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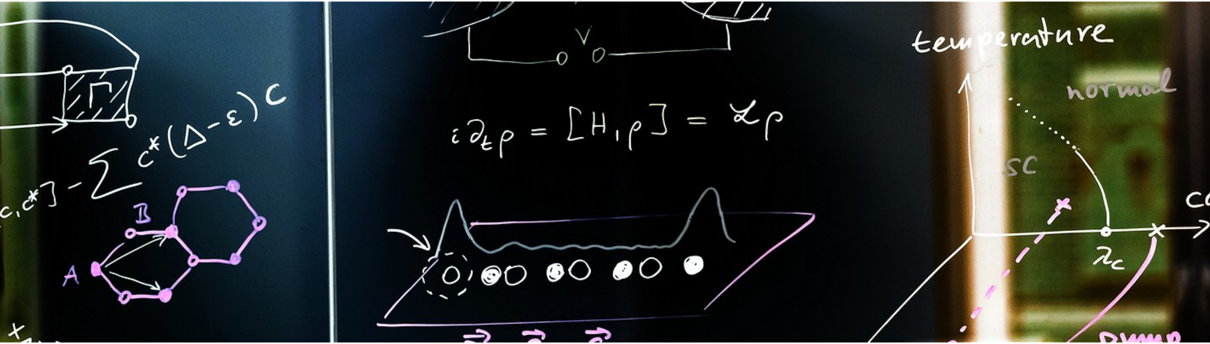


Tjark Sievers – I. Institute of Theoretical Physics 27th June 2024

Superconductivity, flat bands and quantum metric

- Quarter time of my masters thesis

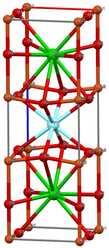
Hamburg - Computational Condensed Matter Theory

Uppsala - Quantum Matter Theory

Routes to High T_C

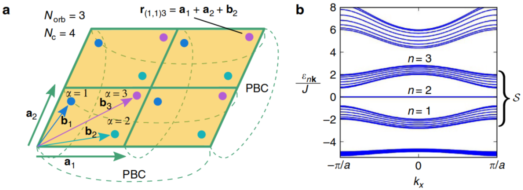
Goal for superconductivity (in terms of technical applications): high transition temperatures

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:

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

In flat bands it is predicted:

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

This is due to the high density of states near the Fermi level and vanishing kinetic energy, so that interaction effects dominate

Even true for cases where the interaction is larger than the band width

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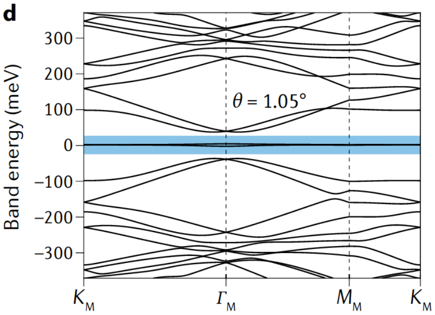
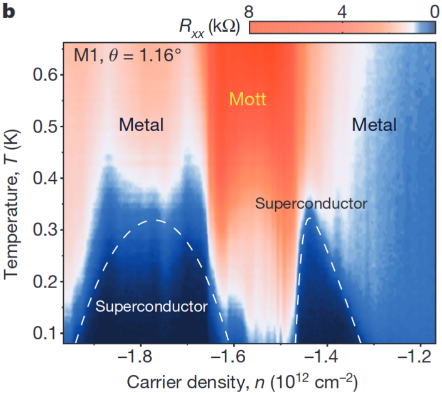
Twisted Bilayer Graphene

Example for such a tunable 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

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

Electrodynamic properties of SC materials captured by:

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

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

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

In single-band BCS theory:

$$D_{S,ij} \sim \sum_{\mathbf{k}} \frac{\partial^2 \epsilon}{\partial k_i \, \partial k_j} \tag{4}$$

Vanishes for a flat band!

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 comprising D_{S}:

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

When constraining to have equal order parameter in all orbitals:

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

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

$\mathcal{M}^{\mathrm{R}}_{ij}$ is the integral over the BZ of a quantity called the quantum metric $g_{i,j}(\mathbf{k})$:

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

Quantum metric determines overlap of Wannier functions, so finite quantum metric means overlap of Wannier functions, so that transport is possible

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

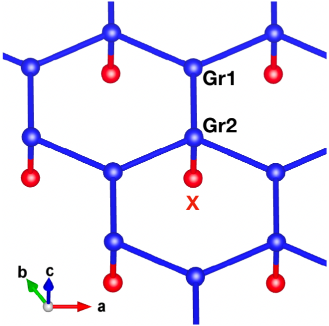
$$\mathcal{M}^{\mathrm{R}}_{ij} \tag{8}$$

Explanation for this connection: for non-zero Chern number, one cannot find exponentially localized Wannier functions

Concretely, for example in lattice systems:

Measures distance between close points on the band

My Model

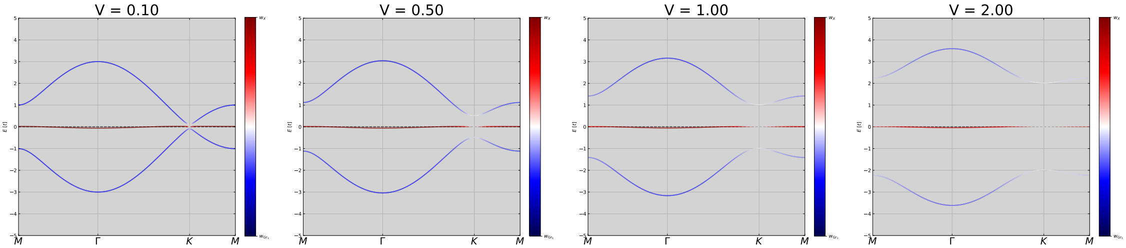


Hexagonal lattice with an additional orbital on one of the sites in the BZ
Material motivation: Graphene on top of a substrate, different substrates give different values of V

Non-interacting Hamiltonian:

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

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 calculate superfluid weight in Hubbard model

BdG Hamiltonian in orbital and band basis

Mean-field energy minimization

Add local Hubbard interaction:

$$H_{\rm int} = U_{\rm X} \sum_i d^\dagger_{i,\uparrow} d^\dagger_{i,\downarrow} d_{i,\downarrow} d_{i,\uparrow} + U_{\rm Gr} \sum_{i,\epsilon=A,B} c^{(\epsilon)\dagger}_{i,\uparrow} c^{(\epsilon)\dagger}_{i,\downarrow} c^{\epsilon}_{i,\downarrow} c^{\epsilon}_{i,\uparrow} \tag{10}$$

What I did so far

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Outlook

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.

- Recent preprint by Niklas [5], DMFT calculations on A3C60, getting superfluid weight and coherence length from a finite-momentum constraint on the pairing

[5] 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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[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.

- Also recent preprint [6] DMFT on Lieb lattice (Flat band system), getting superfluid weight, analysing geometric contribution for finite temperature

[6] Penttilä, Huhtinen, and Törmä, 10.48550/arXiv.2404.12993

Summary

- System with flat bands (Moire materials in particular at the moment) promise high T_{C} SC
- The ability to host a supercurrent (superfluid weight) is determined by quantum geometry
- Quantum geometry encompasses

Quantum metric general

Introduction:

Take Hamiltonian $\{H(\lambda)\}$ with dependence on some parameters $\lambda = (\lambda_1, \lambda_2, \dots)$

Have eigenenergies $E_n(\lambda)$ and eigenstates $|\phi_n(\lambda)\rangle$

Upon infinitesimally varying $\mathrm{d}\lambda$, define quantum distance:

$$\mathrm{d}s^2 = ||\psi(\lambda + \mathrm{d}\lambda)||^2 = \langle \delta\psi | \delta\psi \rangle = \langle \partial_\mu \psi | \partial_\nu \psi \rangle \, \mathrm{d}\lambda^\mu \, \mathrm{d}\lambda^\nu \tag{11}$$

$$= (\gamma_{\mu\nu} + \mathrm{i}\sigma_{\mu\nu}) \, \mathrm{d}\lambda^\mu \, \mathrm{d}\lambda^\nu \tag{12}$$

To ensure that gauge invariance, add term:

$$g_{\mu\nu}(\lambda) := \gamma_{\mu\nu}(\lambda) - \beta_\mu(\lambda)\beta_\nu(\lambda) \tag{13}$$

with Berry connection $\beta_\mu(\lambda)\mathrm{i} \langle \phi(\lambda) | \partial_\mu \phi(\lambda) \rangle$

For two states λ_I and λ_F, quantum distance between them:

$$|\langle \psi(\lambda_F) | \psi(\lambda_I) \rangle| = 1 - \frac{1}{2} \int_{\lambda_I}^{\lambda_F} g_{\mu\nu}(\lambda) \, \mathrm{d}\lambda^\mu \, \mathrm{d}\lambda^\nu \tag{14}$$