Quantum metric and superfluidity

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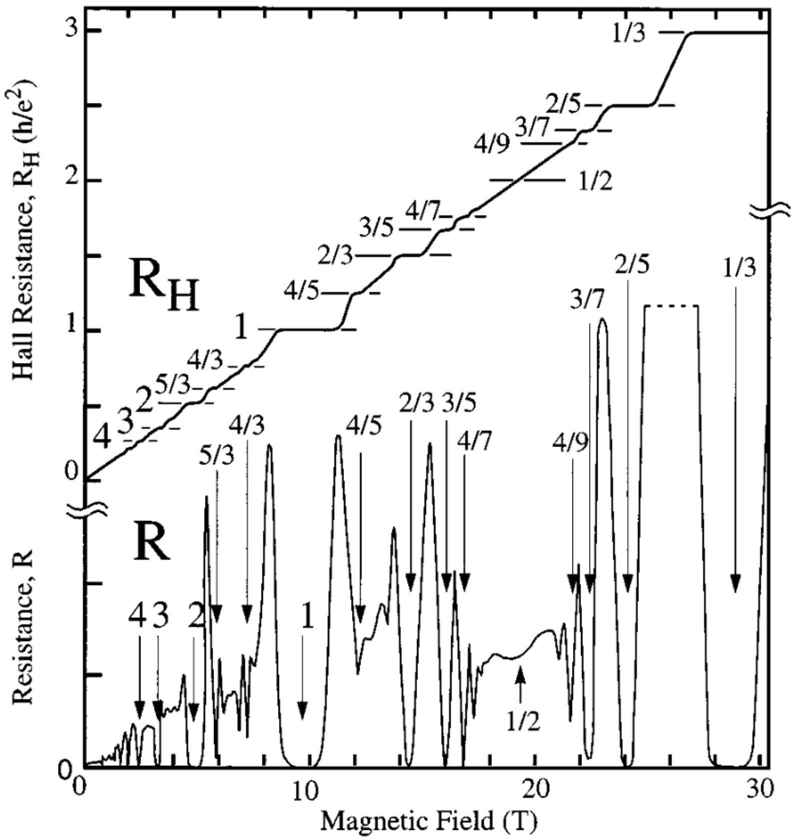
Outline

1) Band structure invariants: quantum metric
2) Flat bands and high-temperature superconductivity
3) The geometric contribution to the superfluid weight
4) Some open questions

Quantum Hall effects

Integer and fractional quantum Hall effects (IQHE and FQHE) in ultrahigh-mobility GaAs/AlGaAs in two dimensional electrons gas

H. L. Stormer, Rev. Mod. Phys. **71**, 875 (1999)



- IQHE: topological band insulator
- FQHE: phase of matter with topological order

A. Bernevig and T. Neupert, arXiv:1506.05805

Band structure invariants

Topological band insulators are characterized by band structure invariants obtained from the wave functions of a noninteracting Hamiltonian

Discrete translational invariance → Bloch plane waves $\Psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} g_{n\mathbf{k}}(\mathbf{r})$

Periodic Bloch functions $g_{n\mathbf{k}}(\mathbf{r}) = g_{n\mathbf{k}}(\mathbf{r}+\mathbf{a}_i)$ $\mathbf{a}_i$ lattice vectors

"Gauge" transformation $g_{n\mathbf{k}}(\mathbf{r}) \to e^{i\phi(\mathbf{k})} g_{n\mathbf{k}}(\mathbf{r})$

Band structure invariants = invariant under gauge transformations

Berry connection

$$\mathbf{A}_n(\mathbf{k}) = i\,\langle g_{n\mathbf{k}} | \boldsymbol{\nabla}_{\mathbf{k}} g_{n\mathbf{k}} \rangle$$

not an invariant $\mathbf{A}_n(\mathbf{k}) \to \mathbf{A}_n(\mathbf{k}) - \boldsymbol{\nabla}_{\mathbf{k}}\phi(\mathbf{k})$

transforms as the EM vector potential

Berry curvature and Chern number

Berry connection
Similar to a vector potential

$$\mathbf{A}_n(\mathbf{k}) = i\,\langle g_{n\mathbf{k}} | \boldsymbol{\nabla}_{\mathbf{k}} g_{n\mathbf{k}} \rangle$$

not an invariant

Berry phase
Similar to a magnetic flux

$$\gamma_n(\mathcal{C}) = \oint_{\mathcal{C}} \mathrm{d}\mathbf{k} \cdot \mathbf{A}_n(\mathbf{k}) = \int_{\mathcal{S}} \mathrm{d}^2\mathbf{k}\,\Omega_n(\mathbf{k})\,, \quad \partial\mathcal{S} = \mathcal{C}$$

Berry curvature
Similar to a magnetic field along the z-axis (2D)

$$\Omega_n(\mathbf{k}) = \hat{z} \cdot \boldsymbol{\nabla}_{\mathbf{k}} \times \mathbf{A}_n(\mathbf{k})$$

Chern number

$$\boxed{C = \frac{1}{2\pi} \int_{\mathrm{B.Z.}} \mathrm{d}^2\mathbf{k}\,\Omega_n(\mathbf{k})}$$

The integral is over the Brillouin zone (B.Z.)

The Chern number C is always an integer!
Topological invariant proportional to the Hall conductance (IQHE)

Kubo-Chern formula $\sigma_{\mathrm{H}} = \dfrac{e^2}{h} C$

D. Thouless, M. Kohmoto, M. Nightingale, and M. den Nijs, PRL **49** 405, (1982)

Quantum geometric tensor

A more comprehensive band structure invariant is the

Quantum Geometric Tensor

J. P. Provost and G. Vallee, Commun. Math. Phys. **76**, 289 (1980)

$$\begin{aligned}\mathcal{B}_{ij}(\mathbf{k}) &= 2\,\langle\partial_{k_i} g_{n\mathbf{k}}|\left(1 - |g_{n\mathbf{k}}\rangle\langle g_{n\mathbf{k}}|\right)|\partial_{k_j} g_{n\mathbf{k}}\rangle \\ &= 2\,\mathrm{Tr}\left[P_n(\mathbf{k})\partial_{k_i}P_n(\mathbf{k})\partial_{k_j}P_n(\mathbf{k})\right] \quad \text{with} \quad P_n(\mathbf{k}) = |g_{n\mathbf{k}}\rangle\langle g_{n\mathbf{k}}|\end{aligned}$$

$$\mathrm{Re}\,\mathcal{B}_{ij}(\mathbf{k}) = \mathrm{Tr}\left[\partial_{k_i}P_n(\mathbf{k})\partial_{k_j}P_n(\mathbf{k})\right] = g_{ij}(\mathbf{k})$$ Quantum metric

$$\mathrm{Im}\,\mathcal{B}_{ij}(\mathbf{k}) = \epsilon_{ij}\Omega_n(\mathbf{k})$$ Berry curvature

Applications of the quantum metric

The quantum metric has found applications in many different contexts:

- Mobility gap in the integer quantum Hall effect (localization length): J. Bellissard, A. van Elst and H. Schulz- Baldes, J. Math. Phys. **35**, 5373 (1994), R. Resta, Eur. Phys. J. B **79**, 121 (2011)
- Localization functional for Wannier functions: N. Marzari et al., Rev. Mod. Phys. **84**, 1419 (2012); Marzari, N., and D. Vanderbilt, Phys. Rev. B **56**, 12847 (1997)
- Superfluidity in flat band systems: SP and P. Törmä, Nat. Comm. **6**, 8944 (2015); P. Törmä, SP and B. A. Bernevig, Nat. Rev. Phys. **4**, 528 (2022)
- Orbital magnetic susceptibility: Y. Gao et al., Phys. Rev. B **91**, 214405 (2015); F. Piéchon et al., Phys. Rev. B **94**, 134423 (2016)
- Current noise: T. Neupert, C. Chamon, and C. Mudry, Phys. Rev. B **87**, 245103 (2013)
- Fractional Chern insulators: R. Roy, Phys. Rev. B **90**, 165139 (2014); T. S. Jackson et al., Nat. Commun. **6**, 8629 (2015); Z. Liu and E. Bergholtz, arXiv:2208.08449
- …….

For an introduction see: Ran Cheng, arXiv:1012.1337

What about disorder?

Disorder is essential to explain the Hall conductance plateaus in the quantum Hall effects

The Kubo-Chern formula can be extended to the disordered case in the framework of noncommutative geometry J. Bellissard, A. van Elst and H. Schulz- Baldes, J. Math. Phys. **35**, 5373 (1994)

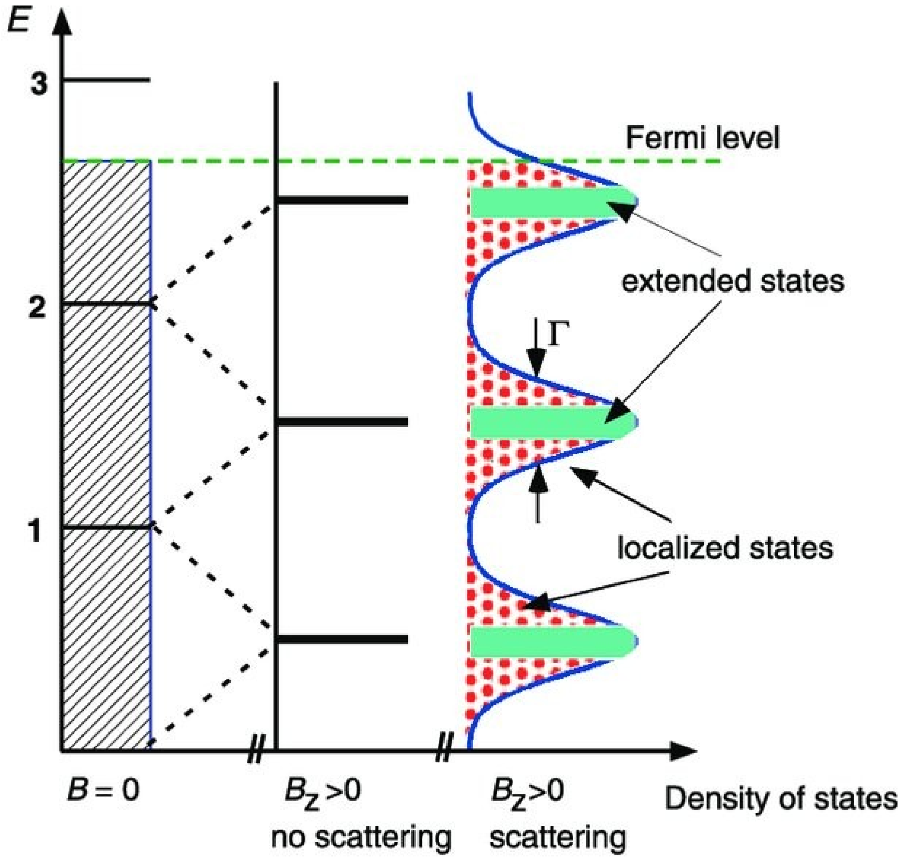
Fourier (Bloch-Floquet-Zak) transform

$P_n(\mathbf{k}) = \vert g_{n\mathbf{k}}\rangle\langle g_{n\mathbf{k}}\vert$	$P = \theta(\mu - H)$
$\boldsymbol{\nabla}_{\mathbf{k}} A(\mathbf{k})$	$-i[\mathbf{r}, A]$
$\int_{\mathrm{B.Z.}} \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \mathrm{Tr}[A(\mathbf{k})]$	$\tau(A) = \lim_{\Lambda\to\infty} \frac{1}{\vert\Lambda\vert} \mathrm{Tr}_\Lambda[A_\Lambda]$
$C = \frac{1}{2\pi i} \int_{\mathrm{B.Z.}} \mathrm{d}^2\mathbf{k}\, \mathrm{Tr}\left[P_n(\mathbf{k})[\partial_{k_1} P_n(\mathbf{k}), \partial_{k_2} P_n(\mathbf{k})]\right]$	$C_{\mathrm{n.c.}} = 2\pi i \tau\big(P\big[[x, P], [y, P]\big]\big)$
$\sum_i \int_{\mathrm{B.Z.}} \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} g_{ii}(\mathbf{k}) = \int_{\mathrm{B.Z.}} \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \mathrm{Tr}\left[\vert\boldsymbol{\nabla}_{\mathbf{k}} P_n(\mathbf{k})\vert^2\right]$	$\boxed{\tau\big(\vert[\mathbf{r}, P]\vert^2\big) = \lim_{\Lambda\to\infty} \frac{1}{\vert\Lambda\vert} \int_\Lambda \mathrm{d}^2\mathbf{r} \int \mathrm{d}^2\mathbf{r}' \,\vert\langle \mathbf{r}\vert P\vert\mathbf{r}'\rangle\vert^2 \vert\mathbf{r} - \mathbf{r}'\vert^2}$

Localization length squared

The noncommutative Chern number $C_{\mathrm{n.c.}}$ is quantized if the localization length is finite (mobility gap)

Density of states and mobility gap

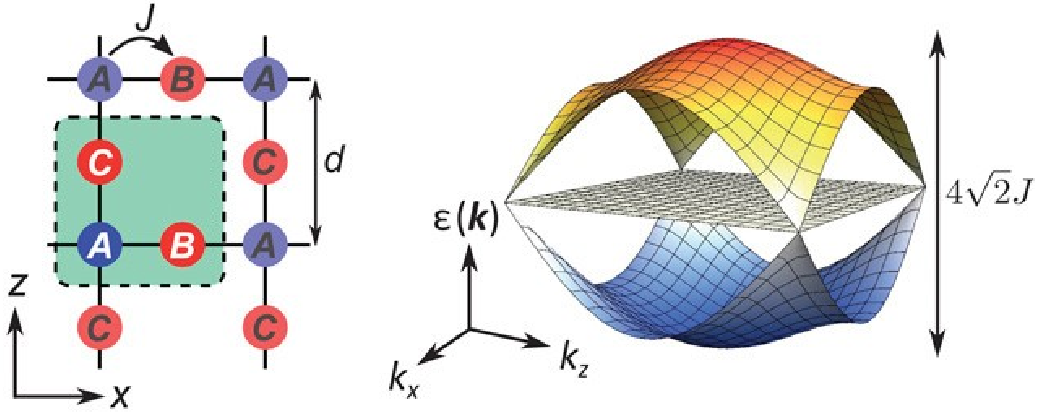


Extended states = diverging localization length

Localized states = finite localization length

Figure from B. Jeckelmann and B. Jeanneret, Rep. Prog. Phys. **64**, 1603 (2001)

2) Flat bands and high-temperature superconductivity

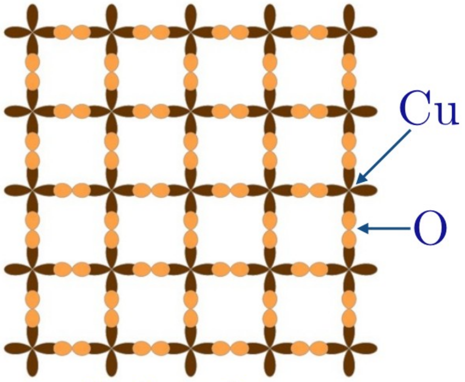


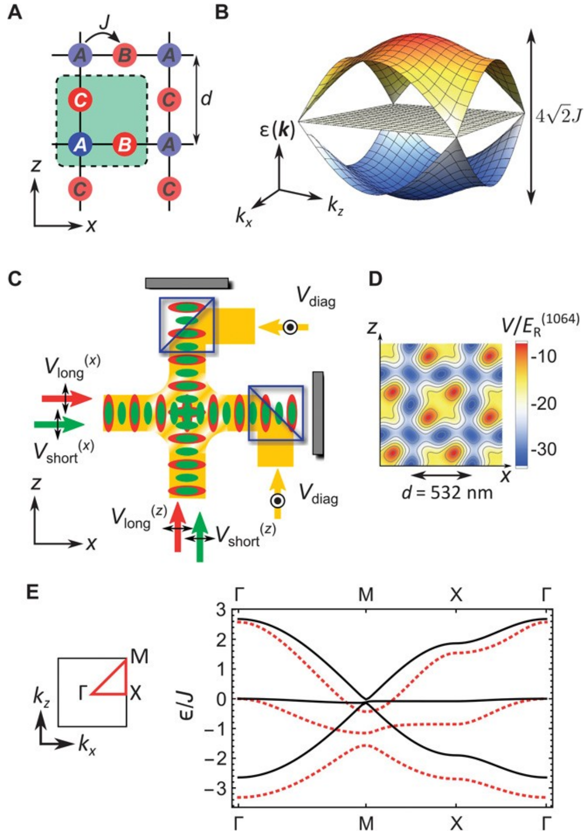
The flat band of the Lieb lattice

Composite lattice with three orbitals per unit cell allows to realize a perfect flat band

The flat band is topologically trivial C=0, but geometrically nontrivial (nonzero quantum metric)

The Lieb lattice is the lattice of the copper-oxide planes of cuprates





S. Taie et al., Science Advances **1**, e1500854 (2015)

H. Ozawa et al., PRL **118**, 175301 (2017)
S. Taie et al., Nat. Comm. **11**, 257 (2020)

Realization of the Harper Hamiltonian in ultracold gases

$$^{87}\mathrm{Rb} \quad |\uparrow\rangle = |F=1, m_F=-1\rangle$$

$$|\downarrow\rangle = |F=2, m_F=1\rangle$$

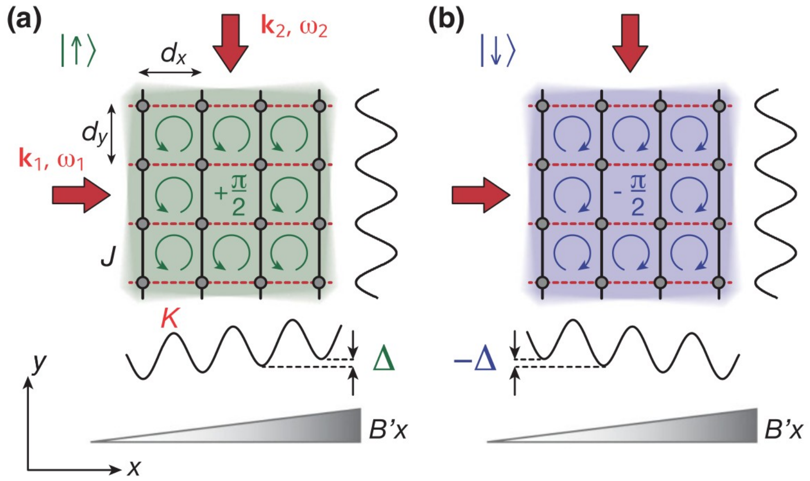
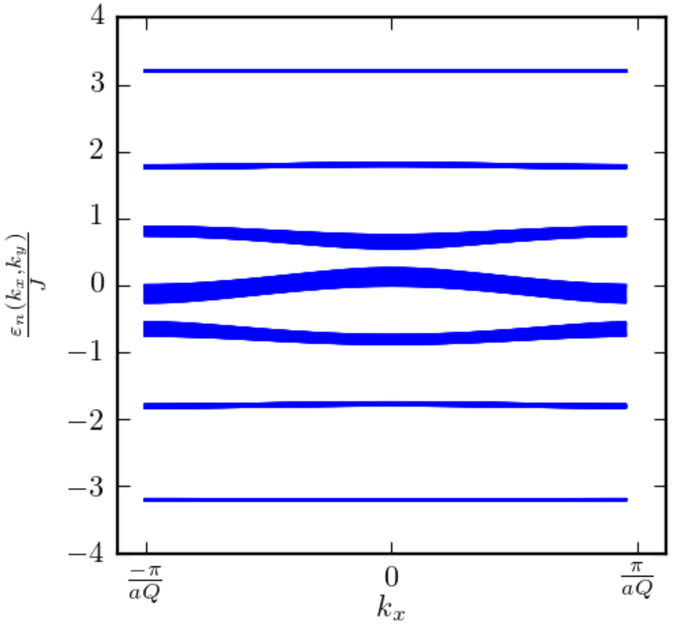


Figure from Ref. 1

[1] Aidelsburger et al., PRL 111, 185301 (2013)
[2] Miyake et al., PRL 111, 185302 (2013)

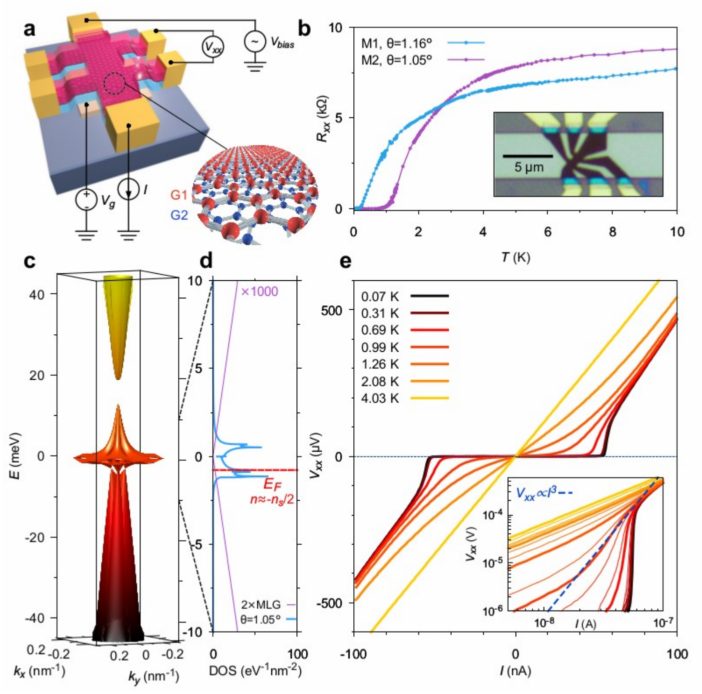
Flux quanta per unit cell $n_\phi = \frac{1}{7}$



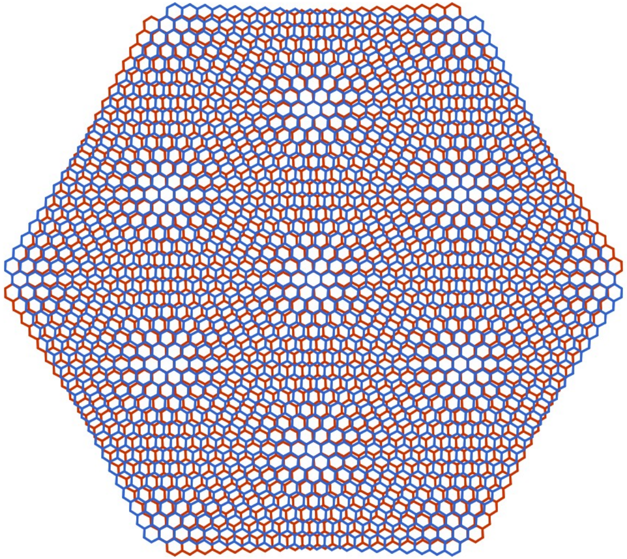
- ✔ Time-reversal symmetry is preserved
- ✔ Lowest bands are quasi-flat (Landau levels)
- ✔ Non-zero (spin) Chern number

Superconductivity in MA-TBG

MA-TBG: Magic **A**ngle**-T**wisted **B**ilayer **G**raphene
Twisiting graphene layers produces quasi-flat bands and (unconventional) superconductivity



From Cao et al., Nature **556**, 43 (2018)



Two graphene layers aligned
with a small twist angle

Flat bands and high-temperature superconductivity

Dispersive band

$$U \ll W \Rightarrow T_\mathrm{c} \propto e^{-\frac{1}{U D(E_\mathrm{F})}}$$

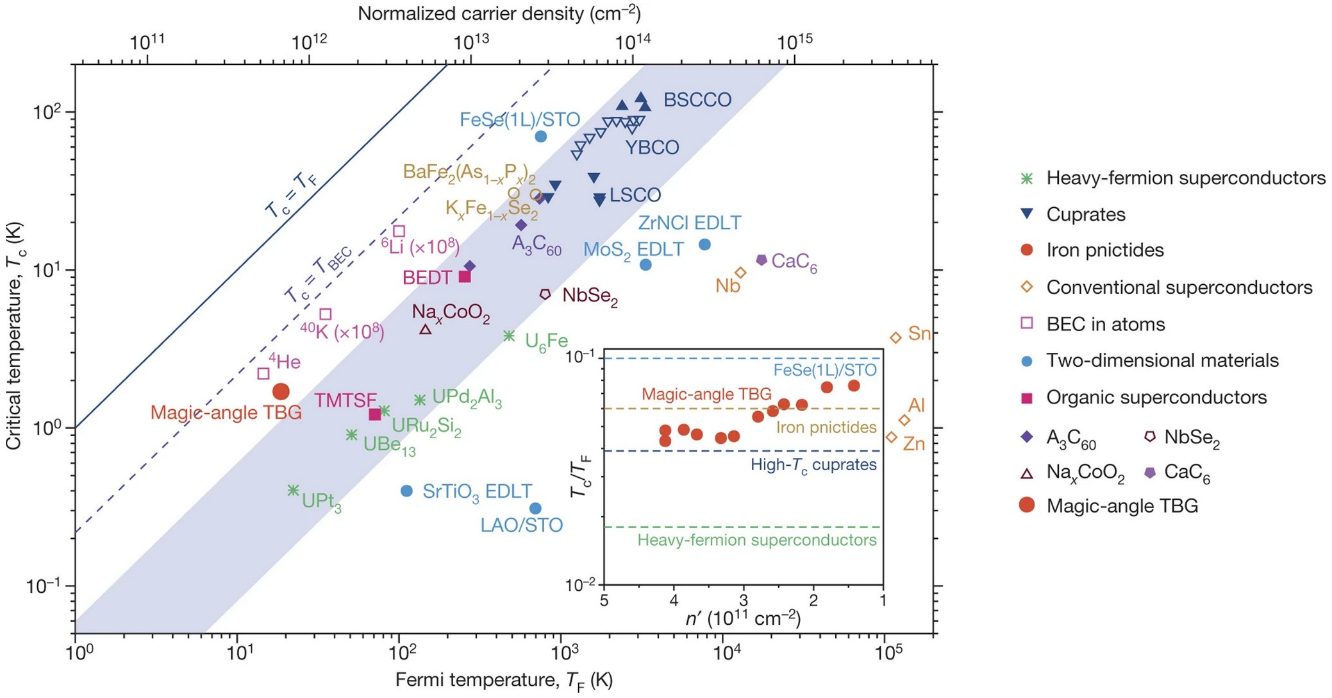
W bandwidth, *U* interaction strength

Flat band

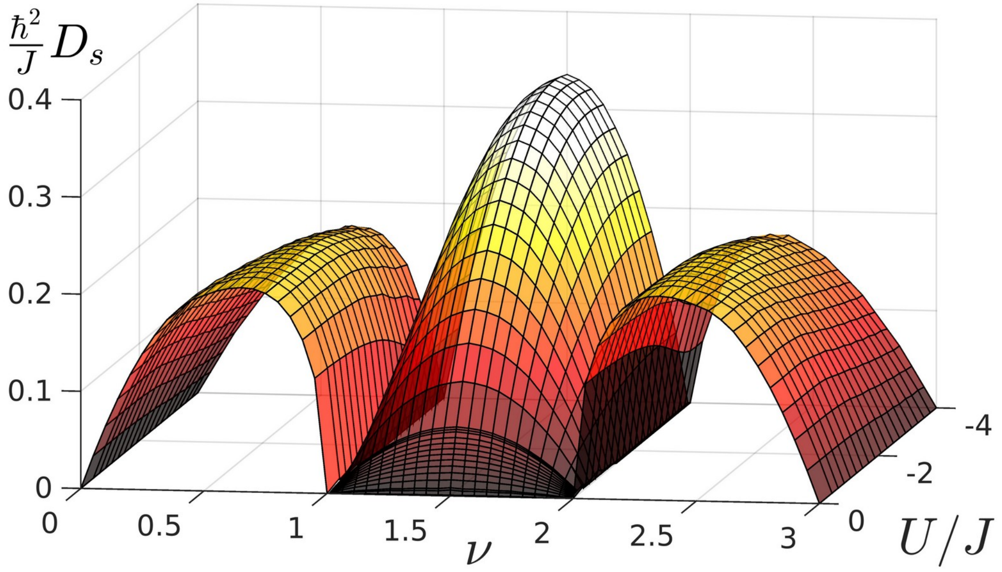
$$U \gg W \Rightarrow T_\mathrm{c} \propto U$$

Kopnin, Heikkilä, Volovik, PRB **83**, 220503(R) (2011)

Critical temperature vs. Fermi temperature in some superconducting materials
Cao et al., Nature **556**, 43 (2018)



3) The geometric contribution to the superfluid weight



In a flat band noninteracting particles are localized (as in an Anderson insulator)

How (superfluid) transport is possible?

Simple answer: two-body problem in a flat band

P. Törmä, L. Liang and SP, PRB **98**, 220511(R) (2018)

P. Törmä, SP and B. A. Bernevig, Nat. Rev. Phys. **4**, 528 (2022)

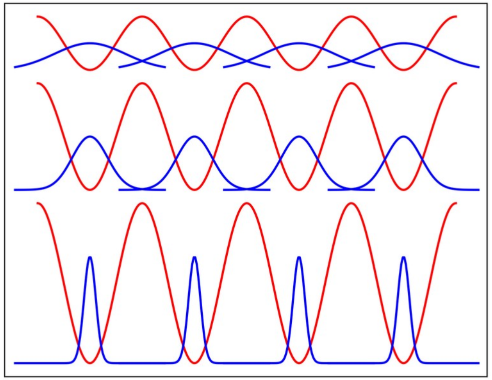
Superfluid density and superfluid weight

Nonzero pairing potential does not guarantee superconductivity

$\Delta \neq 0$

$D_s = 0$

Example of a flat band composed of localized Wannier functions



Definition of superfluid density and superfluid weight

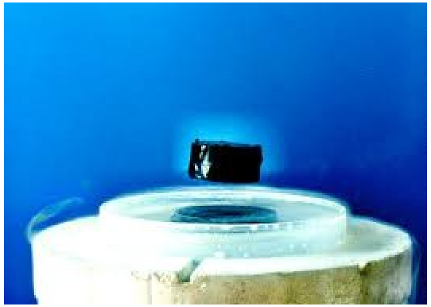
$$\frac{\Delta F}{V} = \frac{1}{2}\rho_s v_s^2 = \frac{1}{8} D_s p_s^2$$

$v_s = \dfrac{\hbar \mathbf{q}}{m}$ Cooper pair velocity

$p_s = 2\hbar \mathbf{q}$ Cooper pair momentum

$\mathbf{J} = \dfrac{1}{4} D_s \hbar \mathbf{q}$ Supercurrent density

$$\left.\begin{array}{r} \Delta \neq 0 \\ D_s \neq 0 \end{array}\right\} \Rightarrow$$



$D_s \propto \lambda_{\mathrm{L}}^{-2}$ Magnetic (or London) penetration depth

Superfluid weight: conventional and geometric

Superfluid weight from free energy $$\frac{\Delta F}{V} = \frac{1}{2}\rho_s v_s^2 = \frac{1}{8} D_s (\hbar \mathbf{q})^2$$

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

Conventional contribution
present in the single band case

Proportional to the effective mass tensor

$$\left(\frac{1}{m_{\mathrm{eff}}}\right)_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon_{n\mathbf{k}}}{\partial k_i \partial k_j}$$

Geometric contribution
present only in the multiband/multiorbital case

Depends essentially on the wavefunctions

For periodic systems, the **Bloch function** and their derivatives $|g_{n\mathbf{k}}\rangle \,, \quad |\boldsymbol{\nabla}_{\mathbf{k}} g_{n\mathbf{k}}\rangle$

See also K. Moon et al., PRB **51**, 5138 (1995)

SP and P. Törmä, Nature Communications **6**, 8944 (2015)
P. Törmä, SP and B. A. Bernevig, Nat. Rev. Phys. **4**, 528 (2022)

Superfluid weight in a flat band

SP and P. Törmä, Nature Communications **6**, 8944 (2015)

Isolated flat-band approximation

bandwidth $W \ll U \ll E_g$ band gap

flat band isolated band

$$\boxed{D_{\mathrm{s},jl} = \frac{4e^2\Delta\sqrt{\nu(1-\nu)}}{\hbar^2}\int_{\mathrm{B.Z.}}\frac{\mathrm{d}^d\mathbf{k}}{(2\pi)^d}\,g_{jl}(\mathbf{k})}$$

Quantum metric of the flat band

Only the geometric contribution survives in the flat band limit

Superfluid weight and Chern number

Superfluid weight in the isolated flat band limit

$$D_{\mathrm{s},jl} = \frac{4e^2\Delta\sqrt{\nu(1-\nu)}}{\hbar^2}\int_{\mathrm{B.Z.}}\frac{\mathrm{d}^d\mathbf{k}}{(2\pi)^d}g_{jl}(\mathbf{k})$$

In two dimensions

$$\mathcal{M}_{jl} = \frac{1}{2\pi}\int_{\mathrm{B.Z.}}\mathrm{d}^2\mathbf{k}\,\mathcal{B}_{jl}(\mathbf{k})$$

Complex positive semidefinite matrix

$$\mathrm{Re}\,\mathcal{M}_{jl} = \frac{1}{2\pi}\int_{\mathrm{B.Z.}}\mathrm{d}^2\mathbf{k}\,g_{jl}(\mathbf{k})$$

$$\mathrm{Im}\,\mathcal{M}_{jl} = \epsilon_{jl}C$$

$$\mathcal{M}\geq 0 \Rightarrow \frac{1}{2}\,\mathrm{Tr}\,\mathrm{Re}\,\mathcal{M} \geq \sqrt{\det\mathrm{Re}\,\mathcal{M}} \geq |C|$$

Chern number

We have shown that:

1) Superfluidity in a flat band has a geometric origin (quantum metric)

2) The flat band superfluid weight is bounded from below by the Chern number

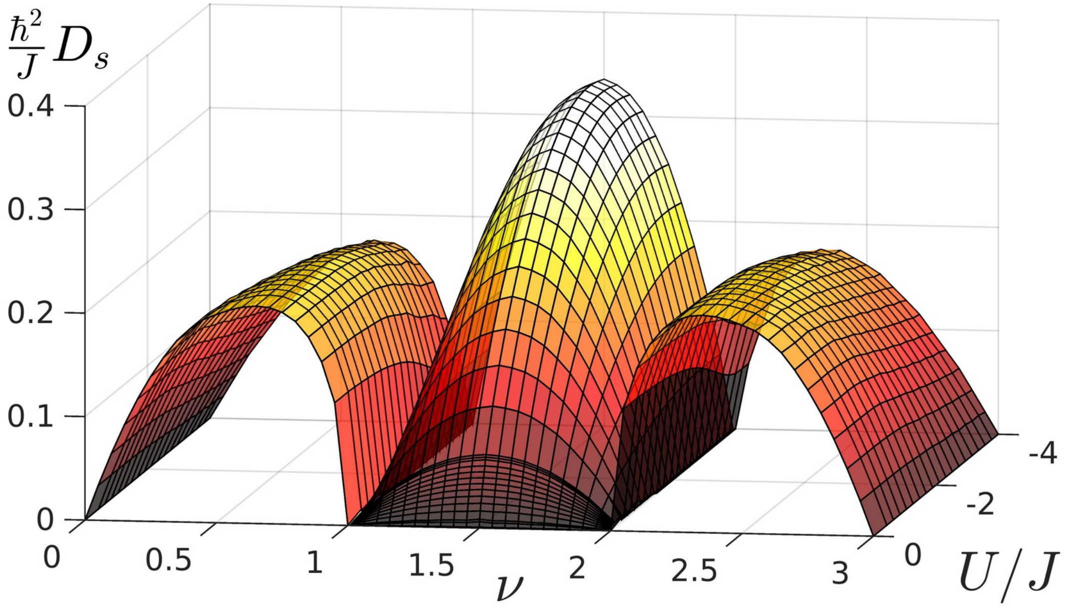
SP, P. Törmä, Nature Communications **6**, 8944 (2015)

Lieb lattice: superfluid weight

A. Julku, SP, T. Vanhala, D.-H. Kim, P. Törmä, Phys. Rev. Lett. **117**, 045303 (2016)

The superfluid of the flat band:
- depends strongly on *U*
- is nonzero and large even if *C=0*

For the dispersive bands it depends weakly on *U*



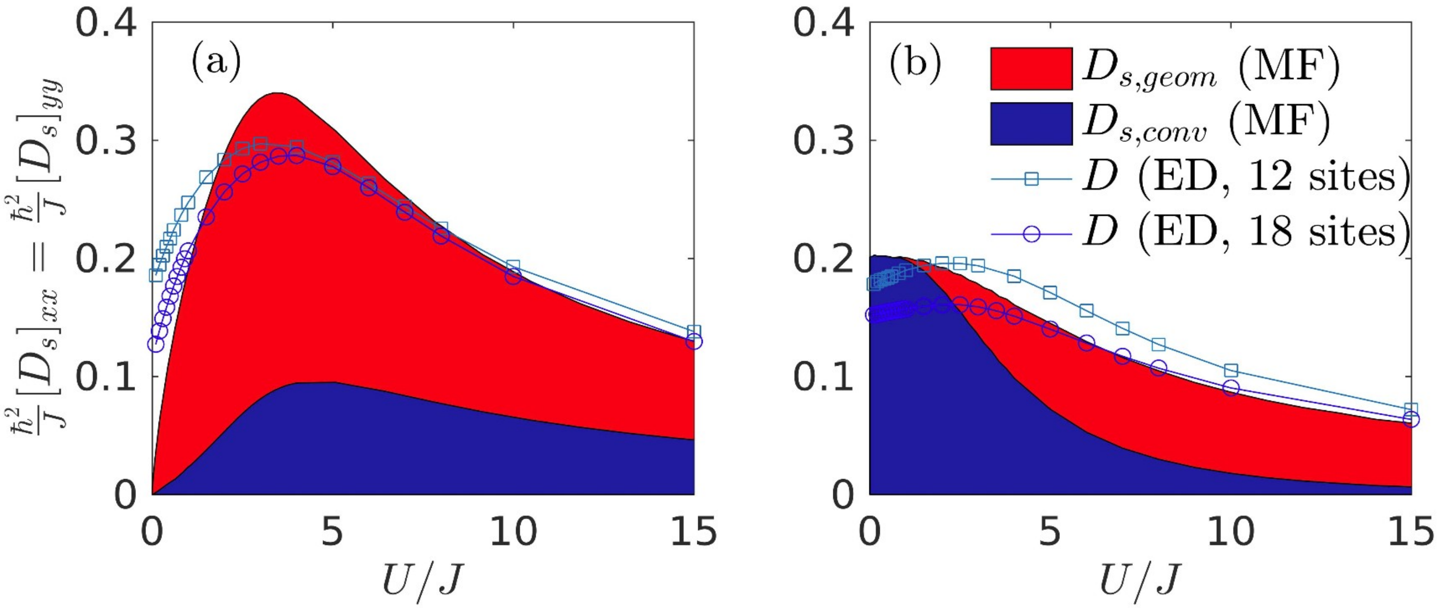
Zero temperature
ν is the filling (1<ν<2 for the flat band)

Lieb lattice: superfluid weight geometric contribution

The large superfluid weight and its strong dependence on *U* within the flat band is explained by the geometric superfluid weight contribution

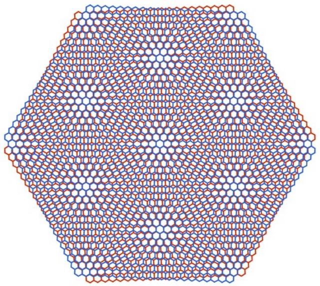
Half-filled flat band (ν = 1.5)

Half-filled upper band (ν = 2.5)

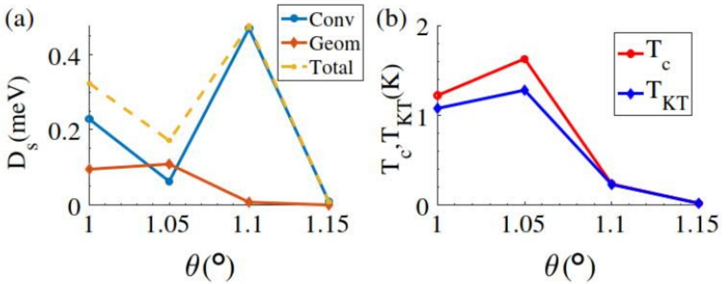


A. Julku, SP, T. Vanhala, D.-H. Kim, P. Törmä, Phys. Rev. Lett. **117**, 045303 (2016)

The geometric contribution in twisted bilayer graphene



MA-TBG: Magic **A**ngle-**T**wisted **B**ilayer **G**raphene
Twisiting graphene layers produces quasi-flat bands and (unconventional) superconductivity



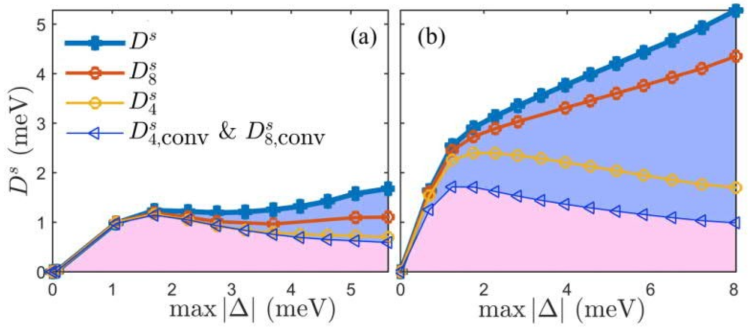
It has been shown that the geometric contribution is important in MA-TBG

1) A. Julku, T. Peltonen, L. Liang, T. Heikkilä, P. Törmä, Phys. Rev. B **101**, 060505 (2020)

2) X. Hu, T. Hyart, D. I. Pikulin, E. Rossi, Phys. Rev. Lett. **123**, 237002 (2019)

3)F. Xie, Z. Song, B. Lian, and B. A. Bernevig, Phys. Rev. Lett. **124**, 167002 (2020)

See also recent reviews: E. Rossi, Current Opinion in Solid State and Materials Science **25**, 100952 (2021); P. Törmä, SP and B. A. Bernevig, Nat. Rev. Phys. **4**, 528 (2022)



From Refs. 1 and 2

Perturbative approach: Schrieffer-Wolff transformation

M. Tovmasyan, SP, P. Törmä, S. Huber, Phys. Rev. B **94**, 245149 (2016)

$$\hat{\mathcal{H}}_{\mathrm{SW}} \approx \hat{\mathcal{H}}_{\mathrm{kin}}\hat{\mathcal{P}} + \hat{\mathcal{P}}\hat{\mathcal{H}}_{\mathrm{int}}\hat{\mathcal{P}} + \hat{\mathcal{H}}^{(2)}_{\mathrm{SW}} + \ldots$$

$\hat{\mathcal{P}}$ Projector on the flat band subspace

BCS wave function is an exact ground state of the projected interaction Hamiltonian

Pair creation operator $\hat{b}_0^\dagger = \sum_{\mathbf{j}} \hat{\mathrm{T}}^+_{\mathbf{j}} = \sum_{\mathbf{j}} \hat{d}^\dagger_{\mathbf{j}\uparrow}\hat{d}^\dagger_{\mathbf{j}\downarrow} = \sum_{\mathbf{k}} \hat{f}^\dagger_{\mathbf{k}\uparrow}\hat{f}^\dagger_{-\mathbf{k}\downarrow}$

Wannier w.f. Bloch w.f.

BCS wave function

$$|\Omega\rangle = u^{N_{\mathrm{c}}} \exp\left(\frac{v}{u}\hat{b}_0^\dagger\right)|\emptyset\rangle = \prod_{\mathbf{j}}\left(u + v\hat{d}^\dagger_{\mathbf{j}\uparrow}\hat{d}^\dagger_{\mathbf{j}\downarrow}\right)|\emptyset\rangle = \prod_{\mathbf{k}}\left(u + v\hat{f}^\dagger_{\mathbf{k}\uparrow}\hat{f}^\dagger_{-\mathbf{k}\downarrow}\right)|\emptyset\rangle$$

Effective spin Hamiltonian

M. Tovmasyan, SP, P. Törmä, S. Huber, Phys. Rev. B **94**, 245149 (2016)

Pseudospin operators: create/annihilate a Cooper pair in a Wannier function

$$\hat{\mathrm{T}}^z_{\mathbf{i}} = \frac{1}{2}(\hat{d}^\dagger_{\mathbf{i}\uparrow}\hat{d}_{\mathbf{i}\uparrow} + \hat{d}^\dagger_{\mathbf{i}\downarrow}\hat{d}_{\mathbf{i}\downarrow} - 1), \quad \hat{\mathrm{T}}^+_{\mathbf{i}} = \left(\hat{\mathrm{T}}^-_{\mathbf{i}}\right)^\dagger = \hat{d}^\dagger_{\mathbf{i}\uparrow}\hat{d}^\dagger_{\mathbf{i}\downarrow}$$

The projected Hamiltonian becomes approximately a ferromagnetic spin Hamiltonian

$$\hat{\mathcal{H}}_{\mathrm{spin}} = -U\sum_{\mathbf{i}\neq\mathbf{j}} J(|\mathbf{i}-\mathbf{j}|)\,\hat{\mathbf{T}}_{\mathbf{i}}\cdot\hat{\mathbf{T}}_{\mathbf{j}}$$

Exchange coupling: overlap of the flat band Wannier functions

$$J(|\mathbf{i}-\mathbf{j}|) = \sum_{\mathbf{m}\alpha} |W_\alpha(\mathbf{m}-\mathbf{i})|^2\,|W_\alpha(\mathbf{m}-\mathbf{j})|^2$$

4) Some open questions

- The BCS wave function is an exact ground states in the flat band limit. Is it unique? Is the relation between superfluid weight and quantum metric exact as well? How about excited states?

- Inequalities between quantum metric and topological invariants are known in few cases (Chern number, 1D winding number, Euler class). Can we find similar inequalities for other topological invariants?

- How about disorder? A. Lau, SP, D. I. Pikulin, E. Rossi, and T. Hyart, arXiv:2203.01058, to appear in Scipost