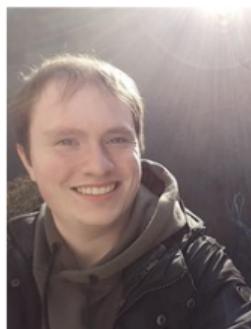


## Hamburg - Computational Condensed Matter Theory



## Uppsala - Quantum Matter Theory



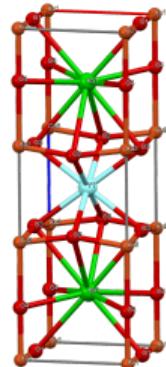
# Routes to High $T_C$

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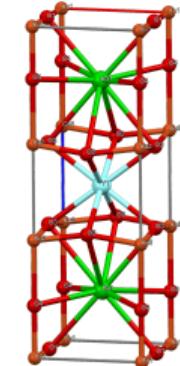
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<sup>1</sup>By Ben Mills - Own work, Public Domain, [Wikimedia Commons](#)

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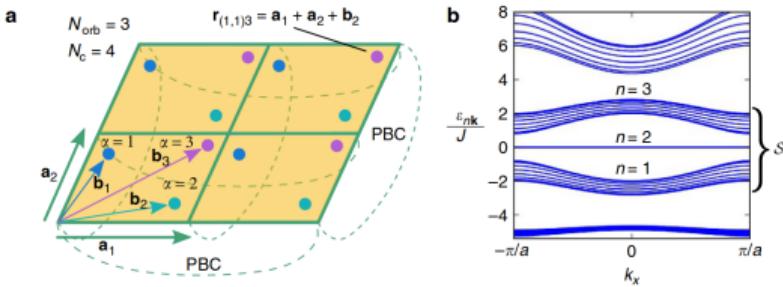
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YBCO unit cell<sup>1</sup>

Simple, tunable systems based on flat bands



Harper-Hubbard model<sup>2</sup>

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

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

# Why Flat Bands?

BCS theory for dispersive bands:

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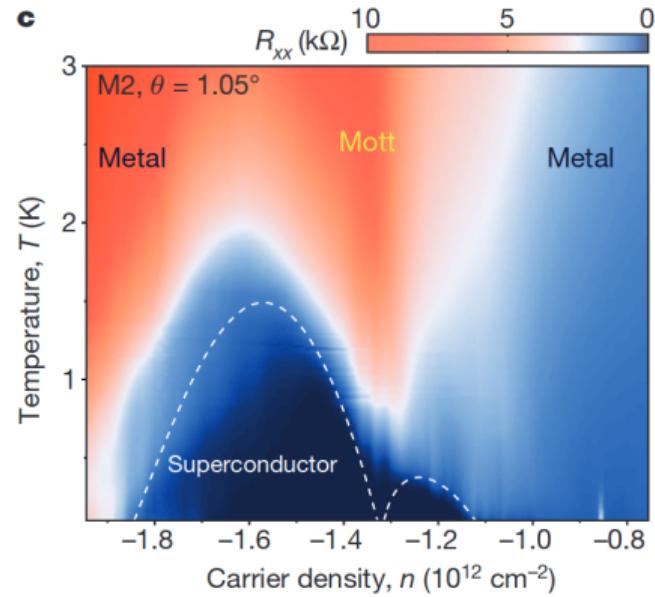
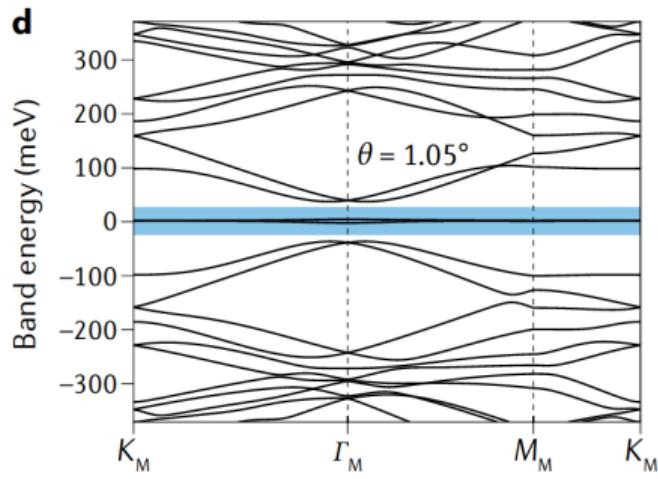
Exponentially enhanced in comparison to dispersive bands

Due to:

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

# Twisted Bilayer Graphene

Example for tunable flat-band system: flat bands can be tuned by changing the twist angle<sup>34</sup>



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

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

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

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London equation:

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

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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

DOI: 10.1038/ncomms9944

OPEN

## Superfluidity in topologically nontrivial flat bands

Sebastiano Peotta<sup>1</sup> & Päivi Törmä<sup>1,2</sup>

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Show<sup>5</sup> there are actually 3 terms making up  $D_S$ :

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- ▶ Geometric:

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

---

<sup>5</sup>Peotta and Törmä, 10.1038/ncomms9944 (2015)

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

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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  $|u_{n\mathbf{k}}\rangle$

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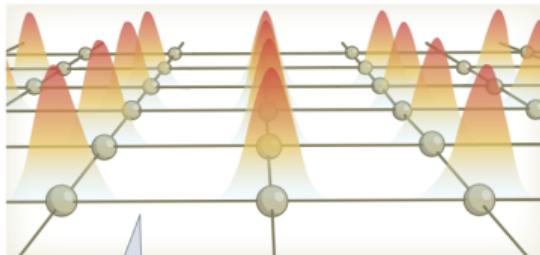
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finite quantum metric  $\rightarrow$  finite overlap of Wannier functions  
 $\rightarrow$  non-localized Cooper pairs  $\rightarrow$  transport in the system is possible

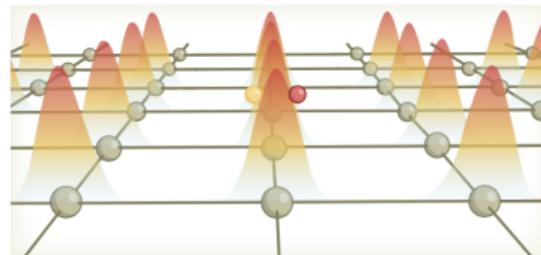
# Wannier Overlap and Transport<sup>6</sup>

**a** Non-interacting particles



Vanishing overlap → localization, flat band

**b** Interacting particles

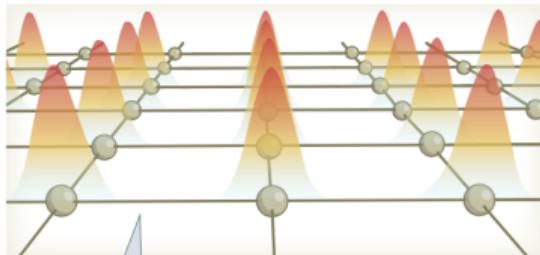


No overlap, remain localized

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

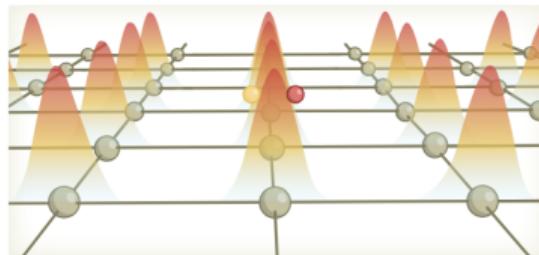
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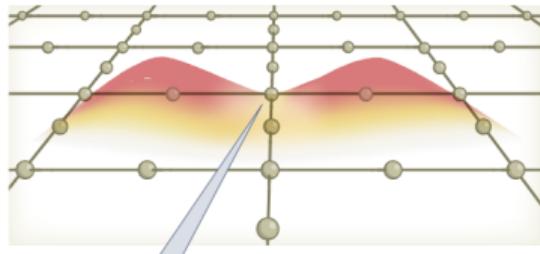


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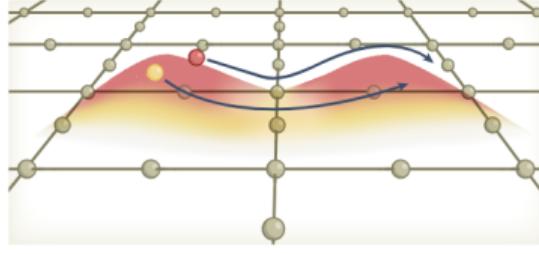
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No overlap, remain localized



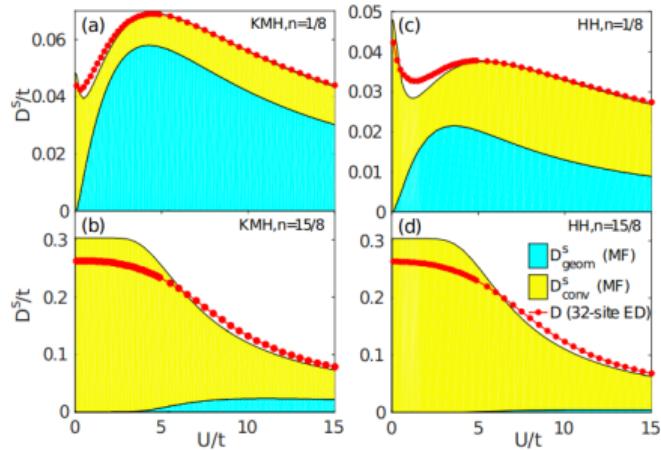
Large overlap and destructive interference → localization, flat band



Interference distorted by interactions → not localized

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

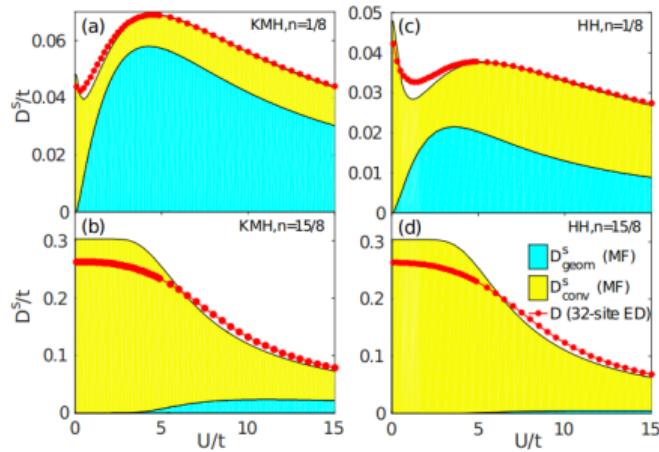
# Examples



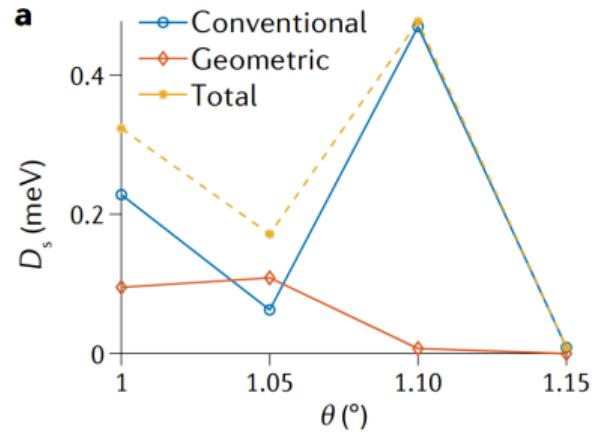
Hubbard models<sup>7</sup> tuned to flat (top) and dispersive band (bottom)

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# Examples



Hubbard models<sup>7</sup> tuned to flat (top) and dispersive band (bottom)

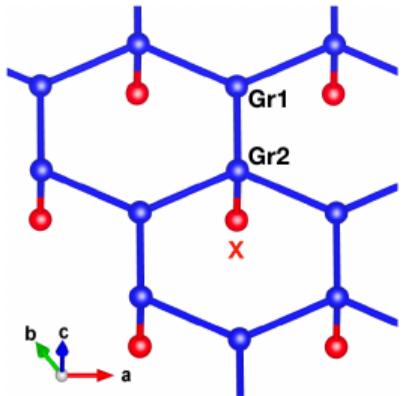


Twisted bilayer Graphene<sup>8</sup>: geometric contribution overtakes at magic angle  $1.05^\circ$

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

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

# My Model

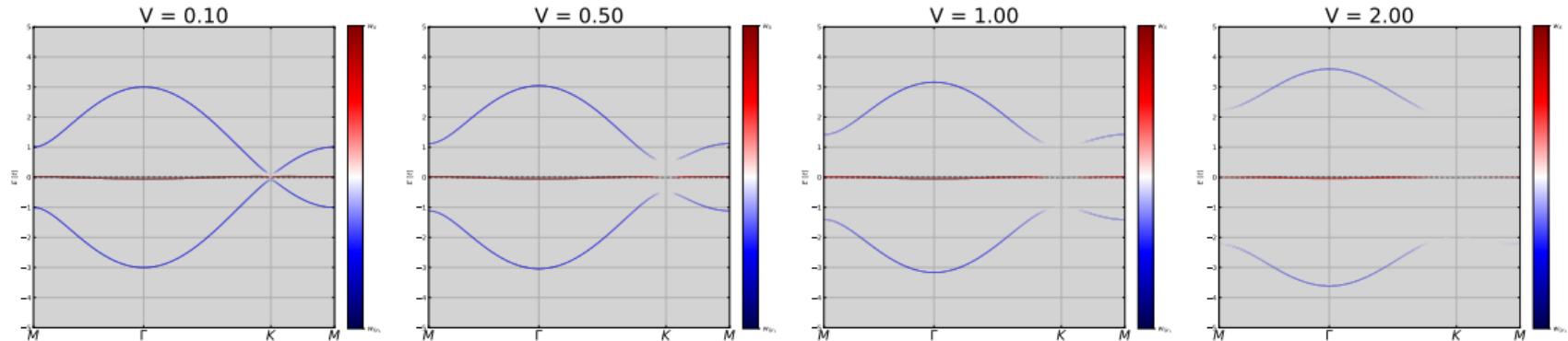


- ▶ Hexagonal lattice with an additional orbital on one of the sites
- ▶ Material motivation: Graphene on top of a substrate

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 ( $U > 0$ ) Hubbard interaction:

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

Mean-field decoupling:

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

with

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

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

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

Task now: find  $\Delta$  self-consistently

Try transforming into band basis and deriving gap equation(s)?

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} \epsilon_{\mathbf{k}} - \mu & G^\dagger \Delta G \\ G^\dagger \Delta^\dagger G & -\epsilon_{\mathbf{k}} + \mu \end{pmatrix} \quad (16)$$

where  $G$  are made up of the Bloch functions

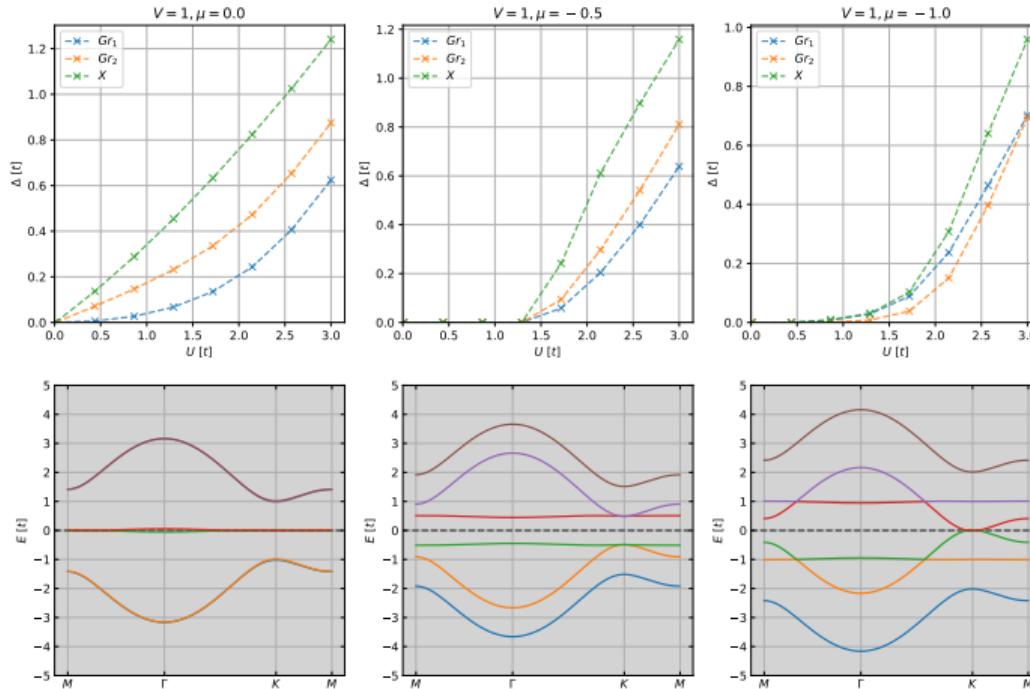
So no closed form like

$$E_{n,\pm}(\mathbf{k}) = \pm \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + |\Delta|^2} \quad (17)$$

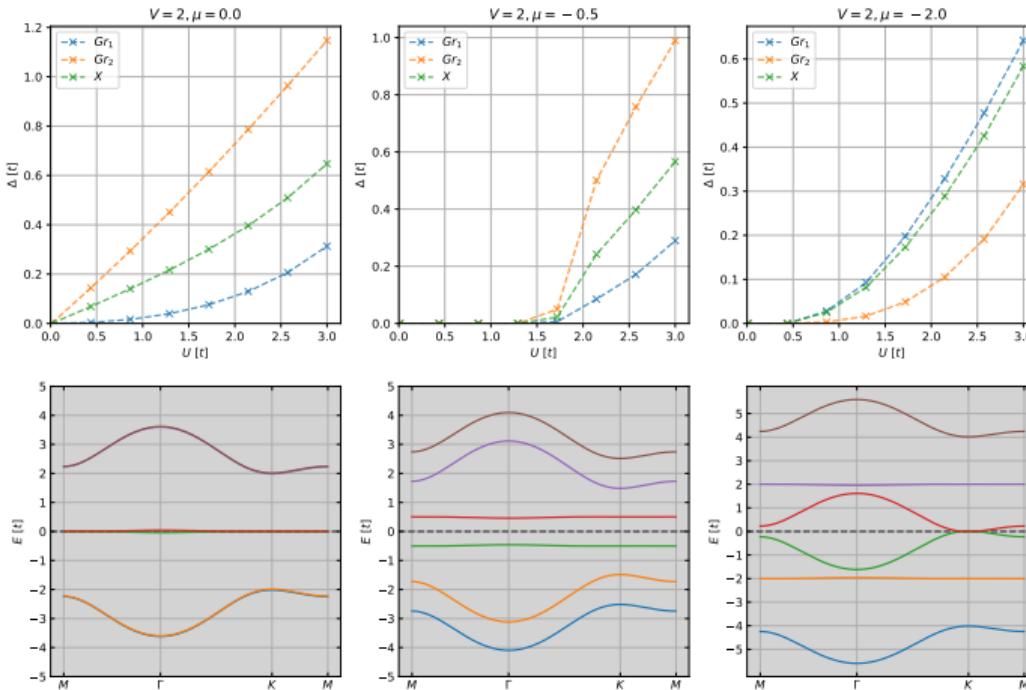
for the BdG energies

- ▶ Mean-field decoupling of interaction terms
- ▶ Self-consistently solve for SC gaps
- ▶ Diagonalize BdG Hamiltonian
- ▶ Calculate superfluid weight from

# Results



# Results



# Outlook

Newer work shows<sup>9</sup>: connection with

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<sup>9</sup>Huhtinen et al., 10.1103/PhysRevB.106.014518 (2022)

# Outlook

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

Niklas Witt<sup>1,2,\*</sup>, Yusuke Nomura<sup>3</sup>, Sergey Brener,<sup>1</sup> Ryotaro Arita<sup>4,5</sup>, Alexander I. Lichtenstein<sup>1,2</sup> and Tim O. Wehling<sup>1,2</sup>

<sup>1</sup>*Institute of Theoretical Physics, University of Hamburg, Notkestraße 9-11, 22607 Hamburg, Germany*

<sup>2</sup>*The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22607 Hamburg, Germany*

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

<sup>4</sup>*Research Center for Advanced Science and Technology,*

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

<sup>5</sup>*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 fullerenes ( $A_3C_{60}$ ). 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 ( $\xi_0$ ) and the London penetration depth ( $\lambda_L$ ), in microscopic theories and from first principles, even in presence of strong electron correlations.

- ▶ DMFT calculations on  $A_3C_{60}$ , getting coherence length and London penetration depth from a finite-momentum constraint on the pairing<sup>10</sup>

<sup>10</sup>Witt et al., 10.48550/arXiv.2310.09063 (2024)

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

Reko P. S. Penttilä,<sup>1</sup> Kukka-Emilia Huhtinen,<sup>1, 2</sup> and Päivi Törmä<sup>1,\*</sup>

<sup>1</sup>*Department of Applied Physics, Aalto University School of Science, FI-00076 Aalto, Finland*

<sup>2</sup>*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.

- ▶ DMFT on Lieb lattice (Flat band system), getting superfluid weight, analysing geometric contribution for finite temperature<sup>11</sup>

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<sup>11</sup>Penttilä, Huhtinen, and Törmä, 10.48550/arXiv.2404.12993 (2024)

# Summary

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- ▶ My work so far: