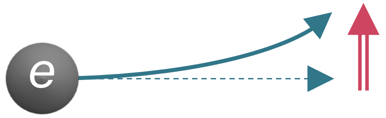
local quantity in BZ $\Omega_n(\boldsymbol{k})$

$C = \int d^2k\,\Omega_n(\boldsymbol{k})$ global structure in BZ

+

■ *Quantum geometry* often leads to interesting physics

e.g., $$\frac{d\boldsymbol{r}}{dt} = \frac{\partial\epsilon_n(\boldsymbol{k})}{\partial\boldsymbol{k}} - e\boldsymbol{E}\times\boldsymbol{\Omega}_n(\boldsymbol{k})$$



by $\Omega_n(\boldsymbol{k})$

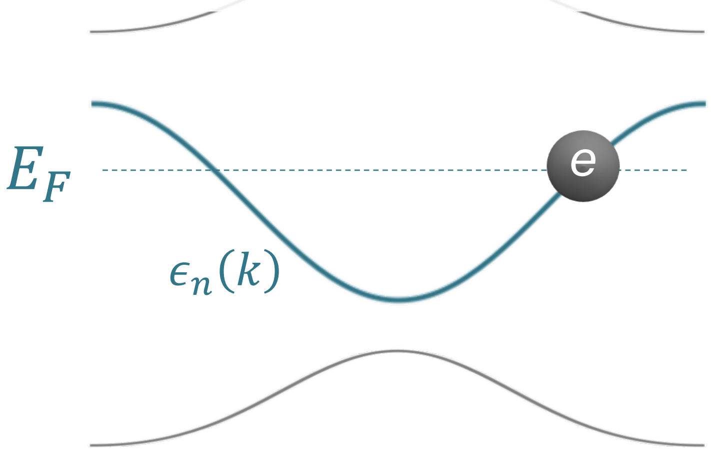
→ various quantized/non-quantized Hall effects

Interesting physics?

Why? → ■ *Quantum geometry* often leads to interesting physics

For many material properties,

A band
in multi-band materials



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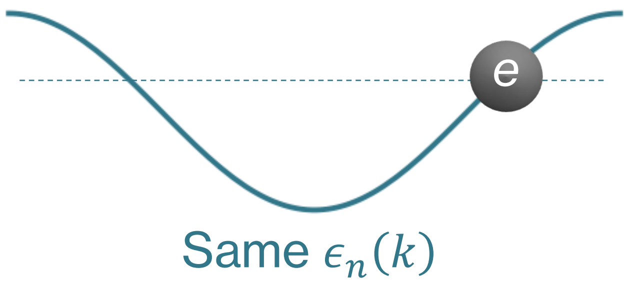
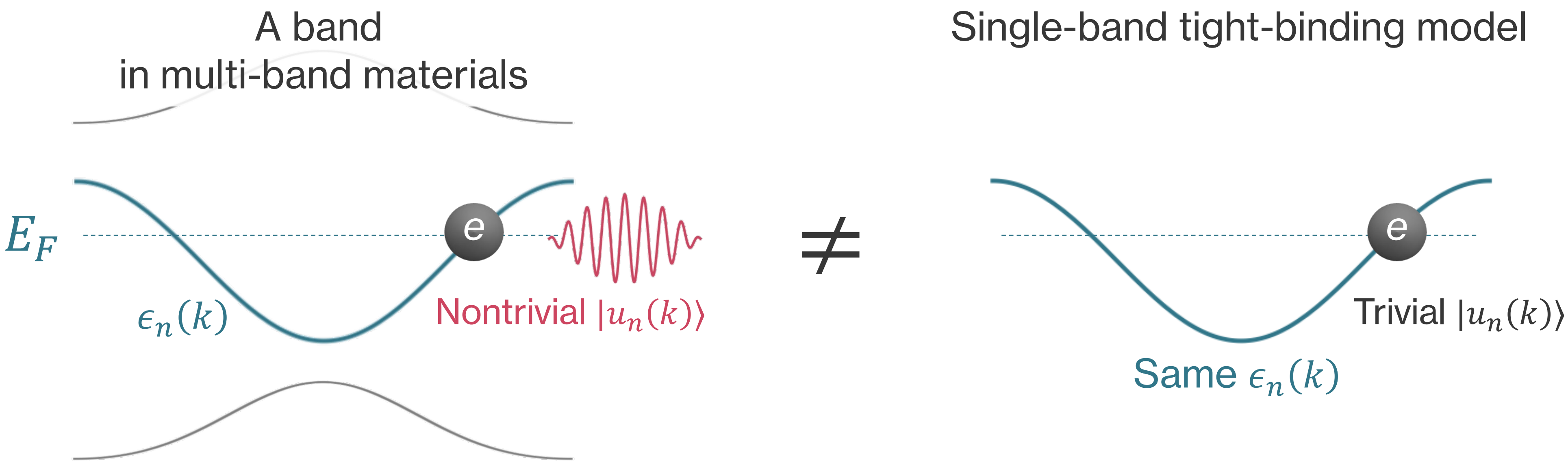
Single-band tight-binding model



Interesting physics?

Why? → ■ ***Quantum geometry* often leads to interesting physics**

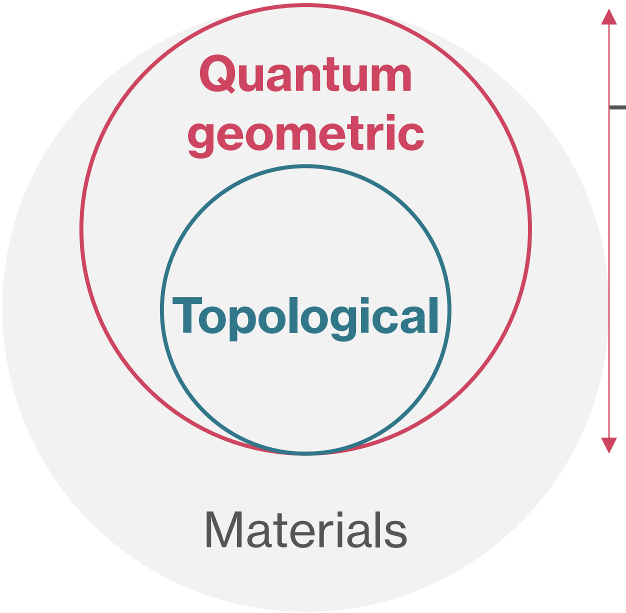
For quantum-geometric phenomena,



meaning **quantum-mechanical phenomena *beyond energy dispersion***
(cf. Drude theory, BCS theory), **triggered by nontrivial wave functions**

Studying quantum-geometric phenomena, not limited to topological ones, would be fruitful!

Recent research focus



Recent research focus

- Interesting physics by quantum geometry?

  In particular, quantum-geometric effects beyond Berry curvature?

Quantum-geometric quantities

Berry curvature, **quantum metric**, their multipoles, their non-Abelian extensions, Shift vector, etc.

e.g., **Berry-curvature dipole**

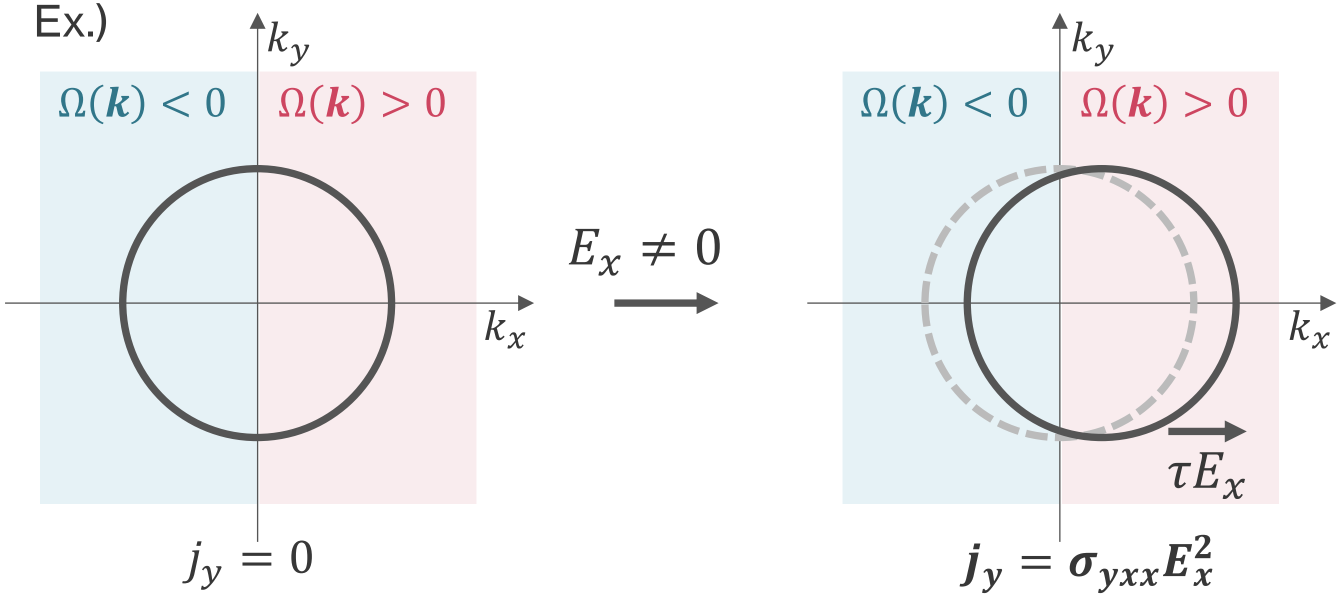
$$\partial_{k_i}\Omega_n(\boldsymbol{k})$$

Nonlinear Hall effect by Berry-curvature dipole

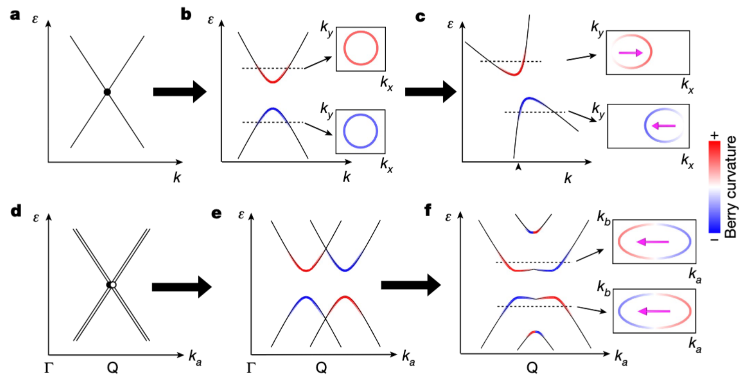
Nonlinear Hall effect: e.g., $j_y = \sigma_{yxx} E_x^2$

Hall current by $\Omega(\boldsymbol{k})$ $\quad j_y = E_x \int d^2k\ \Omega(\boldsymbol{k}) f(\boldsymbol{k})$

Ex.)



I. Sodemann and L. Fu, PRL **115**, 216806 (2015),
Q. Ma *et al.*, Nature **565**, 337 (2019),
K. Kang *et al.*, Nature Materials **18**, 324 (2019).



- Dipolar structure of $\Omega(k)$ → Nonlinear Hall effect (w/ TRS) $\quad D_{ab} = \int_k f_0 (\partial_a \Omega_b).$

- Higher-rank nonlinear Hall effects are induced by Berry-curvature multipoles
  C.-P. Zhang *et al.*, Phys. Rev. B **107**, 115142 (2023).

Quantum-metric effects

■ Quantum metric

$$g_n^{ij}(\boldsymbol{k}) = \mathrm{Re} \sum_{m(\neq n)} A_{nm}^{i}(\boldsymbol{k}) A_{mn}^{j}(\boldsymbol{k})$$

Berry connection $A_{nm}^{i}(\boldsymbol{k}) = -i\langle u_n(\boldsymbol{k}) | \partial_{k_i} u_m(\boldsymbol{k}) \rangle$

cf. $\Omega_n^{ij}(k) = 2\,\mathrm{Im} \sum_{m(\neq n)} A_{nm}^{i}(\boldsymbol{k}) A_{mn}^{j}(\boldsymbol{k})$

"Distance" btw. neighboring Bloch states = How rapidly Bloch state changes at $\boldsymbol{k}$

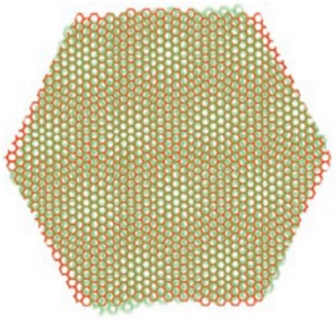
$$ds^2 \equiv 1 - |\langle u_n(\boldsymbol{k} + d\boldsymbol{k}) | u_n(\boldsymbol{k}) \rangle|^2 = g_n^{ij}(\boldsymbol{k})\, dk^i dk^j$$

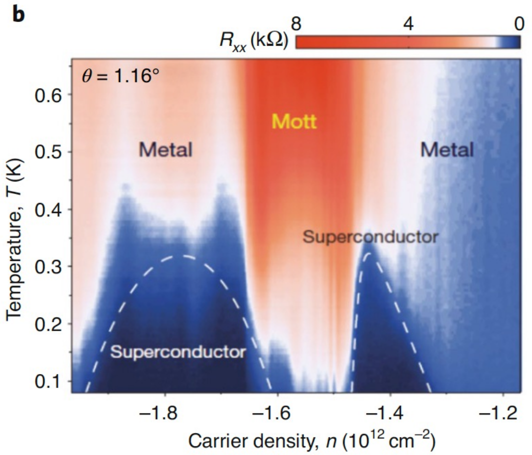
■ Studied in nonlinear optics, current noise, exciton levels, etc.

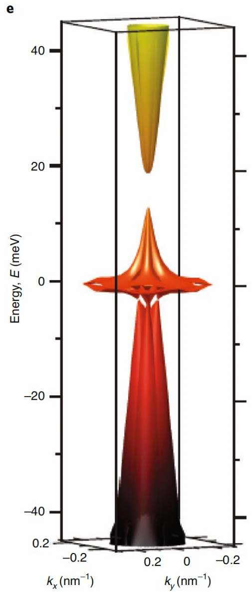
■ Conducting phenomena in (nearly) flat-band systems

- Significant attention after the discovery of **twisted bilayer graphene**
  =Nearly flat-band systems in condensed matter

Review: E. Y. Andrei, A. H. MacDonald, Nat. Materials **19**, 1265 (2020)







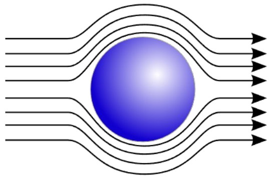
SC properties in nearly-flat band systems

Quantum metric plays an important role in flat-band SC

P. Törmä *et al.*, Nature Reviews Physics **4**, 528 (2022).

- Vanishing group velocity and inverse mass $v^i = \partial_{k_i}\epsilon = 0, \;\; \& \;\; 1/m^{ij} = \partial_{k_i}\partial_{k_j}\epsilon = 0.$
  - **How can flat-band electrons super-conduct?**
- Superfluid weight ↔ penetration depth

London eq. $j^i = D_s A^i = \frac{1}{\lambda^2} A^i$ ⟶ Meissner effect



from Wikipedia

$$D_{s,\mathrm{conv}} = \frac{n}{m} \to 0$$ for flat bands??

- Full expression of the Kubo formula: $D_s = D_{s,\mathrm{conv}} + D_{s,\mathrm{geom}}$

Quantum-geometric contribution enables SC
in flat-band systems!

Quantum-geometric term

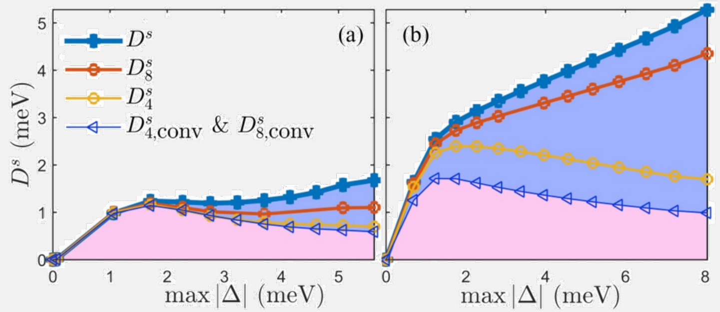
$$\sim \frac{4e^2\Delta\sqrt{\nu(1-\nu)}}{\hbar^2}\int \frac{d^d\mathbf{k}}{(2\pi)^d} g_{jl}(\mathbf{k}),$$

in isolated flat-band limit

SC properties in nearly-flat band systems

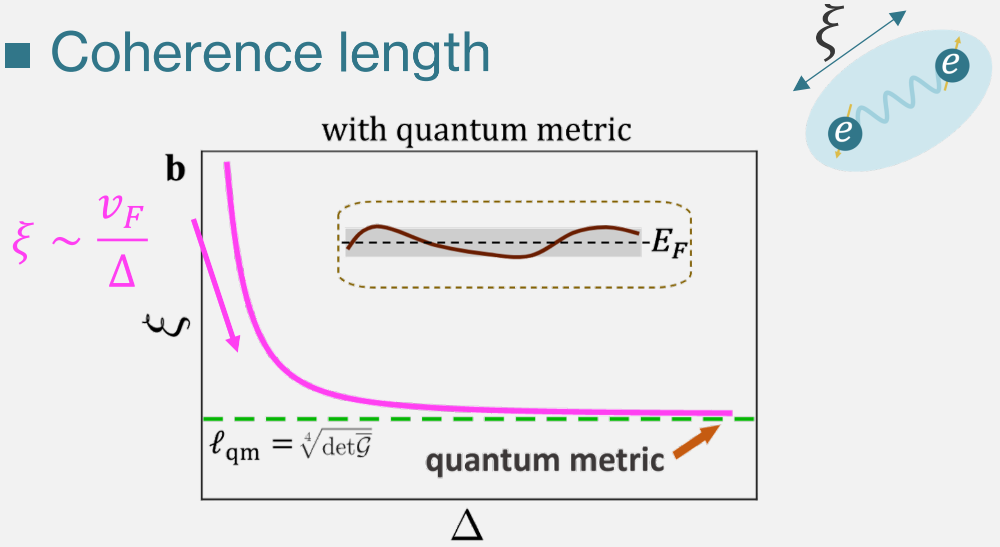
- Superfluid weight $D_s = 1/\lambda^2$

Twisted bilayer graphene



A. Julku *et al*., PRB **101**, 060505 (2020).
X. Hu *et al*., , PRL **123**, 237002 (2019).

- Coherence length



S. Chen and K. T. Law, PRL **132**, 026002 (2024).
J.-X Hu, S. Chen and K. T. Law, arXiv:2308.05686

$$\lambda \to \frac{1}{\sqrt{D_{s,\mathrm{geom}}}} > 0$$

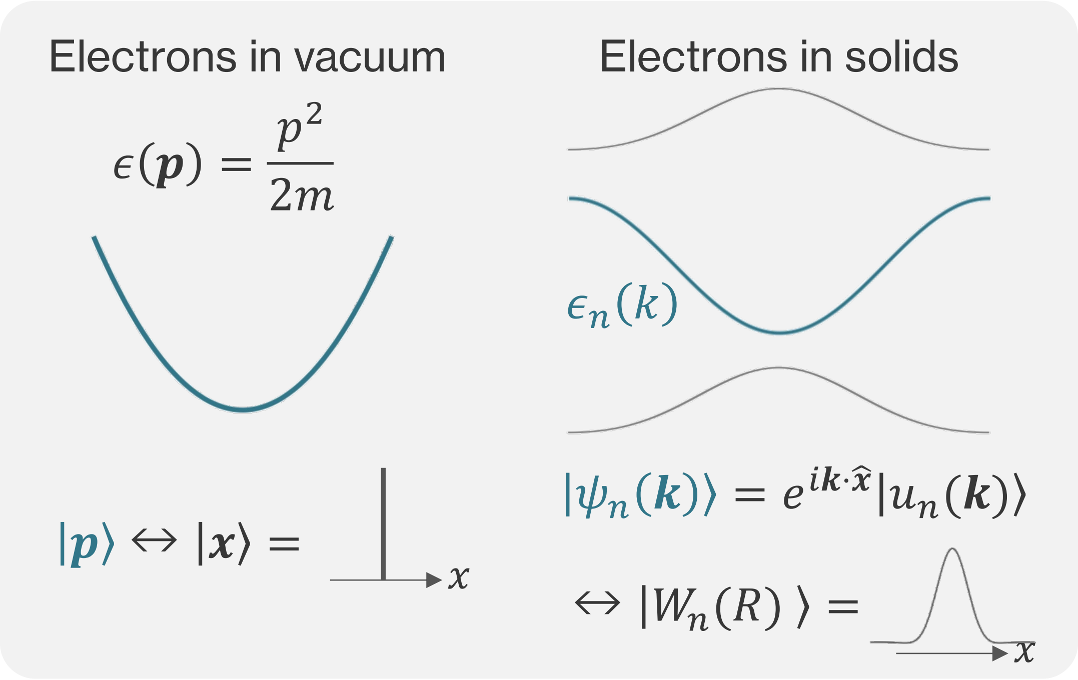
Flat-band limit

$$\xi \to \xi_{\mathrm{geom}} > 0$$

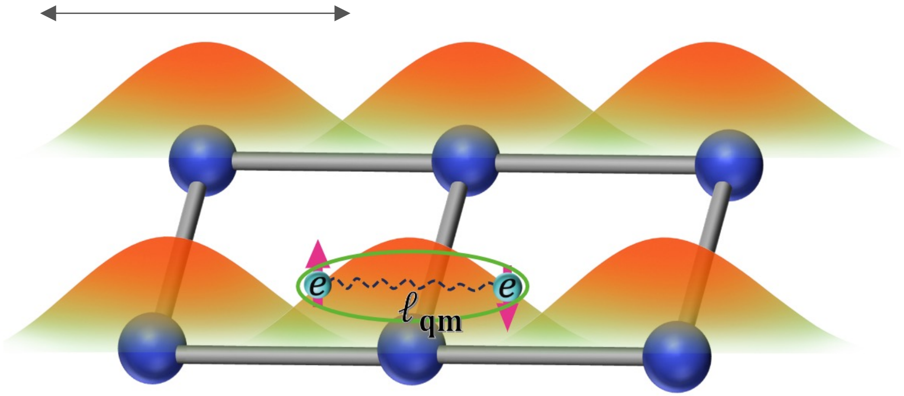
Key to understanding the physics: Length scale related to quantum metric?

SC properties in nearly-flat band systems

- Intuitive understanding: **Overlapping Wannier functions** P. Törmä *et al.*, Nat. Reviews Physics **4**, 528 (2022).



Wannier spread: related to quantum metric



J.-X Hu, S. Chen and K. T. Law, arXiv:2308.05686

Flat-band materials highlight the importance of quantum geometry in SC.

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  - Recent research: Quantum-geometric effects
- Our motivation
- Brief introduction of our previous works
- Today's main topic:

Quantum-geometric effects in thermodynamic responses of SCs

- Summary

Our motivation

Update our understanding of SC by quantum geometry

■ When/where?

Material platform of quantum-geometric SCs

1. Examples other than flat bands?

   Those without twist?
   Bulk superconductors?

2. General conditions?

■ How?

Identify quantum-geometric superconducting properties

1. Equilibrium properties

   Normal-SC, SC-SC phase transitions

   Thermodynamic responses

2. Non-equilibrium properties

Our ambition: "Modern theory of superconductivity"...?

Our efforts

■ When/where?

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■ Taisei Kitamura (D3) addressed many of these questions!

1. "SC in monolayer FeSe enhanced by quantum geometry"
   TK, AD, *et al.*, PRResearch **4**, 023232 (2022).
2. "Quantum geometric effect on FFLO superconductivity"
   TK, AD, and Y. Yanase, PRB **106**, 184507 (2023).
3. "Spin-triplet SC from quantum-geometry-induced ferromagnetic fluctuation"
   TK, AD, and Y. Yanase, PRL **132**, 036001 (2024).

⋮

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Our efforts

■ When/where?

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2. **General conditions?**

■ How?

Identify quantum-geometric superconducting properties

1. Equilibrium properties

   Normal-SC, SC-SC phase transitions

   Thermodynamic responses

2. Non-equilibrium properties

■ Today's topic

AD, TK, and Y. Yanase, arXiv:2310.15558.

- Our recent efforts to study some general aspects regarding equilibrium properties
- Is it possible to **transparently extract quantum-geometric effects?**

Ex.) $D_s = D_{s,\mathrm{conv}} + D_{s,\mathrm{geom}}$

Study Kubo formula and separate terms by hand

$$D^{\mathrm{conv}}_{\mu\nu} = -\sum_{n\sigma\boldsymbol{k}} \langle u_{n\boldsymbol{k}}|\, \partial_\mu H_{0\boldsymbol{k}}\, |u_{n\boldsymbol{k}}\rangle \langle u_{n\boldsymbol{k}}|\, \partial_\nu H_{0\boldsymbol{k}}\, |u_{n\boldsymbol{k}}\rangle \left(\sigma \frac{|\Delta_{\boldsymbol{k}}|^2}{E^3_{n\boldsymbol{k}}} f(\sigma E_{n\boldsymbol{k}}) - \frac{|\Delta_{\boldsymbol{k}}|^2}{E^2_{n\boldsymbol{k}}} f'(\sigma E_{n\boldsymbol{k}})\right),$$

$$D^{\mathrm{geom}}_{\mu\nu} = \sum_{n\neq m\sigma\sigma'\boldsymbol{k}} \langle u_{n\boldsymbol{k}}|\, \partial_\mu H_{0\boldsymbol{k}}\, |u_{m\boldsymbol{k}}\rangle \langle u_{m\boldsymbol{k}}|\, \partial_\nu H_{0\boldsymbol{k}}\, |u_{n\boldsymbol{k}}\rangle \frac{f(\sigma E_{n\boldsymbol{k}}) - f(\sigma' E_{m\boldsymbol{k}})}{\sigma E_{n\boldsymbol{k}} - \sigma' E_{m\boldsymbol{k}}} \left(\sigma\sigma' \frac{|\Delta_{\boldsymbol{k}}|^2}{E_{n\boldsymbol{k}} E_{m\boldsymbol{k}}}\right),$$

$$D^{\mathrm{gap}}_{\mu\nu} = -\sum_{n\sigma\boldsymbol{k}} \langle u_{n\boldsymbol{k}}|\, \partial_\mu \boldsymbol{\Delta}_{\boldsymbol{k}}\, |u_{n\boldsymbol{k}}\rangle \langle u_{n\boldsymbol{k}}|\, \partial_\nu H_{0\boldsymbol{k}}\, |u_{n\boldsymbol{k}}\rangle \left(-\sigma \frac{\Delta_{\boldsymbol{k}}\epsilon_{n\boldsymbol{k}}}{E^3_{n\boldsymbol{k}}} f(\sigma E_{n\boldsymbol{k}}) + \frac{\Delta_{\boldsymbol{k}}\epsilon_{n\boldsymbol{k}}}{E^2_{n\boldsymbol{k}}} f'(\sigma E_{n\boldsymbol{k}})\right),$$

Our efforts

■ When/where?

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AD, TK, and Y. Yanase, arXiv:2310.15558.

- Our recent attempts to study some general aspects regarding equilibrium properties
- Is it possible to **transparently extract quantum-geometric effects?**

- Our strategy: take careful band representation and start from free energy
- Future plan

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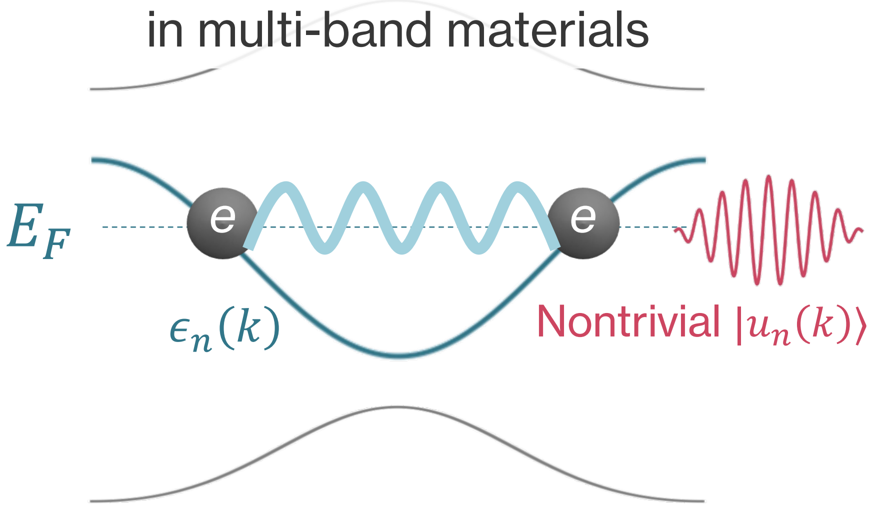
SCs with and without quantum geometry

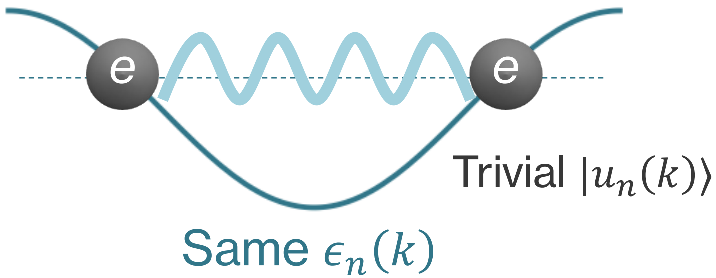
Superconductors with and without quantum geometry:
How are they different?

A band
in multi-band materials



vs.

Single-band model



Normal-state Bloch Hamiltonian

$$H_{\mathrm{N}}(\boldsymbol{k}) = U_{\mathrm{N}}(\boldsymbol{k}) \underbrace{\begin{bmatrix} \ddots & & \\ & \epsilon_n(\boldsymbol{k}) & \\ & & \ddots \end{bmatrix}}_{\hat{\epsilon}(\boldsymbol{k})} U_{\mathrm{N}}(\boldsymbol{k})^{+}$$

$$H_{\mathrm{N}}(\boldsymbol{k}) = \epsilon_n(\boldsymbol{k})\, 1_{1\times 1}$$

SCs with and without quantum geometry

Simplifying assumption (removed later): spin-singlet s-wave pair

$$\Delta_0 \sum_l (c^\dagger_{\boldsymbol{k}\uparrow,l} c^\dagger_{-\boldsymbol{k}\downarrow,l} - c^\dagger_{\boldsymbol{k}\downarrow,l} c^\dagger_{-\boldsymbol{k}\uparrow,l}).$$

Bogoliubov-de Gennes (BdG) Hamiltonian

$$H_{\mathrm{BdG}}(\boldsymbol{k}) = \begin{pmatrix} H_{\mathrm{N}}(\boldsymbol{k}) & \Delta_0 \\ \Delta_0 & -\Theta H_{\mathrm{N}}(-\boldsymbol{k})\Theta^{-1} \end{pmatrix}$$

$$\hat{H} = \frac{1}{2}\sum_{\boldsymbol{k}} \Psi^\dagger(\boldsymbol{k}) H_{\mathrm{BdG}}(\boldsymbol{k}) \Psi(\boldsymbol{k}) + \text{const.},$$

$$[\Psi^\dagger(\boldsymbol{k})]_l = (c^\dagger_{\uparrow,l}(\boldsymbol{k}), c^\dagger_{\downarrow,l}(\boldsymbol{k}), c_{\downarrow,l}(-\boldsymbol{k}), -c_{\uparrow,l}(-\boldsymbol{k})).$$

Time-reversal partner of $H_{\mathrm{N}}(\boldsymbol{k})$ ($\Theta \equiv -is_y K$)

Band representation

Unitary trans. diagonalizing normal-state parts

$$H_{\mathrm{b}}(\boldsymbol{k}) \equiv U_{\mathrm{b}}(\boldsymbol{k}) H_{\mathrm{BdG}}(\boldsymbol{k}) U_{\mathrm{b}}^\dagger(\boldsymbol{k}) = \begin{pmatrix} \hat{\epsilon}(\boldsymbol{k}) & \Delta_{\mathrm{b}}(\boldsymbol{k}) \\ \Delta_{\mathrm{b}}(\boldsymbol{k})^+ & -\hat{\epsilon}_\Theta(-\boldsymbol{k}) \end{pmatrix}$$

$$U_{\mathrm{b}}(\boldsymbol{k}) = \begin{pmatrix} U_{\mathrm{N}}(\boldsymbol{k}) & \\ & \Theta U_N(-\boldsymbol{k})\Theta^{-1} \end{pmatrix}$$

$$[\Delta_{\mathrm{b}}(\boldsymbol{k})]_{nm} = \Delta_0 \langle u_n(\boldsymbol{k}) | \Theta u_m(-\boldsymbol{k}) \rangle,$$

e.g., for time-reversal symmetric normal states,

$$H_{\mathrm{b}}(\boldsymbol{k}) = \bigoplus_n \begin{bmatrix} \epsilon_n(\boldsymbol{k}) & \Delta_0 \\ \Delta_0 & -\epsilon_n(\boldsymbol{k}) \end{bmatrix}$$

$$H_{\mathrm{b}}(\boldsymbol{k}) = \begin{bmatrix} \epsilon_n(\boldsymbol{k}) & \Delta_0 \\ \Delta_0 & -\epsilon_n(\boldsymbol{k}) \end{bmatrix}$$

SCs with and without quantum geometry

Band representation

$$H_{\mathrm{b}}(\boldsymbol{k}) \equiv U_{\mathrm{b}}(\boldsymbol{k}) H_{\mathrm{BdG}}(\boldsymbol{k}) U_{\mathrm{b}}^{\dagger}(\boldsymbol{k}) = \begin{pmatrix} \hat{\epsilon}(\boldsymbol{k}) & \Delta_{\mathrm{b}}(\boldsymbol{k}) \\ \Delta_{\mathrm{b}}(\boldsymbol{k})^{+} & -\hat{\epsilon}_{\Theta}(-\boldsymbol{k}) \end{pmatrix}$$

$$U_{\mathrm{b}}(\boldsymbol{k}) = \begin{pmatrix} U_{\mathrm{N}}(\boldsymbol{k}) & \\ & \Theta U_{N}(-\boldsymbol{k}) \Theta^{-1} \end{pmatrix}$$

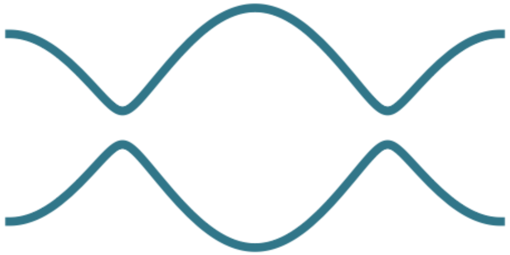
$$[\Delta_{\mathrm{b}}(\boldsymbol{k})]_{nm} = \Delta_0 \langle u_n(\boldsymbol{k}) | \Theta u_m(-\boldsymbol{k}) \rangle ,$$

For time-reversal symmetric normal states,

$$H_{\mathrm{b}}(\boldsymbol{k}) = \bigoplus_n \begin{bmatrix} \epsilon_n(\boldsymbol{k}) & \Delta_0 \\ \Delta_0 & -\epsilon_n(\boldsymbol{k}) \end{bmatrix}$$

$$H_{\mathrm{b}}(\boldsymbol{k}) = \begin{bmatrix} \epsilon_n(\boldsymbol{k}) & \Delta_0 \\ \Delta_0 & -\epsilon_n(\boldsymbol{k}) \end{bmatrix}$$

$$E_n(k) = \pm \sqrt{\epsilon_n(\boldsymbol{k})^2 + \Delta_0^2}$$



Quantum geometry does not appear in
e.g., specific heat, DOS, etc.

Difference appears in responses

The situation changes for the *responses* to the perturbation

- Ex. Response to vector potential $\boldsymbol{A}$ ↔ Cooper-pair momentum $\boldsymbol{q}$

Single-band

$$H_{\mathrm{b}}(\boldsymbol{k}) = \begin{bmatrix} \epsilon_n(\boldsymbol{k}+\boldsymbol{q}) & \Delta_0 \\ \Delta_0 & -\epsilon_n(\boldsymbol{k}-\boldsymbol{q}) \end{bmatrix}$$

$$\epsilon_n(\boldsymbol{k}+\boldsymbol{q}) \simeq \epsilon_n(\boldsymbol{k}) + q_i \partial_{k_i}\epsilon(\boldsymbol{k}) + \frac{1}{2} q_i q_j \partial_{k_i}\partial_{k_j}\epsilon(\boldsymbol{k})$$

- $O(q)$ → Dopper shift of quasiparticle energy, to give "paramagnetic-current" contribution of D_s
- $O(q^2)$ → to give "diamagnetic-current" contribution responsible for $D_s = \frac{n}{m}$ at $T = 0$

$$D_{s,\mathrm{conv}} = \partial_q^2 F = \frac{n}{m}$$

free energy

Difference appears in responses

The situation changes for the *responses* to the perturbation

■ Ex. Response to vector potential $\boldsymbol{A}$ ↔ Cooper-pair momentum $\boldsymbol{q}$

$$[H_\mathrm{b}(\boldsymbol{k})]_{nn} = \begin{bmatrix} \epsilon_n(\boldsymbol{k}+\boldsymbol{q}) & [\Delta_\mathrm{b}(\boldsymbol{k};\boldsymbol{q})]_{nn} \\ [\Delta^*_\mathrm{b}(\boldsymbol{k};\boldsymbol{q})]_{nn} & -\epsilon_n(\boldsymbol{k}-\boldsymbol{q}) \end{bmatrix}$$

$$[\Delta_\mathrm{b}(\boldsymbol{k};\boldsymbol{q})]_{nn} = \Delta_0\langle u_n(\boldsymbol{k}+\boldsymbol{q})|\Theta u_n(-\boldsymbol{k}+\boldsymbol{q})\rangle$$

$$= \Delta_0\langle u_n(\boldsymbol{k}+\boldsymbol{q})|u_n(\boldsymbol{k}-\boldsymbol{q})\rangle \quad \text{(up to phase)}$$

$$= e^{-i\theta_{nn}(k;q)}\left(\Delta_0 - \Delta_0 q_i q_j g_n^{ij}(\boldsymbol{k}) + O(q^3)\right)$$

Quantum metric appears as
additional q *dependence in pair potential*
cf. L. Liang, *et al.*, PRB **96**, 064511 (2017).

$$D_s = D_{s,\mathrm{conv}} + D_{s,\mathrm{geom}}$$

Single-band

$$H_\mathrm{b}(\boldsymbol{k}) = \begin{bmatrix} \epsilon_n(\boldsymbol{k}+\boldsymbol{q}) & \Delta_0 \\ \Delta_0 & -\epsilon_n(\boldsymbol{k}-\boldsymbol{q}) \end{bmatrix}$$

$$\epsilon_n(\boldsymbol{k}+\boldsymbol{q}) \simeq \epsilon_n(\boldsymbol{k}) + q_i\partial_{k_i}\epsilon(\boldsymbol{k}) + \frac{1}{2}q_iq_j\partial_{k_i}\partial_{k_j}\epsilon(\boldsymbol{k})$$

- $O(q)$ → Dopper shift of quasiparticle energy, to give "paramagnetic-current" contribution of D_s
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$$D_{s,\mathrm{conv}} = \partial_q^2 F = \frac{n}{m}$$

free energy

Difference appears in responses

Technical remark

- **Direct expansion of LHS yields gauge-dependent expressions**

$$[\Delta_\mathrm{b}(\boldsymbol{k};\boldsymbol{q})]_{nn} = \Delta_0\langle u_n(\boldsymbol{k}+\boldsymbol{q})|u_n(\boldsymbol{k}-\boldsymbol{q})\rangle$$

$$= \Delta_0\left(1 - 2iq_jA^j_{nn}(\boldsymbol{k}) + q_iq_j\left(g^{ij}_n(\boldsymbol{k}) + 2A^i_{nn}(k)A^j_{nn}(\boldsymbol{k})\right) + O(q^3)\right)$$

- This comes from the gauge dependence of $|u_n(\boldsymbol{k}\pm\boldsymbol{q})\rangle$

When $|u_n(\boldsymbol{k})\rangle \to |u_n(\boldsymbol{k})\rangle e^{i\chi_n(\boldsymbol{k})}$, $\quad \langle u_n(\boldsymbol{k}+\boldsymbol{q})|u_n(\boldsymbol{k}-\boldsymbol{q})\rangle \to e^{-i\chi_n(\boldsymbol{k}+\boldsymbol{q})+i\chi_n(\boldsymbol{k}-\boldsymbol{q})}\langle u_n(\boldsymbol{k}+\boldsymbol{q})|u_n(\boldsymbol{k}-\boldsymbol{q})\rangle$

- RHS can be made gauge-invariant by multiplying a Berry phase factor

$e^{i\theta_{nn}(\boldsymbol{k};\boldsymbol{q})}[\Delta_\mathrm{b}(\boldsymbol{k};\boldsymbol{q})]_{nn}$: gauge invariant

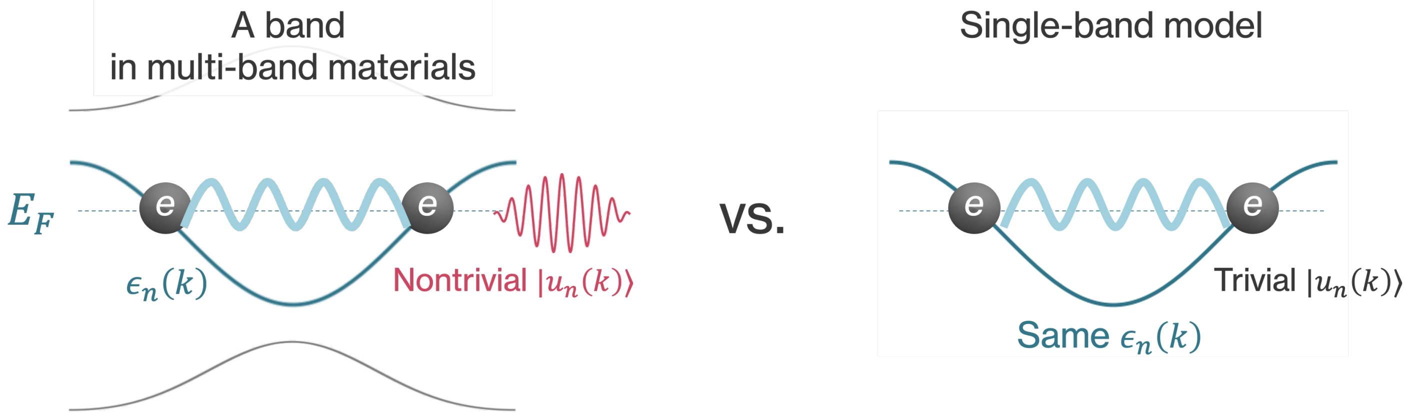
$$\theta_{nn}(\boldsymbol{k};\boldsymbol{q}) = \gamma_n(\boldsymbol{k};\boldsymbol{q}) - \gamma_n(\boldsymbol{k},-\boldsymbol{q}) \qquad \gamma_n(\boldsymbol{k};\boldsymbol{q}) = \int_0^{\boldsymbol{q}} dk'_i\; A^i_{nn}(\boldsymbol{k}+\boldsymbol{k}')\; \left(\to \gamma'_n(\boldsymbol{k};\boldsymbol{q}) = \gamma_n(\boldsymbol{k};\boldsymbol{q}) + \chi_n(\boldsymbol{k}+\boldsymbol{q}) - \chi_n(\boldsymbol{k})\right)$$

- Expansion of $e^{i\theta_{nm}(\boldsymbol{k};\boldsymbol{q})}[\Delta_\mathrm{b}(\boldsymbol{k};\boldsymbol{q})]_{nm}$ is transparent, **ensuring gauge covariance at any order of $\boldsymbol{q}$:**

$$e^{i\theta_{nm}(\boldsymbol{k};\boldsymbol{q})}[\Delta_\mathrm{b}(\boldsymbol{k};\boldsymbol{q})]_{nm} = \sum_{l=0}^{\infty} c^l_{nm}(\boldsymbol{k})q^l \to \sum_{l=0}^{\infty} e^{-i\chi_n(\boldsymbol{k})+i\chi_m(\boldsymbol{k})}c^l_{nm}(\boldsymbol{k})q^l \qquad \text{cf. } \langle u_n(\boldsymbol{k})|O|u_m(\boldsymbol{k})\rangle$$

Quantum-geometric pair potential (QGPP)

Pair potential in band representation is key to quantum-geometric effects.



- The difference appears in response to the perturbation

$$H_{\rm b}(\boldsymbol{k};\boldsymbol{X}) = \begin{bmatrix} \hat{\epsilon}(\boldsymbol{k}+\boldsymbol{q}) & \Delta_{\rm b}(\boldsymbol{k};\boldsymbol{q}) \\ \Delta_{\rm b}(\boldsymbol{k};\boldsymbol{q}) & -\hat{\epsilon}(\boldsymbol{k}-\boldsymbol{q}) \end{bmatrix}$$

Quantum-geometric pair potential (QGPP)

$$e^{i\theta_{nm}(\boldsymbol{k};\boldsymbol{q})}[\Delta_{\rm b}(\boldsymbol{k};\boldsymbol{q})]_{nm} = \Delta_0\delta_{nm} + [\Delta_{\rm g}(\boldsymbol{k};\boldsymbol{q})]_{nm}$$

removable

$$\theta_{nm}(\boldsymbol{k};\boldsymbol{q}) = \gamma_n(\boldsymbol{k};\boldsymbol{q}) - \gamma_m(\boldsymbol{k},-\boldsymbol{q})$$

$$\gamma_n(\boldsymbol{k};\boldsymbol{q}) = \int_0^{\boldsymbol{q}} dk'_i\; A^i_{nn}(\boldsymbol{k}+\boldsymbol{k}')$$

$\underline{n=m}$ $\quad \simeq \left(\Delta_0 - \Delta_0 q_i q_j g^{ij}_n(\boldsymbol{k})\right)$

$\underline{n \neq m}$ $\quad \simeq \Delta_0[2iq_i A^i_{nm}(\boldsymbol{k})]$

- Inter-band pairs also appear
- gauge invariant/covariant

Quantum-geometric effects in free energy

Pair potential in band representation is key to quantum-geometric effects.

Indeed, it is *solely responsible* for quantum-geometric effects to SC thermodynamic responses.

Consider time-reversal-odd external field $\boldsymbol{X} = (\boldsymbol{q}, \boldsymbol{h}, \dots)$

Thermodynamic coeff.

Free energy $$F(X) = F(0) + X_a X_b \, \chi^{X_a X_b} + O(X^4)$$

$$F(\boldsymbol{X}) = -\frac{1}{2\beta}\sum_{\boldsymbol{k}} \mathrm{Tr}\left[\ln\left(1 + e^{-\beta H_{\mathrm{BdG}}(\boldsymbol{k};\boldsymbol{X})}\right)\right] + \mathrm{const.}$$
$$= -\frac{1}{2\beta}\sum_{\boldsymbol{k}} \mathrm{Tr}\left[\ln\left(1 + e^{-\beta H_{\mathrm{b}}(\boldsymbol{k};\boldsymbol{X})}\right)\right] + \mathrm{const.}$$

After removing the phase of pair potential,

Collection of single-band SCs $\Delta_{\mathrm{b}} = \Delta_0 + \Delta_{\mathrm{g}}$

$$H_{\mathrm{b}}(\boldsymbol{k};\boldsymbol{X}) = \begin{bmatrix} \hat{\epsilon}(\boldsymbol{k};\boldsymbol{X}) & \Delta_0 \\ \Delta_0 & -\hat{\epsilon}(\boldsymbol{k};-\boldsymbol{X}) \end{bmatrix} + \begin{bmatrix} 0 & \Delta_{\mathrm{g}}(\boldsymbol{k};\boldsymbol{X}) \\ \Delta_{\mathrm{g}}^{\dagger}(\boldsymbol{k};\boldsymbol{X}) & 0 \end{bmatrix}$$

W/o quantum geometry W/ quantum geometry

Quantum-geometric effects in free energy

Pair potential in band representation is key to quantum-geometric effects.

Indeed, it is *solely responsible* for quantum-geometric effects to SC thermodynamic responses.

Consider time-reversal-odd external field $\boldsymbol{X} = (\boldsymbol{q}, \boldsymbol{h}, \dots)$

Thermodynamic coeff.

Free energy $$F(X) = F(0) + X_a X_b\, \chi^{X_a X_b} + O(X^4)$$

QGPP in response to X: quantum geometry *in the parameter space*

$$[\Delta_{\mathrm{g}}(\boldsymbol{k};\boldsymbol{X})]_{nm} \quad \underline{n=m} \quad \simeq \left(\Delta_0 - \Delta_0 X_i X_j g_n^{X_i X_j}(\boldsymbol{k})\right)$$

$$\underline{n \neq m} \quad \simeq \Delta_0[2iX_i A_{nm}^{X_i}(\boldsymbol{k})]$$

$$g_n^{X_i X_j}(\boldsymbol{k}) = 2\mathrm{Re} \sum_{m(\neq n)} A_{nm}^{X_i}(\boldsymbol{k}) A_{mn}^{X_j}(\boldsymbol{k})$$

$$A_{nm}^{X_i}(\boldsymbol{k}) = -i\langle u_n(\boldsymbol{k};X)|\partial_{X_i} u_m(\boldsymbol{k};\boldsymbol{X})\rangle\Big|_{X\to 0}$$

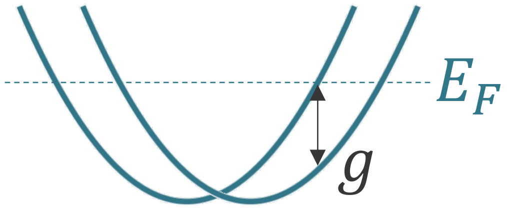
For $X = h$, $\sim \langle n|s|m\rangle/\Delta E_{nm}$

"Quantum-geometric" effects in thermodynamic coeff. other than superfluid weight?

Illustration with two-band model

Usually, namely in weak-coupling SCs, quantum-geometric effects are not significant.

- Setup: two-band model, noncentrosymmetric SC at $T = 0$



$$\chi^{X_iX_j}_{\mathrm{dia}} = \int_{\mathrm{BZ}} \frac{d^dk}{(2\pi)^d} \sum_{n=\pm1} \frac{1}{m_n^{X_iX_j}} \frac{1}{2}\left[1 - \frac{\epsilon_n}{E_n}\right], \quad \chi^{X_iX_j}_{\mathrm{g}} = 4\int_{\mathrm{BZ}} \frac{d^dk}{(2\pi)^d} g^{X_iX_j} \frac{g^2\Delta_0^2}{(E_+ + E_-)E_+E_-},$$

Quantum-geometric contribution for $\Delta_0 \ll g \ll E_F$

	$\chi^{q_iq_j} \leftrightarrow D_S$: superfluid weight	$\chi^{h_iq_j}$: SC Edelstein effect =supercurrent-induced spin	$\chi^{h_ih_j}$: spin susceptibility
$\chi_{\mathrm{dia}}/\chi_{\mathrm{g}}$	$\sim \frac{\Delta_0^2}{E_F^2}\ln\left(\frac{\Delta_0}{g}\right)$	$\sim \Delta_0^2/g^2$	$\sim \Delta_0^2/g^2$

- Platforms require an energy scale comparable with Δ_0
  - Flat-band SCs $W \sim \Delta_0$, BCS-BEC SCs $E_F \sim \Delta_0$,
  - (Nearly) degenerate bands $g \sim \Delta_0$ e.g., PT-sym magnets, $j = \frac{3}{2}$ SCs? ←Future study

General formula of QGPP

- Generalized to arbitrary situations, including...
  - Non-s-wave SCs such as spin-triplet SC, and with other internal DOF
  - Remains valid and gauge covariant for degenerate or entangled bands

Suppressing the argument $\boldsymbol{k}$, $H_{\mathrm{N}}\,|u_n^{(\lambda)}\rangle = \epsilon_n\,|u_n^{(\lambda)}\rangle \quad [\Delta_{\mathrm{b}}]_{n\lambda,n'\lambda'} = \langle u_n^{(\lambda)}|\Delta|u_{n'}^{(\lambda')}\rangle\,,$

$\leftrightarrow \Delta_0[2iq_iA^i_{nm}(\boldsymbol{k})]$

$$\Delta_{\mathrm{g}}(\boldsymbol{X}) = -iX_i\{A^{X_i}_{\mathrm{inter}},\Delta_{\mathrm{b}}\} + \frac{1}{2}X_iX_j\Big(-i[A^{X_i}_{\mathrm{inter};X_j},\Delta_{\mathrm{b}}] - \{A^{X_i}_{\mathrm{inter}},\{A^{X_j}_{\mathrm{inter}},\Delta_{\mathrm{b}}\}\}\Big) + O(X^3),$$

$\leftrightarrow -\Delta_0 q_i q_j g^{ij}_n(\boldsymbol{k})$

covariant derivative
cf. shift vector

$$A^{X_i}_{\mathrm{inter};X_j}(\boldsymbol{X}) \equiv \partial_{X_j}A^{X_i}_{\mathrm{inter}}(\boldsymbol{X}) + i[A^{X_j}_{\mathrm{intra}}(\boldsymbol{X}), A^{X_i}_{\mathrm{inter}}(\boldsymbol{X})],$$

- This implies...
  - Can obtain physical low-energy models in the pseudospin basis with MCBB L. Fu, PRL (2015).
  - Quantum-geometric effects beyond quantum metric?
  - **Possibility of engineering exotic superconducting states?**

Engineering of exotic SC states by QGPP

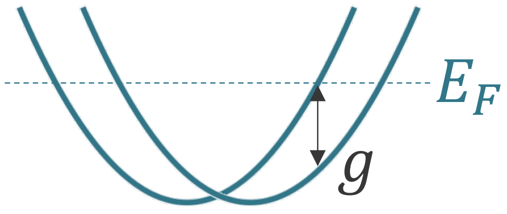
$$\Delta_{\mathrm{g}}(\boldsymbol{X}) = -iX_i\{A^{X_i}_{\mathrm{inter}}, \Delta_{\mathrm{b}}\} + O(X^2)$$

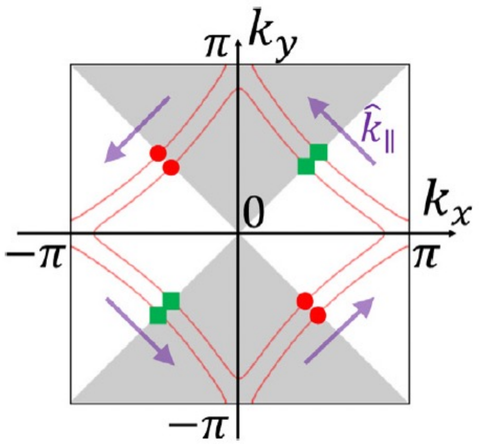
Symmetry of $\boldsymbol{X}$ is encoded to QGPP → e.g., effective chiral SC

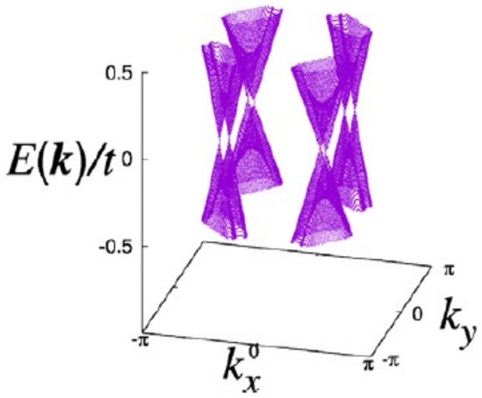
■ Ex. noncentrosymmetric d-wave Rashba SC

- Due to inversion breaking, spin-singlet and triplet Cooper pairs coexist.
- We consider d-wave pairing admixed with p-wave pairing

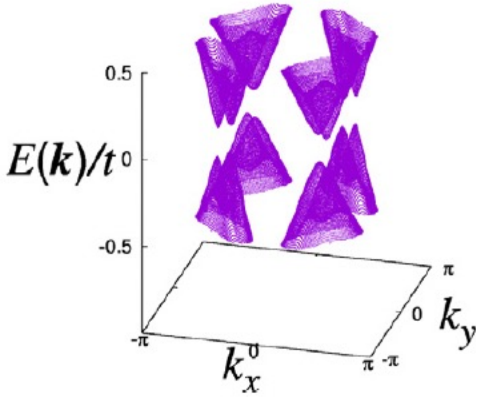
AD and Y. Yanase, PRB **95**, 134507 (2017).



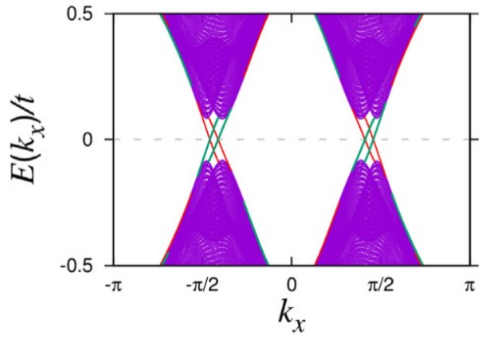




$\boldsymbol{h} = h\hat{z}$ →



$C = 4$

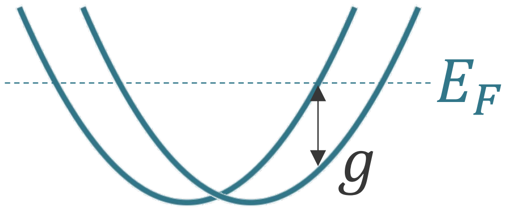


Engineering of exotic SC states by QGPP

$$\Delta_{\mathrm{g}}(\boldsymbol{X}) = -iX_i\{A^{X_i}_{\mathrm{inter}}, \Delta_{\mathrm{b}}\} + O(X^2)$$

Symmetry of $\boldsymbol{X}$ is encoded to QGPP → e.g., effective chiral SC

■ Ex. noncentrosymmetric d-wave Rashba SC



- Due to inversion breaking, spin-singlet and triplet Cooper pairs coexist.
- We consider d-wave pairing admixed with p-wave pairing

AD and Y. Yanase, PRB **95**, 134507 (2017).

$$\Delta_{\mathrm{b}}(\boldsymbol{k}) \to \Delta_{\mathrm{b}}(\boldsymbol{k}) + \Delta_{\mathrm{g}}(\boldsymbol{k};\boldsymbol{X}): \quad \Delta_{\mathrm{b}}(\boldsymbol{k}) = -\left(\psi_0 \mp \frac{d_0}{k_F}\right)(k_x^2 - k_y^2), \quad \Delta_{\mathrm{g}}(\boldsymbol{k}) = -ih\,\frac{d_0}{gk_F^2}\,k_x k_y$$

i.e., $d_{x^2-y^2}$-wave SC → Effectively $d_{x^2-y^2} + id_{xy}$-wave SC by QGPP

■ Some more examples of systems e.g,. with (nearly) degenerate bands are given in our paper

- Non-unitary spin triplet states, anapole SC, ...

Summary

We have introduced QGPP to understand quantum-geometric effects in SCs

AD, TK, and Y. Yanase, arXiv:2310.15558.

- SCs with and without quantum geometry are different by QGPP, which appears in response to external perturbation.
- QGPP is responsible for the quantum-geometric thermodynamic responses.
- QGPP can be used to engineer exotic SC states by external field and quantum geometry
  - Topological SC, chiral SC, non-unitary SC, anapole SC, …

Future plan

- Model studies for e.g., nearly degenerate SCs, $j = \frac{3}{2}$ SCs
- Extension to transport and AC responses & Exploring phenomena induced by quantum-geometry
- Giving exceptions to conventional notions of SCs e.g., spin susceptibility of spin-triplet SCs?