Electronic bands of twisted graphene layers

1. **Origin of Mott Insulating Behavior and Superconductivity in Twisted Bilayer Graphene**
   Authors: Hoi Chun Po, Liujun Zou, Ashvin Vishwanath, and T. Senthil
   arXiv:1803.09742, Phys. Rev. X **8**, 031089 (2018)

2. **Symmetry, Maximally Localized Wannier States, and a Low-Energy Model for Twisted Bilayer Graphene Narrow Bands**
   Authors: Jian Kang and Oskar Vafek
   arXiv:1805.04918, Phys. Rev. X **8**, 031088 (2018)

3. **Maximally-localized Wannier orbitals and the extended Hubbard model for the twisted bilayer graphene**
   Authors: Mikito Koshino, Noah F. Q. Yuan, Takashi Koretsune, Masayuki Ochi, Kazuhiko Kuroki, Liang Fu
   arXiv:1805.06819, Phys. Rev. X **8** 031087 (2018)

Recommended with a Commentary by Francisco Guinea, Imdea Nanoscience, Madrid, and School of Physics and Astronomy, University of Manchester

The recent discovery of insulating behavior and superconductivity in twisted graphene bilayers[1, 2] has attracted a great deal of attention among the contributors to the cond-mat archive, as over 60 entries have been posted in the period March-October 2018 (see also a previous entry in this journal club[3]). There are many reasons for this impact: new broken symmetry phases in a two dimensional system, unconventional superconductivity, and novel features in the electronic bands, among others.

The focus of this commentary is on interesting contributions to the latter issue, the unconventional electronic bands of twisted graphene layers. As it is argued below, these bands show features not encountered before in condensed matter physics. The articles listed above have clarified significantly the mysteries of these bands, although a number of problems remain open. Space considerations prevent a detailed analysis of the many insights into other topics, such as superconductivity itself. Many interesting papers have also been posted in the cond-mat repository recently.

The electronic structure of twisted bilayers was considered shortly after research on graphene began[4]. This seminal paper provides the minimal model for this structure. The basic idea follows the approach which leads from atomistic to tight binding and to continuum

models for single layer graphene, and which finally gives the two dimensional Dirac equation. Ref.[4] describes a hamiltonian in momentum space, where interlayer hopping conserves momentum. The rotation of the crystalline axes of one layer with respect to the other implies that an electron with a given momentum in one layer shows up as a superposition of three waves with three different momenta in the frame of reference appropriate for the other layer. This continuum model describes well situations when the relative displacement of atoms in different layers changes slowly compared to the atomic spacing in each graphene layer. It has the additional advantage that it also describes incommensurate arrangements, where no simple unit cell can be defined.

For large twist angles, this continuum model can be treated perturbatively, as interference effects between interlayer hoppings at different locations effectively decouple the two layers. Experiments further confirmed the validity of the model[5, 6]. Last, but not least, the continuum model has symmetries not present in a real superlattice made from two twisted graphene layers. In the continuum model, electrons in different valleys either in the same or in different layers are decoupled, and the number of electrons per valley is conserved. The electronic bands have spatial symmetries which are not necessarily present in lattice models, as their existence depends on how one plane is rotated with respect to the other. Deviations from these emergent symmetries are quite small in atomistic calculations for low twist angles.

An important advance in the study of the electronic twisted bilayer graphene took place when the model in[4] was systematically studied for small twist angles[7] (by small it is meant angles such that $\theta \lesssim 1^\circ$). Similar results where obtained using tight binding calculations[8]. The detailed results in[7] showed that for certain twist angles, defined as "magic angles" , the effective Fermi velocity of the bands closest to the Dirac energy vanished. As a result, very narrow bands emerged, with bandwiths of a few meV. For these angles, the unit cell of the superlattice contains over 10.000 atoms, and the lattice unit length is $\ell_M \gtrsim 15$nm. The experiments reported in[2, 1] fabricated, in an ingenious way, graphene bilayers with a twist angle of about 1.05°, very close to the largest "magic angle" reported in[7]. The connection between the unusual experimental results reported in[2, 1] and the magic angles intorduced in[7] became very compelling.

The superlattice unit cell can be roughly divided into three interpenetrating lattices with approximate AB, BA and AA stacking between the layers (A and B refer to the two sublattices in a single layer), the AB and BA patterns corresponding the the observed graphite stacking. Numerical calculations suggest that the charge density associated to the low energy bands is mostly localized in the AA regions[8, 9]. If the lattice relaxation is ignored (although it can be important at very small twist angles) these three regions have equal size, see Fig.[1].

In order to consider the role of the electron-electron interaction within the lowest bands, a local description of these bands is convenient, as it allows us to ignore he rest of the electronic structure. The papers at the beginning of this commentary addressed the issue of how to construct a local description of the narrow bands in twisted bilayer graphene at the magic angles. The simplest local model which seems to take into account all the features mentioned previously is a lattice of quantum dots, with four orbitals per spin each (there are two subbands, plus two valleys), placed at the nodes of the triangular lattice where the AA regions are located.

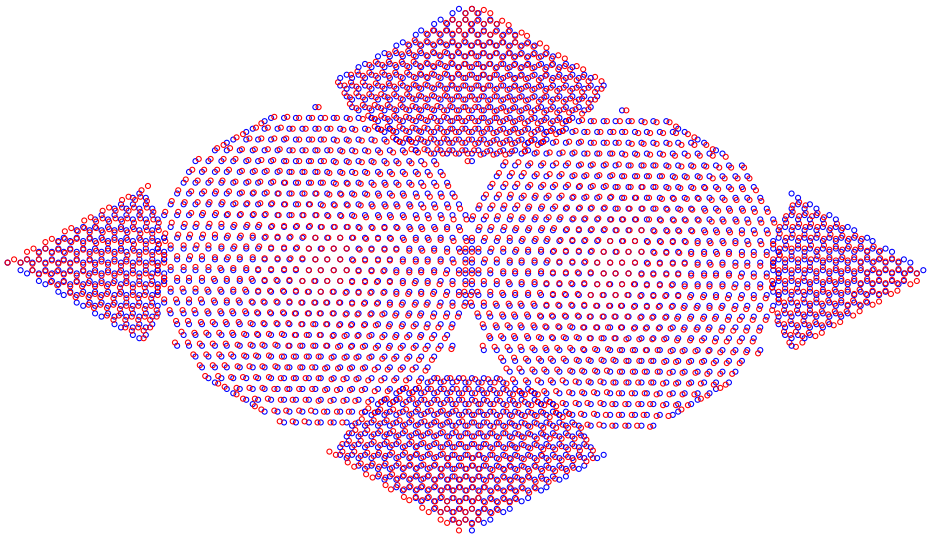

Figure 1: Position of carbon atoms in the unit cell of twisted graphene bilayer. Only pairs of atoms where one atom in one layer has a close neighbor in the other layer are shown. The atoms in the figure form either triangular lattices (AB and BA regions), or honeycomb lattices (AA regions). The twist angle is $\theta \approx 1.35^\circ$ and the number of atoms in the unit cell is 7204.

The actual situation is much more nuanced and complex than the picture obtained from a simple triangular lattice. To start with, a symmetry analysis of the properties of the electronic states at the high symmetry point in the superlattice Brillouin Zone, the Γ, K and M points, showed that the symmetries derived from a model based on a simple triangular lattice do not agree with the features obtained either from the continuum or from tight binding models[10, 11]. In particular, states at K and Γ change differently under certain symmetry operations, while in a triangular lattice they should change in the same way. Moreover, while the charge density of states at K and M are peaked at the AA regions, the states at Γ are more evenly distributed throughout the unit cell. The observed concentration of the integrated density at the AA regions is due to the higher weight of the perimeter of the Brillouin Zone, where the K and M points are located.

All together, a consistent local description of the low energy subbands of twisted bilayer graphene requires the definition of a honeycomb superlattice. This result is consistent with description based on the continuum model mentioned earlier[12, 13], and with tight binding results including details at the atomic scale[11]. The honeycomb structure is provided by the centers of the AB and BA regions. However, Wannier functions whose charge density were peaked at these locations will not explain the observed concentration of charge at the AA regions. The solution of this problem is to define Wannier functions centered at the AB and BA regions but with the maximum value of the charge density is at three lobes around the centers, which lie in the AA regions. The phases of these Wannier functions are also non trivial, as phases in neighboring lobes are shifted by $\pm(2\pi)/3$, in a similar way to atomic $p_x \pm ip_y$ orbitals. As a result, each Wannier function seems to overlap with other Wannier

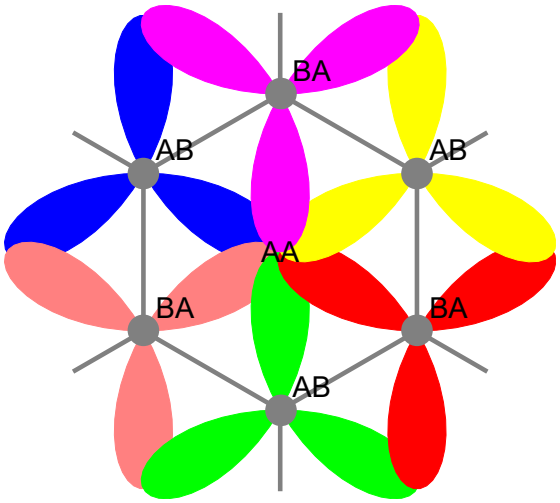

Figure 2: Sketch of the Wannier functions of a twisted graphene bilayer. The functions are defined at the nodes of a honeycomb lattice with the periodicity of the Moiré structure (gray dots, located at regions with AB and BA stacking). Each Wannier function is made up of three lobes, with maximum density at the centers of the hexagons defined by the honeycomb lattice. Six different Wannier functions seem to overlap in these regions (which correspond to AA stacking). Different microscopic phases make these functions mutually orthogonal, see[12] for details.

functions located at the 12 nearest, next nearest and next next nearest neighbors in the honeycomb lattice. The detailed structure of the wavefunctions at the AA regions makes the integrated overlap between Waniier functions centered at different nodes to vanish. A sketch of these unusual functions Wannier is shown in Fig.[2].

It is worth noting that the shape of the Wannier functions, as it is given by integrals of the wavefunctions in momentum space, depends on the choice of phase of these wavefunctions, which can be chosen arbitrarily. The standard procedure is to choose these phases so that the localization in real space of the Wannier functions is maximal[14]. Bands with a non trivial topology, such as those in Hall insulators, do not allow for a smooth choice of phase throughout the Brillouin Zone. The topology of the bands is defined by a non zero index, the Chern number, which, when different from zero, implies singularities in the gauge field whose curl defines the Berry phase. This gauge field also encodes the relation between nearby wavefunctions[15, 16], and its singularities, if not circumvented, lead to Wannier functions which are not exponentially localized. This is the case of the single valley continuum hamiltonians used to describe twisted graphene bilayers, as each valley hamiltonian breaks time reversal invariance. This obstruction to the straightforward definition of localized Wannier functions[13, 17] is overcome by the judicious choice of trial functions described in the previous paragraph.

In summary, twisted bilayer graphene defines a system at the boundary between strongly correlated materials and mesoscopic devices. Its electronic structure shows features not found before in condensed matter physics. The role of these properties in the observed supercon-

ductivity and insulating behavior is not yet fully settled. Another challenging problem is to determine whether other systems share the unusual electronic structure sketched here.

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