Correlated electrons in magic-angle twisted bilayer graphene

A dynamical mean field theory study of twisted bilayer graphene

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In Short

- Magic-angle twisted bilayer graphene exhibits a zoo of highly tuneable, strongly correlated phases providing an unprecedented window into correlated electron physics
- Strong correlation techniques are computationally viable on suitable effective models composed of both localized and delocalized electrons
- Dynamical mean field theory will give access to spectral function and self-energies shedding light in particular on the correlated insulator phases

Take two sheets of graphene and overlay one on top of the other such that one layer is slightly rotated with respect to the other. The interference between the two slightly misaligned layers creates a beautiful, mesmerizing long-wavelength pattern called a Moiré pattern. These emergent patterns are interesting not only for aesthetic reasons, but also for the profound impact that they have on the physics of these structures. For instance, the electronic properties of low-angle twisted bilayer graphene (TBG) are markedly different from those of monolayer graphene as well as unrotated bilayer graphene [1]. In particular, at a relative rotation of ~1.1° between the two layers (also known as the magic angle), the low-energy electronic bands become flat with Fermi velocities of ~10^6 m/s. This places magic-angle twisted bilayer graphene (MATBG) in one of the most interesting classes of materials in modern condensed matter physics—strongly correlated materials.

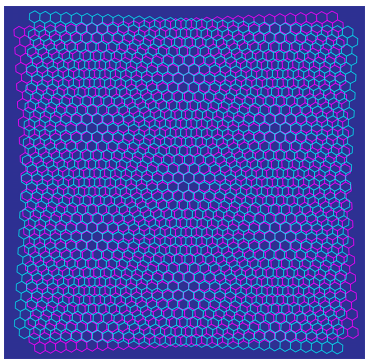

Figure 1: *The Moiré pattern of two relatively rotated honeycomb lattices [1]*

In a strongly correlated material, the behavior of each electron strongly depends on the behavior of all other electrons around it. A faithful description of such a material must simultaneously treat many electrons and all the interactions between them. This is an example of a many-body problem—one of the hardest problems in theoretical physics today. The complexity accompanies some of the most compelling phenomena seen in labs around the world, including unconventional superconductivity and exotic magnetic responses. Where twisted bilayer graphene shines is that it exhibits multiple distinct strongly correlated phases in a highly tuneable setting providing one of the best windows into the nature of correlated electron physics.

It is relatively easy to use an electronic gate to dope (put electrons in to or take electrons out of) a TBG sample. Therein lies the promise of twisted bilayer graphene. In MATBG, multiple distinct superconducting phases occur at different doping levels, interspersed by correlated insulator states. The proximity of superconducting and insulating states in the phase diagram draws immediate comparisons to cuprates, another class of strongly correlated materials, widely studied for their high-temperature superconducting properties.

Four years on since the first demonstration of unconventional superconductivity in twisted bilayer graphene [2], the nature of its superconducting and insulating states is still an open question. For example, it is not yet known whether MATBG has a Mott insulating phase. In this project, we will apply dynamical mean-field theory (DMFT) to answer such questions. DMFT has been widely successful in the study of cuprates in the last few decades and it is the most natural formalism in which to understand the Mott insulator transition in the Hubbard model.

Applying DMFT to TBG is not entirely straightforward. At the center of the issue is that current many-

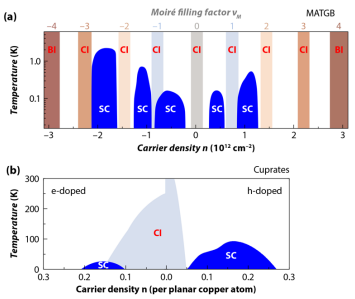

Figure 2: *The low-temperature phase diagram of magic-angle twisted bilayer graphene and cuprates compared [1]*

body techniques (including DMFT) can only be applied to small systems with few degrees of freedom. MATBG, with ~11,000 atoms per Moiré unit cell, is anything but that! The first step, therefore, is to find a suitable effective model that is small enough and captures all the relevant physics. The starting point for this is Bistritzer and MacDonald's seminal continuum model [3]. Unfortunately, the standard procedure of deriving an effective tight-binding model by Wannierizing the low-energy subspace of this continuum model runs into a topological obstruction. The topology of the band structure precludes the existence of a local tight-binding model that respects the symmetries of the model [4].

There have been attempts to circumvent this issue by considering larger subspaces in the Wannierization procedure [5]. The most promising approach involves building sophisticated hybrid models composed of a localized correlated subspace and a delocalized uncorrelated subspace that hybridize with each other. Such a model can be built by projecting onto appropriate Wannier functions, or directly from symmetry considerations [6]. We will apply DMFT to a family of such models in order to gain insight into the low-temperature phase diagram of twisted bilayer graphene.

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More Information

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Project Partners

G. Sangiovanni research group at Julius-Maximilians-Universität Würzburg

Funding

EU Graphene Flagship

DFG Subject Area

307-02