Aalto University
School of Science

Lecture 1: Quantum geometric superfluid stiffness and flat band superconductivity

Päivi Törmä

Aalto University

Winter theory school: New Frontiers in Superconductivity, Florida 2024

10.1.2024

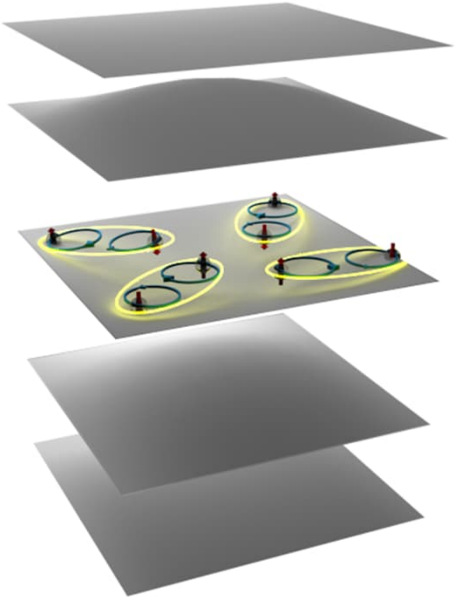
Super C
Room Temperature Superconductivity 2033
Institute Q
erc
HORIZON2020 Marie Skłodowska-Curie actions
ACADEMY OF FINLAND

Lecture material

Peotta, Huhtinen, PT, arXiv:2308.08248 (Varenna Enrico Fermi summer school proceedings)

PT, Peotta, Bernevig, Nat. Rev. Phys. (2022)

And references therein, plus an Essay…



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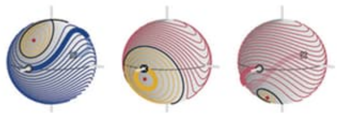

ON THE COVER

Excited-State Phase Diagram of a Ferromagnetic Quantum Gas

December 13, 2023

Topologically distinct Bloch-sphere trajectories (blue, yellow, and red curves) for an atomic spinor Bose-Einstein condensate at three different values of quadratic Zeeman energies (spheres from left to right).

B. Meyer-Hoppe *et al.*

Phys. Rev. Lett. **131**, 243402 (2023)

Issue 24 Table of Contents | More Covers

ESSAY

Essay: Where Can Quantum Geometry Lead Us?

In a new forward-looking Essay, Päivi Törmä highlights the significance and impact of quantum geometry for the future of physics research.

Päivi Törmä

Phys. Rev. Lett. **131**, 240001 (2023)

Current Issue

Vol. 131, Iss. 25 — 22 December 2023

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Vol. 131, Iss. 23 — 8 December 2023

Vol. 131, Iss. 22 — 1 December 2023

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Perspective on quantum geometry

PT, PRL 2023

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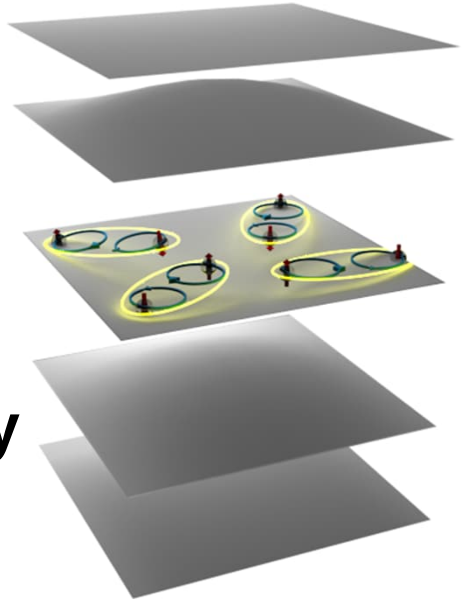

Lecture 1

- Basics of quantum geometry
- Quantum geometry and superconductivity

Lecture 2

- Flat band superconductivity and quantum geometry in twisted bilayer graphene (TBG)
- Non-Fermi liquid normal states in flat bands
- Non-equilibrium transport in flat band superconductors
- DC conductivity in a flat band
- The many-body quantum metric and the Drude weight

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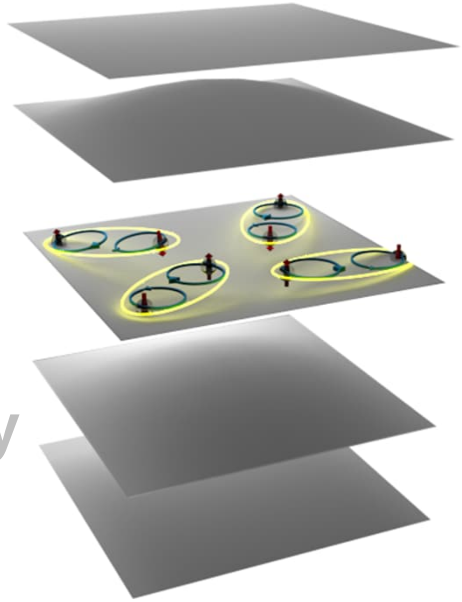

Lecture 1

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- The many-body quantum metric and the Drude weight

Quantum geometric tensor

Metric for the distance between quantum states

Provost, Vallee, Comm. Math. Phys. **76**, 289 (1980)

$$d\ell^2 = ||u(\mathbf{k}+d\mathbf{k}) - u(\mathbf{k})||^2 = \langle u(\mathbf{k}+d\mathbf{k}) - u(\mathbf{k}) | u(\mathbf{k}+d\mathbf{k}) - u(\mathbf{k})\rangle$$

$$\approx \sum_{i,j} \underbrace{\langle \partial_{k_i} u | \partial_{k_j} u \rangle}_{} dk_i dk_j$$

Introduce gauge invariant version $\left(u(\mathbf{k}) \leftrightarrow u(\mathbf{k})e^{i\phi(\mathbf{k})}\right)$

Quantum geometric tensor (Fubini-Study metric)

$$\mathcal{B}_{ij}(\mathbf{k}) = 2\langle \partial_{k_i} u | (1 - |u\rangle\langle u|) | \partial_{k_j} u \rangle$$

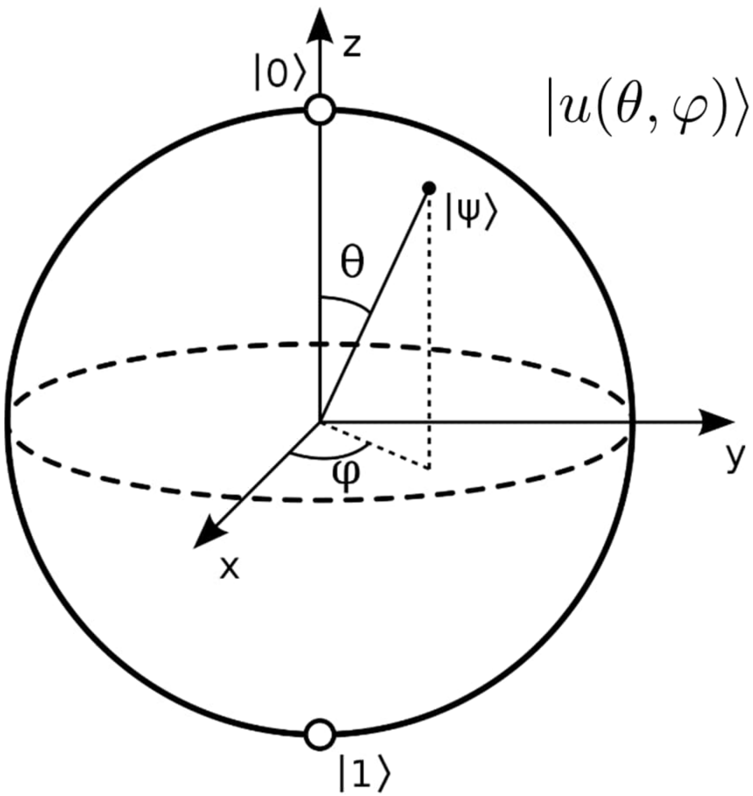
$$\mathrm{Re}\,\mathcal{B}_{ij} = g_{ij}$$ quantum metric $d\ell^2 = \sum_{ij} g_{ij} dk_i dk_j$

$$\mathrm{Im}\,\mathcal{B}_{ij} = [\mathbf{\Omega}_{\mathrm{Berry}}]_{ij}$$ Berry curvature

Chern number: $C = \frac{1}{2\pi}\int_{\mathrm{B.Z.}} \mathrm{d}^2\mathbf{k}\,\Omega_{\mathrm{Berry}}(\mathbf{k})$

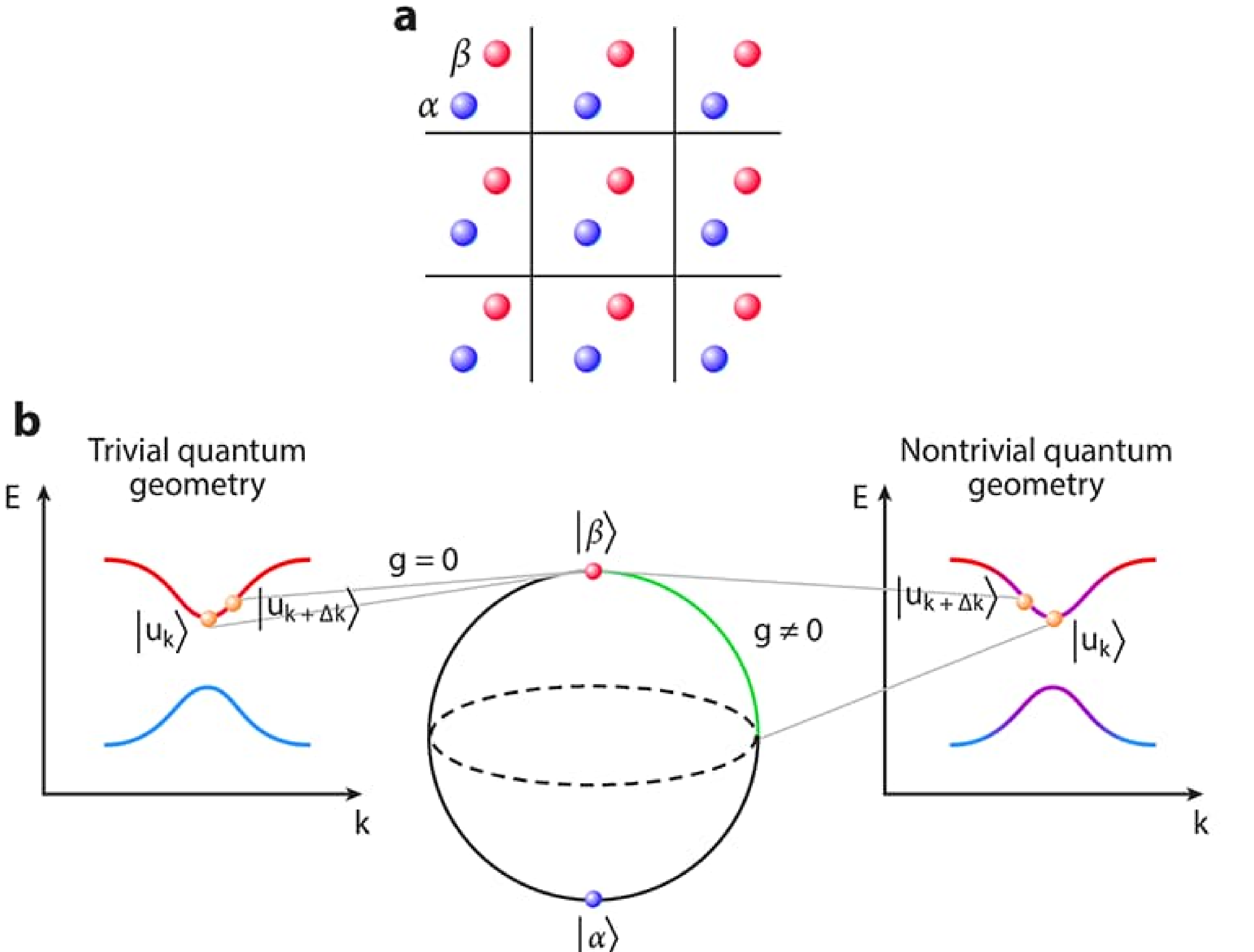
$$\mathcal{B}_{ij}(\mathbf{k}) = 2\langle \partial_{k_i} u | (1 - |u\rangle\langle u|) | \partial_{k_j} u \rangle$$

$\mathrm{Re}\, \mathcal{B}_{ij} = g_{ij}$ quantum metric $\quad d\ell^2 = \sum_{ij} g_{ij} dk_i dk_j$



$$|u(\theta,\varphi)\rangle = e^{-i\varphi/2}\cos(\theta/2)\,|0\rangle + e^{i\varphi/2}\sin(\theta/2)\,|1\rangle$$

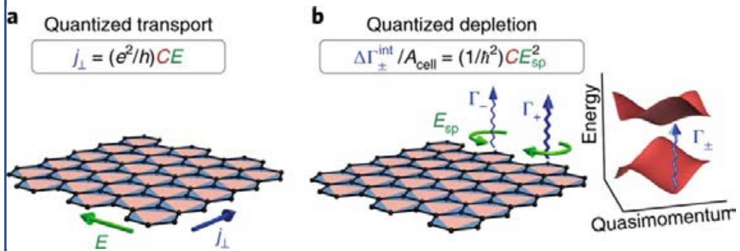
$$g_{\varphi\varphi} = \sin^2\theta$$



a
β
α
b
Trivial quantum geometry
Nontrivial quantum geometry
E
k
E
k
|β⟩
|α⟩
g = 0
g ≠ 0
|u_k⟩
|u_{k+Δk}⟩
|u_{k+Δk}⟩
|u_k⟩

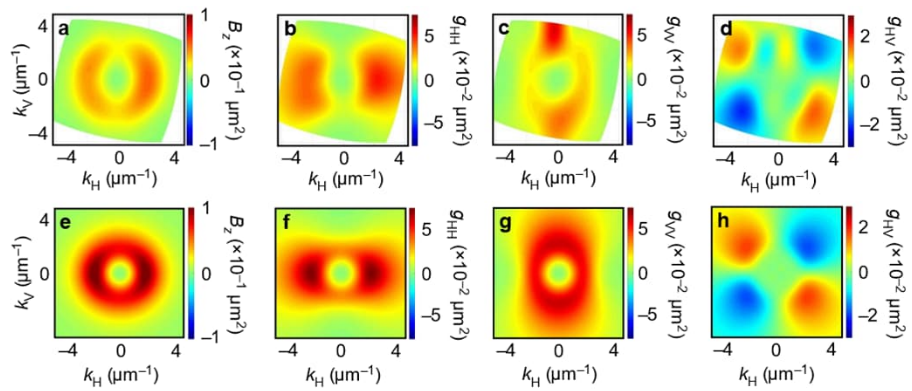
Quantum Geometric Tensor (QGT) observation

Optical lattices



Asteria, Tran, Ozawa, Tarnowski, Rem, Fläschner, Sengstock, Goldman, Weitenberg, *Nature Physics* **15**, 449 (2019)

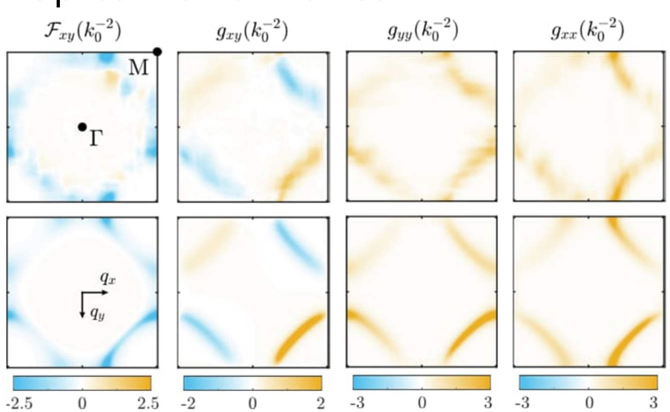
Microcavity polaritons



Gianfrate, Bleu, Dominici, Ardizzone, De Giorgi, Ballarini, Lerario, West, Pfeiffer, Solnyshkov, Sanvitto, Malpuech, *Nature* **578**, 381 (2020)

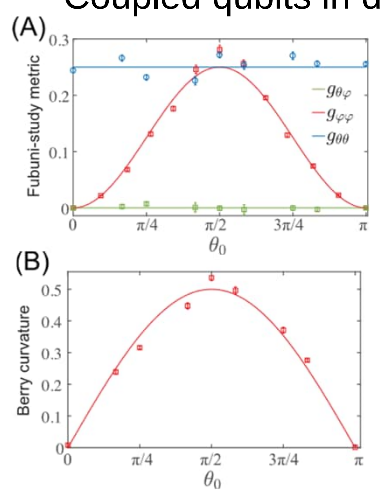
Ren, Liao, Li, Li, Bleu, Malpuech, Yao, Fu, Solnyshkov, *Nat Commun* **12**, 689 (2021)

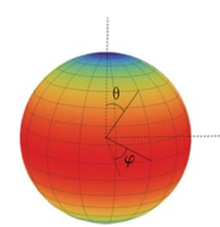
Optical Raman Lattice



Yi, Yu, Yuan, Jiao, Yang, Jiang, Zhang, Chen, Pan, *Phys. Rev. Research* **5**, L032016 (2023)

Coupled qubits in diamond





Yu, Yang, Gong, Cao, Lu, Liu, Plenio, Jelezko, Ozawa, Goldman, Zhang, Cai, *National Science Review* **7**, 254 (2020)

Quantum Geometric Tensor (QGT) observation

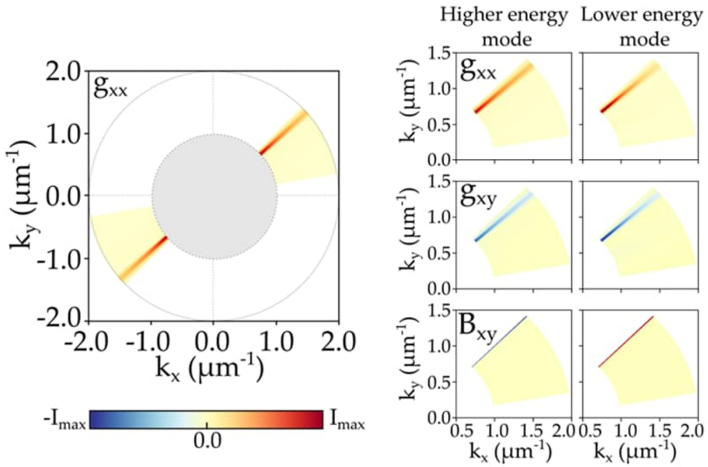
Javier Cuerda

Jani Taskinen

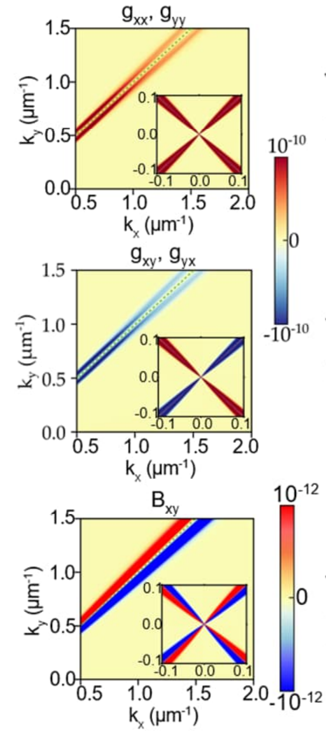
Plasmonic lattices

Cuerda, Taskinen, Källman, Grabitz, PT, *arXiv*:2305.13174, *arXiv*:2305.13244 (2023)

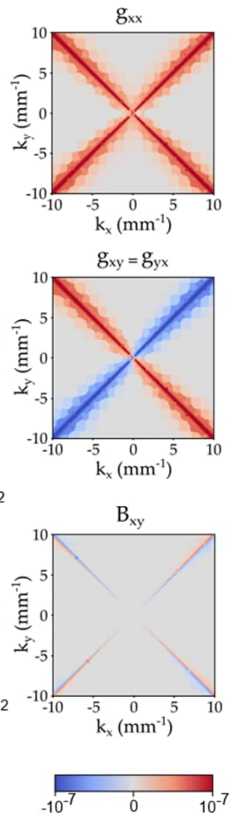
Experiments



Two-band model



T-matrix



The first observation of non-Hermitian Berry curvature!!

The first observation of quantum metric in a plasmonic lattice

Quantum geometric tensor (QGT) with projectors

$$\mathcal{B}_{ij}(\mathbf{k}) = 2\langle \partial_{k_i} u|(1 - |u\rangle\langle u|)|\partial_{k_j} u\rangle$$

$\mathrm{Re}\,\mathcal{B}_{ij} = g_{ij}$ quantum metric $d\ell^2 = \sum_{ij} g_{ij} dk_i dk_j$

$\mathrm{Im}\,\mathcal{B}_{ij} = [\mathbf{\Omega}_{\mathrm{Berry}}]_{ij}$ Berry curvature

Projector to the band(s) of interest: $P(\mathbf{k}) = |u_{n\mathbf{k}}\rangle \langle u_{n\mathbf{k}}|$

$$P(\mathbf{k}) = P^{\dagger}(\mathbf{k}) = P^2(\mathbf{k}) \qquad P(\mathbf{k}) = I - \sum_{m \neq n} |u_{m\mathbf{k}}\rangle \langle u_{m\mathbf{k}}|$$

(In this lecture) The periodic Bloch function: $|u_{n\mathbf{k}}\rangle$

The projector is gauge invariant: $|u_{n\mathbf{k}}\rangle \to \mathrm{e}^{i\theta(\mathbf{k})} |u_{n\mathbf{k}}\rangle$

$$\boxed{\mathcal{B}_{ij}(\mathbf{k}) = 2\mathrm{Tr}\left[P(\mathbf{k})\partial_{k_i} P(\mathbf{k})\partial_{k_j} P(\mathbf{k})\right]}$$

$$\mathcal{B}_{ij}(\mathbf{k}) = 2\mathrm{Tr}\big[P(\mathbf{k})\partial_{k_i}P(\mathbf{k})\partial_{k_j}P(\mathbf{k})\big]$$

is positive semidefinite complex matrix; i.e. of the form where b is an arbitrary vector:

$$\sum_{ij} b_i^* A_{ij} b_j \geq 0$$

The real part is the quantum metric:

$$g_{ij}(\mathbf{k}) = \mathrm{Re}\,\mathcal{B}_{ij}(\mathbf{k}) = \mathrm{Tr}\big[\partial_{k_i}P(\mathbf{k})\partial_{k_j}P(\mathbf{k})\big]$$

And the imaginary one is the Berry curvature:

$$\begin{aligned}\Phi_{\mathrm{Berry}} &= \oint_\gamma \mathrm{d}\mathbf{k}\cdot\mathcal{A}(\mathbf{k}) = \int_S \mathrm{d}\mathbf{S}\cdot\nabla_{\mathbf{k}}\times\mathcal{A}(\mathbf{k}) \\ &= \frac{1}{2}\int_S \mathrm{d}S_l\epsilon^{lmn}\mathrm{Im}\,\mathcal{B}_{nm}(\mathbf{k})\end{aligned}$$

Berry connection:

$$\mathcal{A}(\mathbf{k}) = i\left\langle u_{n\mathbf{k}}\middle|\nabla_{\mathbf{k}}u_{n\mathbf{k}}\right\rangle$$

Quantum geometric tensor in physics

Quantum metric

$$\mathcal{B}_{ij}(\mathbf{k}) = 2\langle \partial_{k_i} u|(1-|u\rangle\langle u|)|\partial_{k_j} u\rangle$$
$$\mathrm{Re}\,\mathcal{B}_{ij} = g_{ij} \qquad d\ell^2 = \sum_{ij} g_{ij} dk_i dk_j$$
$$\mathrm{Im}\,\mathcal{B}_{ij} = [\mathbf{\Omega}_{\mathrm{Berry}}]_{ij}$$

Theory

- Quantum information
  Bengtsson, Życzkowski (2006)
- Quantum phase transition
  S. J. Gu (2006)
- Signatures in current noise
  Neupert, Chamod, Murdy, PRB (2013)
- Fractional Chern insulators
  Dobardžić, Milovanović, Regnault, PRB (2013)
  Roy, PRB (2014)
- **Superconductivity (our work, since 2015)**
- Excitons in transition metal dichalcogenides
  Srivastava, Imamoglu, PRL (2015)
- Orbital paramagnetism
  Gao, Yang, Niu, PRB (2016)
  Piéchon, Raoux, Fuchs, Montambaux, PRB (2016)
- Photonic systems
  Ozawa, PRB (2018)
- **Plus increasing number of works since 2019: especially on superconductivity, Fractional Chern insulators, various transport phenomena, even electron-phonon coupling (Bernevig et al. 2023)**

Berry curvature (Chern number)

- (Fractional) quantum Hall effect
- Topological insulators
- Topological semimetals
- Topological defects and textures
- Topological superconductors
- etc

Perspective on quantum geometry
PT, PRL 2023

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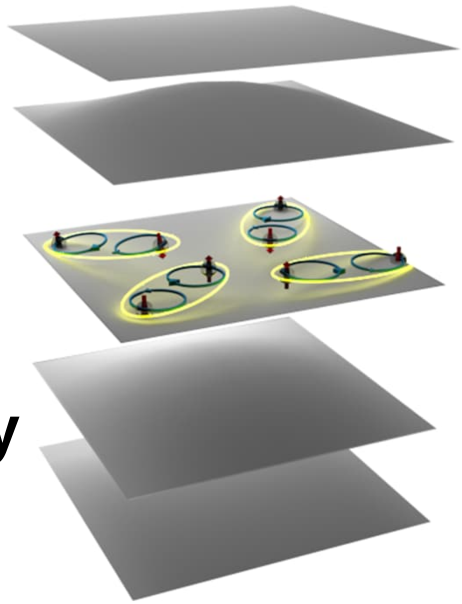

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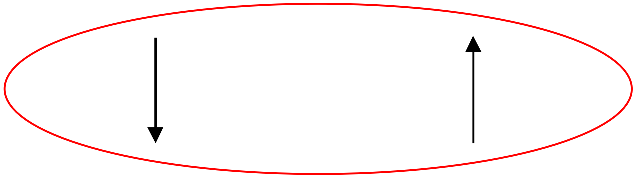
Superconductivity: Cooper pair formation competes with kinetic energy



Weak interaction U
Large kinetic energy (Fermi level)
Low critical temperature

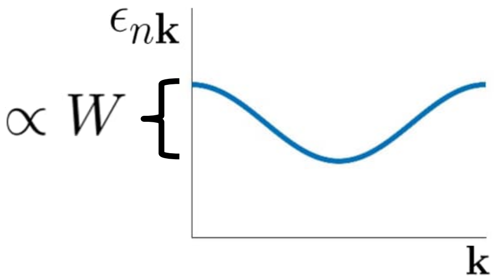
$$T_c \propto e^{-1/(U n_0(E_f))}$$

Constituents: interactions, density of states (DOS)

Remove the kinetic energy/maximize DOS:
interaction effects dominate!

Flat bands: interactions dominate

Dispersive band U<<W:



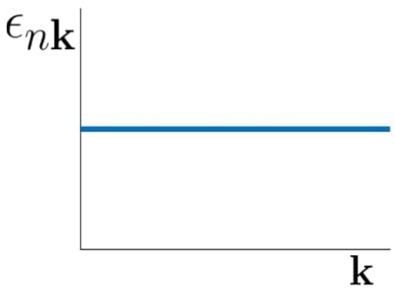
$$\psi_n(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r})$$

(periodic part of) the Bloch function

T_c for Cooper pairing

$$T_c \propto e^{-1/(U n_0(E_f))}$$

Flat band U>>W:



$\epsilon_{n\mathbf{k}} =$ constant

Group velocity: $\frac{\partial \epsilon_{n\mathbf{k}}}{\partial k} = 0$

No interactions: insulator at any filling

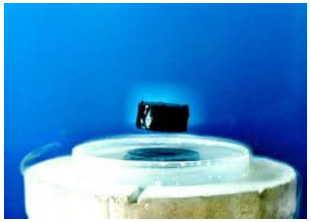
$$T_c \propto U V_{\mathrm{flat\ band}}$$

High T_c for pairing
(Khodel, Shaginyan, Volovik, Kopnin, Heikkilä)

This is the critical temperature for Cooper pairing

$$\Delta(\mathbf{r}) = \langle \psi_\sigma(\mathbf{r}) \psi_{\sigma'}(\mathbf{r}) \rangle \qquad \Delta(\mathbf{r}) = |\Delta(\mathbf{r})|$$

Superfluid weight: supercurrent and Meissner Effect



Supercurrent

$$\mathbf{j} = -D_s \mathbf{A}$$

Current

$$\mathbf{j} = \sigma \mathbf{E} \qquad \mathbf{E} = -\partial \mathbf{A}/\partial t$$

Order parameter phase gradient $\Delta(\mathbf{r}) = |\Delta(\mathbf{r})| \mathrm{e}^{2i\phi(\mathbf{r})}$

$\nabla\phi - e\mathbf{A}/\hbar$ Invariant under gauge transformations

Free energy change associated with phase gradient

$$\Delta F = \frac{\hbar^2}{2e^2} \int \mathrm{d}^3\mathbf{r} \sum_{ij} [D_s]_{ij} \partial_i \phi(\mathbf{r}) \partial_j \phi(\mathbf{r})$$

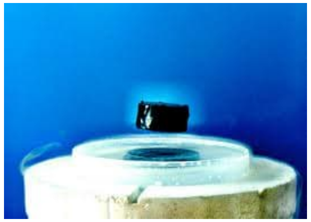
London equation and penetration depth

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{j}$$

$$\nabla^2 \mathbf{B} = \mu_0 D_s \mathbf{B}$$

$$\lambda_L = (\mu_0 D_s)^{-1/2}$$

Superfluid weight: supercurrent and Meissner Effect



Supercurrent

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Conventional BCS: $\quad D_s = \frac{e^2 n_{\mathrm{p}}}{m_{\mathrm{eff}}} \left(1 - \left(\frac{2\pi\Delta}{k_{\mathrm{B}}T} \right)^{1/2} \mathrm{e}^{-\Delta/(k_{\mathrm{B}}T)} \right)$

Zero at a flat band!!!

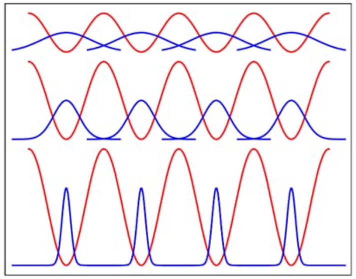
n_{p} Particle density

$$\frac{1}{m_{\mathrm{eff}}} \propto J \propto \partial_{k_i} \partial_{k_j} \epsilon_{\mathbf{k}}$$

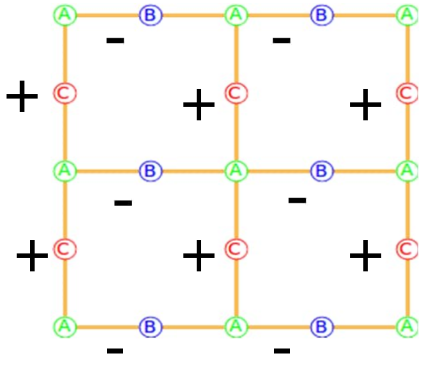
Bandwidth $\qquad i, j = x, y, z$

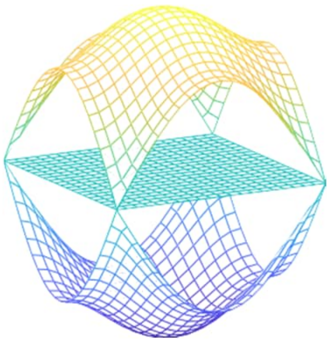
Flat bands

Trivial: the extreme atomic limit



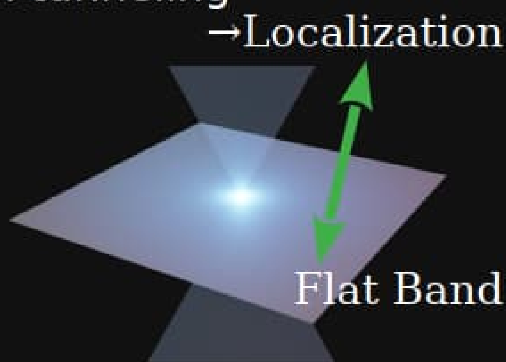
Non-trivial: due to interference effects

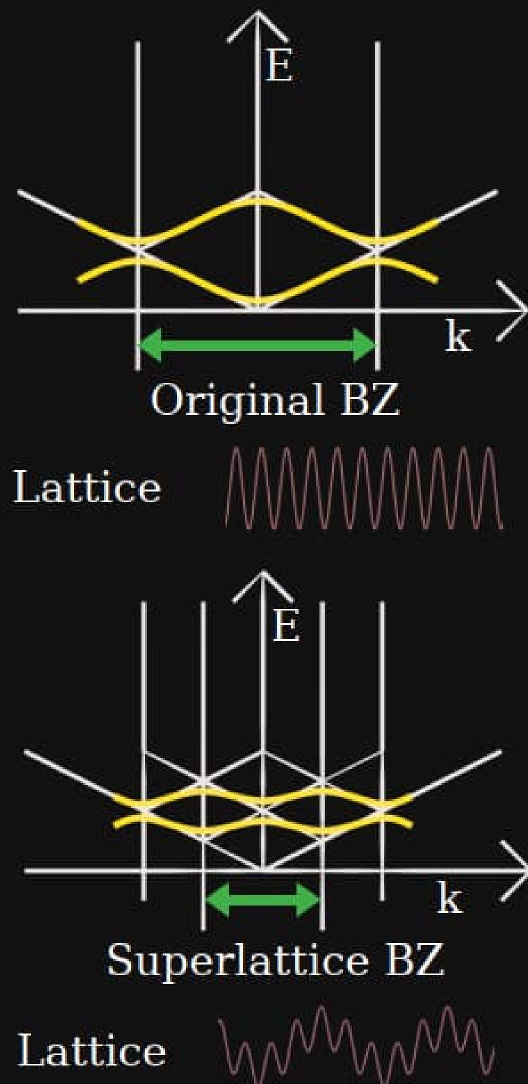


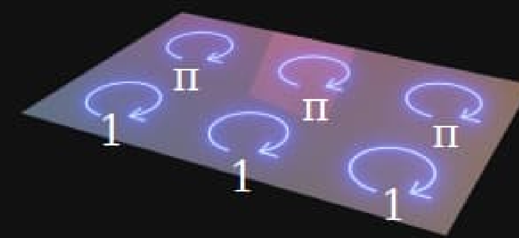


Formation of flat bands

Destructive interference in tunneling





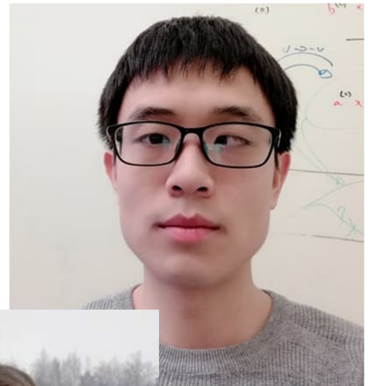


Landau levels

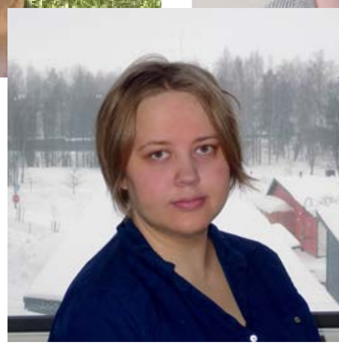
Review: Leykam, Andreanov, Flach, Advances in Physics 2018

Superfluidity and quantum geometry

Sebastiano Peotta



Long Liang



Kukka-Emilia Huhtinen

Andrei Bernevig

Sebastian Huber

Murad Tovmasyan

Jonah Herzog-Arbeitman

Aaron Chew

Aleksi Julku

Dong-Hee Kim

Tuomas Vanhala

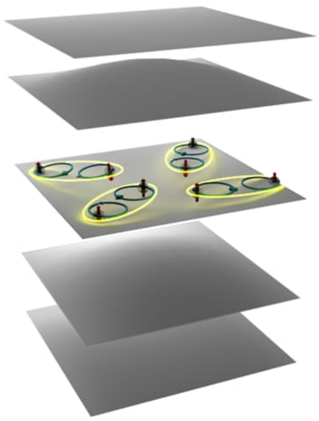
Ari Harju

Topi Siro

Peotta, PT, Nat Comm 2015
Julku, Peotta, Vanhala, Kim, PT, PRL 2016
Tovmasyan, Peotta, PT, Huber, PRB 2016
Liang, Vanhala, Peotta, Siro, Harju, PT, PRB 2017
Liang, Peotta, Harju, PT, PRB 2017
Tovmasyan, Peotta, Liang, PT, Huber, PRB 2018
PT, Liang, Peotta, PRB(R) 2018
Huhtinen, Herzog-Arbeitman, Chew, Bernevig, PT, PRB 2022
Herzog-Arbeitman, Chew, Huhtinen, PT, Bernevig, arXiv 2022

Our multiband approach

MULTIBAND BCS MEAN-FIELD THEORY
multiband two-component attractive
Fermi-Hubbard model –U < 0



$$H = -\sum_{ij\alpha\beta\sigma} t^{\sigma}_{i\alpha j\beta} c^{\dagger}_{i\alpha\sigma} c_{j\beta\sigma} - U \sum_{i\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} - \mu \sum_{i\alpha\sigma} n_{i\alpha\sigma}$$

Introduce supercurrent

$$\Delta(\mathbf{r}) \to \Delta(\mathbf{r}) e^{2i\mathbf{q}\cdot\mathbf{r}}$$

$$\nabla\phi - e\mathbf{A}/\hbar$$

$2\mathbf{q}$ Cooper pair momentum

$$\langle j_i(\omega, \mathbf{q})\rangle = -\sum_j \chi_{ij}(\omega, \mathbf{q}) A_j(\omega, \mathbf{q})$$

$$[D_s]_{ij} = \frac{e^2}{V} \frac{\mathrm{d}^2\Omega}{\mathrm{d}q_i \mathrm{d}q_j}\Big|_{\mathbf{q}=\mathbf{0}}$$

$$D_s = \lim_{\mathbf{q}\to 0} \chi(\omega = 0, \mathbf{q})$$

$i, j = x, y, z$

Superfluid weight in a multiband system

$$D_s = D_{s,\mathrm{conventional}} + D_{s,\mathrm{geometric}}$$

$$i, j = x, y, z$$

$$\propto \partial_{k_i} \partial_{k_j} \epsilon_{\mathbf{k}}$$

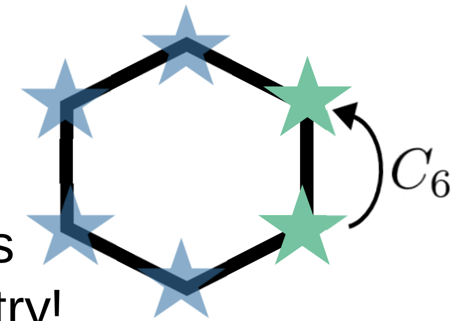
Can be nonzero also in a flat band
Present only in a multiband case
Proportional to the quantum metric

$$[D_{s,\mathrm{geometric}}]_{ij} \propto U g_{ij}$$

Peotta, PT, Nat Comm 2015
Liang, Vanhala, Peotta, Siro, Harju, PT, PRB 2017
Huhtinen, Herzog-Arbeitman, Chew, Bernevig, PT, PRB 2022

Superfluid weight and quantum metric

Isolated flat band: $W \ll U \ll E_{\text{band gap}}$



Uniform pairing: $\Delta_{\text{orbital }\#} = \Delta$ Valid when orbitals related by symmetry!

$$\Rightarrow \quad [D_s]_{ij} = \frac{4e^2 U\nu(1-\nu)}{(2\pi)^{d-1} N_{\text{orb}} \hbar^2} \mathcal{M}^{\text{R,min}}_{ij}$$

$$\Delta = \frac{U}{N_{\text{orb}}} \sqrt{\nu(1-\nu)}$$

$$\mathcal{M}^{\text{R}}_{ij} = \frac{1}{2\pi} \int_{\text{B.Z.}} \mathrm{d}^d \mathbf{k} \, \underbrace{\mathrm{Re}\, \mathcal{B}_{ij}(\mathbf{k})}_{\text{quantum metric } g_{ij}}$$

$$[D_s]_{ij} = \frac{2e^2}{\pi \hbar^2} \frac{\Delta^2}{U N_{\text{orb}}} \mathcal{M}^{\text{R,min}}_{ij}$$

Mean-field → Peotta, PT, Nat Comm 2015

Mean-field → Huhtinen, Herzog-Arbeitman, Chew, Bernevig, PT, PRB 2022

Exact many-body → Herzog-Arbeitman, Chew, Huhtinen, PT, Bernevig, arXiv 2022

Finite temperature, general case (non-isolated flat band)

$$D_s = D_{s,\mathrm{conventional}} + D_{s,\mathrm{geometric}}$$

$$D_{\mathrm{s,conventional},jl} = \frac{e^2}{\hbar^2}\int\frac{\mathrm{d}^d\mathbf{k}}{(2\pi)^d}\sum_n\left[-\frac{\beta}{2\cosh^2(\beta E_{n\mathbf{k}}/2)}+\frac{\tanh(\beta E_{n\mathbf{k}}/2)}{E_{n\mathbf{k}}}\right]\frac{\Delta^2}{E_{n\mathbf{k}}^2}\partial_j\varepsilon_{n\mathbf{k}}\partial_l\varepsilon_{n\mathbf{k}}$$

$$D_{\mathrm{s,geometric},jl} = \frac{e^2\Delta^2}{\hbar^2}\int\frac{\mathrm{d}^d\mathbf{k}}{(2\pi)^d}\sum_{n\neq m}\left[\frac{\tanh(\beta E_{n\mathbf{k}}/2)}{E_{n\mathbf{k}}}-\frac{\tanh(\beta E_{m\mathbf{k}}/2)}{E_{m\mathbf{k}}}\right]\times$$
$$\frac{(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}})^2}{E_{m\mathbf{k}}^2-E_{n\mathbf{k}}^2}\left[\,\langle\partial_j u_{n\mathbf{k}}|u_{m\mathbf{k}}\rangle\,\langle u_{m\mathbf{k}}|\partial_l u_{n\mathbf{k}}\rangle+(j\leftrightarrow l)\right]$$

The geometric contribution originates from the interband part of the current operator

$$D_{\mathrm{s,geometric},jl} = \frac{e^2\Delta^2}{\hbar^2}\int \frac{\mathrm{d}^d\mathbf{k}}{(2\pi)^d} \sum_{n\neq m}\left[\frac{\tanh(\beta E_{n\mathbf{k}}/2)}{E_{n\mathbf{k}}} - \frac{\tanh(\beta E_{m\mathbf{k}}/2)}{E_{m\mathbf{k}}}\right]\times$$
$$\frac{(\varepsilon_{n\mathbf{k}}-\varepsilon_{m\mathbf{k}})^2}{E_{m\mathbf{k}}^2 - E_{n\mathbf{k}}^2}\left[\langle \partial_j u_{n\mathbf{k}}|u_{m\mathbf{k}}\rangle \langle u_{m\mathbf{k}}|\partial_l u_{n\mathbf{k}}\rangle + (j \leftrightarrow l)\right]$$

Superfluid weight from linear response (current-current correlator):

$$\langle j_i(\omega,\mathbf{q})\rangle = -\sum_j \chi_{ij}(\omega,\mathbf{q})A_j(\omega,\mathbf{q})$$
$$D_s = \lim_{\mathbf{q}\to 0}\chi(\omega=0,\mathbf{q})$$

Expectation value of the current operator:

$$\langle u_{m\mathbf{k}}|\nabla_{\mathbf{k}}\tilde{K}^{\uparrow}(\mathbf{k})|u_{n\mathbf{k}}\rangle = \nabla_{\mathbf{k}}\epsilon_{n\mathbf{k}}\delta_{nm} + (\epsilon_{n\mathbf{k}}-\epsilon_{m\mathbf{k}})\langle u_{m\mathbf{k}}|\nabla_{\mathbf{k}} u_{n\mathbf{k}}\rangle$$

$$\hat{H} = \hat{H}_0 + \hat{H}_{\mathrm{int}} \qquad \hat{H}_0 = \sum_{\mathbf{i}\alpha,\mathbf{j}\beta}\sum_{\sigma}\hat{c}^{\dagger}_{\mathbf{i}\alpha\sigma}K^{\sigma}_{\mathbf{i}\alpha,\mathbf{j}\beta}\hat{c}_{\mathbf{j}\beta\sigma}$$

Lower bound for flat band superfluidity

Peotta, PT, Nat Comm 2015

The quantum geometric tensor $\mathcal{B}_{ij}$
is complex positive semidefinite

➡ $$\boxed{D_s \geqslant \int_{B.Z.} d^d\mathbf{k}|\mathbf{\Omega}_{\mathrm{Berry}}(\mathbf{k})| \geqslant C}$$

Time reversal symmetry assumed; C is a spin Chern number

Constituents: interactions, density of states (DOS)
and Bloch functions = quantum geometry and topology

Lower bound for flat band superfluidity

The quantum geometric tensor $\mathcal{B}_{ij}$
is complex positive semidefinite

$$\Rightarrow \boxed{D_s \geqslant \int_{B.Z.} d^d\mathbf{k}|\mathbf{\Omega}_{\text{Berry}}(\mathbf{k})| \geqslant C}$$

$$\Omega_{\text{Berry}}(\mathbf{k}) = i\hat{z}\cdot\nabla_{\mathbf{k}} \times \langle u_{n\mathbf{k}}|\nabla_{\mathbf{k}} u_{n\mathbf{k}}\rangle$$

Berry curvature: $\Omega(\mathbf{k}) = i\hat{z}\cdot\nabla\times\langle u_{n\mathbf{k}}|\partial_{\mathbf{k}} u_{n\mathbf{k}}\rangle$

Chern number: $C = \frac{1}{2\pi}\int_{B.Z.} d^2\mathbf{k}\ \Omega(\mathbf{k})$

Time reversal symmetry assumed; C is a spin Chern number

Mean-field results confirmed by:
exact diagonalization, DMFT, DMRG, perturbation theory

The Cooper problem: two particles

PHYSICAL REVIEW VOLUME 104, NUMBER 4 NOVEMBER 15, 1956

Letters to the Editor

PUBLICATION of brief reports of important discoveries in physics may be secured by addressing them to this department. The closing date for this department is five weeks prior to the date of issue. No proof will be sent to the authors. The Board of Editors does not hold itself responsible for the opinions expressed by the correspondents. Communications should not exceed 600 words in length and should be submitted in duplicate.

Bound Electron Pairs in a Degenerate Fermi Gas*

LEON N. COOPER
Physics Department, University of Illinois, Urbana, Illinois
(Received September 21, 1956)

IT has been proposed that a metal would display superconducting properties at low temperatures if the one-electron energy spectrum had a volume-independent energy gap of order $\Delta \simeq kT_c$, between the ground state and the first excited state.[1,2] We should like to point out how, primarily as a result of the exclusion principle, such a situation could arise.

Consider a pair of electrons which interact above a

$=(1/V)\exp[i(\mathbf{k}_1\cdot\mathbf{r}_1+\mathbf{k}_2\cdot\mathbf{r}_2)]$ which satisfy periodic boundary conditions in a box of volume V, and where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the coordinates of electron one and electron two. (One can use antisymmetric functions and obtain essentially the same results, but alternatively we can choose the electrons of opposite spin.) Defining relative and center-of-mass coordinates, $\mathbf{R}=\frac{1}{2}(\mathbf{r}_1+\mathbf{r}_2)$, $\mathbf{r}=(\mathbf{r}_2-\mathbf{r}_1)$, $\mathbf{K}=(\mathbf{k}_1+\mathbf{k}_2)$ and $\mathbf{k}=\frac{1}{2}(\mathbf{k}_2-\mathbf{k}_1)$, and letting $\mathcal{E}_K+\epsilon_k=(\hbar^2/m)(\frac{1}{4}K^2+k^2)$, the Schrödinger equation can be written

$$(\mathcal{E}_K+\epsilon_k-E)a_{\mathbf{k}}+\sum_{\mathbf{k}'}a_{\mathbf{k}'}(\mathbf{k}|H_1|\mathbf{k}')\times\delta(\mathbf{K}-\mathbf{K}')/\delta(0)=0 \quad (1)$$

where

$$\Psi(\mathbf{R},\mathbf{r})=(1/\sqrt{V})e^{i\mathbf{K}\cdot\mathbf{R}}\chi(\mathbf{r},K),$$
$$\chi(\mathbf{r},K)=\sum_{\mathbf{k}}(a_{\mathbf{k}}/\sqrt{V})e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (2)$$

and

$$(\mathbf{k}|H_1|\mathbf{k}')=\left(\frac{1}{V}\int d\mathbf{r}e^{-i\mathbf{k}\cdot\mathbf{r}}H_1e^{i\mathbf{k}'\cdot\mathbf{r}}\right)_{0\ \text{phonons}}.$$

We have assumed translational invariance in the metal. The summation over $\mathbf{k}'$ is limited by the exclusion principle to values of k_1 and k_2 larger than q_0, and by the delta function, which guarantees the conservation of the total momentum of the pair in a single scattering.

$$T_c \propto e^{-1/(Un_0(E_f))}$$

The two-body problem in a multiband lattice

PT, Liang, Peotta, PRB(R) 2018

$$[T_1 + T_2 + \lambda V(1,2)]\,|\psi(1,2)\rangle = E|\psi(1,2)\rangle$$

The Cooper problem Add the Fermi sea: instability of the Fermi sea towards pairing.

Now we claim
Flat band No Fermi sea but large degeneracy: instability towards breaking the degeneracy, and thus towards ordered states, is given by the pair effective mass.

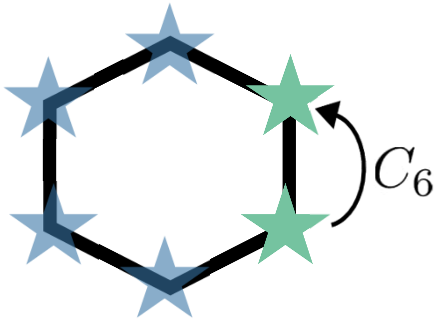
Quantum metric and the two-body effective mass

PT, Liang, Peotta, PRB(R) 2018

$$E_b = \lambda \sum_{\mathbf{k}} \int \mathrm{d}\mathbf{x}\, V(\mathbf{x}) |u_{\mathbf{k}+\frac{\mathbf{q}}{2}}(\mathbf{x}) u_{\mathbf{k}-\frac{\mathbf{q}}{2}}(\mathbf{x})|^2$$

periodic part of the Bloch function

For uniform pairing $V(\mathbf{x}) = 1$ we get approximately



$$\left[\frac{1}{m^*}\right]_{ij} \simeq \frac{-\lambda}{N_{\mathrm{c}} N_{\mathrm{orb}}} \sum_{\mathbf{k}} g_{ij}(\mathbf{k})$$

$$D^s_{ij} \simeq n(1/m^*)_{ij}$$

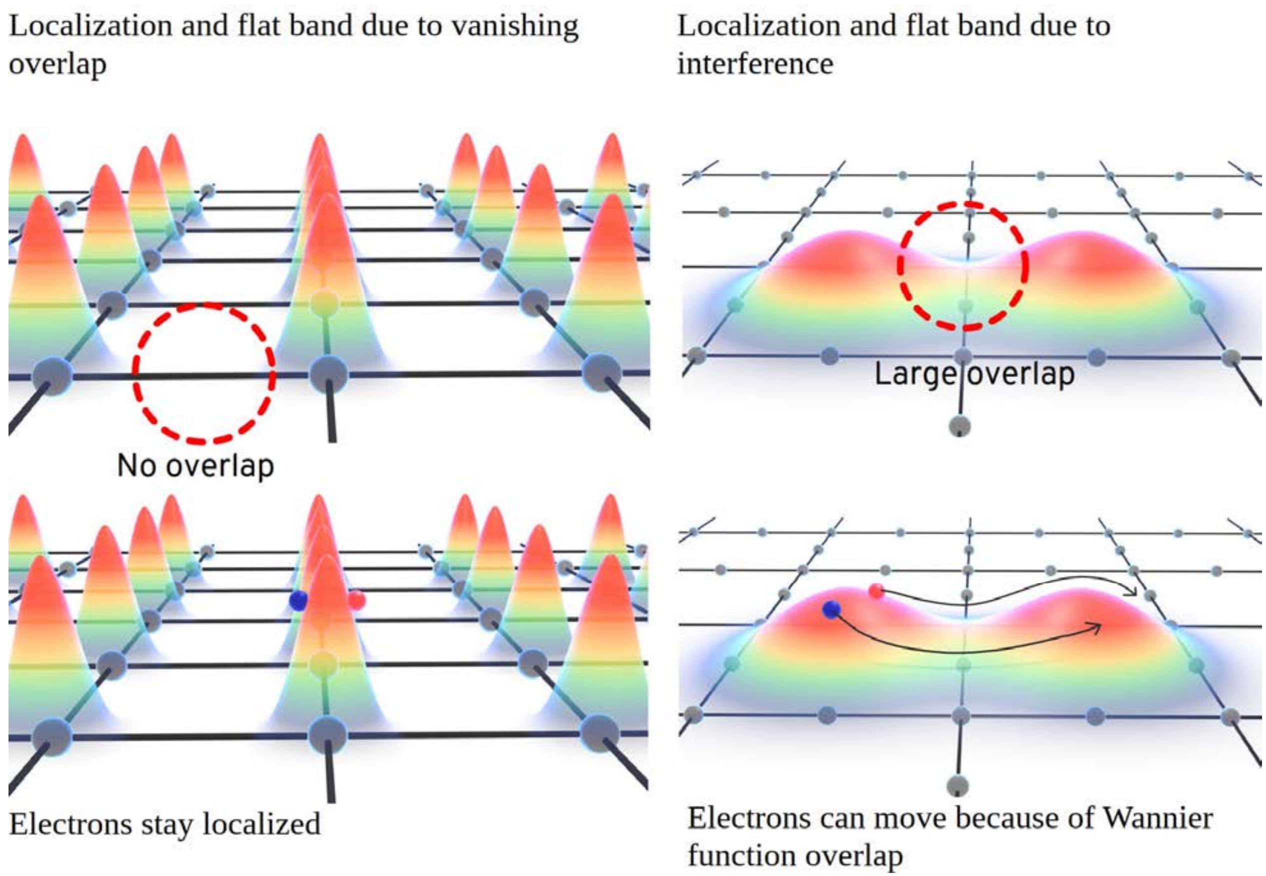
quantum metric

Same as the multiband BCS result!

Why can there be transport in a flat band?

Non-interacting

Interacting



$C \neq 0 \Leftrightarrow$ non-localized $w(\mathbf{r}) = \mathcal{F}[u(\mathbf{k})]$

Brouder, Panati, Calandra, Marzari, PRL 2007

$$D_s \propto g_{ij} \geqslant C$$

Quantum geometric superconductivity: confirmed beyond mean-field

BCS-state is the exact ground state at T=0

Julku, Peotta, Vanhala, Kim, PT, PRL 2016
Tovmasyan, Peotta, PT, Huber, PRB 2016

Exact diagonalization, DMFT, QMC, DMRG

Julku, Peotta, Vanhala, Kim, PT, PRL 2016
Liang, Vanhala, Peotta, Siro, Harju, PT, PRB 2017
Mondaini, Batrouni, Grémaud, PRB 2018
Hofmann, Berg, Chowdhury, PRB 2020
Peri, Song, Bernevig, Huber, PRL 2021
Chan, Grémaud, Batrouni, PRB 2022 (x 2)
Herzog-Arbeitman, Peri, Schindler, Huber, Bernevig, PRL 2022
Hofmann, Berg, Chowdhury, PRL 2023

Preformed pairs

Tovmasyan, Peotta, Liang, PT, Huber, PRB 2018

Perturbation theory with a Hamiltonian projected to a flat band

Tovmasyan, Peotta, Törmä, Huber, PRB 2016

$$H = \frac{|U|}{2}\sum_{i\alpha}(\overline{n}_{i\alpha\uparrow} - \overline{n}_{i\alpha\downarrow})^2$$

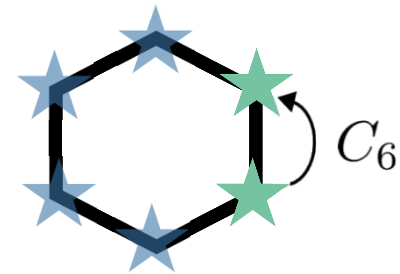
Exact results on the excitations possible! …. next ….

Quantum geometric superconductivity: exact results on Cooper pair mass and excitations

Project to the flat band and assume the uniform pairing condition

$$\overline{c}^\dagger_{\mathbf{k}\alpha\sigma} = \sum_\beta c^\dagger_{\mathbf{k}\beta\sigma} P^\sigma_{\beta\alpha}(\mathbf{k}) \qquad \frac{1}{N_c}\sum_{\mathbf{k}} P_{\alpha\alpha}(\mathbf{k}) = \frac{N_f}{N_{\mathrm{orb}}}$$

$$P^\sigma(\mathbf{k}) = \sum_{n\in\mathcal{B}} |u_{n\mathbf{k}\sigma}\rangle\langle u_{n\mathbf{k}\sigma}|$$



$$\Rightarrow \quad H = \frac{|U|}{2}\sum_{i\alpha}(\overline{n}_{i\alpha\uparrow} - \overline{n}_{i\alpha\downarrow})^2$$

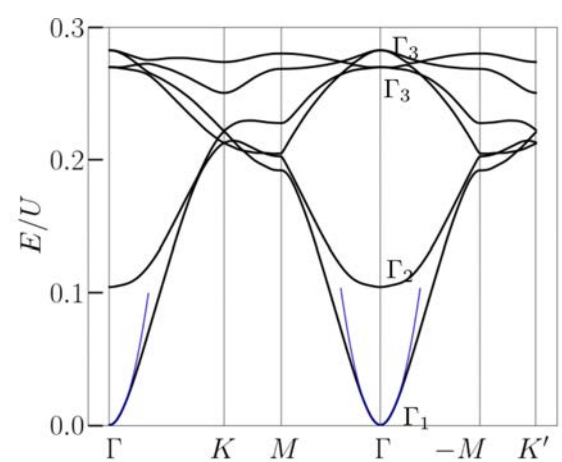
Ground state $|n\rangle \propto \eta^{\dagger n}|0\rangle \qquad \eta^\dagger = \sum_{\mathbf{k}\alpha} \overline{c}^\dagger_{\mathbf{k}\alpha\uparrow}\overline{c}^\dagger_{-\mathbf{k}\alpha\downarrow}$

Cooper pair excitations governed by an effective single particle Hamiltonian

$$h_{\alpha\beta}(\mathbf{q}) = -\frac{|U|}{N_c}\sum_{\mathbf{k}} P_{\alpha\beta}(\mathbf{k}+\mathbf{q})P_{\beta\alpha}(\mathbf{k})$$

- Single particles immobile
- Cooper pair mass from quantum geometry
- Leggett and Goldstone modes

$$\left[\frac{1}{m^*}\right]_{ij} = \frac{|U|}{N_{\mathrm{orb}}}\mathcal{M}^{\mathrm{R,min}}_{ij}$$

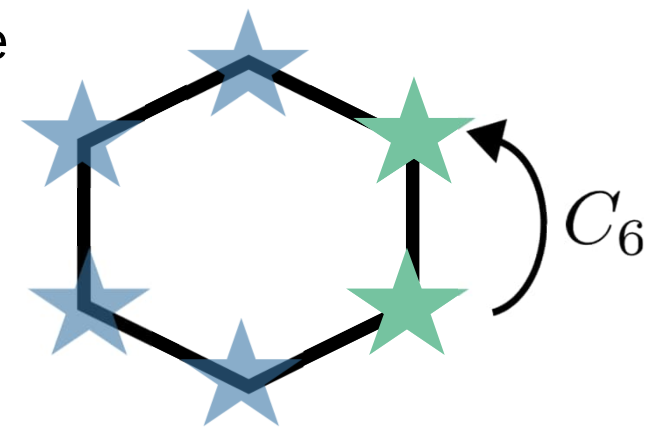


Herzog-Arbeitman, Chew, Huhtinen, PT, Bernevig, arXiv 2022

Uniform Pairing Condition from symmetry

Are uniform pairing flat bands just fine-tuning?

- No! Uniform pairing is guaranteed by space group symmetry and the orbitals

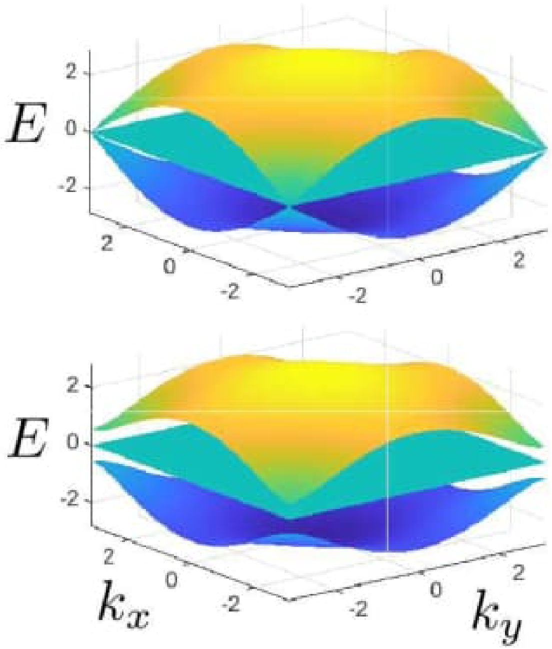


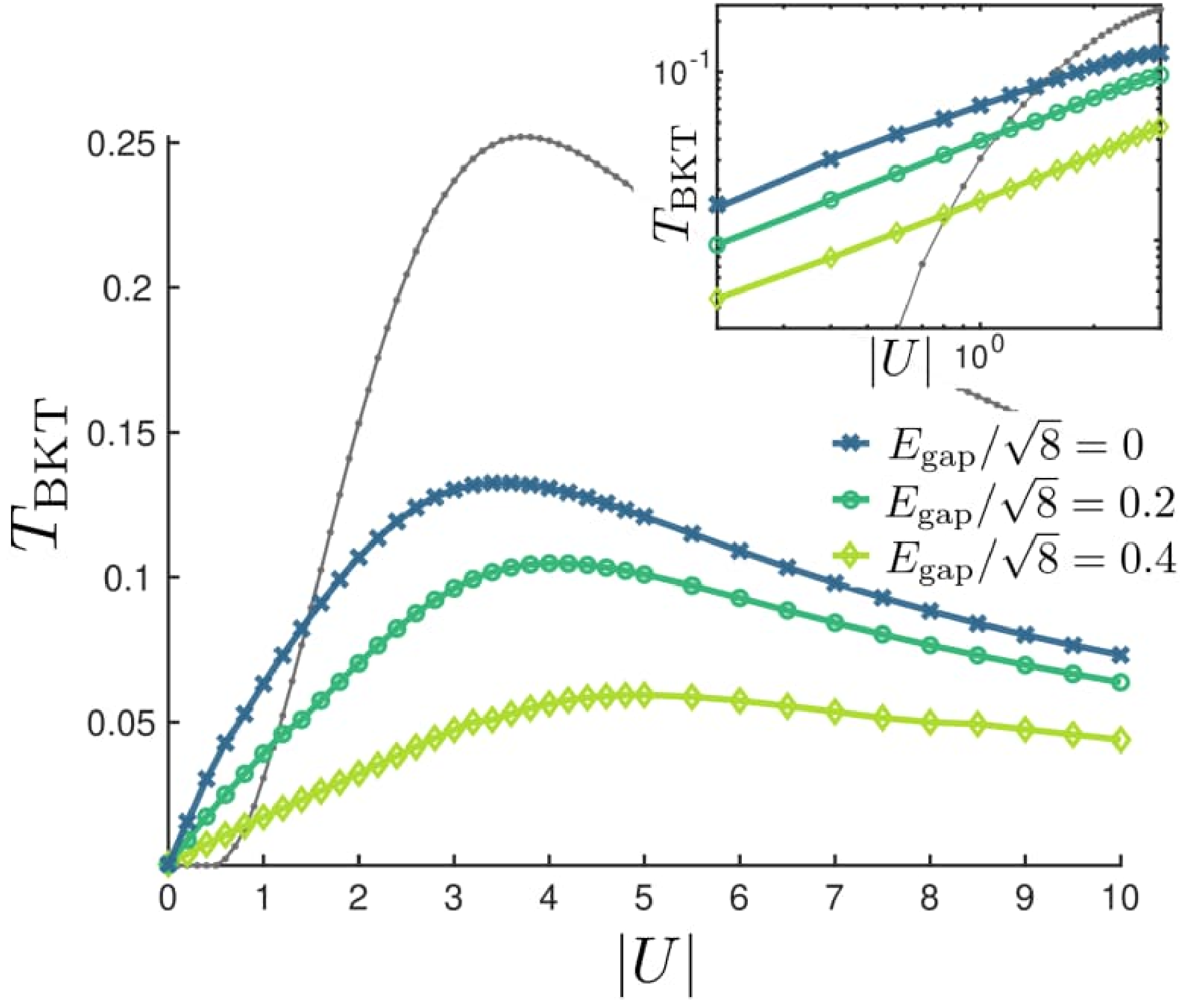
Intuition: orbitals related by symmetry have uniform pairing

Precise statement: Orbitals forming an irrep of the site-symmetry group of a single Wyckoff position have uniform pairing

Non-isolated bands:
Band touchings **increase** the critical temperature

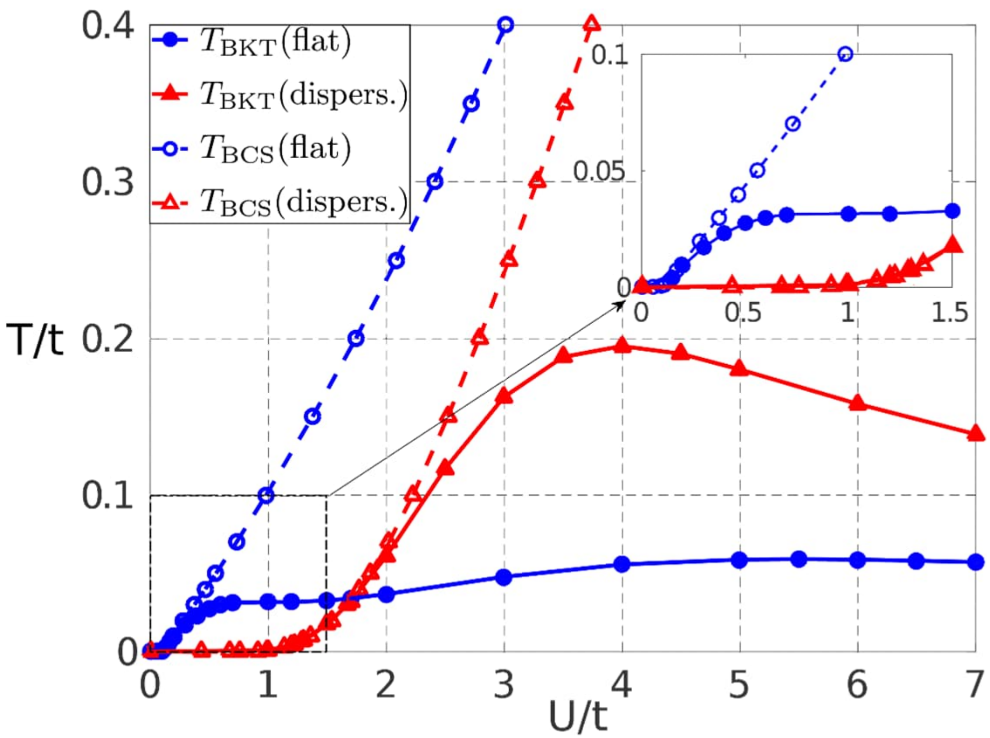
$$T_{\mathrm{BKT}} = \frac{\pi}{8}\sqrt{\det D^s(T_{\mathrm{BKT}})}$$





Huhtinen, Herzog-Arbeitsman, Chew, Bernevig, PT, PRB (2022)

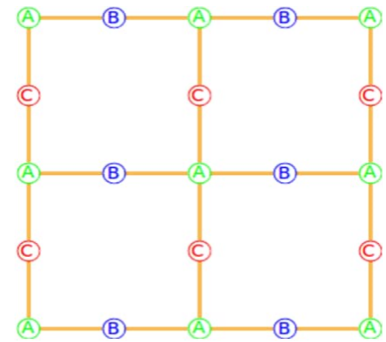
Haldane-Hubbard model



Liang, Vanhala, Peotta, Siro, Harju, PT, PRB 2017

- Linear dependence of Δ, T_c, D_s on U
- Dramatic effect for small U

Devil in the details (devil in the supplementary)



The first mean-field results:

(Peotta, PT, 2015)

Isolated flat band: $W \ll U \ll E_{\text{band gap}}$

Uniform pairing: $\Delta_{\text{orbital }\#} = \Delta$

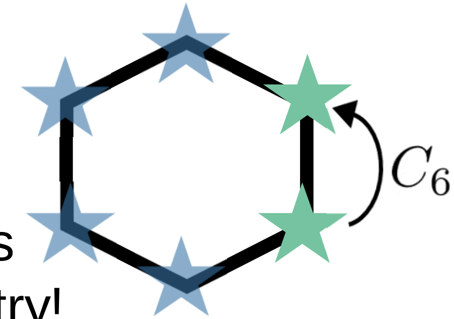
$i, j = x, y, z$

$$[D_s]_{ij} = \frac{4e^2 U \nu(1-\nu)}{(2\pi)^d N_{\text{orb}} \hbar^2} \int_{\text{B.Z.}} \mathrm{d}^d\mathbf{k} \underbrace{\mathrm{Re}\,\mathcal{B}_{ij}(\mathbf{k})}_{\text{quantum metric } g_{ij}}$$

Problem: D_s is independent of orbital positions (basis independence), while QGT depends on them!

Superfluid weight and quantum metric

Isolated flat band: $W \ll U \ll E_{\text{band gap}}$



Uniform pairing: $\Delta_{\text{orbital }\#} = \Delta$ Valid when orbitals related by symmetry!

$$[D_s]_{ij} = \frac{4e^2 U\nu(1-\nu)}{(2\pi)^{d-1} N_{\text{orb}} \hbar^2} \mathcal{M}_{ij}^{\mathrm{R,min}}$$

$$\Delta = \frac{U}{N_{\text{orb}}}\sqrt{\nu(1-\nu)}$$

$$\mathcal{M}_{ij}^{\mathrm{R}} = \frac{1}{2\pi}\int_{\mathrm{B.Z.}} \mathrm{d}^d\mathbf{k}\, \underbrace{\mathrm{Re}\,\mathcal{B}_{ij}(\mathbf{k})}_{\text{quantum metric } g_{ij}}$$

$$[D_s]_{ij} = \frac{2e^2}{\pi\hbar^2}\frac{\Delta^2}{U N_{\text{orb}}}\mathcal{M}_{ij}^{\mathrm{R,min}}$$

Mean-field → Peotta, PT, Nat Comm 2015; Huhtinen, Herzog-Arbeitman, Chew, Bernevig, PT, PRB 2022

Exact many-body → Herzog-Arbeitman, Chew, Huhtinen, PT, Bernevig, arXiv 2022

Complete equation for the superfluid weight

$$\left.\frac{\mathrm{d}^2\Omega}{\mathrm{d}q_i\mathrm{d}q_j}\right|_{\mathbf{q}=\mathbf{0}} = \left.\frac{\partial^2\Omega}{\partial q_i\partial q_j}\right|_{\mathbf{q}=\mathbf{0}} - [\mathrm{d}_i\mathrm{Im}(\Delta)]^T\mathbf{A}[\mathrm{d}_j\mathrm{Im}(\Delta)]\Big|_{\mathbf{q}=\mathbf{0}}$$

Conserved Not conserved Not conserved

TRS: $\Delta_\alpha(\mathbf{q}) = \Delta^*_\alpha(-\mathbf{q})$

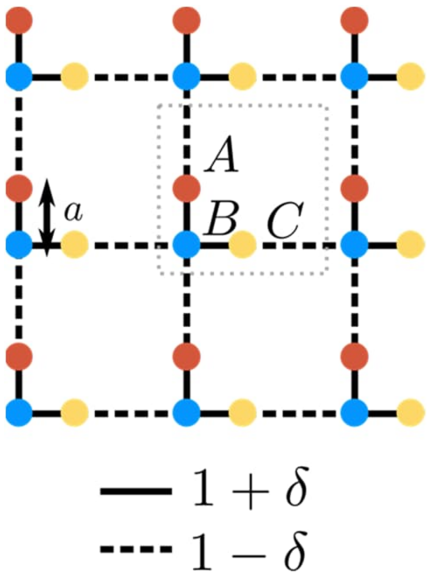
$$\mathbf{A} = \begin{pmatrix} \frac{\partial^2\Omega}{\partial\mathrm{Im}\Delta_2\partial\mathrm{Im}\Delta_2} & \cdots & \frac{\partial^2\Omega}{\partial\mathrm{Im}\Delta_2\partial\mathrm{Im}\Delta_{N_{\mathrm{orb}}}} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2\Omega}{\partial\mathrm{Im}\Delta_{N_{\mathrm{orb}}}\partial\mathrm{Im}\Delta_2} & \cdots & \frac{\partial^2\Omega}{\partial\mathrm{Im}\Delta_{N_{\mathrm{orb}}}\partial\mathrm{Im}\Delta_{N_{\mathrm{orb}}}} \end{pmatrix}$$

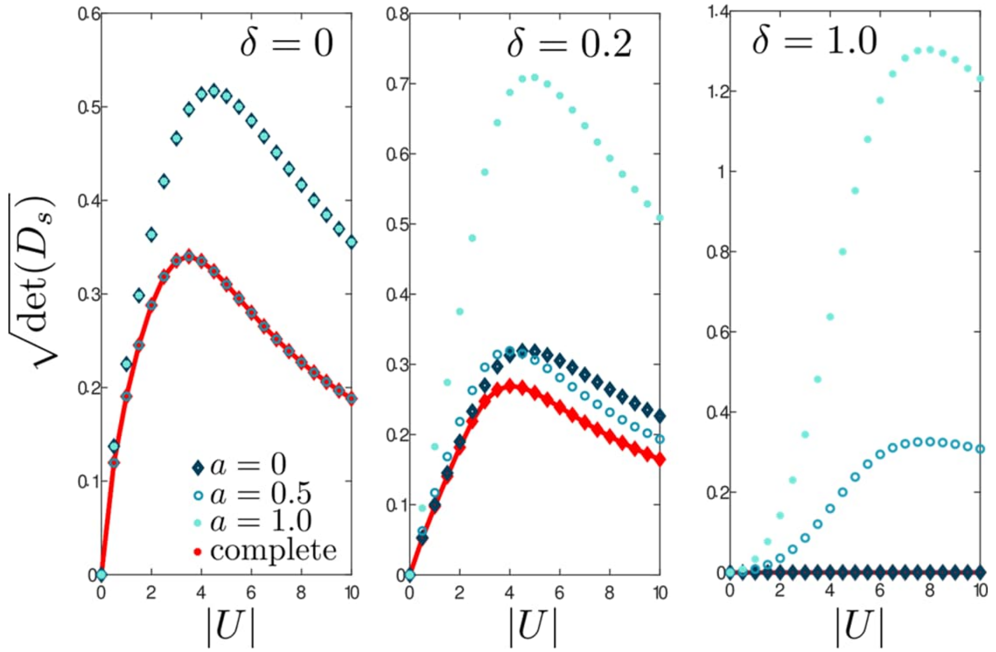
$$\mathrm{d}_i\mathrm{Im}(\Delta) = \left(\frac{\mathrm{d}\,\mathrm{Im}\Delta_2}{\mathrm{d}q_i}, \ldots, \frac{\mathrm{d}\,\mathrm{Im}\Delta_{N_{\mathrm{orb}}}}{\mathrm{d}q_i}\right)^T$$

- The minimal quantum metric, i.e. the one with the smallest possible trace, is related to the superfluid weight in isolated flat bands with TRS and uniform pairing.

When the orbitals are at high-symmetry positions, the quantum metric is guaranteed to be minimal

Example: the Lieb lattice





At worst, $\frac{1}{V}\frac{\partial^2\Omega}{\partial q_i \partial q_j}\Big|_{\boldsymbol{q}=\boldsymbol{0}}$ **can give an incorrectly nonzero superfluid weight.**

When the orbitals are at high-symmetry positions, the quantum metric is guaranteed to be minimal

Superfluid weight: the general case

Non-isolated band, non-TRS results exist as well (but more cumbersome)

Note: whether to use free energy or grand potential is subtle in the non-TRS case (for TRS, they produce the same result since $\mu(q) = \mu(-q)$)

$$[D_s]_{ij} = \frac{e^2}{V}\frac{\mathrm{d}^2 F}{\mathrm{d}q_i \mathrm{d}q_j}\bigg|_{\mathbf{q}=\mathbf{0}} \qquad [D_s]_{ij} = \frac{e^2}{V}\frac{\mathrm{d}^2 \Omega}{\mathrm{d}q_i \mathrm{d}q_j}\bigg|_{\mathbf{q}=\mathbf{0}}$$

Peotta, PT, Nat Comm 2015 (the first paper)
PT, Peotta, Bernevig 2022 (easy-to-access review)
Huhtinen, Herzog-Arbeitman, Chew, Bernevig, PT, PRB 2022 (corrections identified)
Peotta, Huhtinen, PT, arxiv:2308.08248 (pedagogical review)

Up-to-date basis-independent formulas

Basis-independent formulas can be derived also based on RPA (Peotta, NJP 2022; Minh, Peotta, arXiv 2023)