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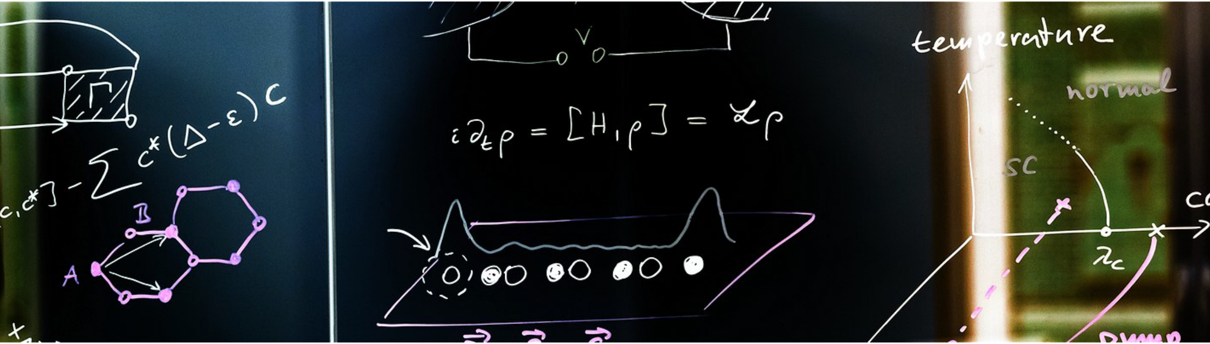

Tjark Sievers – I. Institute of Theoretical Physics
27th June 2024

Superconductivity, flat bands and quantum metric

Hamburg - Computational Condensed Matter Theory

Uppsala - Quantum Matter Theory

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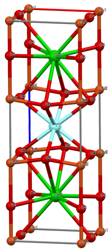
Routes to High T_C

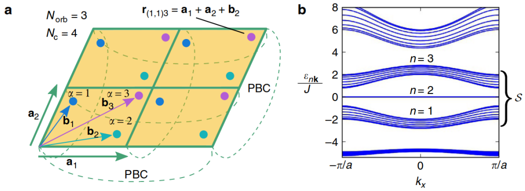
Goal for superconductivity (in terms of technical applications): high transition temperatures

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



YBCO unit cell[1]

Implement simple and tunable systems following theory guidelines based on flat bands



Harper-Hubbard model[2]

[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:

$$T_C \propto \exp\left(-\frac{1}{U n_0(E_\mathrm{F})}\right) \tag{1}$$

In flat bands it is predicted:

$$T_C \propto U \tag{2}$$

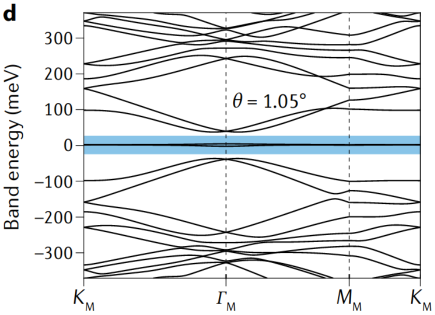
Exponentially enhanced in comparison to dispersive bands

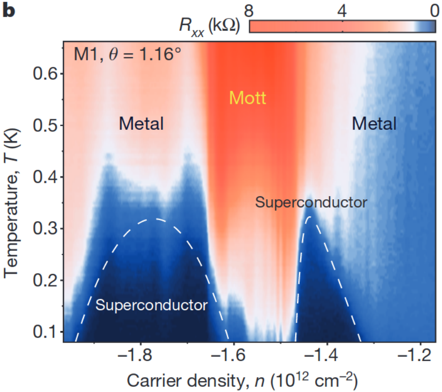
Due to:

- High density of states near Fermi level
- Vanishing kinetic energy, so that interaction effects dominate

Twisted Bilayer Graphene

Example for tunable flat-band system: flat bands can be tuned by changing the twist angle[3]





[3] Plots from Cao et al., 10.1038/nature26160 (2018)

Transport in Flat-Band Systems

Only one aspect of superconductivity: below T_C, there is pairing. But this does not necessarily mean there is a supercurrent!

London equation:

$$\mathbf{j} = -D_\mathrm{S}\mathbf{A} \tag{3}$$

with current density $\mathbf{j}$, vector potential $\mathbf{A}$, superfluid weight D_S

Describes properties of SC, e.g. perfect diamagnetism and conductivity. So $|D_\mathrm{S}| > 0$ needed for SC

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]

Show[4] there are actually 3 terms making up D_{S}:

- Conventional:

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

- Geometric:

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

[4] Peotta and Törmä, 10.1038/ncomms9944 (2015)

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

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

Quantum metric can be connected to the overlap of Wannier functions

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

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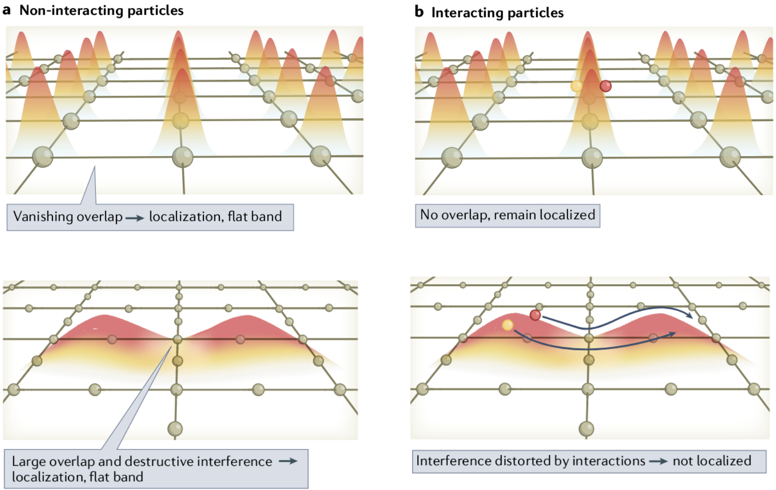
Wannier Overlap and Transport[5]



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

A Connection to Topology

Lower bound for $\mathcal{M}_{ij}^{\mathrm{R}}$ given by Chern number $\mathcal{C}$:

$$\det \mathcal{M}_{ij}^{\mathrm{R}} \geq \mathcal{C}^2 \tag{8}$$

Explanation for this connection: topological invariants provide obstruction to full localization of Wannier functions

Quantum Metric in Lattice Systems

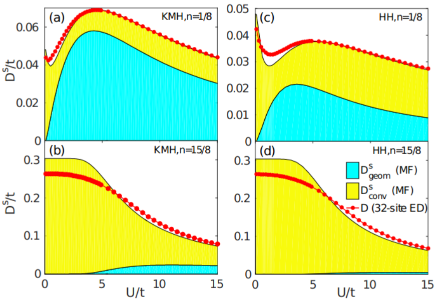
In lattice system, the quantum metric can be expressed as:

$$g_{ij}(\mathbf{k}) = \mathrm{Tr}\left[\partial_i P(\mathbf{k})\, \partial_j P(\mathbf{k})\right] \tag{9}$$

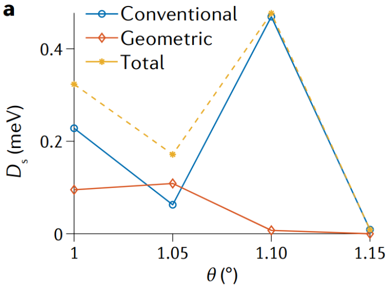
using the projector to the band n of interest $P(\mathbf{k}) = |u_{n\mathbf{k}}\rangle \langle u_{n\mathbf{k}}|$, expressed with the periodic Bloch functions $|u_{n\mathbf{k}}\rangle$

It measures the distance between infinitesimally close wavefunctions in $\mathbf{k}$-space.

Examples



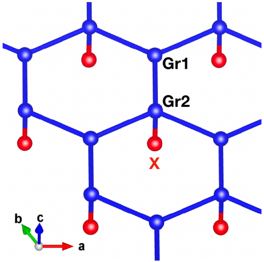
Different Hubbard models[6] tuned to flat (a, c) and dispersive band (b, d)



In twisted bilayer Graphene[7], geometric contribution overtakes at magic angle 1.05°

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

My Model

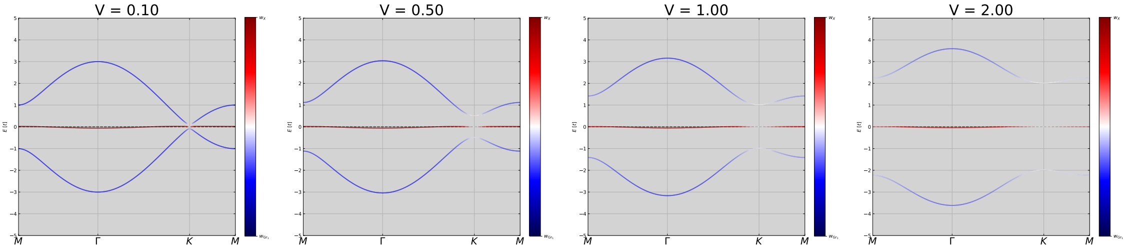


- Hexagonal lattice with an additional orbital on one of the sites
- Material motivation: Graphene on top of a substrate

Non-interacting Hamiltonian:

$$H_0 = -t_{\mathrm{X}} \sum_{\langle ij \rangle, \sigma\sigma'} d^{\dagger}_{i,\sigma} d_{j,\sigma'} - t_{\mathrm{Gr}} \sum_{\langle ij \rangle, \sigma\sigma'} c^{\dagger}_{i,\sigma} c_{j,\sigma'} + V \sum_{i,\sigma\sigma'} d^{\dagger}_{i,\sigma} c^{(\mathrm{Gr2})}_{i,\sigma'} \tag{10}$$

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



Important features:

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

How to actually go about calculating superfluid weight, so:

Mean-Field decoupling, BdG Hamiltonian in orbital and band basis

Mean-field energy minimization

What goes into superfluid weight now?

Outlook

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

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(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.

- DMFT calculations on A3C60, getting coherence length and London penetration depth from a finite-momentum constraint on the pairing[8]

[8] Witt et al., 10.48550/arXiv.2310.09063 (2024)

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

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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[9]

[9] Penttilä, Huhtinen, and Törmä, 10.48550/arXiv.2404.12993 (2024)

Summary

- System with flat bands promise high T_{C} superconductivity
- Superfluid weight ($\hat{=}$ capacity to host a supercurrent) is determined by quantum geometry
- Quantum geometry encompasses distances and curvatures in the space (or manifold) formed by the electronic Bloch functions, that is, the eigenfunctions of the band.