Strongly correlated states in twisted graphene bilayers

When a periodic pattern is overlaid on a copy of the same pattern with a small twist angle, a large-scale interference forms which is also called Moiré pattern. Such Moiré patterns that are produced by overlaying two graphene sheets are a hot topic of current research. For a discrete set of so-called "magic" twist angles these two overlaid graphene sheets form very flat conduction bands at the Fermi energy [1][2]. Although graphene is usually considered to be weakly interacting, the impact of correlations on the properties of a material are determined by the ratio between interaction strengths and bandwidth. Thus, the discovery of flat bands in twisted bilayer graphene opens the possibility to study correlation effects in this two-dimensional system. This has been confirmed in 2018, when unconventional superconductivity and correlated insulating states have been observed in twisted bilayer graphene at a magic angle [3][4]. The unconventional superconductivity resembles the high-T_C cuprates, as it emerges from an insulating strongly correlated state in two dimensions upon doping. Thus, the discovery of superconductivity in twisted bilayer graphene provides a new possibility to probe and understand unconventional superconductivity in two dimensions and thus advance our knowledge also about high-T_C cuprates.

In this project, we plan to theoretically analyze strongly correlated states in bilayer graphene. After setting up a suitable model for the band structure of twisted bilayer graphene including the flat bands at the Fermi energy, we will use real-space dynamical mean field theory (*R*DMFT) to analyze correlation effects. Dynamical mean field theory (DMFT) takes into account local correlations exactly and has been widely used to study strongly correlated phases of matter [5]. The extension to *R*DMFT [6] makes it possible to take into account inhomogeneities of the lattice such as impurities or open boundaries. For twisted bilayer graphene, this aspect becomes important because the twisting leads to a Moiré pattern, where different atoms in a unit cell behave differently. Thus, *R*DMFT gives us the possibility to analyze the impact of strong correlations separately for each atom within the Moiré pattern. *R*DMFT yields a set of coupled quantum impurity problems that must be solved self-consistently. As a fast impurity solver, we use the numerical renormalization group (NRG), which yields accurate spectral functions on the real-frequency axis for a wide range of interaction parameters and temperatures [7]. One of our first goals is to double-check for magnetic instabilities, and preliminary investigations in this respect by a static mean-field theory are under way in Cergy-Pontoise.

The group at the Université de Cergy-Pontoise is among the pioneers of twisted graphene bilayers [2] and Robert Peters an expert for (*R*)DMFT using the NRG [8]. We are already collaborating on single-layer graphene sheets and -nanostructures. The visit of Robert Peters at the beginning of 2019 will provide us with an opportunity to push the topical project on twisted graphene bilayers forward.

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