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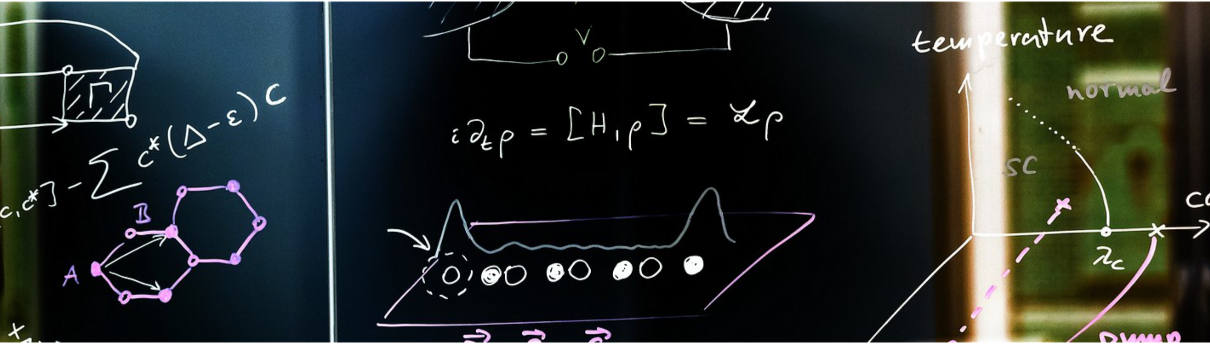


Tjark Sievers – I. Institute of Theoretical Physics

27th June 2024

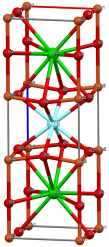
Superconductivity, flat bands and quantum metric

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 cell[1]

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

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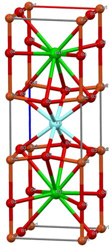
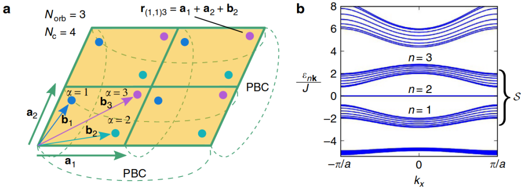


YBCO unit cell[1]

Simple, tunable systems based on flat bands



Harper-Hubbard model[2]

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[1] By Ben Mills - Own work, Public Domain, Wikimedia Commons
[2] Peotta and Törmä, 10.1038/ncomms9944 (2015)

Why Flat Bands?

BCS theory for dispersive bands:

$$T_C \propto \exp\left(-\frac{1}{Un_0(E_\mathrm{F})}\right) \tag{1}$$

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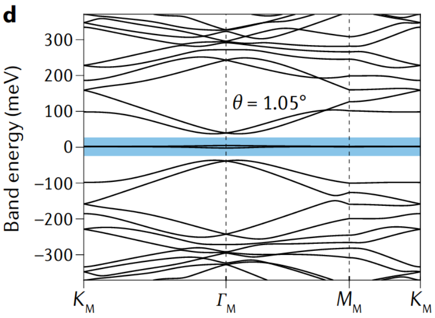
Exponentially enhanced in comparison to dispersive bands

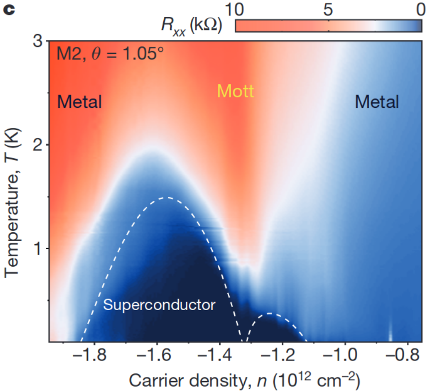
Due to:

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

Twisted Bilayer Graphene[3,4]

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





[3] Cao et al., 10.1038/nature26160 (2018)
[4] Band 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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$$\mathbf{j} = -D_{\mathrm{S}}\mathbf{A} \tag{3}$$

with current density $\mathbf{j}$, vector potential $\mathbf{A}$, superfluid weight D_{S}. Non-zero D_{S} needed for SC

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In single-band BCS theory:

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

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[1] & Päivi Törmä[1,2]

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Show[5] there are actually 3 terms making up D_{S}:

- Conventional:

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- Geometric:

$$D_{\mathrm{S},2,ij} + D_{\mathrm{S},3,ij} \sim U \mathcal{M}_{ij}^{\mathrm{R}} \tag{6}$$

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

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

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$$g_{ij}(\mathbf{k}) = \mathrm{Tr}\left[\partial_i P(\mathbf{k})\, \partial_j P(\mathbf{k})\right] \tag{8}$$

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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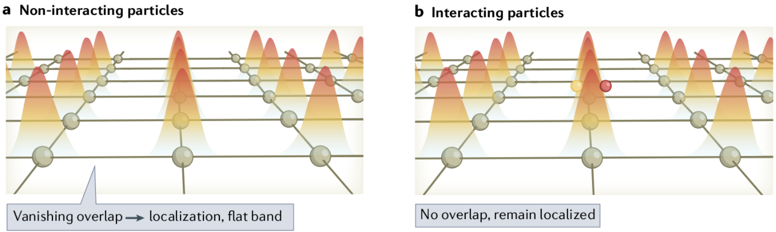
Determining factor for finite quantum metric: mixing between bands

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

Wannier Overlap and Transport[6]



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

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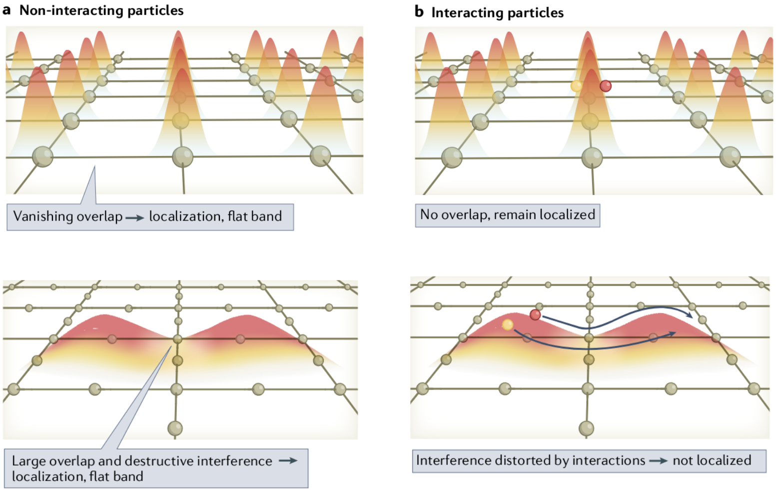

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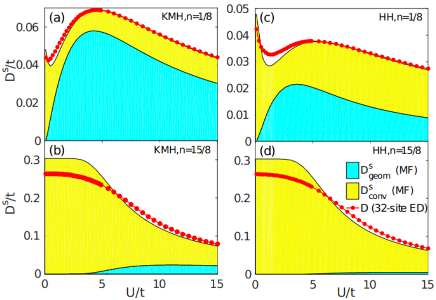
Examples



Hubbard models[7] tuned to flat (top) and dispersive band (bottom)

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

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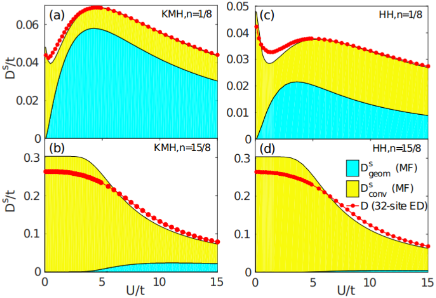

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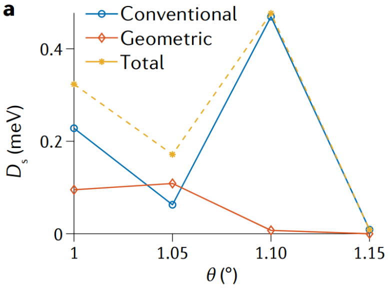
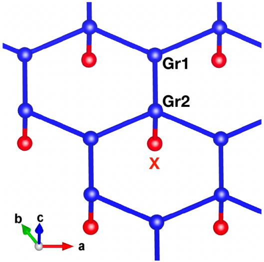


Twisted bilayer Graphene[8]: geometric contribution overtakes at magic angle 1.05°

[7] Liang et al., 10.1103/PhysRevB.95.024515 (2017)
[8] Törmä, Peotta, and Bernevig, 10.1038/s42254-022-00466-y (2022)

My Model

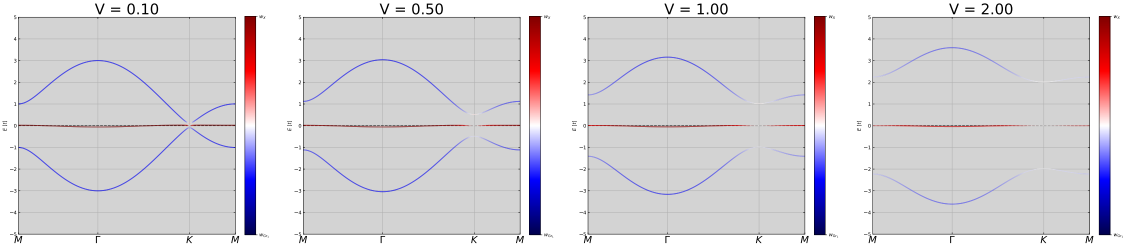


- Hexagonal lattice with an additional orbital on one of the sites
- Material motivation: Graphene on top of a substrate

Non-interacting Hamiltonian:

$$H_0 = -t_{\mathrm{X}} \sum_{\langle ij\rangle,\sigma\sigma'} d^\dagger_{i,\sigma} d_{j,\sigma'} - t_{\mathrm{Gr}} \sum_{\langle ij\rangle_{\mathrm{Gr}},\sigma\sigma'} c^\dagger_{i,\sigma} c_{j,\sigma'} + V \sum_{i,\sigma\sigma'} d^\dagger_{i,\sigma} c^{(\mathrm{Gr2})}_{i,\sigma'} \tag{9}$$

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



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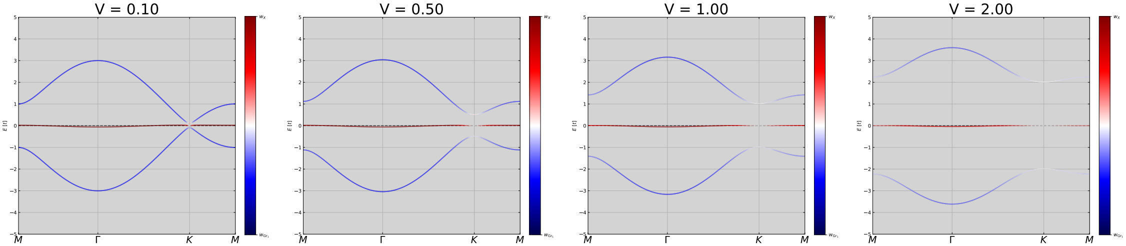

- Flat band
- Bands are mixed between the Graphene and X orbitals
- V determines this mixing

Add attractive Hubbard interaction:

$$H_{\mathrm{int}} = -U_{\mathrm{X}} \sum_i d^\dagger_{i,\uparrow} d^\dagger_{i,\downarrow} d_{i,\downarrow} d_{i,\uparrow} - U_{\mathrm{Gr}} \sum_i c^\dagger_{i,\uparrow} c^\dagger_{i,\downarrow} c_{i,\downarrow} c_{i,\uparrow} \tag{10}$$

Add attractive Hubbard interaction:

$$H_{\text{int}} = -U_{\text{X}} \sum_{i} d_{i,\uparrow}^{\dagger} d_{i,\downarrow}^{\dagger} d_{i,\downarrow} d_{i,\uparrow} - U_{\text{Gr}} \sum_{i} c_{i,\uparrow}^{\dagger} c_{i,\downarrow}^{\dagger} c_{i,\downarrow} c_{i,\uparrow} \tag{10}$$

Mean-field decoupling:

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

with

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

Write:

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

with Nambu spinor

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

and BdG Hamiltonian

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

Superfluid weight[9]:

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

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

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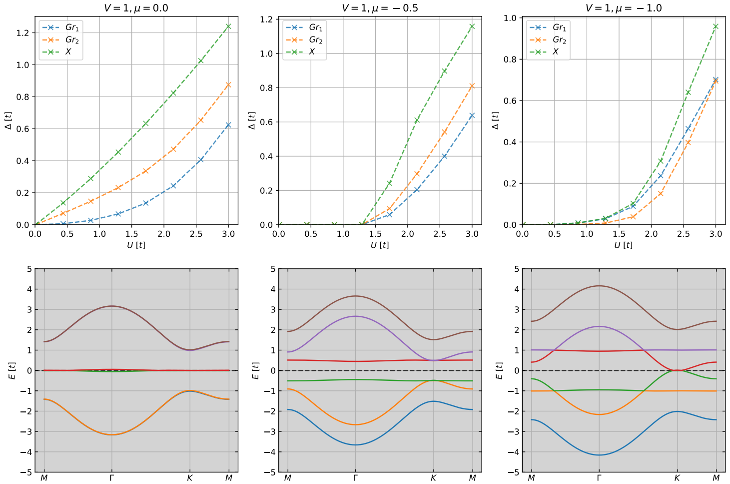
Self-consistently find Δ_α: minimize free energy

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

[9] Liang et al., 10.1103/PhysRevB.95.024515 (2017)

Results



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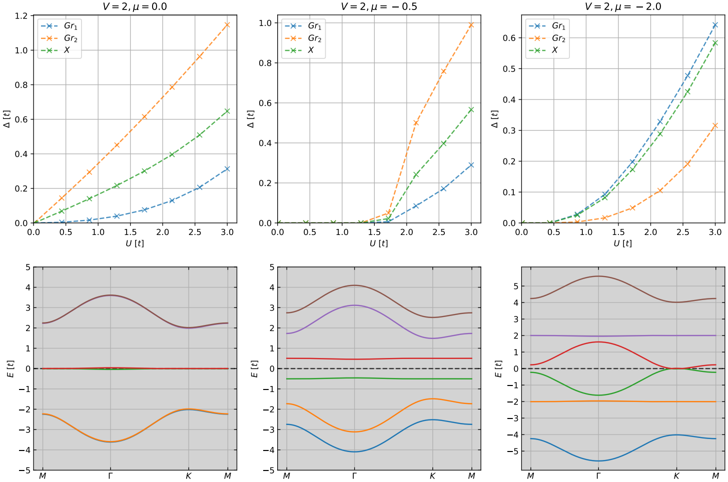

Outlook

Revisiting flat band superconductivity: Dependence on minimal quantum metric and band touchings

Kukka-Emilia Huhtinen,[1,*] Jonah Herzog-Arbeitman,[2] Aaron Chew,[2] Bogdan A. Bernevig,[2,3,4] and Päivi Törmä[1,†]
[1]*Department of Applied Physics, Aalto University School of Science, FI-00076 Aalto, Finland*
[2]*Department of Physics, Princeton University, Princeton, New Jersey 08540, USA*
[3]*Donostia International Physics Center, P. Manuel de Lardizabal 4, 20018 Donostia-San Sebastian, Spain*
[4]*IKERBASQUE, Basque Foundation for Science, 48009 Bilbao, Spain*

(Received 21 March 2022; revised 18 June 2022; accepted 22 June 2022; published 26 July 2022)

A central result in superconductivity is that flat bands, though dispersionless, can still host a nonzero superfluid weight due to quantum geometry. We show that the derivation of the mean field superfluid weight in previous literature is incomplete, which can lead to severe quantitative and even qualitative errors. We derive the complete equations and demonstrate that the minimal quantum metric, the metric with minimum trace, is related to the superfluid weight in isolated flat bands. We complement this result with an exact calculation of the Cooper pair mass in attractive Hubbard models with the uniform pairing condition. When the orbitals are located at high-symmetry positions, the Cooper pair mass is exactly given by the quantum metric, which is guaranteed to be minimal. Moreover, we study the effect of closing the band gap between the flat and dispersive bands, and develop a mean field theory of pairing for different band-touching points via the S-matrix construction. In mean field theory, we show that a nonisolated flat band can actually be beneficial for superconductivity. This is a promising result in the search for high-temperature superconductivity as the material does not need to have flat bands that are isolated from other bands by the thermal energy. Our work resolves a fundamental caveat in understanding the relation of multiband superconductivity to quantum geometry, and the results on band touchings widen the class of systems advantageous for the search of high-temperature flat band superconductivity.

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

Niklas Witt[1,2,*] Yusuke Nomura[3] Sergey Brener,[1] Ryotaro Arita[4,5] Alexander I. Lichtenstein[1,2] and Tim O. Wehling[1,2]

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[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, Meguru-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.

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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 SC gap self-consistently, found that the pairing is different in the three orbitals