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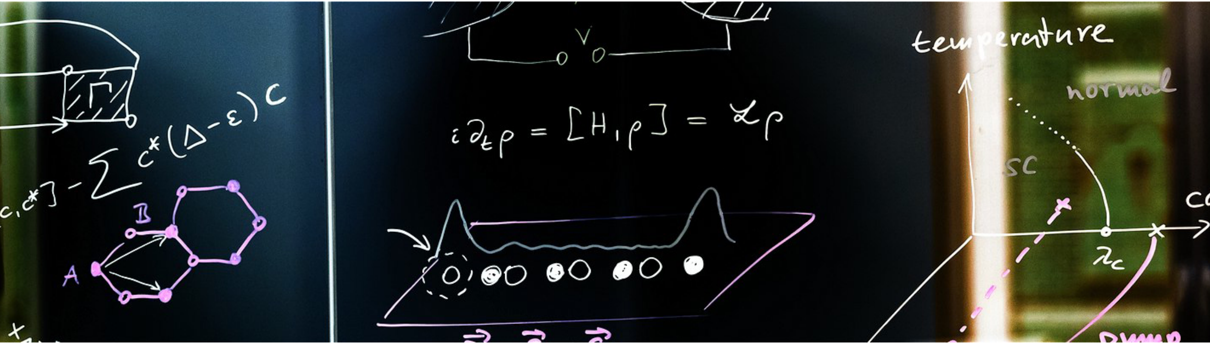


Tjark Sievers – I. Institute of Theoretical Physics 27th June 2024

Superconductivity, flat bands and quantum metric

- Quarter time of my masters thesis

Hamburg - Computational Condensed Matter Theory

Uppsala - Quantum Matter Theory

From review

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

Routes to achieve that:

- Explore classes of materials that show high T_C (e.g. Cuprates)
- More recent: take simpler and more tunable systems following simple theory guidelines based on flat bands and quantum geometry

In BCS theory for dispersive bands:

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

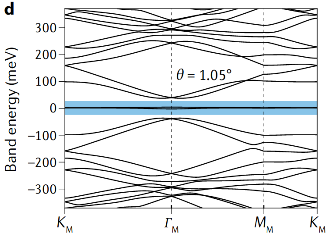
In flat bands it is predicted (energy dispersion is constant as function of momentum $\mathbf{k}$):

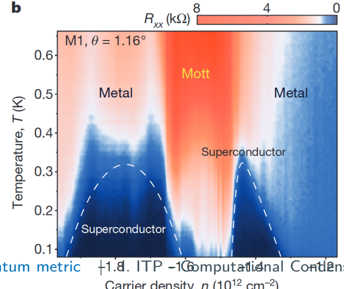
$$T_C \propto U \tag{2}$$

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

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

Twisted bilayer materials, in particular twisted bilayer graphene: flat bands can be tuned by changing the twist angle





Critical temperature is only one aspect of superconductivity: under this temperature, there is Cooper pairing, but this does not necessarily mean there is a supercurrent

Especially in flat-band systems: group velocity for the non-interacting particles $v_g = \frac{\partial \epsilon}{\partial \mathbf{k}}$, so these dont move

Electrodynamic properties of SC materials captured by:

$$\mathbf{j} = -D_S \mathbf{A} \tag{3}$$

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

Describes quantitative description of phenomena of SC (perfect diamagnetism, perfect conductivity), so non-zero superfluid weight is criterion of superconductivity

In single-band BCS theory:

$$D_{s,ij} \sim \int \frac{\partial^2 \epsilon}{\partial k_i \, \partial k_j} \tag{4}$$

Vanishes for a flat band!

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

Introduction:

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

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

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

$$\begin{aligned} \mathrm{d}s^2 &= ||\psi(\lambda + \mathrm{d}\lambda)||^2 = \langle \delta\psi | \, \delta\psi \rangle = \langle \partial_\mu \psi | \, \partial_\nu \psi \rangle \, \mathrm{d}\lambda^\mu \, \mathrm{d}\lambda^\nu \qquad (5) \\ &= (\gamma_{\mu\nu} + \mathrm{i}\sigma_{\mu\nu}) \, \mathrm{d}\lambda^\mu \, \mathrm{d}\lambda^\nu \qquad (6) \end{aligned}$$

To ensure that gauge invariance, add term:

$$g_{\mu\nu}(\lambda) := \gamma_{\mu\nu}(\lambda) - \beta_\mu(\lambda)\beta_\nu(\lambda) \qquad (7)$$

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

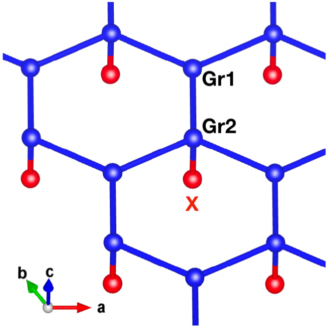
For two states λ_I and λ_F, quantum distance between them:

$$| \, \langle \psi(\lambda_F) | \psi(\lambda_I) \rangle \, | = 1 - \frac{1}{2} \int_{\lambda_I}^{\lambda_F} g_{\mu\nu}(\lambda) \, \mathrm{d}\lambda^\mu \, \mathrm{d}\lambda^\nu \qquad (8)$$

Concretely, for example in lattice systems:

Measures distance between close points on the band

Model:



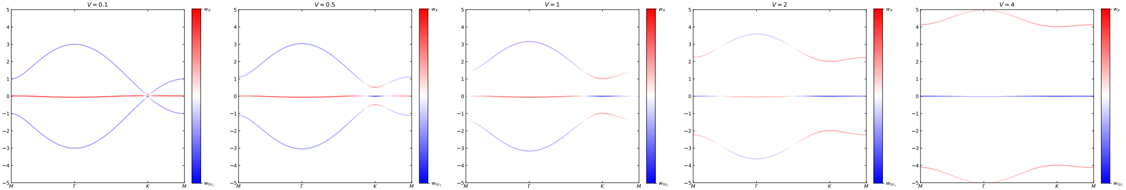
Hexagonal lattice with an additional orbital on one of the sites in the BZ

Non-interacting Hamiltonian:

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

$$+ V \sum_{i,\sigma\sigma'} \left(d^{\dagger}_{i,\sigma} c^{(A)}_{i,\sigma'} + c^{(A),\dagger}_{i,\sigma} d_{i,\sigma'} \right) \tag{10}$$

Band structure:



Important feature:

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

Add local Hubbard interaction:

$$H_{\text{int}} = U_{\text{X}} \sum_{i} d_{i,\uparrow}^{\dagger} d_{i,\downarrow}^{\dagger} d_{i,\downarrow} d_{i,\uparrow} + U_{\text{Gr}} \sum_{i,\epsilon=A,B} c_{i,\uparrow}^{(\epsilon)\dagger} c_{i,\downarrow}^{(\epsilon)\dagger} c_{i,\downarrow}^{\epsilon} c_{i,\uparrow}^{\epsilon} \tag{11}$$

Outlook

Recent preprint by Niklas [3], DMFT calculations on A3C60, getting superfluid weight and coherence length from a finite-momentum constraint on the pairing

Also recent preprint by Peotta/Törma [4] DMFT on Lieb lattice (Flat band system), getting superfluid weight, analysing geometric contribution for finite temperature

Summary

- Flat bands offer a route