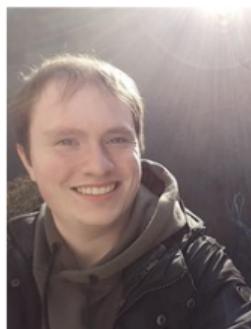


Hamburg - Computational Condensed Matter Theory

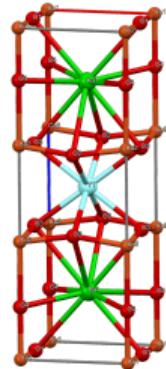


Uppsala - Quantum Matter Theory



Routes to High T_C

Explore classes of materials that show high T_C
(e.g. Cuprates)

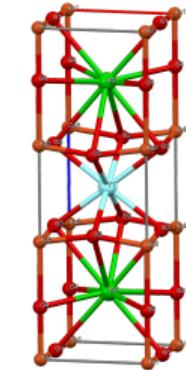


YBCO unit cell¹

¹By Ben Mills - Own work, Public Domain, [Wikimedia Commons](#)

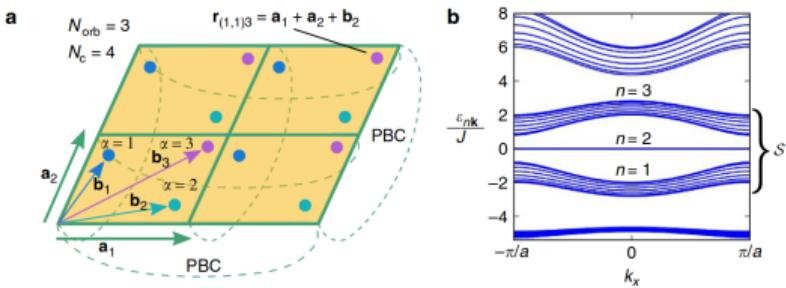
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YBCO unit cell¹

Simple, tunable systems based on flat bands



Harper-Hubbard model²

¹By Ben Mills - Own work, Public Domain, [Wikimedia Commons](#)

²Peotta and Törmä, [10.1038/ncomms9944](https://doi.org/10.1038/ncomms9944) (2015)

Why Flat Bands?

BCS theory for dispersive bands:

$$T_C \propto \exp\left(-\frac{1}{Un_0(E_F)}\right) \quad (1)$$

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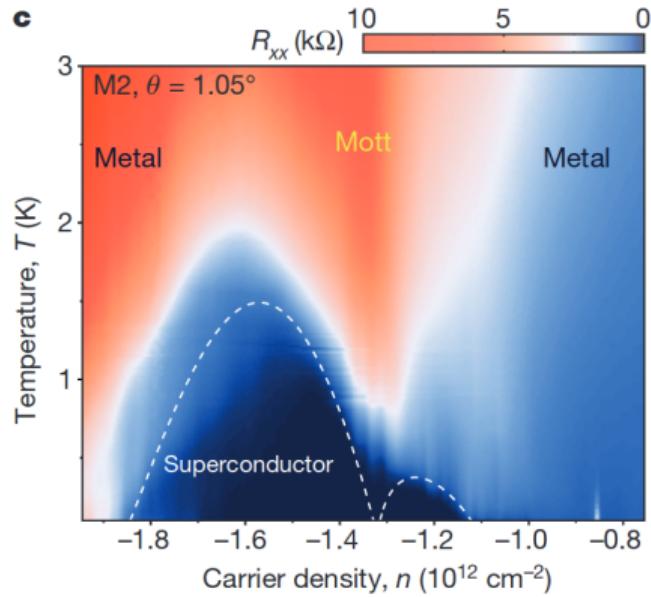
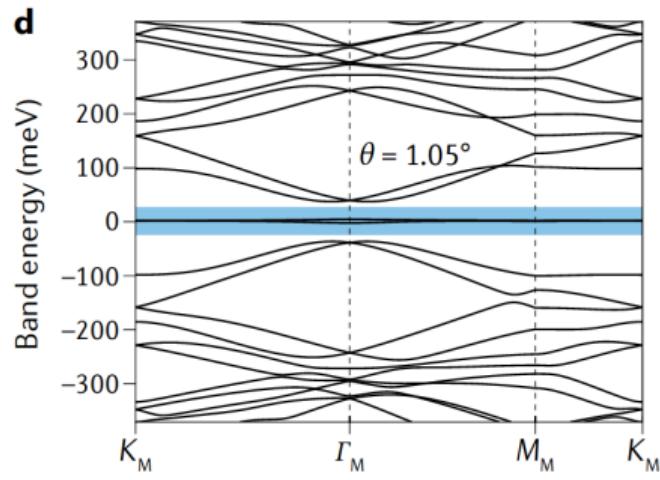
Exponentially enhanced in comparison to dispersive bands

Due to:

- ▶ High DOS near Fermi level
- ▶ Vanishing kinetic energy, interaction effects dominate

Twisted Bilayer Graphene³⁴

Example for tunable flat-band system: flat bands can be tuned by changing the twist angle



³Cao et al., 10.1038/nature26160 (2018)

⁴Band structure taken from Törmä, Peotta, and Bernevig, 10.1038/s42254-022-00466-y (2022)

Transport in Flat-Band Systems

Below T_C , there is pairing. Does not necessarily mean there is a supercurrent!

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$$\mathbf{j} = -D_S \mathbf{A} \quad (3)$$

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In single-band BCS theory:

$$D_{S,ij} \sim \sum_{\mathbf{k}} \frac{\partial^2 \epsilon}{\partial k_i \partial k_j} \quad \text{Vanishes for a flat band!} \quad (4)$$

And Yet!

ARTICLE

Received 17 Sep 2015 | Accepted 19 Oct 2015 | Published 20 Nov 2015

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OPEN

Superfluidity in topologically nontrivial flat bands

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Show⁵ there are actually 3 terms making up D_S :

- Conventional:

$$D_{S,1,ij} \sim \sum_{\mathbf{k}} \frac{\partial^2 \epsilon}{\partial k_i \partial k_j} \quad (5)$$

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- ▶ Geometric:

$$D_{S,2,ij} + D_{S,3,ij} \sim U \mathcal{M}_{ij}^R \quad (6)$$

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\mathcal{M}_{ij}^R related to a quantity called the **quantum metric** $g_{ij}(\mathbf{k})$:

$$\mathcal{M}_{ij}^R \sim \int_{\text{BZ}} d^2\mathbf{k} g_{ij}(\mathbf{k}) \quad (7)$$

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with projector to the band n of interest $P(\mathbf{k}) = |u_{n\mathbf{k}}\rangle \langle u_{n\mathbf{k}}|$, Bloch functions $|u_{n\mathbf{k}}\rangle$

Determining factor for finite quantum metric: mixing between bands

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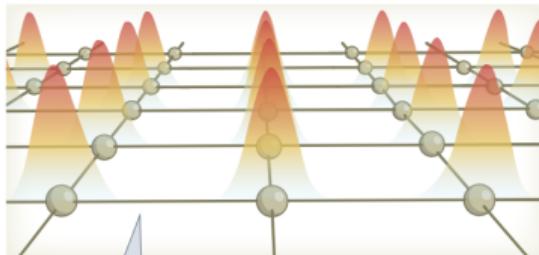
with projector to the band n of interest $P(\mathbf{k}) = |u_{n\mathbf{k}}\rangle \langle u_{n\mathbf{k}}|$, Bloch functions $|u_{n\mathbf{k}}\rangle$

Determining factor for finite quantum metric: mixing between bands

finite quantum metric \rightarrow finite overlap of Wannier functions
 \rightarrow non-localized Cooper pairs \rightarrow transport in the system is possible

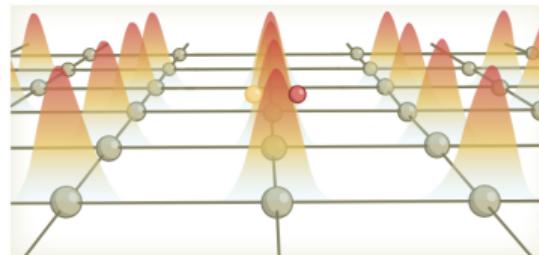
Wannier Overlap and Transport⁶

a Non-interacting particles



Vanishing overlap → localization, flat band

b Interacting particles

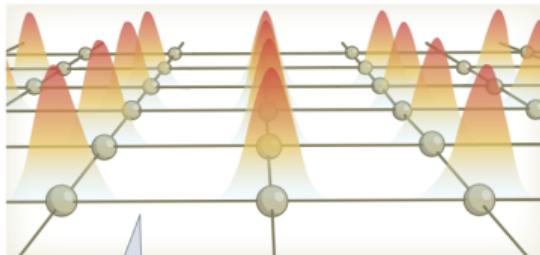


No overlap, remain localized

⁶Graphic from Törmä, Peotta, and Bernevig, 10.1038/s42254-022-00466-y (2022)

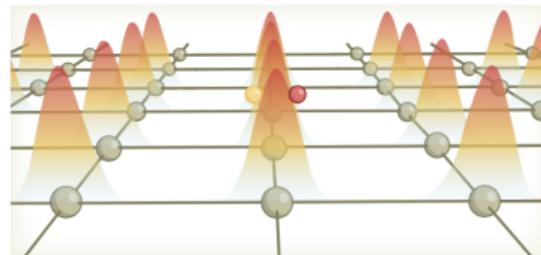
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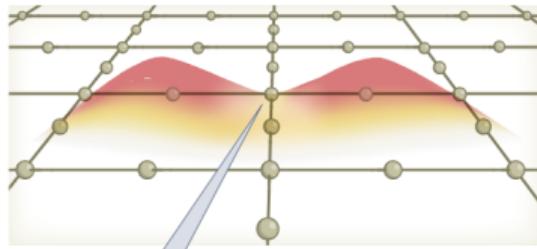


Vanishing overlap → localization, flat band

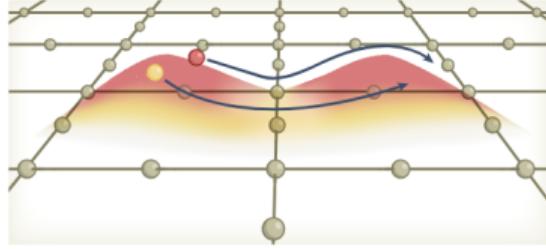
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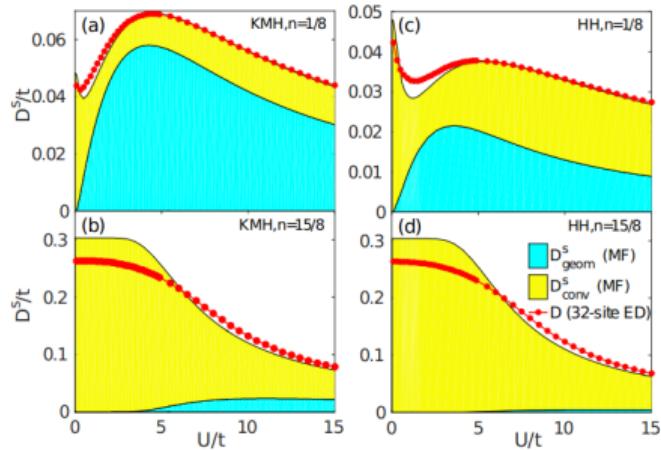
Large overlap and destructive interference → localization, flat band



Interference distorted by interactions → not localized

⁶Graphic from Törmä, Peotta, and Bernevig, 10.1038/s42254-022-00466-y (2022)

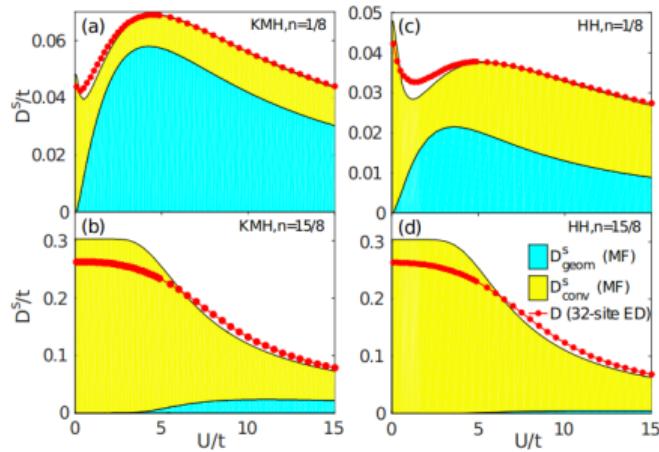
Examples



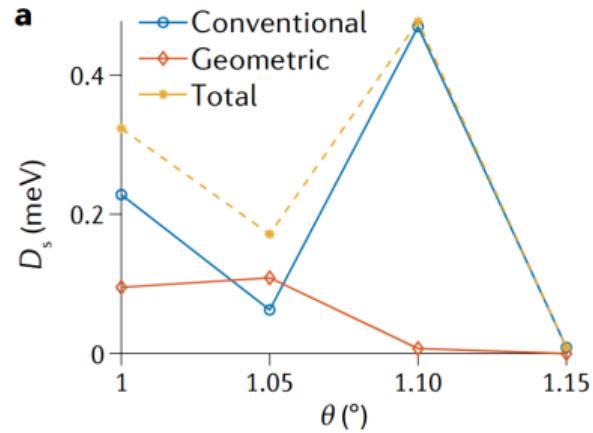
Hubbard models⁷ tuned to flat (top) and dispersive band (bottom)

⁷Liang et al., 10.1103/PhysRevB.95.024515 (2017)

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Hubbard models⁷ tuned to flat (top) and dispersive band (bottom)

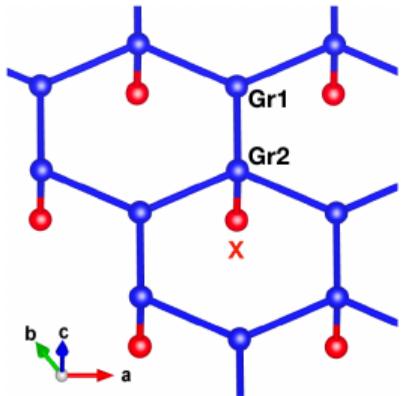


Twisted bilayer Graphene⁸: geometric contribution overtakes at magic angle 1.05°

⁷Liang et al., 10.1103/PhysRevB.95.024515 (2017)

⁸Törmä, Peotta, and Bernevig, 10.1038/s42254-022-00466-y (2022)

My Model

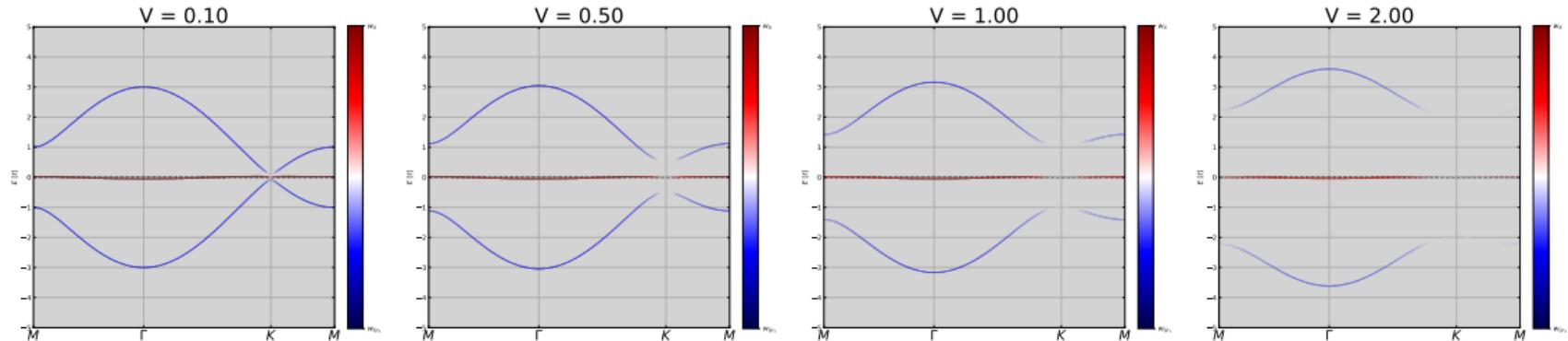


- ▶ Hexagonal lattice with an additional orbital on one of the sites
- ▶ Material motivation: Graphene on top of a substrate

Non-interacting Hamiltonian:

$$H_0 = -t_X \sum_{\langle ij \rangle, \sigma\sigma'} d_{i,\sigma}^\dagger d_{j,\sigma'} - t_{\text{Gr}} \sum_{\langle ij \rangle_{\text{Gr}}, \sigma\sigma'} c_{i,\sigma}^\dagger c_{j,\sigma'} + V \sum_{i,\sigma\sigma'} d_{i,\sigma}^\dagger c_{i,\sigma'}^{(\text{Gr2})} \quad (9)$$

Band structure ($t_{Gr} = 1$, $t_X = 0.01$):



- ▶ Flat band
- ▶ Bands are mixed between the Graphene and X orbitals
- ▶ V determines this mixing

Add attractive Hubbard interaction:

$$H_{\text{int}} = -U_X \sum_i d_{i,\uparrow}^\dagger d_{i,\downarrow}^\dagger d_{i,\downarrow} d_{i,\uparrow} - U_{\text{Gr}} \sum_i c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger c_{i,\downarrow} c_{i,\uparrow} \quad (10)$$

Mean-field decoupling:

$$H_{\text{int}} \approx \sum_{\alpha, \mathbf{k}} (\Delta_\alpha c_{\mathbf{k}\alpha\uparrow}^\dagger c_{-\mathbf{k}\alpha\downarrow}^\dagger + \Delta_\alpha^* c_{-\mathbf{k}\alpha\downarrow} c_{\mathbf{k}\alpha\uparrow}) \quad (11)$$

with

$$\Delta_\alpha = -U_\alpha \sum_{\mathbf{k}'} \langle c_{-\mathbf{k}'\alpha\downarrow} c_{\mathbf{k}'\alpha\uparrow} \rangle \quad (12)$$

Write:

$$H_{\text{MF}} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} \mathcal{H}(\mathbf{k}) \Psi_{\mathbf{k}} \quad (13)$$

with Nambu spinor

$$\Psi_{\mathbf{k}} = \begin{pmatrix} c_{1,\mathbf{k}\uparrow} \\ c_{2,\mathbf{k}\uparrow} \\ c_{3,\mathbf{k}\uparrow} \\ c_{1,-\mathbf{k}\downarrow}^{\dagger} \\ c_{2,-\mathbf{k}\downarrow}^{\dagger} \\ c_{3,-\mathbf{k}\downarrow}^{\dagger} \end{pmatrix} \quad (14)$$

and BdG Hamiltonian

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} H_{0,\uparrow}(\mathbf{k}) - \mu & \Delta \\ \Delta^{\dagger} & -H_{0,\downarrow}^*(-\mathbf{k}) + \mu \end{pmatrix} \quad (15)$$

Superfluid weight:

$$D_{S,ij} = \sum_{\mathbf{k}} \sum_{m,n,p,q} C_{pq}^{mn} {}_{\uparrow} \langle m | \partial_i H_{0\uparrow}(\mathbf{k}) | n \rangle {}_{\uparrow} {}_{\downarrow} \langle q | \partial_j H_{0\downarrow}(-\mathbf{k}) | p \rangle {}_{\downarrow} \quad (16)$$

C_{pq}^{mn} depends on the eigenvalues and eigenvectors of the BdG Hamiltonian, $|m\rangle_\sigma$ are the Bloch functions

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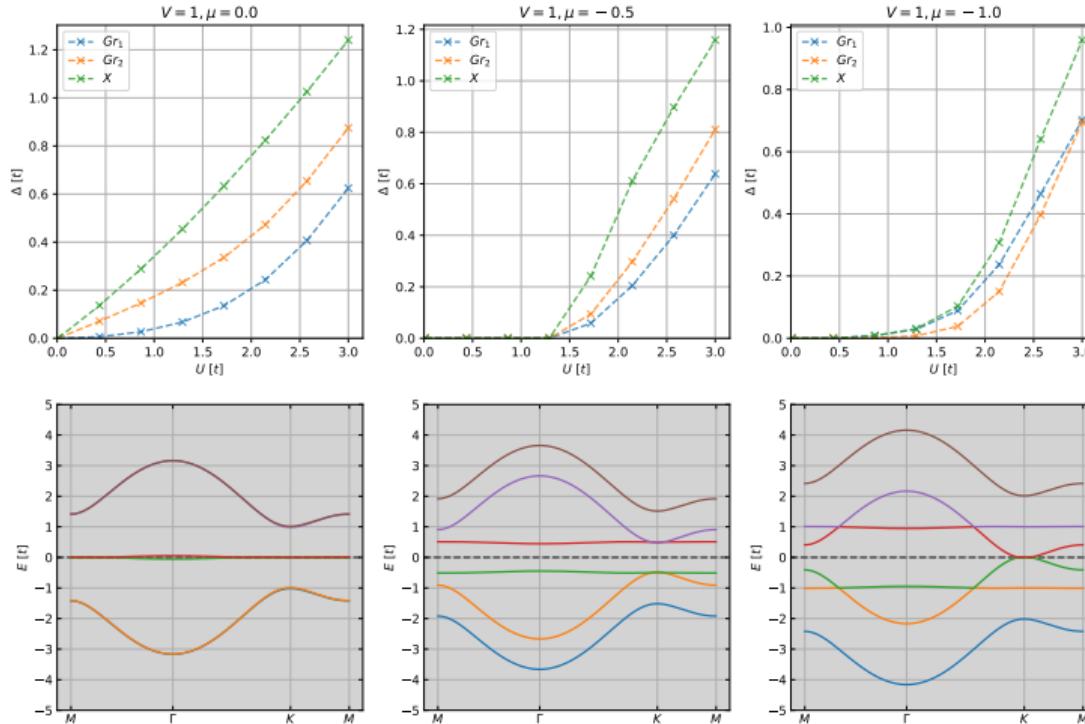
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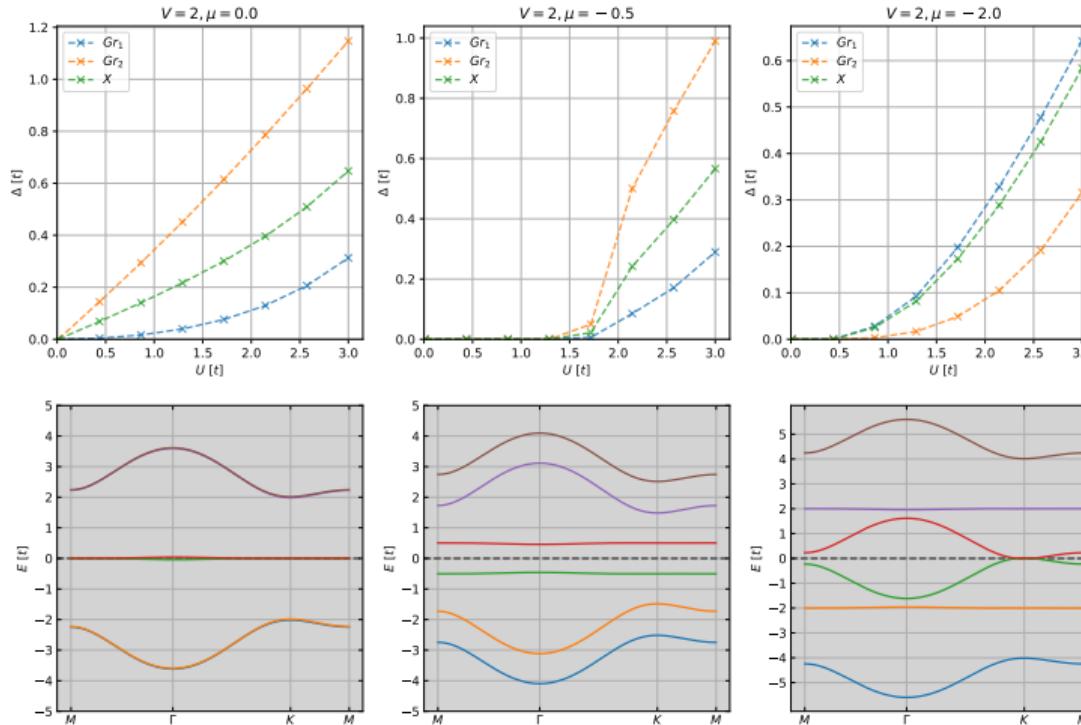
Self-consistently find Δ_α : minimize free energy

$$F = - \sum_{\mathbf{k}, i \in \text{occ}} |E_{\mathbf{k},i}| + \sum_\alpha \frac{|\Delta_\alpha|^2}{U_\alpha} \quad (17)$$

Results



Results



Outlook

Outlook

Bypassing the lattice BCS-BEC crossover in strongly correlated superconductors: resilient coherence from multiorbital physics

Niklas Witt^{1,2,*}, Yusuke Nomura³, Sergey Brener,¹ Ryotaro Arita^{4,5}, Alexander I. Lichtenstein^{1,2} and Tim O. Wehling^{1,2}

¹*Institute of Theoretical Physics, University of Hamburg, Notkestraße 9-11, 22607 Hamburg, Germany*

²*The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22607 Hamburg, Germany*

³*Institute for Materials Research (IMR), Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan*

⁴*Research Center for Advanced Science and Technology,*

The University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8904, Japan

⁵*RIKEN Center for Emergent Matter Science (CEMS), 2-1 Hirosawa, Wako, Saitama 351-0198, Japan*

(Dated: April 5, 2024)

Superconductivity emerges from the spatial coherence of a macroscopic condensate of Cooper pairs. Increasingly strong binding and localization of electrons into these pairs compromises the condensate's phase stiffness, thereby limiting critical temperatures – a phenomenon known as the BCS-BEC crossover in lattice systems. In this study, we report on an enhancement of superconductivity beyond the limits of the lattice BCS-BEC crossover realized in a multiorbital model of alkali-doped fullerides (A_3C_{60}). We show how strong correlations and multiorbital effects lead into a localized superconducting regime characterized by a short coherence length but robust stiffness and a domeless rise in critical temperature with increasing pairing interaction. These insights are derived from the development of a theoretical framework to calculate the fundamental length scales of superconductors, namely the coherence length (ξ_0) and the London penetration depth (λ_L), in microscopic theories and from first principles, even in presence of strong electron correlations.

Flat-band ratio and quantum metric in the superconductivity of modified Lieb lattices

Reko P. S. Penttilä,¹ Kukka-Emilia Huhtinen,^{1, 2} and Päivi Törmä^{1,*}

¹*Department of Applied Physics, Aalto University School of Science, FI-00076 Aalto, Finland*

²*Institute for Theoretical Physics, ETH Zurich, CH-8093, Switzerland*

Flat bands may offer a route to high critical temperatures of superconductivity. It has been predicted that the quantum geometry of the bands as well as the ratio of the number of flat bands to the number of orbitals determine flat band superconductivity. However, such results have assumed at least one of the following: an isolated flat band, zero temperature, mean-field theory, and/or uniform pairing. Here, we explore flat band superconductivity when these assumptions are relaxed. We consider an attractive Hubbard model for different extensions of the Lieb lattice. The superconducting order parameter, critical temperature, superfluid weight, and Berezinskii-Kosterlitz-Thouless temperature are calculated within dynamical mean-field theory. We find that while the flat-band ratio and quantum geometry are good indicators of superconductivity near zero temperature, at finite temperatures the behavior is more complicated. Our results suggest that the properties of the other bands near the flat band(s) are crucial.

Summary

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- ▶ Superfluid weight ($\hat{=}$ capacity to host supercurrent) is determined by quantum geometry
- ▶ Quantum geometry: distances in the space formed by electronic Bloch functions
- ▶ My work so far: solved system for gap self-consistently, found that the pairing is different in the three orbitals