Quantum Geometry

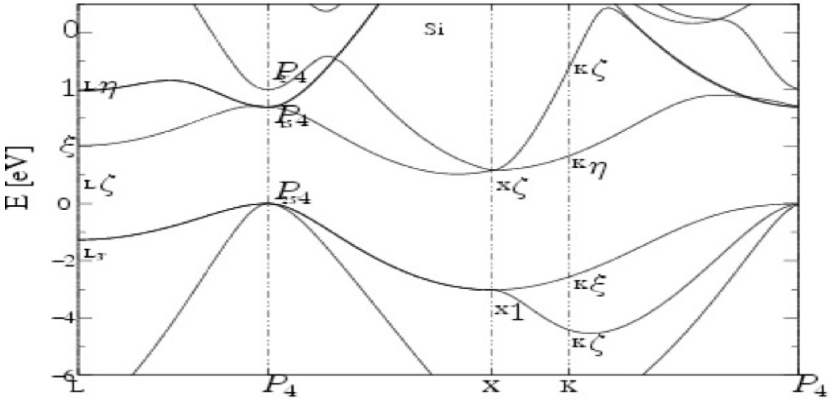
1. What
2. When
3. Where

Quantum Geometry and the Opinion of Referee A

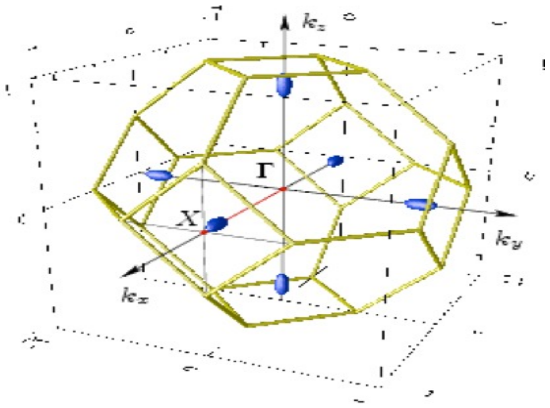
Note also that the geometric part …. cannot be observed experimentally, and thus predictions of this quantity are irrelevant.

The topological perspective of EPC put forward by the authors does not lead to any new verifiable predictions and it remains a mathematical exercise of rewriting existing equations…. Therefore the manuscript should not be published in any form.

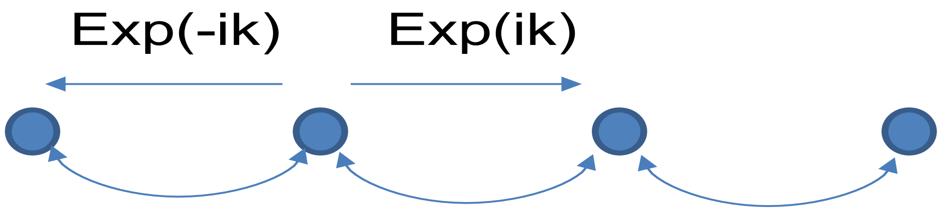
Non-Interacting Electrons In Periodic Structures Form Bands And ”Disperse”: Concept of Bloch State

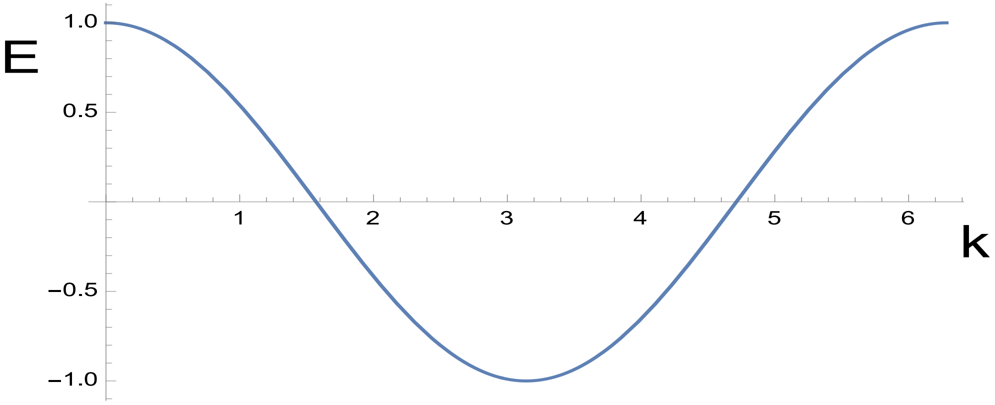


(a) Band diagram of silicon.



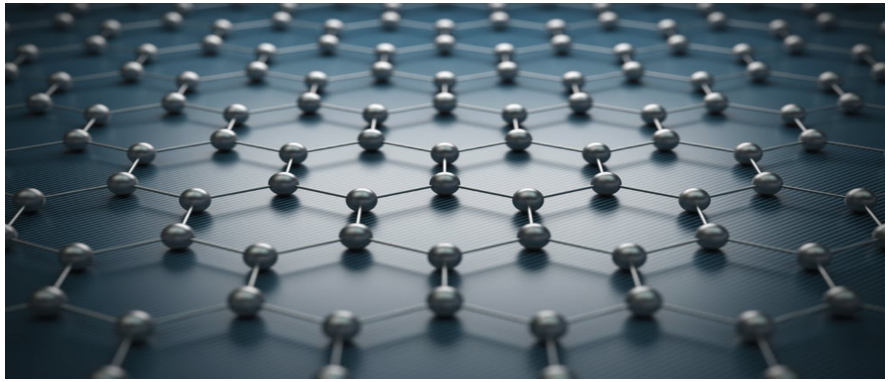
(b) First conduction band valleys.

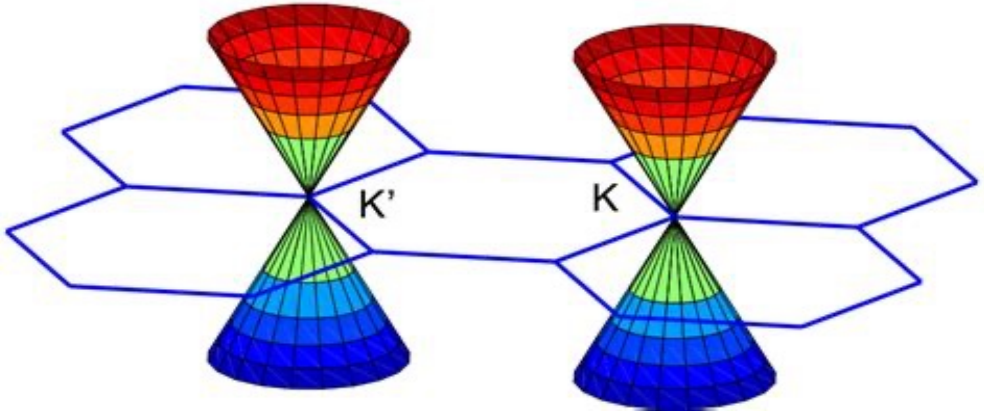


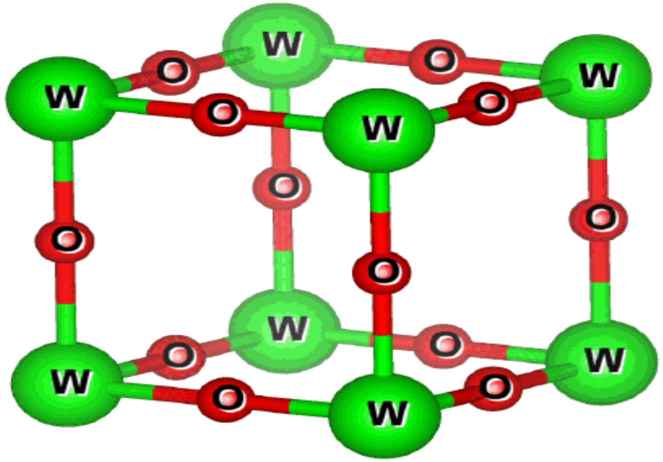


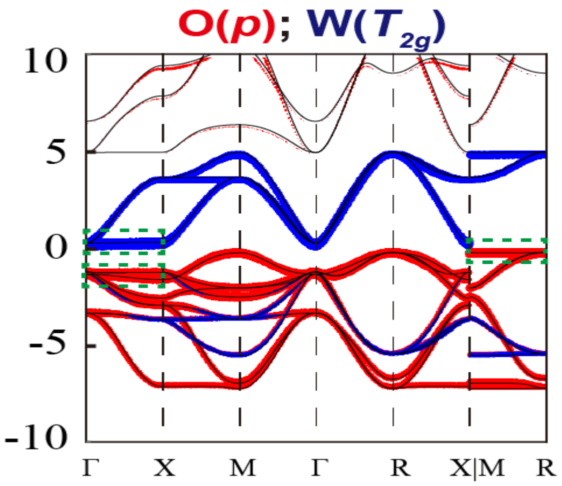
Adding interactions becomes exponetially hard (without a “smart/lucky/good” basis chance - quasiparticles)

Band Dispersions Depend on the Underlying Lattice and Orbitals





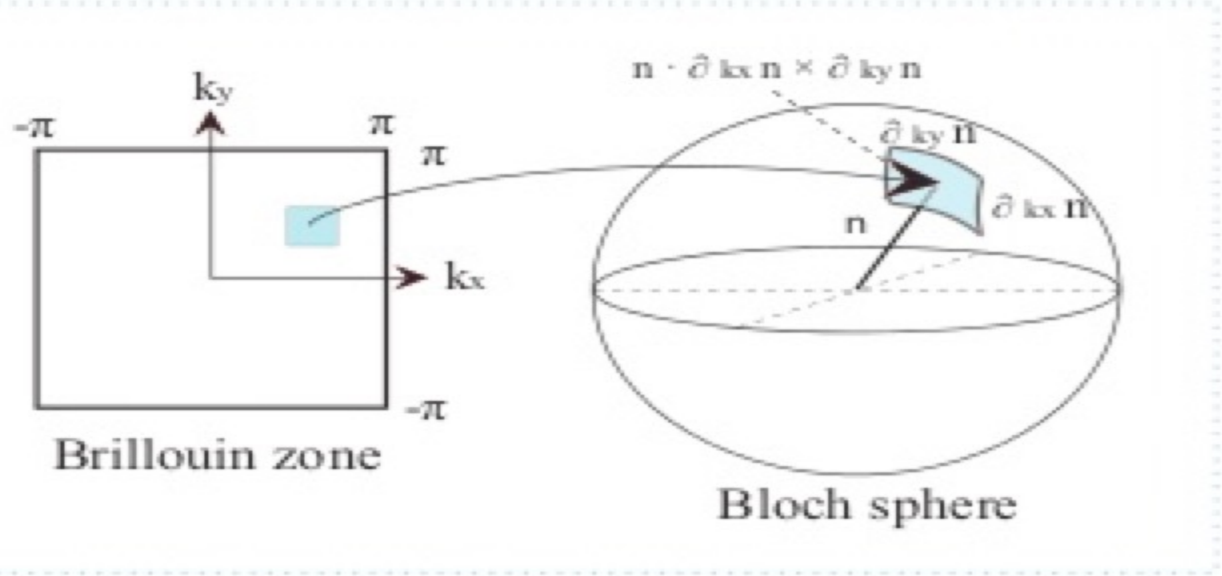




Schrodinger Eq for Electrons in a band: Energy $E(\vec{k})$ **; Wavefunction** $\psi(\vec{k})$

How Topology Meets Materials Classifies Maps Into Integer Classes

$$\boxed{\psi(\vec{k}) : T^2 \to S^2}$$



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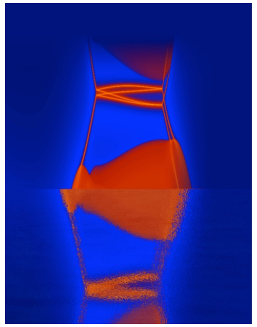
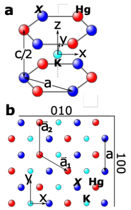
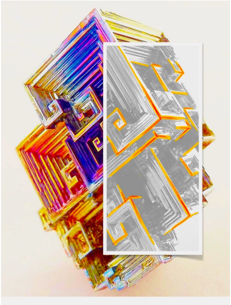
1

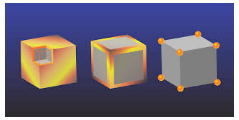
Integers cannot change adiabatically

Exotic Surface and Hinge States



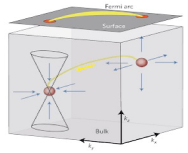


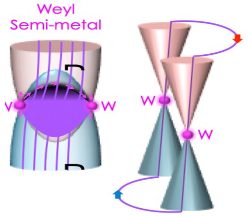


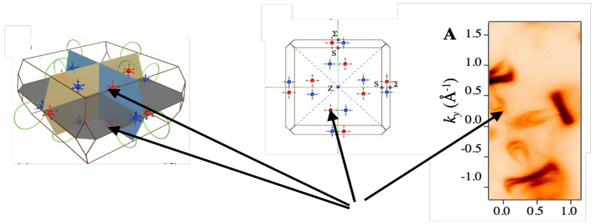


Weyl Semimetals And Fermi Arcs

Conyers Herrings







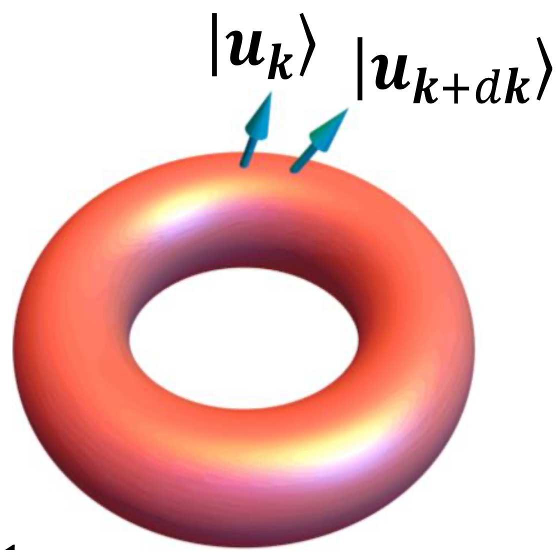
$$A_j = iU^\dagger(\mathbf{k})\partial_j U(\mathbf{k})$$

$$\mathcal{F}_{ij} = \partial_{k_i} A_j - \partial_{k_j} A_i - i[A_i, A_j]$$

+ Symmetries Gives Myriad of Topology

Nontrivial F is usually defined/tantamount to absence of localized Wannier Orbitals

A, F Are Not The Only Quantity(ies) that Characterize bands



$$d^2(\mathbf{k}, \mathbf{k}+d\mathbf{k}) = \frac{1}{2}\mathrm{Tr}\left(\tilde{u}_{\mathbf{k}}\tilde{u}_{\mathbf{k}}^{\dagger} - \tilde{u}_{\mathbf{k}+d\mathbf{k}}\tilde{u}_{\mathbf{k}+d\mathbf{k}}^{\dagger}\right)^2$$

$$d^2(\mathbf{k}, \mathbf{k} + d\mathbf{k}) = g_{ij}(\mathbf{k}) dk_i dk_j$$

The New Form Is Symmetric (in i, j)

$$g_{ij}(\mathbf{k}) = \frac{1}{2}\left(\partial_{k_i} u^\dagger(\mathbf{k})\partial_{k_j} u(\mathbf{k}) + \partial_{k_j} u^\dagger(\mathbf{k})\partial_{k_i} u(\mathbf{k})\right)$$
$$+ u^\dagger(\mathbf{k})\partial_{k_i} u(\mathbf{k}) u^\dagger(\mathbf{k})\partial_{k_j} u(\mathbf{k}) \,,$$

$$= \mathrm{Tr}\ \partial_i P(\mathbf{k})\partial_j P(\mathbf{k}) \qquad\qquad P(\mathbf{k}) = U(\mathbf{k})U^\dagger(\mathbf{k})$$

Its trace over the bands is called the Fubini-Study Metric

Resta, Brouder, Vanderbilt

The Fubini Study metric and the Berry Curvature Together can be placed as the real and imaginary part of a single tensor, the Quantum Geometric Tensor

$$\mathfrak{G}_{ij} = \mathfrak{g}_{ij} - \frac{i}{2}\mathcal{F}_{ij}$$

$$\mathrm{Re}[\mathfrak{G}_{ij}] = \mathfrak{g}_{ij} \qquad \mathrm{Im}\,\mathfrak{G}_{ij} = -\tfrac{1}{2}\mathcal{F}_{ij}$$

$$\boxed{\mathfrak{G}_{ij} = \partial_i U^\dagger(\mathbf{k})(1 - P(\mathbf{k}))\partial_j U(\mathbf{k})}$$

To higher order, entering in nonlinear effects, other cumulants exists, having their own bounds.

Pioneering work on both theory and applications by Grushin, de Juan, Moore, Orenstein, Vanderbilt, Pesin, Morimoto, Guinea, others.

Still very new, much to be discovered

Early Bounds/Relations Between Quantum Geometry and Physical Quantities

Wannier function localization functional

$$F = \sum_n \left[\langle 0n|\hat{\mathbf{r}}^2|0n\rangle - |\langle 0n|\hat{\mathbf{r}}|0n\rangle|^2 \right] \geq \frac{\Omega_c}{(2\pi)^2} \int d^2k \, \mathrm{tr}\, g(\mathbf{k})$$

Clearer quantum geometry and topology have connections.
Topological states do not admit localized Wannier descriptions

$$H = \frac{-\hbar^2}{2M_e} \frac{\partial^2}{\partial x^2} + V(x)$$

$$[l_\alpha]^2 = \frac{1}{N} \sum_R \langle R\alpha | (\hat{r} - R)^2 | R\alpha \rangle \leq \frac{\hbar^2}{2M_e E_g}$$

(Vanderbilt, Resta, Kivelson, Souza and others)

Quantum geometry and Localization

- Real space structure of a Bloch band = quantum geometric tensor

$$\mathcal{G}_{ij}(\mathbf{k}) = \langle \mathbf{k}|r_i r_j|\mathbf{k}\rangle - \langle \mathbf{k}|r_i|\mathbf{k}\rangle \langle \mathbf{k}|r_j|\mathbf{k}\rangle = \underline{g_{ij}(\mathbf{k})} + \frac{i}{2}\epsilon_{ij}\underline{f(\mathbf{k})}$$

- Semi-classically, $g_{ii}(\mathbf{k})$ is the wavepacket size, $f(\mathbf{k})$ is its angular momentum

- Interacting flat bands known to be sensitive to band geometry:

Neupert, Sheng, Chamon, Regnault, BAB, Haldane, Hughes, Vishwanath, Todadri, Parker, Fu, Roy

$f(\mathbf{k}) \longrightarrow$ Fractional Quantum Hall, Fractional Chern Insulator

$g(\mathbf{k}) \longrightarrow$ Flat band superconductor, itinerant ferromagnetism

Peotta, Törmä, Song, Lieb, Tasaki, Volovik

Quantum Geometry beyond Berry curvature

Atomic limit

$f(\mathbf{k}) = g(\mathbf{k}) = 0$

B-field

Band inversion

$g(\mathbf{k}) = f(\mathbf{k}) = \frac{C}{2\pi}$

(topology, obstructed bands)

$f(\mathbf{k}) \to \frac{m}{2|m|}\delta(\mathbf{k})$

$g(\mathbf{k}) \to 1/2\mathbf{k}^2$

Lowest Landau level

Chiral TBG/
"Vortexable"

bipartite lattice
flat bands

Strained TBG

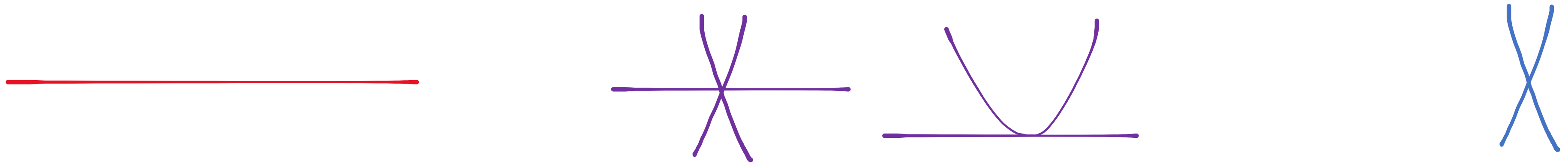
Massive 2D Dirac
$m \to 0$

Gapped, uniform geometry

Lieb lattice, Kagome

Gapless, divergent geometry

$E(\mathbf{k})$

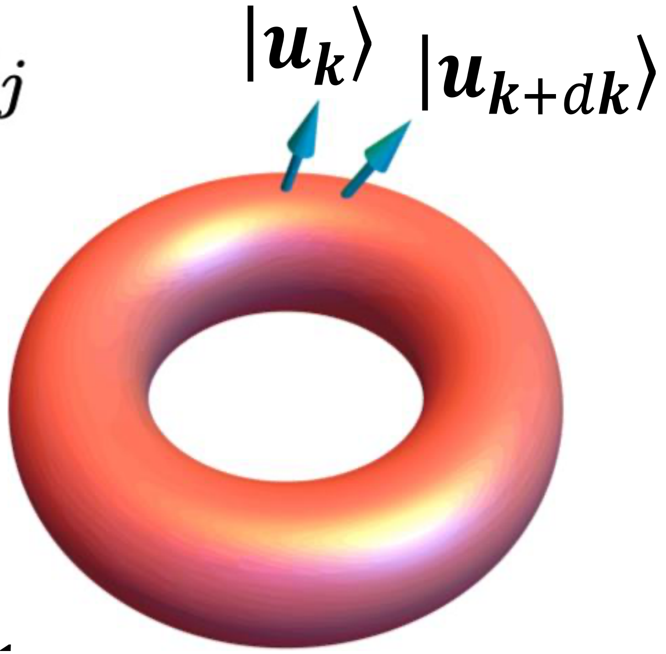


Metric Tensor and Fubini-Study Metric Are Bounded By Topology

But not only!!!

$$\boxed{d^2(\mathbf{k},\mathbf{k}+d\mathbf{k}) = \frac{1}{2}\mathrm{Tr}\left(\tilde{u}_{\mathbf{k}}\tilde{u}^{\dagger}_{\mathbf{k}} - \tilde{u}_{\mathbf{k}+d\mathbf{k}}\tilde{u}^{\dagger}_{\mathbf{k}+d\mathbf{k}}\right)^2}$$

$$d^2(\mathbf{k},\mathbf{k}+d\mathbf{k}) = g_{ij}(\mathbf{k})dk_i dk_j$$



$$\mathrm{Tr}\ \partial_i P(\mathbf{k})\partial_j P(\mathbf{k})$$

Topology

$$\mathfrak{G}_{ij} = \mathfrak{g}_{ij} - \frac{i}{2}\mathcal{F}_{ij} > 0$$

Quantum metric is bounded from below by topology

$$\sum_{ij} c_i^\dagger \mathfrak{G}_{ij} c_j \geq 0$$

$$c_x = 1 \text{ and } c_y = i \qquad \operatorname{tr} g = g_{xx} + g_{yy} \geq -\mathcal{F}_{xy}$$

$$c_x = 1 \text{ and } c_y = -i \qquad \operatorname{tr} g \geq \mathcal{F}_{xy}$$

$$\operatorname{tr} g \geq |\mathcal{F}_{xy}|$$

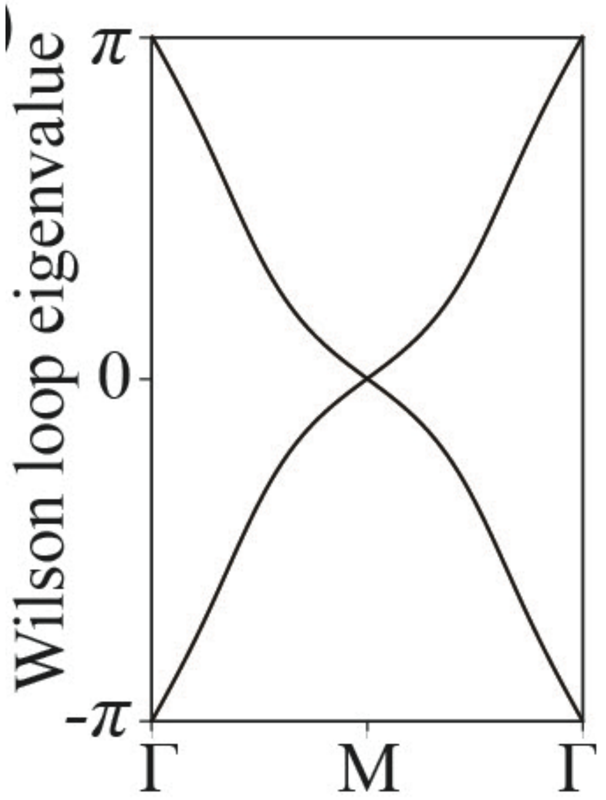
(Torma, Peotta, Heikkila, others before)

New Bounds: Euler Class, Twisted Bilayer Graphene; 2 Bands Per Valley Per Spin

Jarillo-Hererro, Andrei, Efetov, Young, Dean, Tutuc, Yazdani, Kim, Yacoby….

$$\mathcal{F}_{xy} = \partial_{k_x} A_y(\mathbf{k}) - \partial_{k_y} A_x(\mathbf{k}) - i[A_x(\mathbf{k}), A_y(\mathbf{k})] = \begin{pmatrix} 0 & i f_{xy} e^{\frac{i}{2}(\theta_{1\mathbf{k}} - \theta_{2\mathbf{k}})} \\ -i f_{xy} e^{\frac{i}{2}(\theta_{2\mathbf{k}} - \theta_{1\mathbf{k}})} & 0 \end{pmatrix}$$

$$\mathbf{A}(\mathbf{k}) = \begin{pmatrix} \frac{1}{2}\partial_{\mathbf{k}}\theta_{1\mathbf{k}} & i\mathbf{a}(\mathbf{k}) e^{\frac{i}{2}(\theta_{1\mathbf{k}} - \theta_{2\mathbf{k}})} \\ -i\mathbf{a}(\mathbf{k}) e^{\frac{i}{2}(\theta_{2\mathbf{k}} - \theta_{1\mathbf{k}})} & \frac{1}{2}\partial_{\mathbf{k}}\theta_{2\mathbf{k}} \end{pmatrix}$$



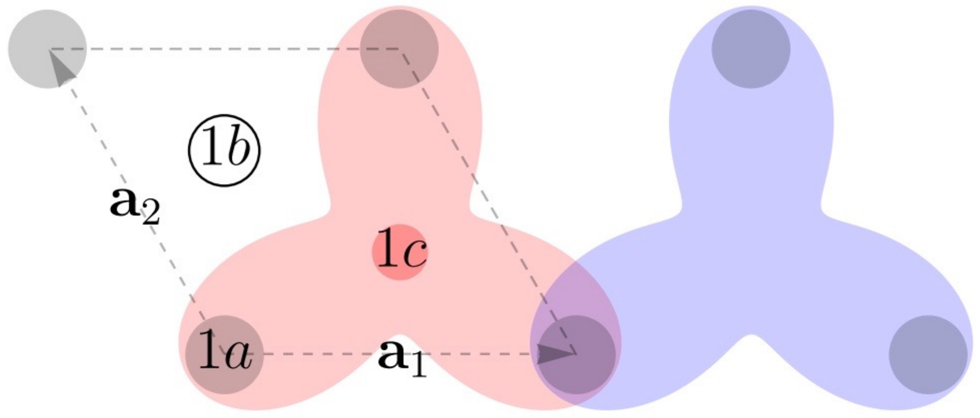
$$e_2 = \frac{1}{2\pi} \int_{\mathrm{BZ}'} d^2k\, f_{xy}$$

$$\frac{1}{4\pi} \int_{\mathrm{BZ}} d^2k\, \mathrm{tr}\, g(\mathbf{k}) \geq \frac{1}{2\pi} \int_{\mathrm{BZ}'} d^2k\, |f_{xy}| \geq \left| \frac{1}{2\pi} \int_{\mathrm{BZ}'} d^2k\, f_{xy} \right| = |e_2|$$

(Xie, Song, BAB, Bohm-Jung Yang, Ahn, Rossi, Pikulin, Torma, Peotta)

Quantum Metric Can Have Nontrivial Bounds Even In Absence of Topology (Obstructed Atomic Insulators)

If wannier center has moved away from the atoms, nontrivial quantum metric



Comes from the impossibility of fully localizing the orbital on-site; even though localized

Bounded from below by the Real Space Indicators and other quantities

These indicate the Wannier center position.

$$\delta_1 = m(^1E) - m(A), \quad \delta_2 = m(^2E) - m(A)$$

$$(\delta_{1c,1}, \delta_{1c,2}) \ = \ (-1,-1)$$

$$G = \frac{1}{2}\int \frac{d^2k}{(2\pi)^2} \mathrm{Tr}\, \nabla P \cdot \nabla P \ \geq \ \frac{a^2}{9\Omega_c}(\delta_{1c,1}^2 - \delta_{1c,1}\delta_{1c,2} + \delta_{1c,2}^2) \ .$$

Herzog-Arbeitman, Song, Peri, BAB, Torma, Hukkinen, Hughes, Refael, Huber others

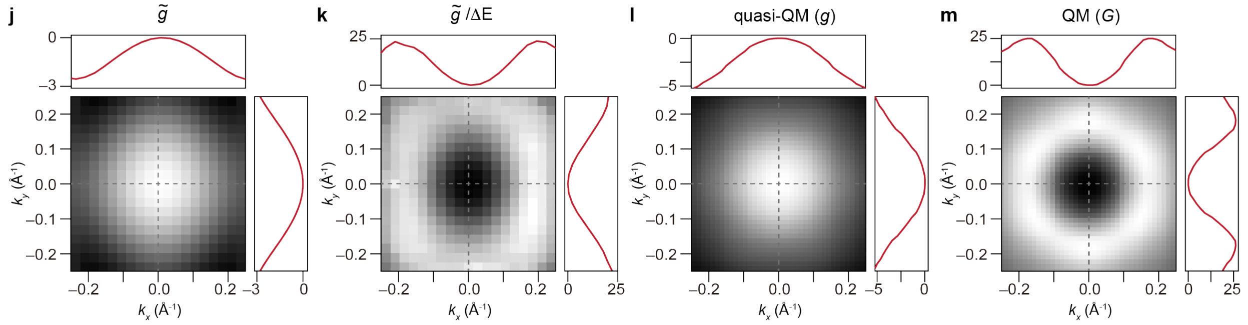
Quantum Geometry Direct Measurements

For Nearest neighbor (not yet published, approximation similar to the ”Gaussian approximation” given later

$$g_{xx}^{n} + g_{yy}^{n} \approx \tilde{g}^{n} = \frac{1}{2}\left(-a^{2}(E_n - E_0) - \left(\partial_{k_x}^{2} + \partial_{k_y}^{2}\right) E_n\right)$$

Checkelsky, Yang, Comin

All these can be obtained from Arpes

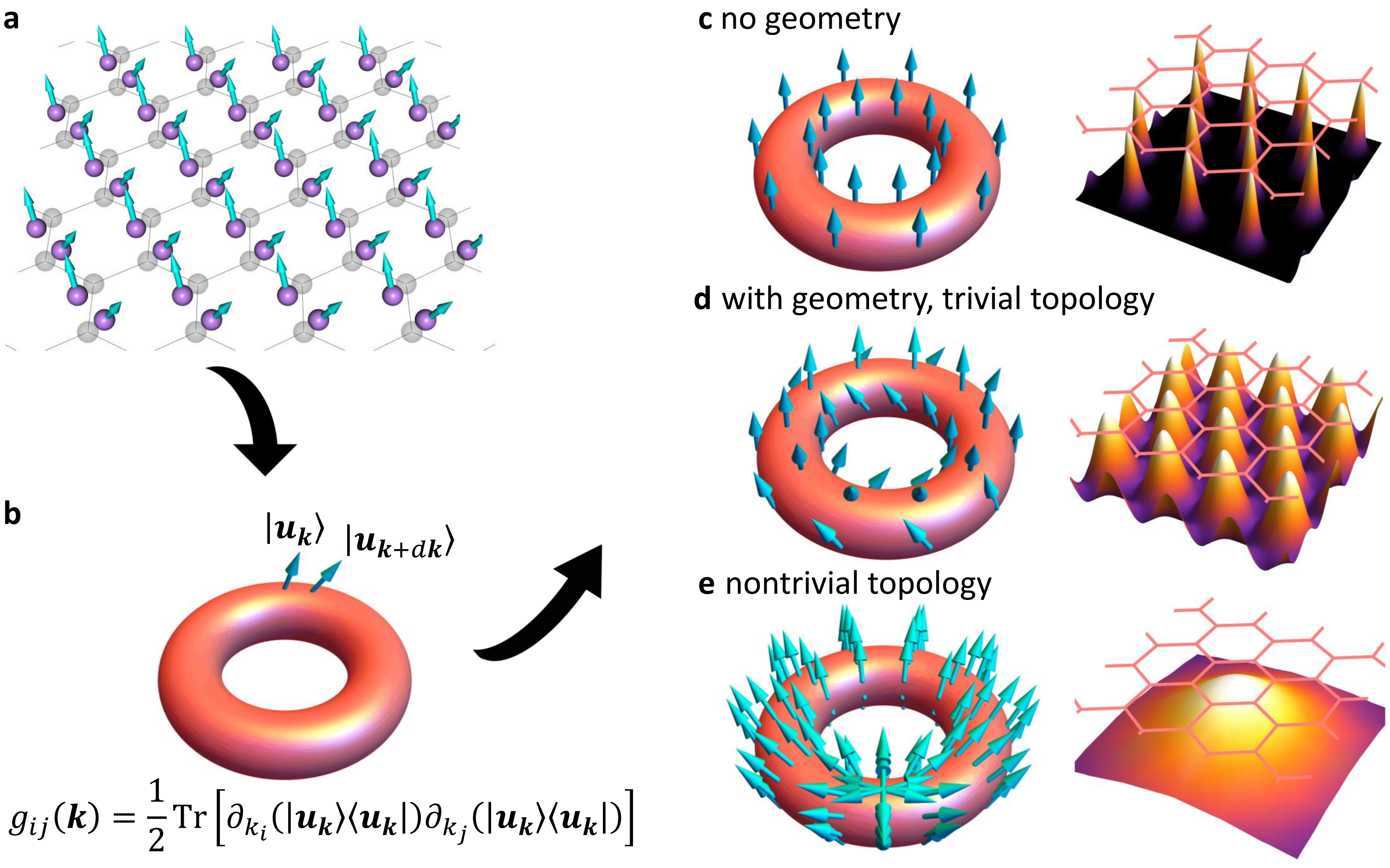


High-quality planar microcavity with embedded quantum wells that support 2D strongly coupled exciton–photon bands

The polarized polariton eigenstates are exactly determined by a Fourier space mapping of polarization-resolved photoluminescence. They exhibit non-zero Berry curvature and a non-zero quantum metric.

D. Sanvitto, Malpuech, 2020
Refael

Integrated optical conductivity also measures quantum geometry (Martin, Resta)



a
b
$|\boldsymbol{u_k}\rangle$
$|\boldsymbol{u_{k+dk}}\rangle$
$$g_{ij}(\boldsymbol{k}) = \frac{1}{2}\mathrm{Tr}\left[\partial_{k_i}(|\boldsymbol{u_k}\rangle\langle\boldsymbol{u_k}|)\partial_{k_j}(|\boldsymbol{u_k}\rangle\langle\boldsymbol{u_k}|)\right]$$
c no geometry
d with geometry, trivial topology
e nontrivial topology

Quantum Geometry Effects Can Appear in Both Flat and dispersive bands

Flat bands: quantum geometry and Berry phases are everything.
QG Bounds the superfluid weight, stiffness of collective modes. Berry Curvatures gives the spread in low magnetic field

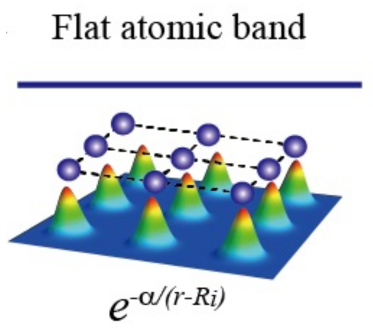
Peotta, Törmä, Tasaki, Gao, Niu,
Xiao, Yang, Parker, Vishwanath, Calugaru, Arbeitman, Yu, Hu, BAB

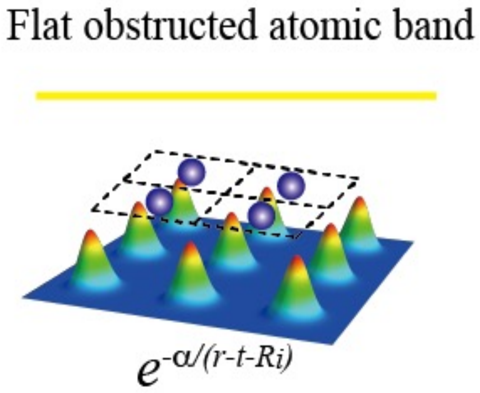
Dispersive bands: quantum geometry is dominated the electron-phonon coupling at least in 3 famous cases (and the number is going up)

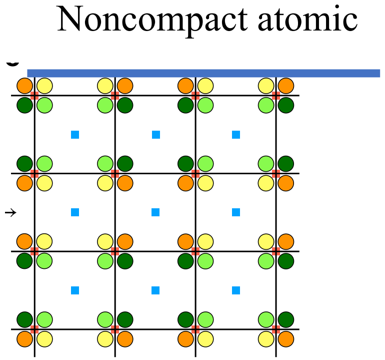
First, Start With Flat Bands

(E. Andrei, J. Checkelsky, MacDonald, Altman, Balents, Bergman, Levitov, Todadri, Vishwanath, Zalatel
Houck, Titus, Huber, BAB, Calugaru, Herzog-Arbeitman…)

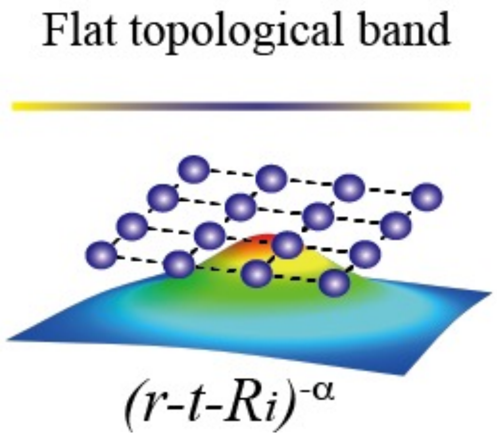
Quantum Geometry: Where does it appear and how it links to physical observables?

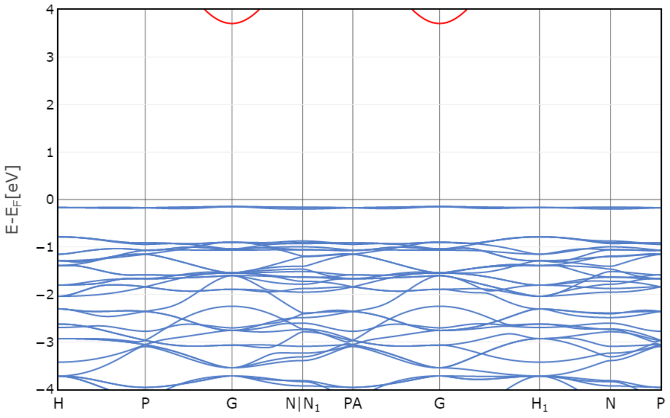






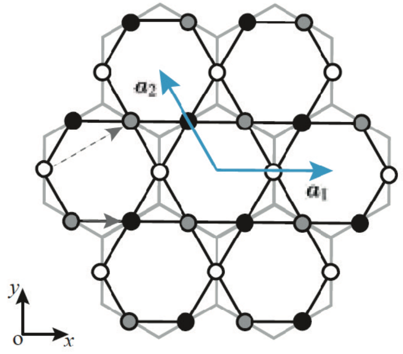
Schindler, BAB

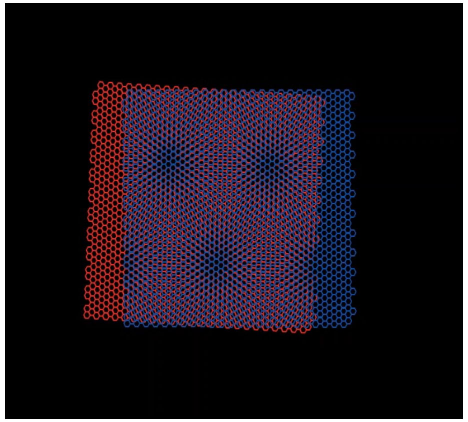


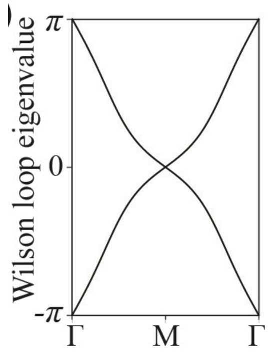


$Al_{12}Ca_8O_{24}S_2$
ICSD:67589

Localized Wannier functions originated from no hopping







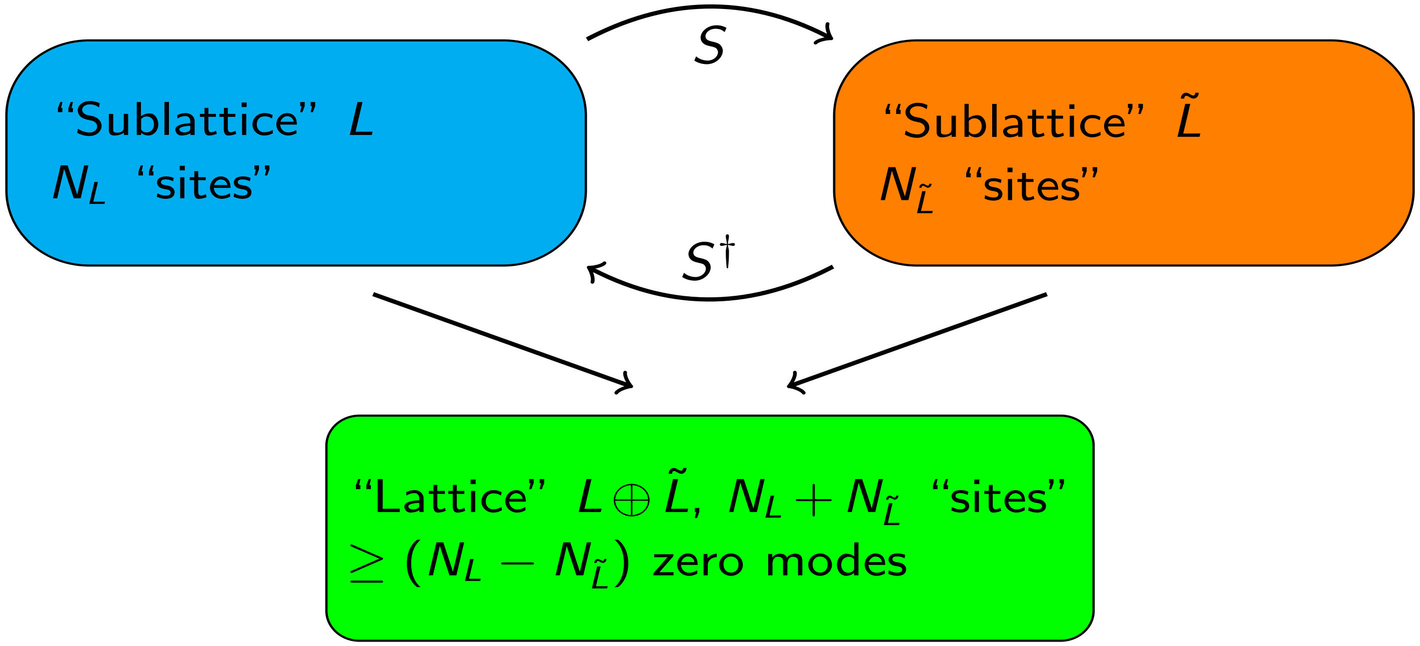
Delocalized Wannier functions originated from lattice geometry: Line graph, TBG, bipartite lattice…

Myriad of bands with nontrivial quantum geometry

Generalized Flat Band Construction: All flat bands w/o particle hole

Chiral (Lieb 1989)
Calugaru et al (2020)

$$S^{\dagger}_{\mathbf{k},\alpha}\phi_{\mathbf{k},\alpha} = 0$$



Generalized/Beyond Chiral

$$\begin{array}{cc} & \begin{array}{cc} N_L & N_{\tilde{L}} \end{array} \\ H_{\mathbf{k}} = & \begin{pmatrix} A_{\mathbf{k}} & S_{\mathbf{k}} \\ S^{\dagger}_{\mathbf{k}} & B_{\mathbf{k}} \end{pmatrix} \begin{array}{c} N_L \\ N_{\tilde{L}} \end{array} \end{array}$$

Calugaru Chew et al, Nat Phys 2021

$A_{\mathbf{k}}$ has k-independent eigenvalue **a** with degeneracy n_a

If $N_{\tilde{L}} < n_a \leq N_L$, then the Hamiltonian in Eq. (3) has at least $n_a - N_{\tilde{L}}$ flat bands of energy a irrespective of $B_{\mathbf{k}}$.

Calugaru

Classification of Topology of Flat Bands

Proof: The non-flat pair of bands have same symmetry eigenvalues at high symmetry points

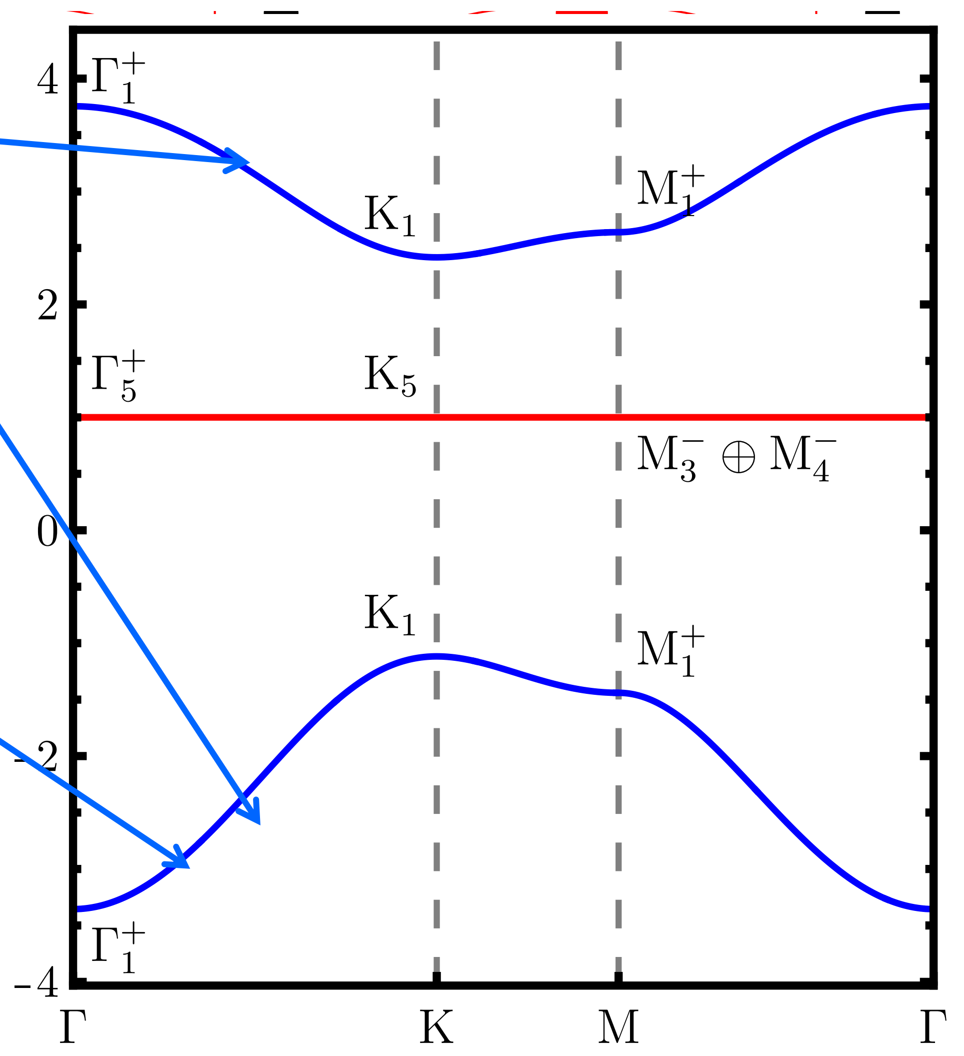
All bands form = $L \oplus \tilde{L}$ orbitals

The smaller lattice orbitals $\tilde{L}$ = nonzero energy bands.

We have $L \oplus \tilde{L} = \tilde{L} \oplus \text{FB} \oplus \tilde{L}$

Knowing ONLY the orbitals on the two lattice - an immediate way of obtaining the FB eigenvalues!

$$\boxed{\mathcal{B}_{\mathrm{FB}} = \mathcal{BR}_L \boxminus \mathcal{BR}_{\tilde{L}}}$$



Not always expressible as sums of atomic limits (BRs): Topological

(Po et al, 2017, Bradlyn et al, 2017; with C2T, Ahn, BJ Yang)

Flat band database

Regnault, Yuanfeng Xu, Vergniory, Elcoro, Song, Houck, BAB

Compound:	Space Group:	ICSD:
O7 Pb2 Sb2	*Fd-3m* (227)	27120

Materials Data

Crystallographic data

Cell Length A	10.4
Cell Length B	10.4
Cell Length C	10.4
Cell Angle α	90
Cell Angle β	90
Cell Angle γ	90

External links:

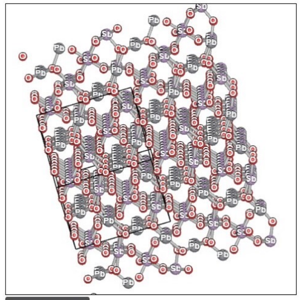
See ICSD 27120 on the Topological Material Database.
For more information we refer to Materials Project.

Tags:

Manually tagged as flat band
Belong to the best flat bands

Add to my compounds

Lattice Structure



Export POSCAR

Topological Classification

With SOC	ES (SM)
Without SOC	ESFD (SM)

Magnetic properties

None

Superconductivity

Unknown

Nbr of valence electrons

120

Theory ICSD

No

Has f-electrons

No

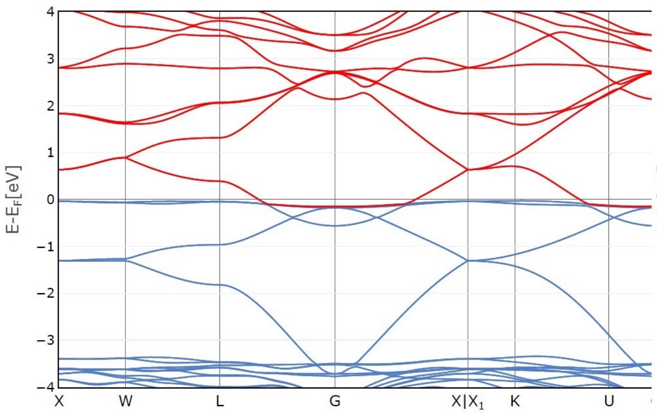
Sublattices summary

Pyrochlore
Kagome
Bipartite
Split

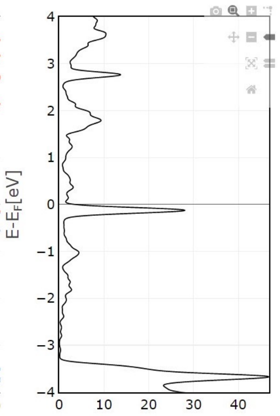
With SOC

Hide

Band Structure



Density of States



https://www.topologicalquantumchemistry.fr/flatbands/

Without SOC — Show

Information about isolated, connected sets of bands (with SOC) — Show

Information about isolated, connected sets of bands (without SOC) — Show

Sublattices

Rigorous Kagome sublattices:

- Atom type: Sb, Miller indices: (1, -1, 1), Unit cell coordinates: [1/8, 1/8, 5/8](c) [3/8, 3/8, 5/8](c) [1/8, 3/8, 7/8](c), Additional atoms: Pb:[3/8, 1/8, 3/8](d)
  Equivalent Kagome sublattices: +
- Atom type: Pb, Miller indices: (1, -1, -1), Unit cell coordinates: [1/8, 1/8, 1/8](d) [3/8, 3/8, 1/8](d) [3/8, 1/8, 3/8](d), Additional atoms: Sb:[5/8, 3/8, 3/8](c)
  Equivalent Kagome sublattices: +

Bipartite lattices:

- Threshold: 1.5 Å
  Decoupling distance: 1.2 x nearest neighbor distance set by O [1/2, 1/2, 7/10]], [Sb(c), [3/8, 3/8, 5/8]]], [[O(b), [1/2, 1/2, 0](f) - Pb [3/8, 3/8, 1/8](d)
  Nbr atoms in sublattice A: 12
  Nbr atoms in sublattice B: 4
  Atoms of the sublattice A: O:[3/10, 1/2, 1/2](f) O:[1/2, 3/10, 1/2](f) O:[1/2, 1/2, 7/10](f) O:[7/10, 1/2, 1/2](f) O:[1/2, 7/10, 1/2](f) O:[1/2, 1/2, 3/10](f) O:[0.9500, 3/4, 3/4](f) O:[3/4, 0.9500, 3/4](f) O:[3/4, 3/4, 0.5500](f) O:[0.5500, 3/4, 3/4](f) O:[3/4, 0.5500, 3/4](f) O:[3/4, 3/4, 0.9500](f)
  Atoms of the sublattice B: Sb:[3/8, 3/8, 5/8](c) Sb:[5/8, 5/8, 5/8](c) Sb:[5/8, 3/8, 3/8](c) Sb:[3/8, 5/8, 3/8](c)
- Threshold: 1.5 Å
  Decoupling distance: 1.2 x nearest neighbor distance set by O [1/2, 1/2, 7/10]], [Sb(c), [3/8, 3/8, 5/8]]], [[O(b), [1/2, 1/2, 0](f) - Pb [3/8, 3/8, 1/8](d)
  Split lattice
  Nbr atoms in sublattice A: 2
  Nbr atoms in sublattice B (medium sublattice): 4
  Atoms of the sublattice A: O:[0, 0, 0](b) O:[1/4, 1/4, 1/4]](b)
  Atoms of the sublattice B: Pb:[3/8, 3/8, 1/8](d) Pb:[1/8, 1/8, 1/8](d) Pb:[1/8, 3/8, 3/8](d) Pb:[3/8, 1/8, 3/8](d)

Ni_3In, Ni_3Ga, Ni_3Al, Ni_3Si, Ni_3Ge

https://www.topologicalquantumchemistry.com/flatbands/

(Regnault et al, 2022) Co_3W, Co_3Mo

Most Flat band "Kagome" materials available there

- Theory:
  - correlation: D. D. Sante, *et al.*, Phys. Rev. Research **5**, L012008 (2023)
  - structural: A. A. Mousa, *et al.*, Mater. Chem. Phys. **249**, 123104 (2020); G. Y. Guo, *et al.*, Phys. Rev. B **66**, 054440 (2002); G. Y. Guo, *et al.*, J. Magn. Magn., **239**, 91 (2002); L. S. Hsu, *et al.*, J. Appl. Phys. **92**, 1419 (2002);
- Exp:
  - flat band: L. Ye, *et al.*, arXiv: 2106.10824 (2021);
  - Structural: L. S. Hsu, *et al.*, J. Phys. Chem. Solids **60**, 1627 (1999);
  - Optical: L. S. Hsu, *et al.*, J. Alloys Compd. **377**, 29 (2004);
  - Electronic: S. M. Hayden, *et al.*, Phys. Rev. B **33**, 4977 (1986);
  - Alloy: S. Ochial, *et al.*, Acta Metall. 32, 289 (1984);
  - Catalytic: P. Czaja, *et al.*, J. Alloys Compd. **927**, 167076 (2022).

Inspiration from: Andrei, Checkelsky, Regnault, Cava, Moll, Schoop, Ong, Yazdani

J. G. Checkelsky:

- Theory:
  - Fe_3Sn_2: S. Fang, *et al.*, Phys. Rev. B **105**, 035107 (2022);
- Exp:
  - FeSn: M. Kang, *et al.*, Nature Mater. 19, 163 (2020); H. Inoue, *et al.*, Appl. Phys. Lett. **115**, 072403 (2019); M. Han, *et al.*, Nature Commun. **12**, 5345 (2021);
  - CoSn: M. Kang, *et al.*, Nature Commun. **11**, 4004 (2020);
  - Fe_3Sn_2: C. Lee, *et al.*, arXiv: 2212.02498 (2022); L. Ye, *et al.*, Nature Commun. 10, 4870 (2019); L. Ye, *et al.*, Nature **555**, 638 (2018);
  - AV_3Sb_5 (A = K, Rb, Cs): H. Li, et al., arXiv: 2303.07254 (2023); M. Kang, *et al.*, Nature Mater. **22**, 186 (2023); M. Kang, et al., arXiv: 2202.01902; M. Kang, et al., arXiv: 2202.01902
  - Ni_3In: L. Ye, *et al.*, arXiv: 2106.10824 (2021);

135 Family (KV3Sb5, RbV3Sb3, CsV3Sb3)

- Experiment: CDW: H. Li *et al.*, Nat. Phys. **18**, 265 (2022), E. Uykur *et al.*, npj Quantum Mater. **7**, 1 (2022), H. Luo *et al.*, Nat Commun **13**, 273 (2022), S. Cho *et al.*, Phys. Rev. Lett. **127**, 236401 (2021), N. Ratcliff *et al.*, Phys. Rev. Mater. **5**, L111801 (2021), B. R. Ortiz *et al.*, Phys. Rev. X **11**, 041030 (2021), M. Kang *et al.*, (2021), H. Zhao *et al.*, Nature **599**, 216 (2021), K. Nakayama *et al.*, Phys. Rev. B **104**, L161112 (2021), Z. Liu *et al.*, Phys. Rev. X **11**, 041010 (2021), N. N. Wang *et al.*, Phys. Rev. Res. **3**, 043018 (2021), Z. X. Wang *et al.*, Phys. Rev. B **104**, 165110 (2021), H. Li *et al.*, Phys. Rev. X **11**, 031050 (2021), Z. Liang *et al.*, Phys. Rev. X **11**, 031026 (2021), F. H. Yu *et al.*, Nat Commun **12**, 3645 (2021), B. Q. Song *et al.*, arXiv:2105.09248 (2021), D. W. Song *et al.*, arXiv:2104.09173 (2021), Z. Wang *et al.*, arXiv:2104.05556 (2021).
  - Chiral: C. Mielke *et al.*, Nature **602**, 245 (2022), Y.-X. Jiang *et al.*, Nat. Mater. **20**, 1353 (2021), Z. Wang *et al.*, Phys. Rev. B **104**, 075148 (2021), N. Shumiya *et al.*, Phys. Rev. B **104**, 035131 (2021).
- Theory: CDW: M. M. Denner, R. Thomale, and T. Neupert, Phys. Rev. Lett. **127**, 217601 (2021), X. Feng *et al.*, Science Bulletin **66**, 1384 (2021), H. Tan *et al.*, Phys. Rev. Lett. **127**, 046401 (2021), Y.-P. Lin and R. M. Nandkishore, Phys. Rev. B **104**, 045122 (2021).
- Experiment: Superconductivity: Y. Wang *et al.*, arXiv:2012.05898 (2023), C. C. Zhu *et al.*, Phys. Rev. B **105**, 094507 (2022), A. Tsirlin *et al.*, SciPost Physics **12**, 049 (2022), L. Yin *et al.*, Phys. Rev. B **104**, 174507 (2021), H. Chen *et al.*, Nature **599**, 222 (2021), H.-S. Xu *et al.*, Phys. Rev. Lett. **127**, 187004 (2021), N. N. Wang *et al.*, Phys. Rev. Res. **3**, 043018 (2021), W. Duan *et al.*, Sci. China Phys. Mech. Astron. **64**, 107462 (2021), C. Mu *et al.*, Chinese Phys. Lett. **38**, 077402 (2021), F. Du *et al.*, Phys. Rev. B **103**, L220504 (2021), K. Y. Chen *et al.*, Phys. Rev. Lett. **126**, 247001 (2021), F. H. Yu *et al.*, Nat Commun **12**, 3645 (2021), S. Ni *et al.*, Chinese Phys. Lett. **38**, 057403 (2021), B. Q. Song *et al.*, arXiv:2105.09248 (2021), T. Wang *et al.*, arXiv:2105.07732 (2021), B. R. Ortiz *et al.*, Phys. Rev. Mater. **5**, 034801 (2021), C. C. Zhao *et al.*, arXiv:2102.08356(2021), Q. Yin *et al.*, Chin. Phys. Lett. **38**, 037403 (2021), B. R. Ortiz *et al.*, Phys. Rev. Lett. **125**, 247002 (2020).
  - AHE E. M. Kenney *et al.*, J. Phys.: Condens. Matter **33**, 235801 (2021), S.-Y. Yang *et al.*, Science Advances **6**, eabb6003 (2020).
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Heavy Fermion Link: Checkelsky, BAB, Si, Coleman, Buehler-Paschen, To Appear

166

And many others!

- Theory: 166, flatband, Kagome: G. Venturini, Zeitschrift für Kristallographie **221**, 511(2006), Daniel C. Fredrickson *et al.*, J. Am. Chem. Soc. **130**, 8195 (2008); N.V. Baranov *et al.*, Phys. Met. Metallogr. **112**, 711(2011); P. M. Neves *et al.*, arXiv: 2303.02524 (2023); Y. Wang *et al.*, arXiv: 2303.03359 (2023); M. Jovanovic, *et al.*, J. Am. Chem. Soc. **144**, 10978 (2022)
  - CDW: H. Tan *et al.*,arXiv: 2302.07922 (2023);

  Exp: CDW: Arachchige H. W. S. *et al.*, Phys. Rev. Lett. **129**, 216402 (2022); T. Hu *et al.*, arXiv: 2211.03412; S. Kang *et al.*, arXiv: 2302.14041 (2023), M. Tuniz *et al.*, arXiv: 2302.10699 (2023), S. Cheng *et al.*, arXiv: 2302.12227 (2023), Y. Hu *et al.*, arXiv: 2304.06431 (2023); Z. Guguchia, *et al.*, arXiv: 2304.06436 (2023), S. Cao *et al.*, arXiv: 2304.08197 (2023), A. Korshunov, *et al.*, arXiv: 2304.09173 (2023); S. Lee *et al.*, arXiv: 2304.11820 (2023); X. Zhang *et al.*, Materials **15**, 7372 (2022). Y. Wang *et al.*, Chem. Mater. **34**, 7337 (2022); Y. Wang *et al.*, 2204.09637 (2023); M. Sinha *et al.*, ACS Cent. Sci. **7**, 1381 (2021);
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- Exp: Magnetic: S. X. M. Riberolles, *et al.*, arXiv: 2303.01613 (2023); X. Huang, *et al.*, arXiv: 2303.00627 (2023); C. Mielke III, *et al.*, Commun. Phys. **5**, 107 (2022); S. X. M. Riberolles, *et al.*, Phys. Rev. X **12**, 021043 (2022); H. Bhandari, *et al.*, arXiv: 2304.11502 (2023); K. Guo, *et al.*, arXiv: 2210.12117 (2022); F. Kabir, *et al.*, Phys. Rev. Mater. **6**, 064404 (2022); M. Wenzel, *et al.*, Phys. Rev. B **106**, L241108 (2022); J. Lee, *et al.*, Phys. Rev. Mater. **6**, 083401 (2022); G. Pokharel, et al., Phys. Rev. Mater. **6**, 104202 (2022); X. Zhang, *et al.*, Phys. Rev. Mater. **6**, 105001 (2022); E. Rosenberg, *et al.*, Phys. Rev. B **106**, 115139 (2022); H. Ishikawa, *et al.*, J. Phys. Soc. Jpn **90**, 124704 (2021); H. Zhang, *et al.*, Phys. Rev. B **101**, 100405(R) (2020); X. Y. Li, *et al.*, J. Appl. Phys. **123**, 203903 (2018); F. Canepa, *et al.*, J. Alloys Compd. **383**, 10 (2004); A. Szytuła, *et al.*, J. Alloys Compd. **366**, L16 (2004); G. K. Marasinghe, *et al.*, J. Appl. Phys. **91**, 7863 (2002); Y. Janssen, et al., Physica B Condens. **294**, 208 (2001); T. Mazet, *et al.*, J. Alloys Compd. **325**, 67 (2001); J. M. Cadogan, *et al.*, J. Appl. Phys. **87**, 6046 (2000); M. F. Fedyna, *et al.*, Neorganicheskie Materialy **35**, 461 (1999); G. Venturini, *et al.*, J. Alloys Compd. **236**, 102 (1996); F. Weitzer, *et al.*, J. Appl. Phys. **73**, 8447 (1993); G. Venturini, *et al.*, J. Alloys Compd. **200**, 51 (1993); G. Venturini, *et al.*, J. Magn. Magn. **94**, 35 (1991);

Exp: Dirac: Y. Hu *et al.*, Sci. Adv. **8**, add2024 (2022); H. Li *et. al.*, Nature Phys. **18**, 644 (2022); S. Peng *et al.*, Phys. Rev. Lett. **127**, 266401 (2021)

- AHE: D. C. Jones, *et al.,* arXiv: 2203.17246 (2023); H. Zhou, *et al.,* Phys. Rev. Mater. **7**, 024404 (2023); L. Min *et al.*, Commun. Phys. **5**, 63 (2022); W. Ma, *et al.,* Phys. Rev. B **103**, 235109 (2021); L. Gao, *et al.,* Appl. Phys. Lett. **119**, 092405 (2021); G. Dhakal, *et al.,* Phys. Rev. B **103**, L161115 (2021);
- Thermoelectric: S. Roychowdhury, *et al.,* Adv. Mater. **34**, 2201350 (2022);
- other: C. Liu, et al., Surf. Interfaces **39**, 102866 (2023); T. Y. Yang, *et al.,* Quantum Front. **1**, 14 (2022); H. Zhang, *et al.,* Appl. Phys. Lett. **121**, 202401 (2022); X. X. Chen, *et al.,* Int. J. Mod. Phys. B **30**, 1650068 (2016); T. Braun, *et al.,* J. Solid State Chem. **318**, 123742 (2023); P. Wang, *et al.,* Chinese Phys. Lett. **37**, 087102 (2020); L. Eichenberger, *et al.,* Phys. Rev. B **101**, 020408 (2020); L. Romaka, *et al.,* J. Alloys Compd. **509**, 8862 (2011); I. Oshchapovsky, *et al.,* Acta Cryst. **66**, i82 (2010); G. Venturini, J. Alloy Compd. **322**, 190 (2001); T. Mazet, *et al.,* Solid State Commun. **110**, 407 (1999); P. Schobinger, *et al.,* J. Alloy Compd **256**, 92 (1997); B. Malaman, *et al.,* Mater. Res. Bull. **23**, 1629 (1988); V. W. Buchholz, *et al.,* Z. anorg. allg. Chem. **482**, 40 (1981);

Usual reasons - given in models of SG 191 FeGe and related - for flat bands need revisiting (no s-orbital Kagome/line graph/Mielke, different counting/physics) - trigonal Ge spoils Kagome!

A high degree of caution must be exercised with the physics of all these realistic flat bands/Diracs; especially theoretical interpretation

Geometric Limit of the Orbital Magnetic Moment

- Berry phase first appeared in the generalized Onsager relation

(LL/Hofstadter spectrum) $$\mathrm{Area}(E) = B(n + \frac{1}{2} - \frac{\gamma_B}{2\pi})$$ (band topology)

- In atomic physics, $H(B) = H + \mu_0 L_z B$ defines spin magnetic moment
  - In Bloch bands, semi-classical calculations generalize $\mu_0 L_z \to \mu_n(\mathbf{k})$

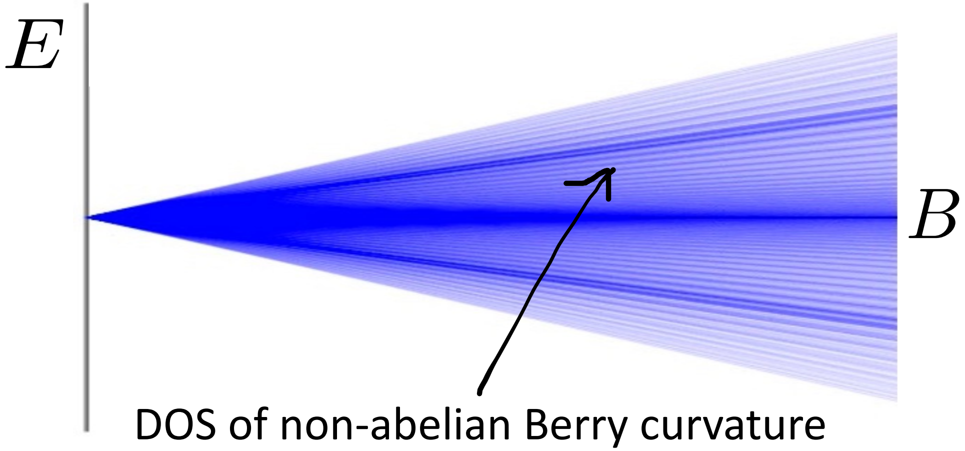
Gau, Niu

- Topological limit $h(\mathbf{k}) \to \Delta(1 - P(\mathbf{k}))$ reveals a flat band Onsager formula:

$$E_0 \to E_0 + B\Delta f(\mathbf{k})$$

flat bands in flux dispersive according to topology

Bohm-Jung Yang, Jonah Arbeitman, Calugaru, others



DOS of non-abelian Berry curvature

Herzog-Arbeitman

Strongly Correlated quantum geometric flat bands

Huhtinen Torma

In Mean-Field, it is possible to prove (Peotta and Torma; Huhtinen, Arbeitman BAB Torma):

$$[D_s]_{ij} = \frac{8e^2\Delta}{\hbar^2}\sqrt{\nu(1-\nu)}\int \frac{d^2k}{(2\pi)^2} g_{ij}(\mathbf{k}) \qquad [D_s]_{ij} = \frac{1}{V}\frac{\partial^2\Omega(\mathbf{q})}{\partial q_i \partial q_j}\Big|_{\mathbf{q}=0}$$

In GL, it should be 1/m = 0. Band delocalization provides stiffness

- Can we make more exact statements, beyond mean field?
- Exact results possible in flat band lattice Hubbard models with quantum geometry

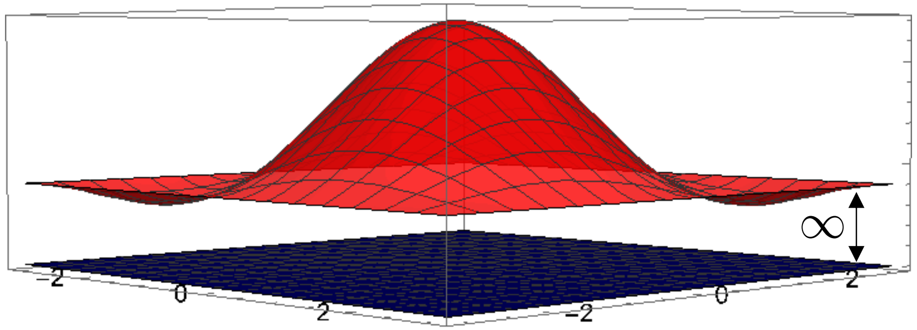
(Vafek, Kang, Lian, Song, BAB, Calugaru, Vishwanath, Regnault, Crepel, Zaletel)

Projecting into the Flat band limit

- Tovmasyan Peotta Torma and Huber identified a nontrivial strong coupling limit of the Hubbard model.

$$P_{\alpha\beta}(\mathbf{k}) = [U(\mathbf{k})U^\dagger(\mathbf{k})]_{\alpha\beta}$$

(Hermitian projector into the flat bands)



- Positive semi-definite Hubbard Hamiltonian

$$H = \frac{|U|}{2}\sum_{\mathbf{R}\alpha}(\bar{n}_{\mathbf{R},\alpha,\uparrow} - \bar{n}_{\mathbf{R},\alpha,\downarrow})^2$$

"Uniform Pairing condition"

$$\frac{1}{V}\sum_{\mathbf{k}} P_{\alpha\alpha}(\mathbf{k}) = \frac{N_{flat}}{N_{orb}} \equiv \epsilon$$

Projected attractive Hubbard

$$H = \frac{\epsilon|U|}{2}\bar{N} - |U|\sum_{\mathbf{R}\alpha}\bar{n}_{\mathbf{R},\alpha,\uparrow}\bar{n}_{\mathbf{R},\alpha,\downarrow}$$

Enlarged Many-body Symmetry Group

$$H = \frac{|U|}{2} \sum_{\mathbf{R}\alpha} (\bar{n}_{\mathbf{R},\alpha,\uparrow} - \bar{n}_{\mathbf{R},\alpha,\downarrow})^2$$

- Hamiltonian possesses an eta symmetry (introduced by Yang)

$$\eta^\dagger = \sum_{\mathbf{k}\alpha} \bar{c}^\dagger_{\mathbf{k},\alpha,\uparrow} \bar{c}^\dagger_{-\mathbf{k},\alpha,\downarrow} = \sum_{\mathbf{R}\alpha} \bar{c}^\dagger_{\mathbf{R},\alpha,\uparrow} \bar{c}^\dagger_{\mathbf{R},\alpha,\downarrow}$$

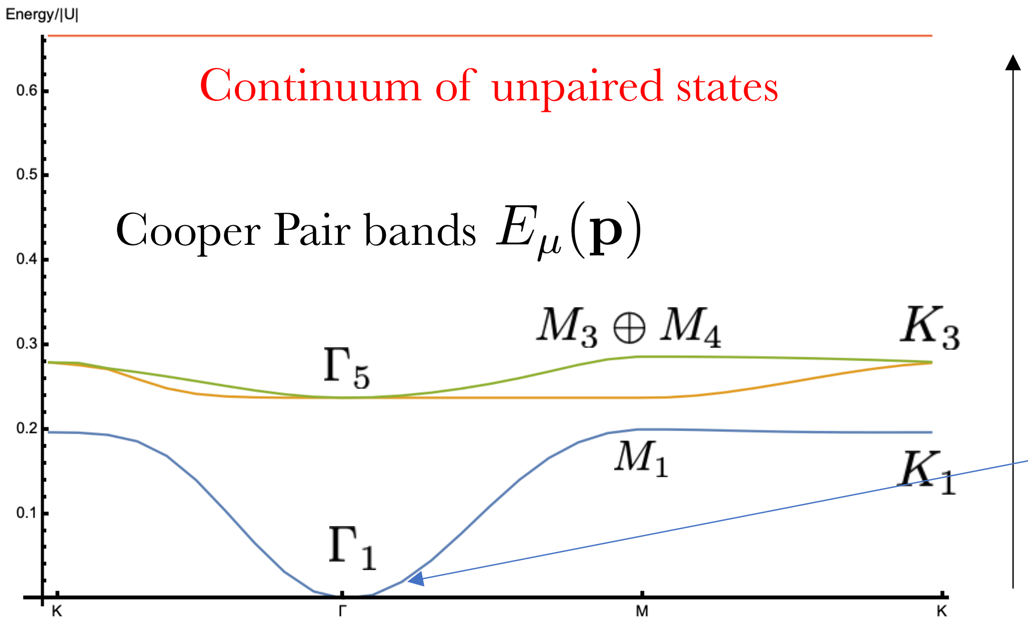
Arbeitman, Huhkinen Chew Torma BAB, Calugaru et al

- $|n\rangle \propto \eta^{\dagger n} |0\rangle$ are all ground states

Cooper Pair Excitations (Spin Wave For Repulsive U)

- Straightforward calculation of the excitation matrix

$$[H, \gamma^\dagger_{\mathbf{p}+\mathbf{k},m,\sigma}\gamma^\dagger_{-\mathbf{k},n,\sigma'}]\,|n\rangle = \sum_{\mathbf{k}'m'n'} \gamma^\dagger_{\mathbf{p}+\mathbf{k}',m',\sigma}\gamma^\dagger_{-\mathbf{k}',n',\sigma'}\,|n\rangle\,[R^{\sigma\sigma'}(\mathbf{p})]_{\mathbf{k}'m'n',\mathbf{k}mn}$$



- Quadratic: $E_0(\mathbf{p}) = g_{ij}p_ip_j + \ldots$

where g_{ij} is the minimal quantum metric

Arbeitman, Huhkinen Chew Torma BAB.
Calugaru et al

Relevance to TBG

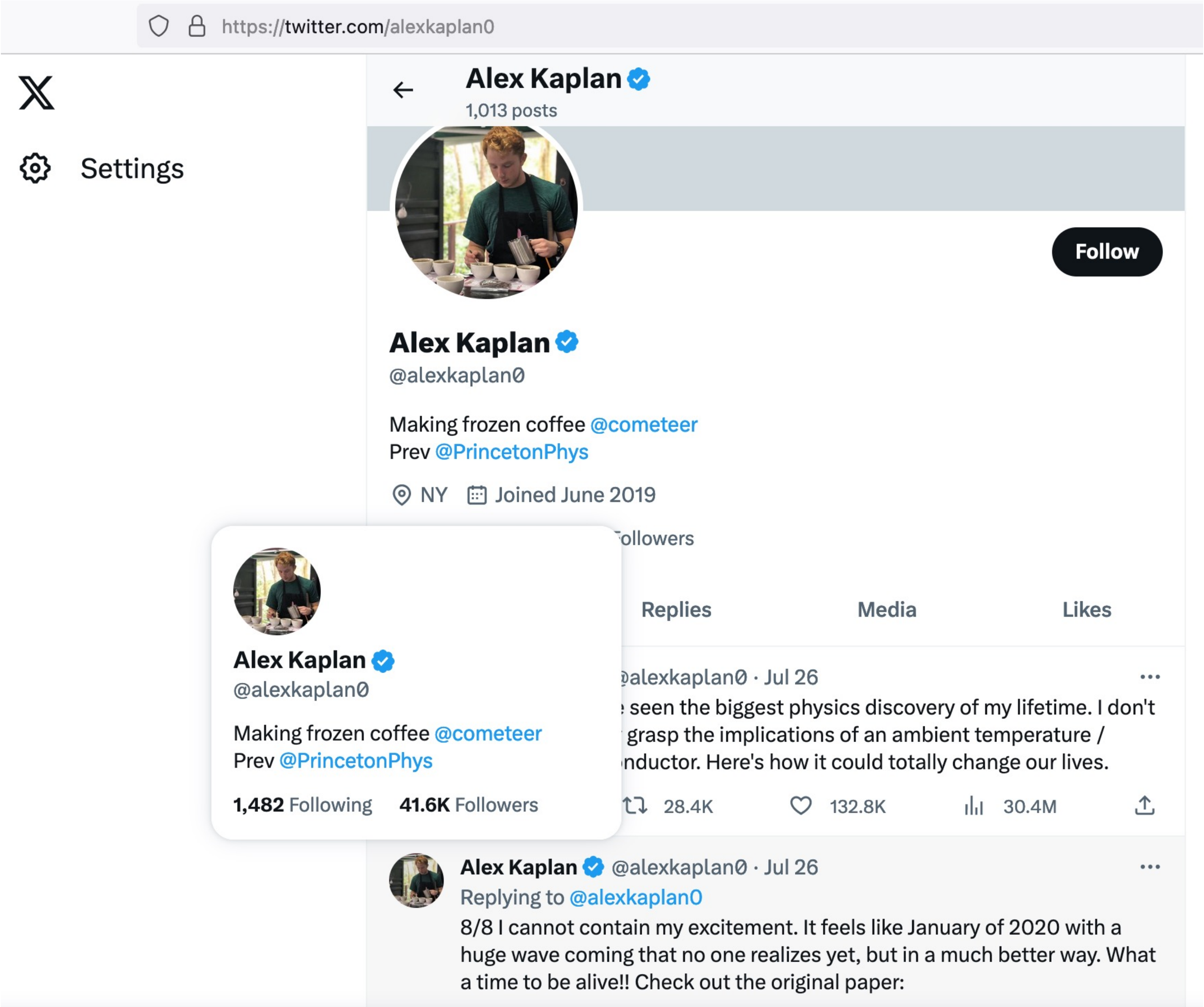
Evidence for Dirac flat band superconductivity enabled by quantum geometry

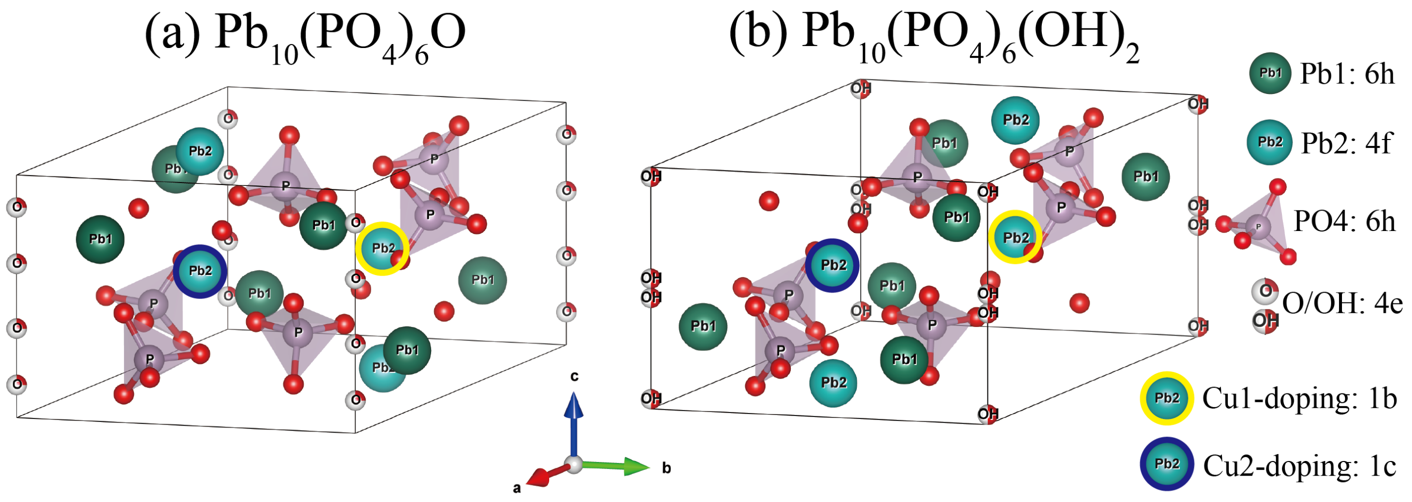
Haidong Tian, Xueshi Gao, Yuxin Zhang, Shi Che, Tianyi Xu, Patrick Cheung, Kenji Watanabe, Takashi Taniguchi, Mohit Randeria, Fan Zhang, Chun Ning Lau & Marc W. Bockrath

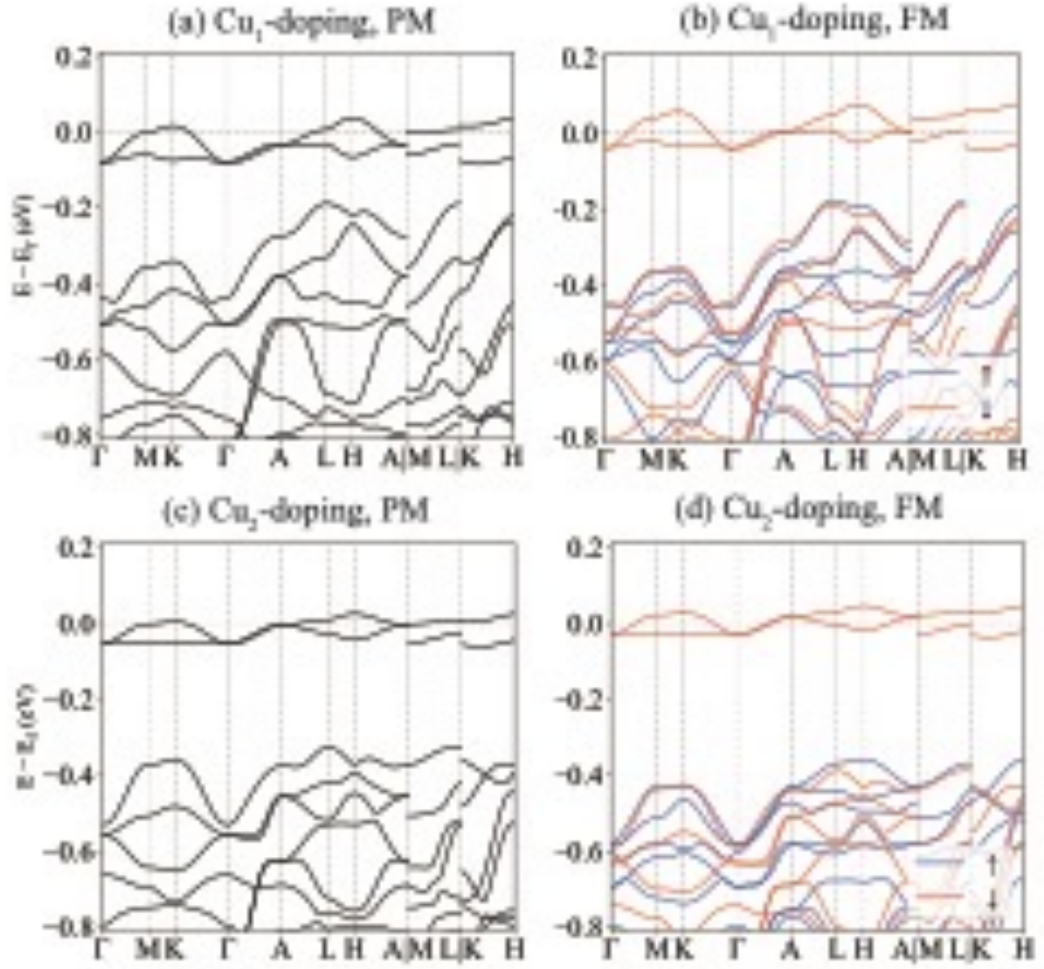
- Dramatically reduced critical velocity (characteristic of flat bands)
  - Measured from R vs J plots to determine SC state critical current
- Correlation-dominated superfluid weight "from quantum geometry" (CAUTION WITH THE INTERPRETATION)
  - Calculated from critical current and coherence length measurements
  - Also tracks the measured Tc as a function of density, unlike the BCS formula

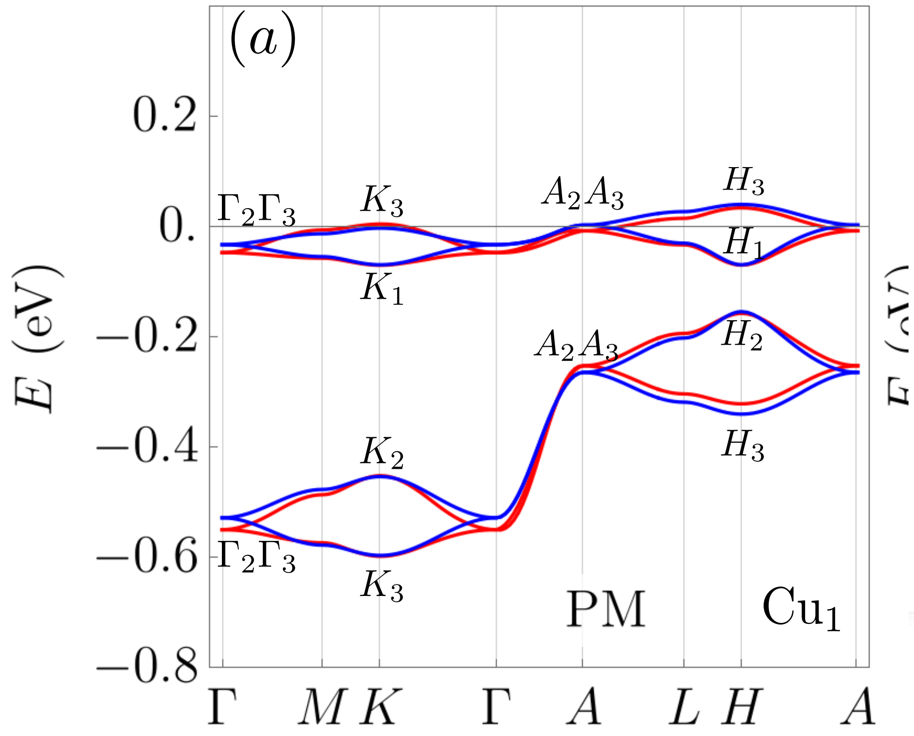

(b)
Name per
Person's hand
Levitation
Magnet
Superconductor
pellet

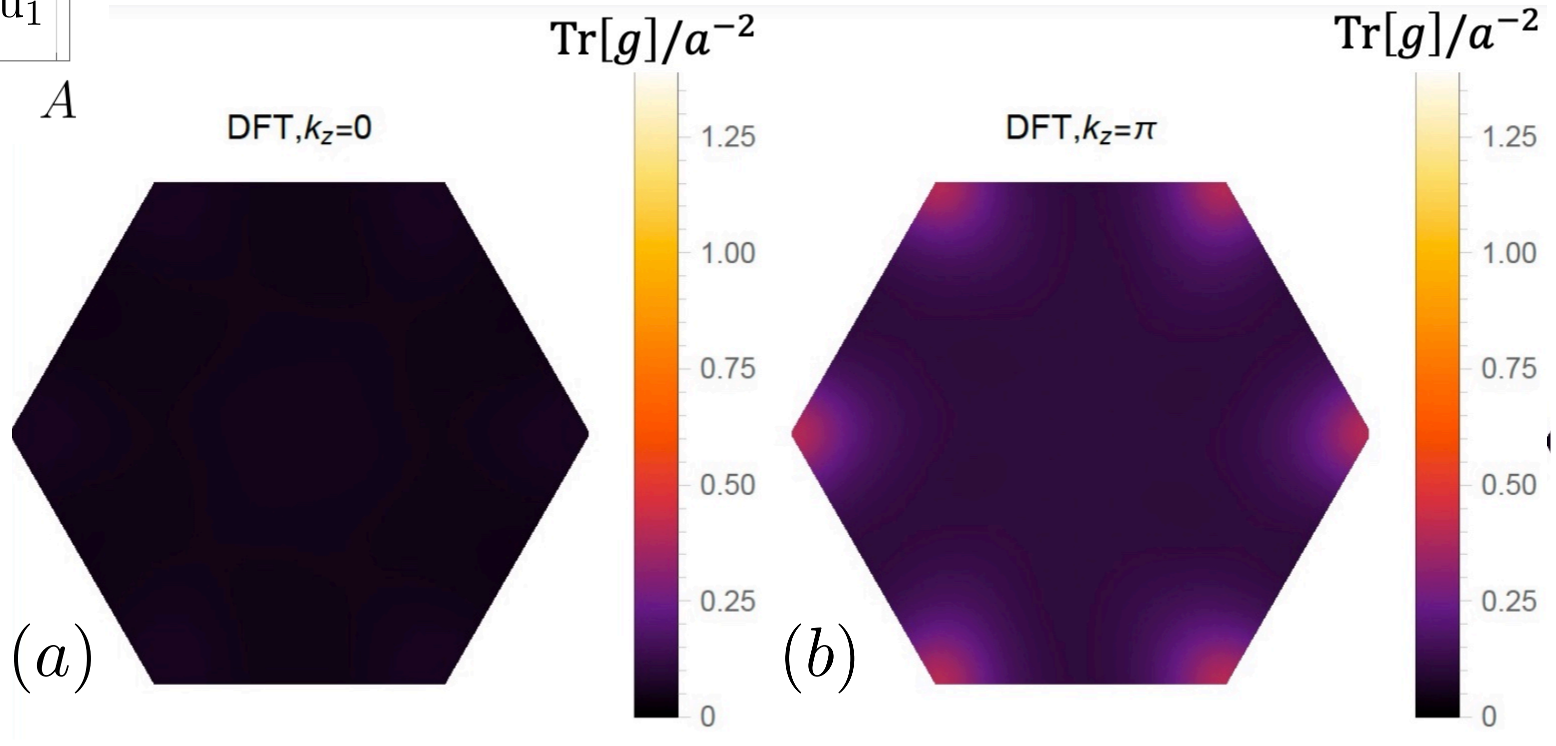
The Twitter Superconductor




(a) $Pb_{10}(PO_4)_6O$
(b) $Pb_{10}(PO_4)_6(OH)_2$
Pb1: 6h
Pb2: 4f
PO4: 6h
O/OH: 4e
Cu1-doping: 1b
Cu2-doping: 1c
a
b
c


(a) Cu_1-doping, PM
(b) Cu_1-doping, FM
(c) Cu_2-doping, PM
(d) Cu_2-doping, FM
$E-E_F$ (eV)
Γ M K Γ A L H A|M L|K H


(a)
0.2
0.
−0.2
−0.4
−0.6
−0.8
E (eV)
Γ2Γ3
K3
K1
A2A3
H3
H1
H2
H3
K2
Γ2Γ3
K3
PM
Cu1
Γ
M
K
Γ
A
L
H
A


Tr[g]/a^−2
DFT, kz=0
1.25
1.00
0.75
0.50
0.25
0
(a)
Tr[g]/a^−2
DFT, kz=π
1.25
1.00
0.75
0.50
0.25
0
(b)

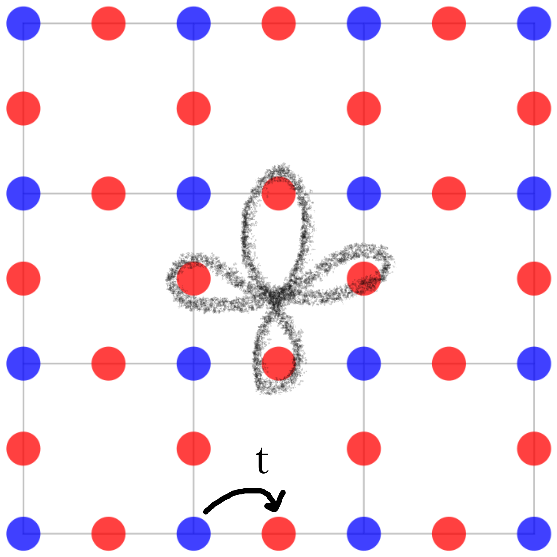
Gapless bands and Singular geometry: Heavy Fermion Mapping, mirroring TBG

Yazdani, Nadj-Perge, Ilani and Herrero, Young

Band localization length^2

- Excitation mass "universal" $$\frac{1}{m} \propto U \int d^2k\, (\partial P)^2$$
  - Naively enhanced by gapless flat band where $\partial P \to \infty$ at a singular band touching (BJ Yang, Calugaru, …)

E.g. Lieb

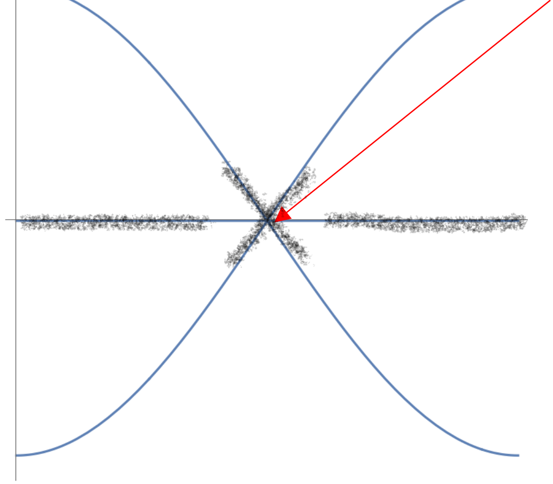


- Cutoff momentum scale $\Lambda \sim U/t$ set by interactions
- A finite length scale emerges associated with an obstructed heavy fermion which condense into Cooper pairs dressed by conduction electrons

$$\int_\Lambda d^2k\, (\partial P)^2 = \log\frac{1}{\Lambda} + \text{const} \to \log\frac{t}{U}$$

- Superfluid weight is log-enhanced by the singular quantum geometry

Flat band quantum metric diverges!



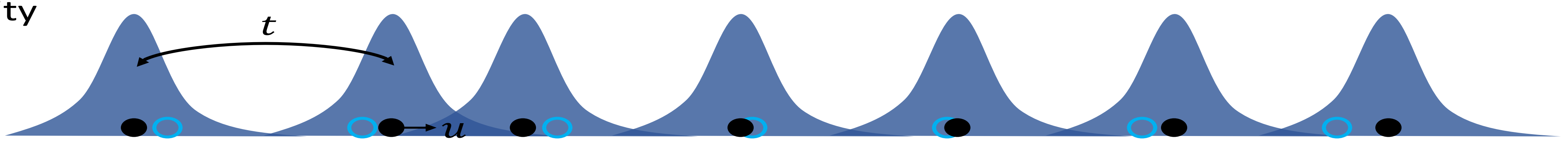
We know topology appears on metallic Fermi surfaces and not only in insulators

We know for flat bands, only topology and quantum geometry can exist

Can Quantum Geometry appear in dispersive bands or is it overwhelmed by the kinetic part?

We now look at electron-phonon coupling.

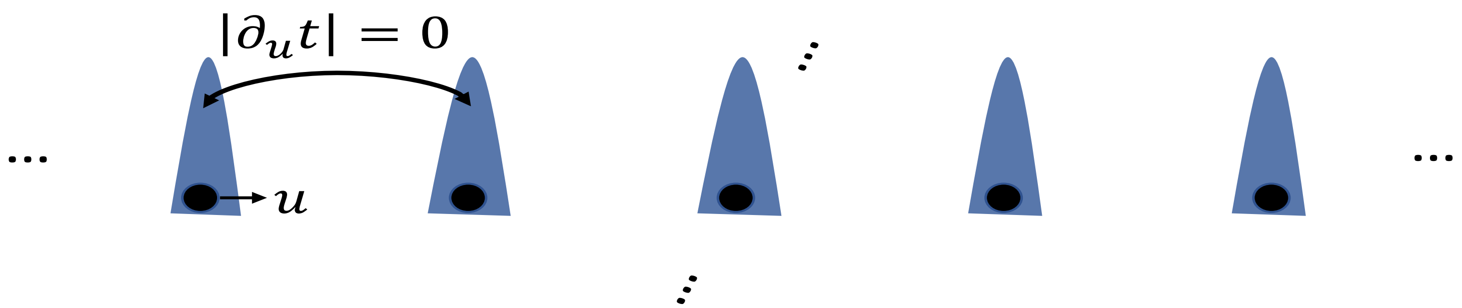
Reality



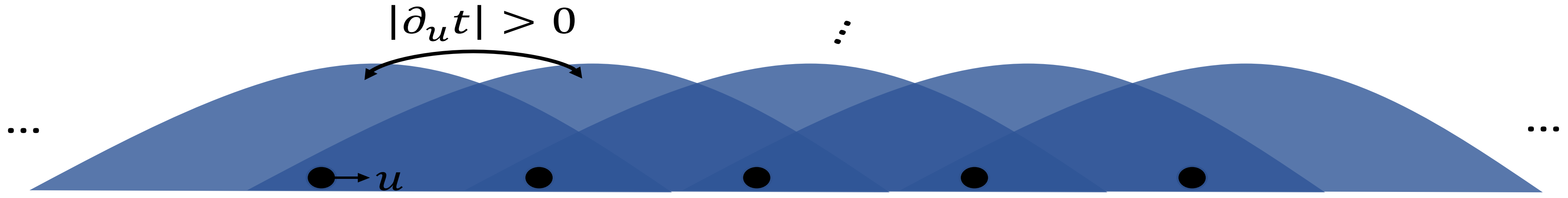
EPC$\sim \partial_u t$

Intuition: Why EPC cares about band geometry/topology

Trivial Geometry/Topology: $|\partial_u t|$ can be small



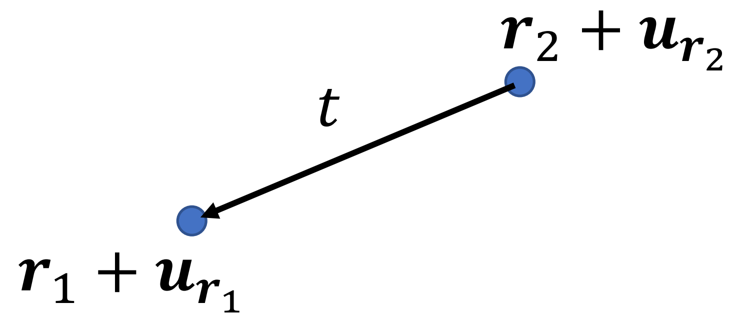
Nontrivial Geometry /Topology: $|\partial_u t|$ is typically large



Tight-Binding + Two-Center approximations

Mitra (1969)

- Hopping between two atoms at $\boldsymbol{r}_1 + \boldsymbol{u}_{\boldsymbol{r}_1}$ and $\boldsymbol{r}_2 + \boldsymbol{u}_{\boldsymbol{r}_2}$:



$$t(\boldsymbol{r}_1 + \boldsymbol{u}_{\boldsymbol{r}_1} - \boldsymbol{r}_2 - \boldsymbol{u}_{\boldsymbol{r}_2})$$

- EPC in atomic basis $\sim \nabla_{\boldsymbol{r}} t(\boldsymbol{r})$

EPC constant λ

McMillan (1968)

$$\Gamma_{nm}(\boldsymbol{k}_1, \boldsymbol{k}_2) = \frac{\hbar}{2} \sum_{\boldsymbol{\tau},i} \frac{1}{m_{\boldsymbol{\tau}}} \mathrm{Tr}\left[P_n(\boldsymbol{k}_1) F_{\boldsymbol{\tau}i}(\boldsymbol{k}_1, \boldsymbol{k}_2) P_m(\boldsymbol{k}_2) F^{\dagger}_{\boldsymbol{\tau}i}(\boldsymbol{k}_1, \boldsymbol{k}_2)\right]$$

$$\lambda = 2 \int_0^{\infty} d\omega \, \frac{\alpha^2 F(\omega)}{\omega} = \frac{2}{N\,\hbar} \frac{\mathrm{DOS}(\mu)}{\langle \omega^2 \rangle} \boxed{\langle \Gamma \rangle}$$

$\sim$ average phonon line width

A Novel Approximation

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(Princeton)

Christopher Ciccarino
(Stanford)

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Ion Errea
(University of the Basque Country, DIPC)

Prineha Narang
(UCLA)

- Gaussian Approximation:

$$t(\boldsymbol{r}) = t_0\, e^{\frac{\gamma\, r^2}{2}} \qquad \text{with } \gamma < 0$$

- EPC $\sim \nabla_{\boldsymbol{r}} t(\boldsymbol{r}) = \gamma\, \boldsymbol{r}\, t(\boldsymbol{r})$

F. T.

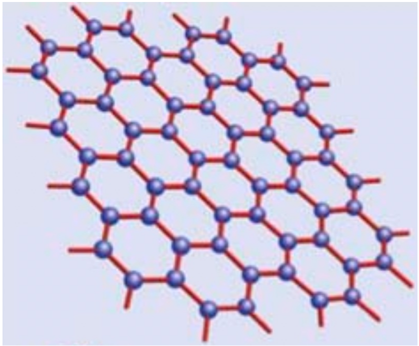
$$\gamma \nabla_{\boldsymbol{k}} h(\boldsymbol{k}) = \underbrace{\gamma \sum_n P_n(\boldsymbol{k}) \nabla_{\boldsymbol{k}} E_n(\boldsymbol{k})}_{\text{energetic}} + \underbrace{\boxed{\gamma \sum_n E_n(\boldsymbol{k}) \nabla_{\boldsymbol{k}} P_n(\boldsymbol{k})}}_{\text{geometric}}$$

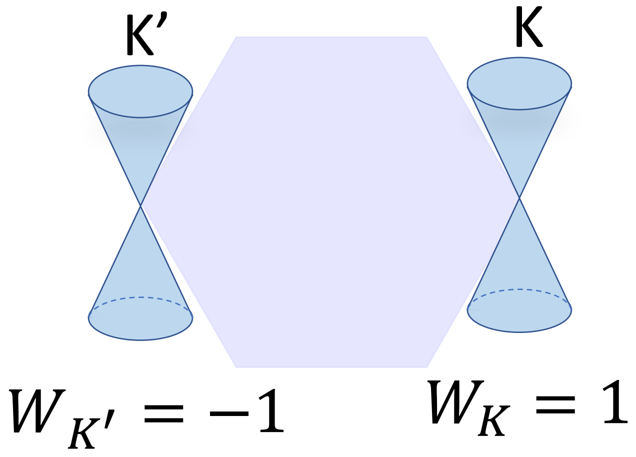
Geometric contribution λ_{geo} to λ

$$h(\mathbf{k}) = \sum\nolimits_n E_n(\mathbf{k}) P_n(\mathbf{k})$$

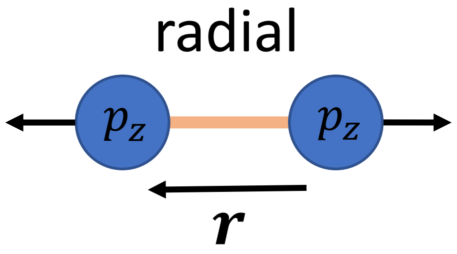
Graphene

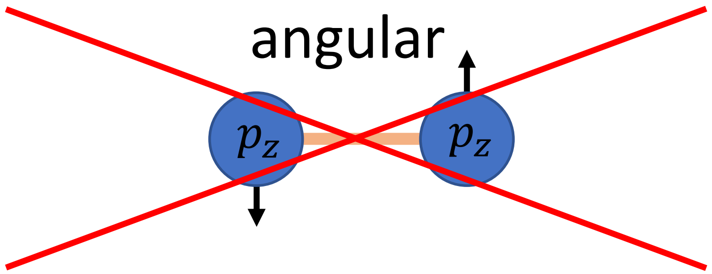
- Electrons: Carbon atom, one p_z orbital per atom, nearest-neighboring hopping
  Review: Neto et al (2009)





- EPC: Gaussian approximation $\nabla_{\boldsymbol{r}} t(\boldsymbol{r}) = \gamma\, \boldsymbol{r}\, t(\boldsymbol{r})$ exact
  Jiabin Yu, Ciccarino, Bianco, Errea, Narang, BAB





Combined with nearest-neighbor and symmetries (Thingstad, et al. (2020))

Graphene

- $\lambda = \lambda_E + \lambda_{geo}$
  - $\lambda_E = \mathrm{A}\int_{FS} d\sigma_{\boldsymbol{k}}\, |\nabla_{\boldsymbol{k}} E_{n_F}(\boldsymbol{k})|$
  - $\lambda_{geo} = \mathrm{A}\int_{FS} d\sigma_{\boldsymbol{k}} \frac{\Delta\mathrm{E}^2(\boldsymbol{k})}{|\nabla_{\boldsymbol{k}} E_{n_F}(\boldsymbol{k})|} \mathrm{Tr}[g_{n_F}(\boldsymbol{k})]$

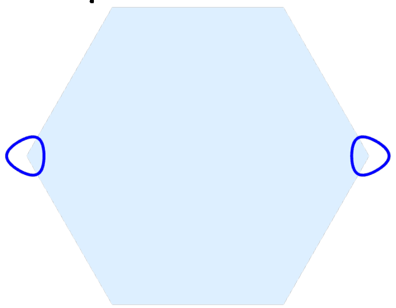
$\mathrm{A} = \frac{1}{4\pi^2}\frac{\Omega\,\gamma^2}{\langle\omega^2\rangle\, m_C}$: Material-dependent

$\Delta\mathrm{E}(\boldsymbol{k})$: Energy difference between two bands

- $\lambda_{geo} \geq \lambda_{topo}$

$$\lambda_{topo} = \pi^2 \mathrm{A} \frac{(|W_{K'}| + |W_K|)^2}{\int_{FS} d\sigma_{\boldsymbol{k}} \left|\nabla_{\boldsymbol{k}} E_{n_F}(\boldsymbol{k})\right| / \Delta\mathrm{E}^2(\boldsymbol{k})}$$ for FS enclosing K and K'

$\mu = -1$ eV

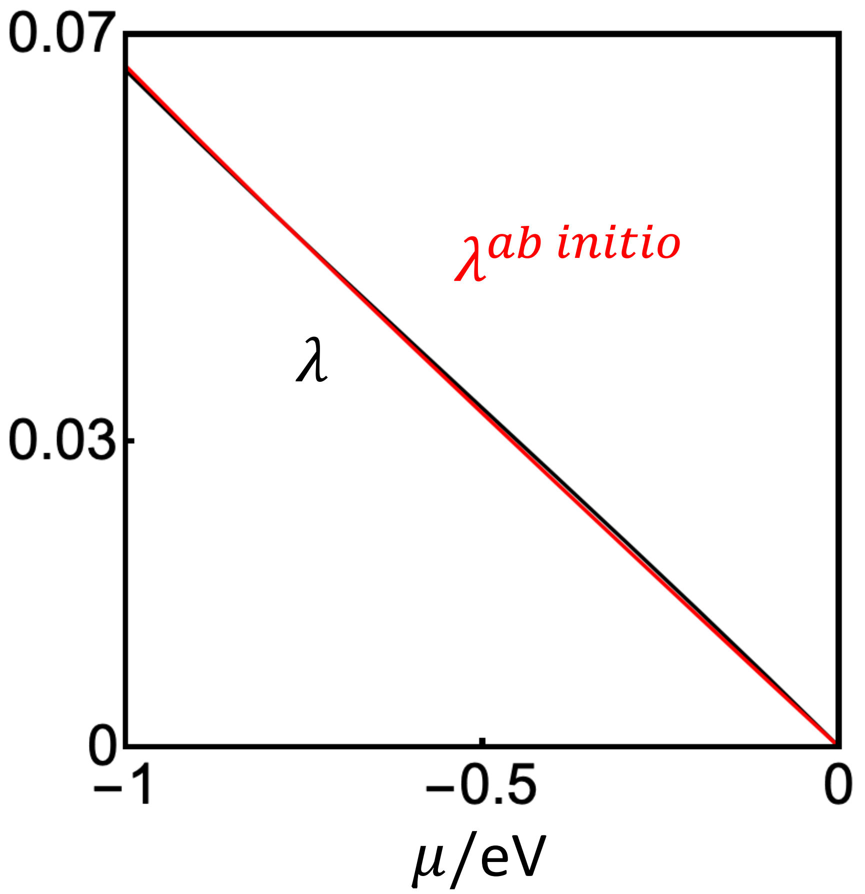


Roughly half of EPC comes from band geometry/topology!

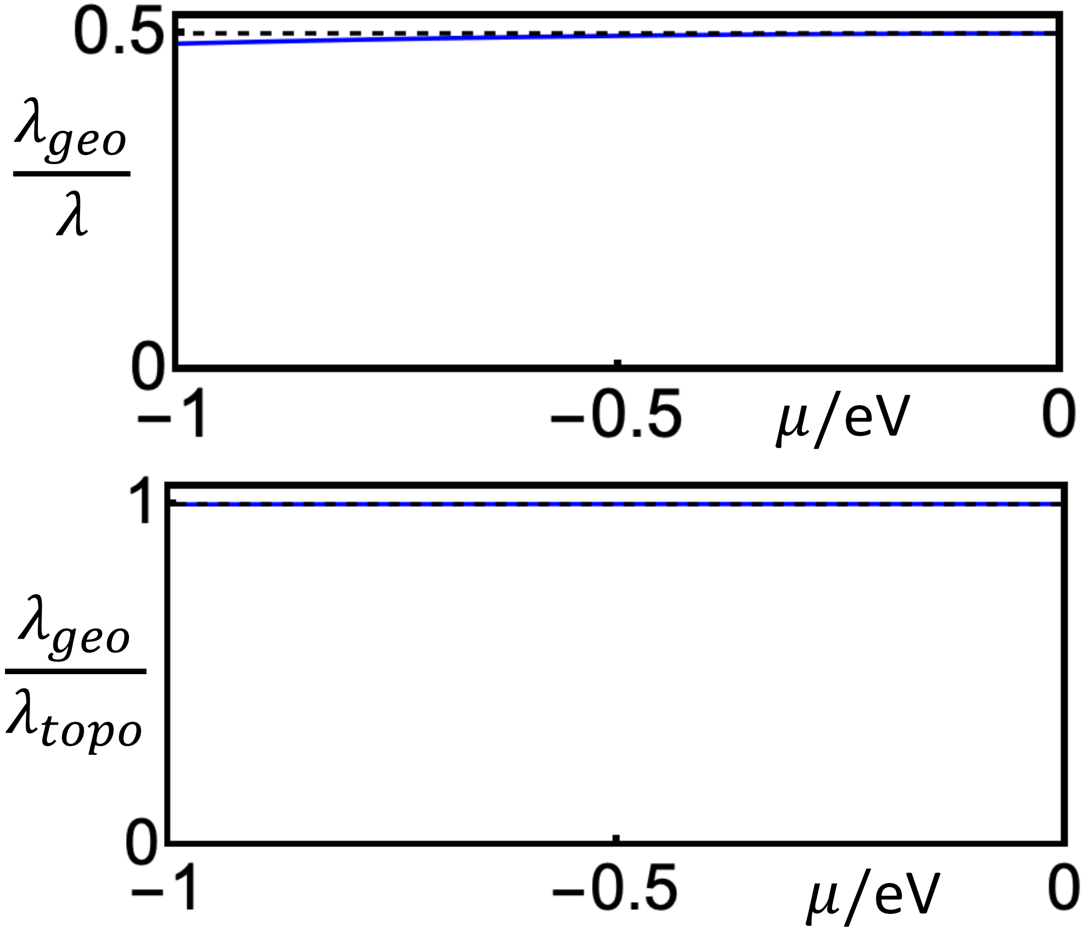
Graphene

JY, Ciccarino, Bianco, Errea, Narang, Bernevig

Approximation is good.

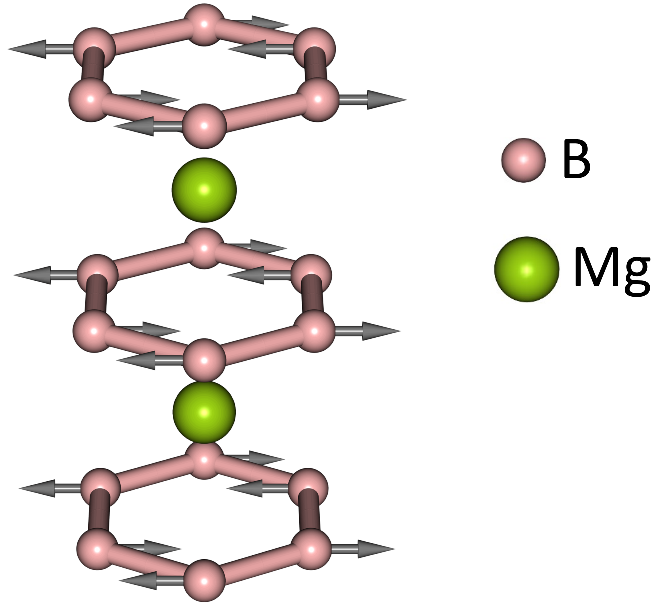


Analytic: $\frac{\lambda_{geo}}{\lambda} \to \frac{\lambda_{topo}}{\lambda} \to \frac{1}{2}$ as $\mu \to 0$



Roughly half of EPC supported by band geometry/topology!

MgB_2: 3D Phonon-mediated Superconductor



P6/mmm

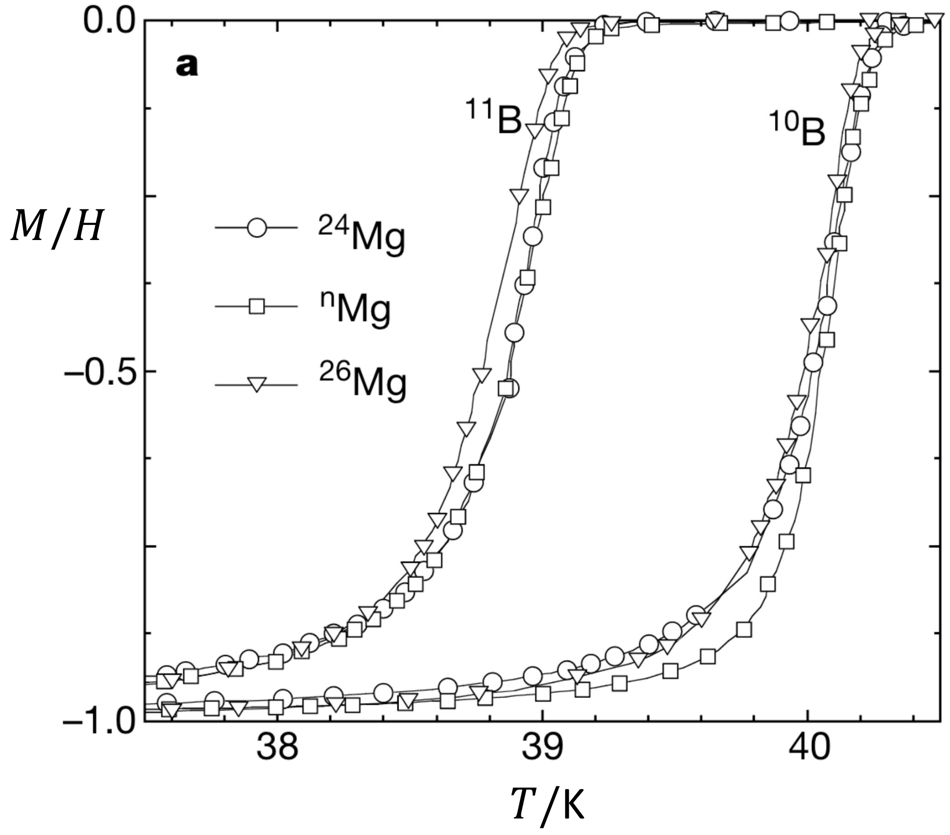
Superconducting $T_c = 39\text{K}$

Nagamatsu, et al. (2001)

Dominant phonons E_{2g}

Kong, et al. (2001)

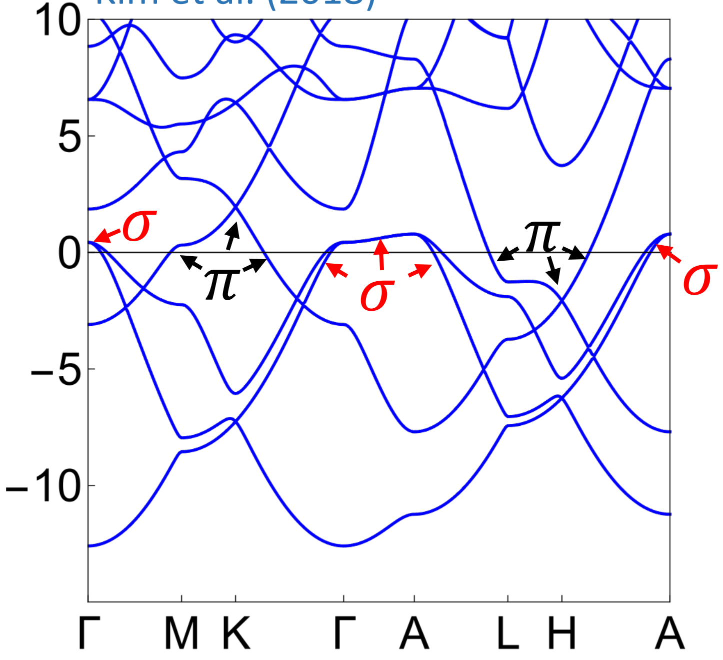
Bud'ko, et al. (2001), Hinks, et al. (2001)

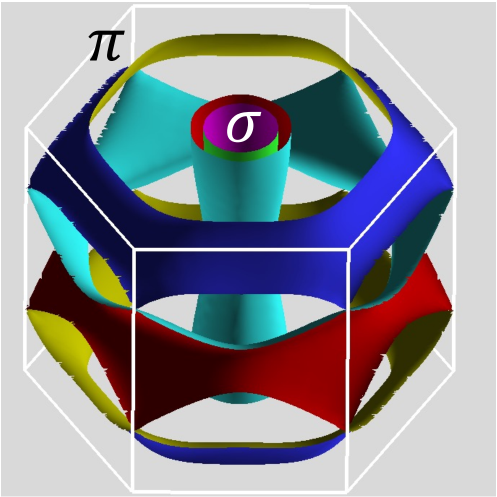


EPC is strong!

MgB_2: Normal phase

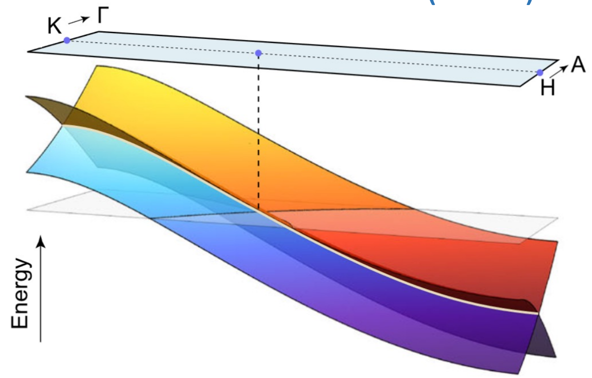
Kim et al. (2018)





- π−bonding: p_z of B

Jin et al. (2019)



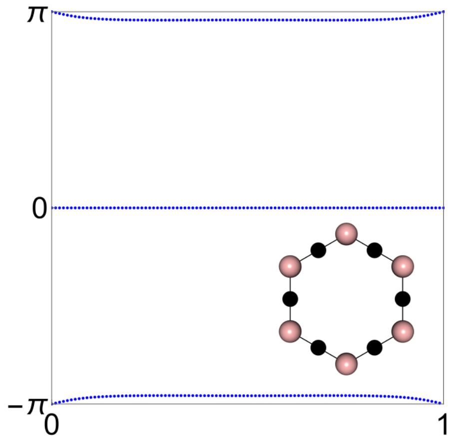
like graphene + k_z dispersion

Nodal lines carry winding numbers

- σ-bonding: p_x, p_y of B

Jiabin Yu, Ciccarino, Bianco, Errea, Narang, BAB

Obstructed atomic limit



Effective Euler number

$$\Delta\mathcal{N} = 1$$

w_2 and $\mathcal{N}$ in other systems (Fang et al, (2015), Zhao, et al. (2017), Ahn, et al. (2018), Ahn, et al. (2019), ...)

MgB_2: Geometric/Topological Contributions to EPC Constant

- $\lambda = \lambda_\pi + \lambda_\sigma \qquad \lambda_{\pi/\sigma} = \lambda_{\pi/\sigma,E} + \lambda_{\pi/\sigma,geo} \qquad \lambda_{\pi/\sigma,geo} \geq \lambda_{\pi/\sigma,topo}$

- $\lambda_{\pi,E}, \lambda_{\pi,geo}, \lambda_{\pi,topo}$ are similar as graphene, $\lambda_{\sigma,E}$ is negligible

- $\lambda_{\sigma,geo} = \mathrm{A} \int_{FS} d\sigma_{\boldsymbol{k}} \frac{\Delta E^2(0)}{|\nabla_{\boldsymbol{k}} E_{n_F}(\boldsymbol{k})|} \sum_{\alpha}^{\text{parity-odd}} \mathrm{Tr}[\boxed{g_{n_F,\alpha}(0)}]$

Orbital-selective Fubini-Study metric

FS+ phonon form factor

- $\lambda_{\sigma,topo} = \mathrm{A}' \left[\int_{FS} d\sigma_{\boldsymbol{k}} \frac{|\nabla_{\boldsymbol{k}} E_{n_F}(\boldsymbol{k})|}{|\boldsymbol{k}_{\parallel}|^2} \right]^{-1} (\Delta\mathcal{N})^2$

MgB_2: Numerical Results

λ ($\lambda^{ab\ initio}$)	0.78 (0.67)	λ_π	0.16	λ_σ	0.62
λ_E	0.07	$\lambda_{\pi,E}$	0.07	$\lambda_{\sigma,E}$	0.00
λ_{geo}	0.71	$\lambda_{\pi,geo}$	0.09	$\lambda_{\sigma,geo}$	0.62
λ_{topo}	0.32	$\lambda_{\pi,topo}$	0.01	$\lambda_{\sigma,topo}$	0.31

- $\frac{\lambda_{geo}}{\lambda} \approx 92\%$, $\frac{\lambda_{topo}}{\lambda} \approx 44\%$
- $\frac{\lambda_{\sigma,geo}}{\lambda} \approx 79\%$, $\frac{\lambda_{\sigma,topo}}{\lambda} \approx 40\%$

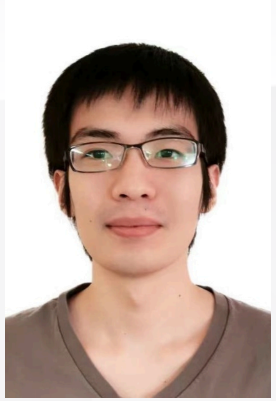
λ mainly from band geometry of σ-bonding

➢ Quantum Geometry Is Fundamental to EPC In Multiband Systems

Kagome SG 191: LEGO building blocks, soft flat phonons, CDW formation Quantum Geometry In Electron-Phonon Coupling: MgB2, Graphene, and Kagome Materials ScV6Sn6

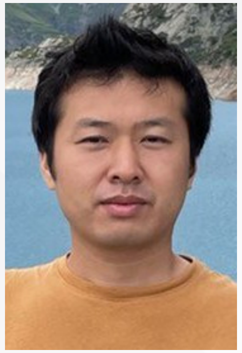
Thy: arXiv:2304.09173

Exp: arXiv:2304.09173


Haoyu Hu


Yi Jiang


Dumitru Calugaru


Xiaolong Feng


D Subires


Santiago Blanco-Canosa


Claudia Felser

A. Korshunov, A. Rajapitamahuni, C. Yi, **S. Roychowdhury**, M. G. Vergniory, J. Strempfer, **C. Shekhar**, E. Vescovo, D. Chernyshov, A. H. Said, A. Bosak


Jiabin Yu


Christopher Ciccarino


Raffaello Bianco


Ion Errea

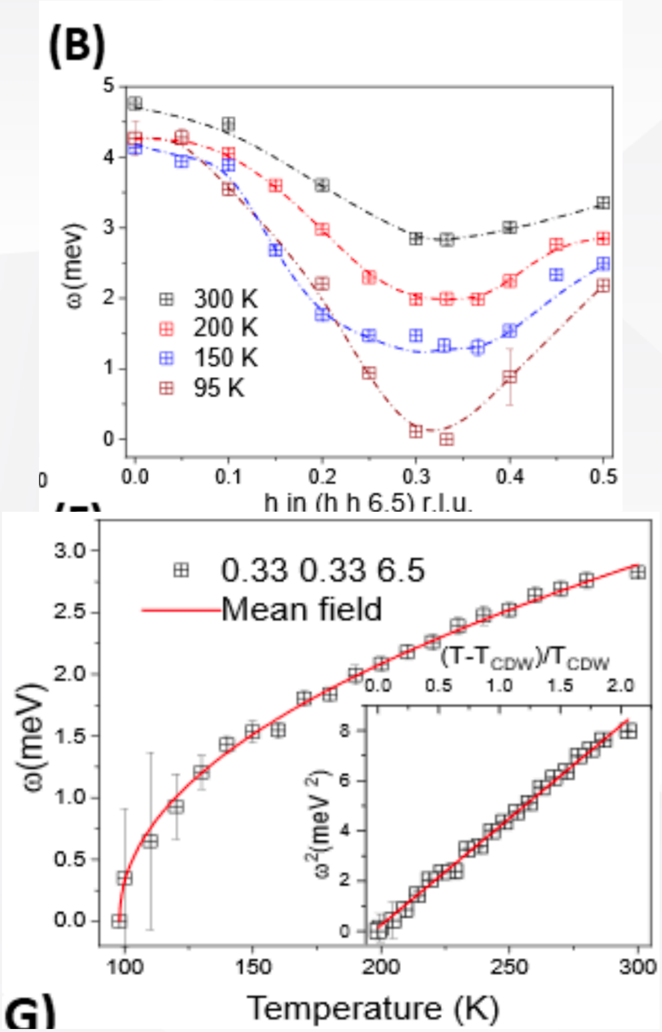

Prineha Narang

arXiv:2305.02340

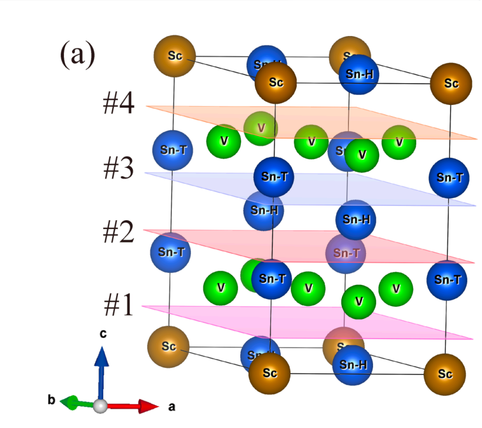

Jonah H. Arbeitman

El-Phonon Coupling Quantum Geometric Approximation in other Systems (David Mandrus Compound)

ScV6Sn6: Remarkable CDW



- BS/orbitals very similar to MgFe6Ge6 BUT different electron number => Fermi level NOT at flat bands



➢Multiple phonons near $H = (1/3,1/3,1/2)$ soften as T lowered

➢H phonon collapses at CDW Tc= 95 K (w mean-field)

➢CDW appears at different wavevector $\bar{K} = (1/3,1/3,1/3)$ (1st-order transition)

Puzzle

Exp: arXiv: 2304.09173 (2023).
A. Korshonov, H. Hu, et al & B. A. B, S. Blanco-Canosa

Thy: arXiv: 2305.15469 (2023)
H. Hu, Y. Jiang, D. Calugaru, X. Feng, et al & B. A. B.

X

Origin of soft phonon

➢Electron-phonon coupling from new (Gaussian) approximation (explained soon)

Jiabin Yu, et al, arXiv: 2305.15469 (2023) MgB2, Graphene

➢Dominant electron-phonon coupling

$$\tilde{g}\sum_{\mathbf{R},\sigma} u_{ez}(\mathbf{R}) c^\dagger_{\mathbf{R},e,\sigma} c_{\mathbf{R},e,\sigma}$$

$$c_{\mathbf{R},e,\sigma} = \frac{1}{\sqrt{2}}\left(c_{\mathbf{R},(Sn_1^T,p_z),\sigma} - c_{\mathbf{R},(Sn_2^T,p_z),\sigma}\right);$$

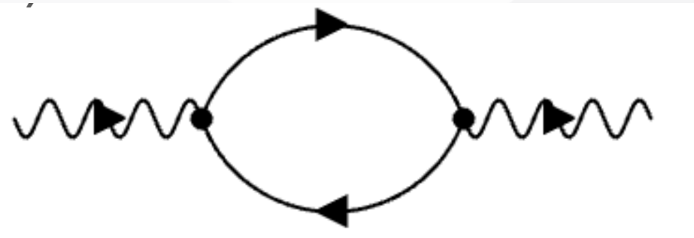
$$u_{ez}(\mathbf{R}) = \frac{1}{\sqrt{2}}(u_{Sn_1^T,z}(\mathbf{R}) - u_{Sn_2^T,z}(\mathbf{R}))$$

➢Quantum geometry: Wannier centers of mirror-even electron orbitals and mirror-even phonon orbitals are the same.

➢Strong 'on-site' coupling between two molecular orbitals with same Wannier center

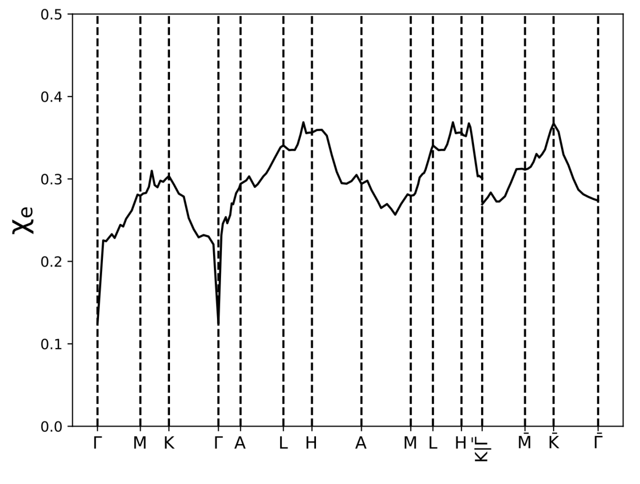
Origin of soft phonon

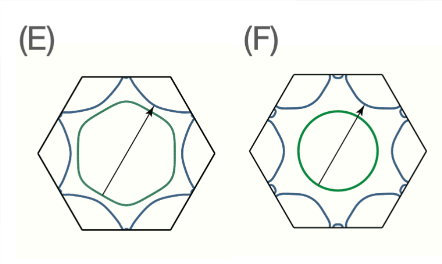
➢One-loop correction to the phonon propagators



$$\Phi^{corr}_{ez,ez}(\mathbf{q}) = -\tilde{g}^2 \chi_e(\mathbf{q}, i\Omega_n = 0)$$

➢The behavior of charge susceptibility of mirror-even electron orbital

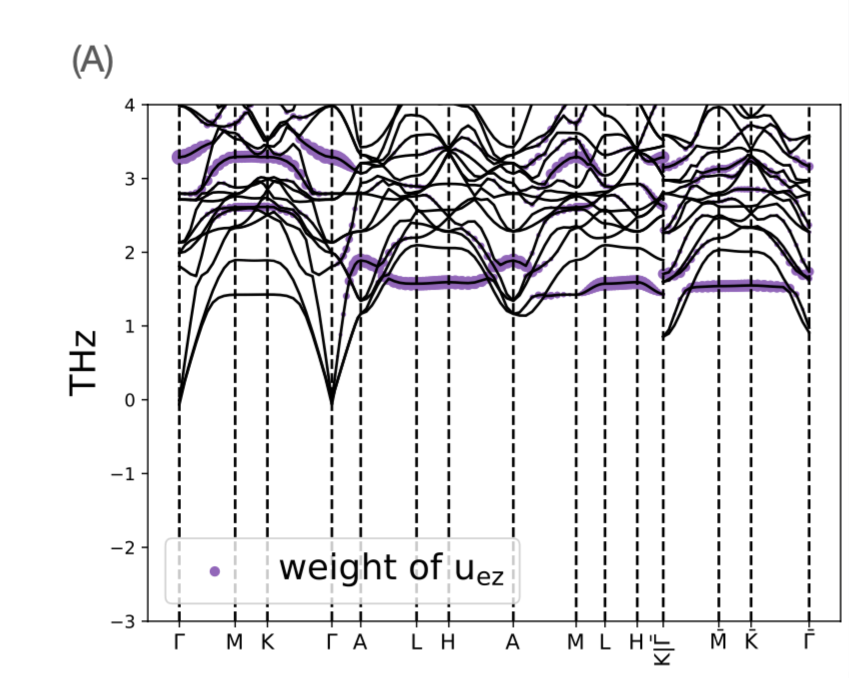


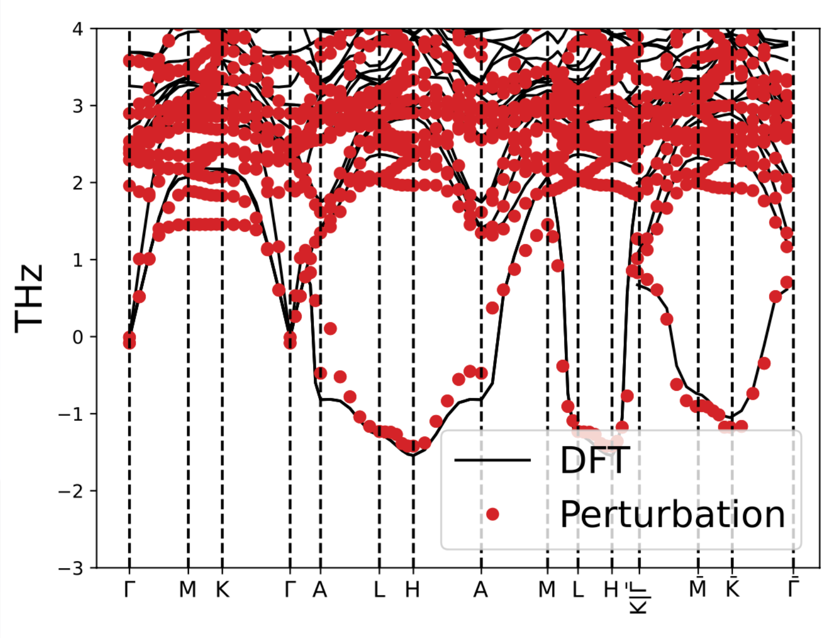


$$\chi_e(\mathbf{R}) \approx \chi^{on\text{-}site}\delta_{\mathbf{R},\mathbf{0}} + \sum_{i=1,\ldots,6} \chi^{xy}\delta_{\mathbf{R},\mathbf{R}_i^{xy}} + \sum_{i=1,2} \chi^{z}\delta_{\mathbf{R},\mathbf{R}_i^{z}}$$

Origin of soft phonon

Low-T phonon = Non-interaction (high T) phonon + correction from electron-phonon coupling





High-T (non-interacting) phonon spectrum DFT

Almost flat

Low-T phonon spectrum from DFT and analytic one-loop calculation

Weak in-plane dispersion from the one-loop correction

X


Dumitru Calugaru


Jonah H. Arbeitman


Jiabin Yu


Haoyu Hu


Yi Jiang