Science Bulletin 63 (2018) 1087–1091

Contents lists available at ScienceDirect

Science Bulletin

journal homepage: www.elsevier.com/locate/scib

Article

Inter-valley spiral order in the Mott insulating state of a heterostructure of trilayer graphene-boron nitride

Guo-Yi Zhu [a], Tao Xiang [b,c], Guang-Ming Zhang [a,c,*]

[a] State Key Laboratory of Low-Dimensional Quantum Physics and Department of Physics, Tsinghua University, Beijing 100084, China
[b] Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China
[c] Collaborative Innovation Center of Quantum Matter, Beijing 100084, China

ARTICLE INFO

Article history:
Received 3 June 2018
Received in revised form 19 June 2018
Accepted 20 June 2018
Available online 20 July 2018

Keywords:
Moire superlattice
Mott phase
Valley
Fermi surface nesting
Multilayer graphene

ABSTRACT

Recent experiment has shown that the ABC-stacked trilayer graphene-boron nitride Moire super-lattice at half-filling is a Mott insulator. Based on symmetry analysis and effective band structure calculation, we propose a valley-contrasting chiral tight-binding model with local Coulomb interaction to describe this Moire super-lattice system. By matching the positions of van Hove points in the low-energy effective bands, the valley-contrasting staggered flux per triangle is determined around $\pi/2$. When the valence band is half-filled, the Fermi surfaces are found to be perfectly nested between the two valleys. Such an effect can induce an inter-valley spiral order with a gap in the charge excitations, indicating that the Mott insulating behavior observed in the trilayer graphene-boron nitride Moire super-lattice results predominantly from the inter-valley scattering.

1. Introduction

The Moire super-lattice in the van der Waals heterostructure composed of multi-layer graphenes and hexagonal boron nitrides (hBN) has recently attracted great interest [1–6]. Both graphenes and hBN have hexagonal lattice structures, but the original lattice periodicity is ruined due to the mismatch between their lattice constants. Nevertheless, the periodicity can be restored on a much larger length scale, i.e., the Moire wave length ($L_M \simeq 15$ nm), upon which a triangular Moire super-lattice emerges [2–4]. On the other hand, bilayer graphene with a small twisted angle can also form the Moire band structure [7–10]. In the magic-angle twisted bilayer graphene, the Moire bandwidth is reduced dramatically and the local Coulomb repulsion becomes relatively significant, leading to the observation of the Mott insulating state as well as the unconventional superconductivity around the half-filling [11,12]. Meanwhile, it has been reported that a Mott insulating state also exists in the ABC-stacked trilayer graphene-hBN heterostructure [13]. In this experiment the low energy bandwidth is about 10 meV while a Mott gap $\sim$2 meV is observed at half filling. The comparable energy scale renders such a system in an intermediate coupling regime, therefore the role of band structure cannot be overemphasized.

In this paper, we will investigate the physical origin of the Mott insulating behavior observed in the trilayer-graphene-hBN heterostructure. Based on the symmetry analysis and effective band structure calculation, we propose a minimal tight-binding model with local Coulomb interaction. This model defined on a triangular lattice characterizes an interacting electron system in a staggered fictitious magnetic field for each of the two degenerate valley degrees of freedom. By matching the van Hove point positions of the effective low-energy bands, the staggered flux of each triangle is close to $\pi/2$. At half-filling, the two valley Fermi surfaces are found to be perfectly nested. Such an effect leads to a novel correlated insulating state with an inter-valley spiral order and a charge excitation gap, giving a natural explanation to the experimental observation.

2. Moire band structure

The ABC-stacked trilayer graphene (TLG) has the same Bravais lattice as in the monolayer graphene. But the electron and hole touching at zero energy support chiral quasiparticles with 3π Berry phase, generalizing the low-energy band structure of the monolayer and bilayer graphene [14]. The hBN also forms a honeycomb lattice but has a lattice constant about 1.8% larger than that of the

* Corresponding author.
E-mail address: gmzhang@mail.tsinghua.edu.cn (G.-M. Zhang).

https://doi.org/10.1016/j.scib.2018.06.022

graphene. Thus the heterostructure of TLG and hBN can form a triangular Moire super-lattice shown in Fig. 1a, which contains three interlaced regions. The region shaded by blue circles shows the maximal alignment between the TLG and hBN, denoted as the α zone; and the regions shaded by yellow or green triangles have a larger misalignment between the TLG and hBN, denoted as β and β' zone, respectively. The β zone differs from the β' zone by a sub-lattice exchange, defined by the C_6 rotation along the z-axis or the M_y mirror reflection with respect to the x-z plane. Each unit cell of the Moire super-lattice includes the α, β and β' zone. The TLG-hBN heterostructure possesses the threefold rotational symmetry along the z-axis C_3, the mirror reflection symmetry with respect to the y-z plane M_x, and the time reversal symmetry $\mathcal{T}$.

For both TLG and hBN, the honeycomb lattice can be bipartitioned into two triangular sub-lattices. A Dirac cone is generated in the electronic structure at the charge neutral point (CNP). The Dirac fermions become massive when the sublattice symmetry $C_2 \cdot \mathcal{T}$ which relates the two sub-lattices is broken [15,16]. In the hBN, boron and nitrogen atoms each form one of the sub-lattices, which breaks the symmetry between these two sub-lattices. This leads to a large energy gap (about 2.3 eV) in the low-lying excitations [15]. In contrast, the TLG itself is invariant under the sublattice symmetry, which protects the triple Dirac points near the Brillouin zone (BZ) corners. Thus the low-energy physics is dominated by the TLG, while hBN just contributes to a Moire scattering potential under second order perturbation. Such a Moire potential modulation folds the bands in the original BZ of the graphene layers into many mini-bands in the mini-Brillouin zones (mBZ), as displayed in Fig. 1b. As the mBZ is smaller by four order of magnitude than the original BZ, the bandwidth of the mini-bands is significantly suppressed. And the mini-bands near the charge neutral point (CNP) mainly originate from the low-energy valleys (K and K' shown in Fig. 1b) in the original TLG [17].

There are two crucial points about the Moire modulation of the band structure. First, the two valleys originally connected within one band are now significantly separated into two degenerate bands, because the valley distance in the original BZ is significantly longer than the characteristic wave vector of the Moire potential. This is the reason why the valley degree of freedom enters into the superlattice as the internal degrees of freedom of electrons. Second, as the triple Dirac cones are in fact split by trigonal warping process in the TLG [14], the splitting distance is relatively small in the original BZ, but quite comparable to the scale of the folded mBZ (Fig. 2a and b). As a result, the flat dispersion between the Dirac cones dominate most area of the mBZ, which further suppresses the kinetic energy. Moreover, the Dirac point is gapped out by the interplay between the hBN and TLG, which breaks the sub-lattice symmetry. A valence band is thus separated from the other mini-bands by the Moire band gap (Fig. 2c), which has fourfold degenerate associated with the spin and valley degrees of freedom. Electrons around the valleys K and K' are related to each other by either one of the following transformations: the time-reversal symmetry $\mathcal{T}$, mirror reflection M_x, and C_6 rotation.

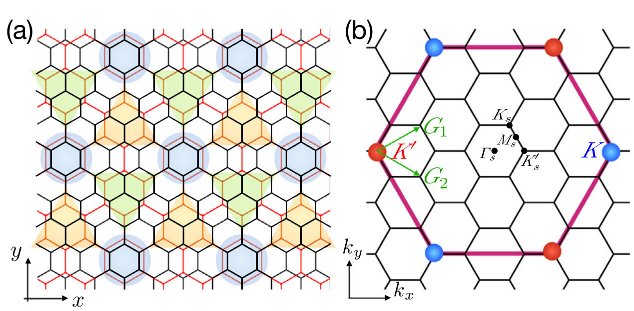

Fig. 1. Super-lattice structure and Brillouin Zone. (a) Super-lattice formed by the TLG (black lines) and hBN (red lines). For the sake of clearness, we exaggerate the lattice constant mismatch to 33%. The Moire pattern is composed of three interlaced regions shaded by blue, yellow, and green. (b) The Brillouin zone of the TLG on the original lattice (marked by the purple hexagon) is folded into many mini-Brillouin zone by the Moire periodic potential.

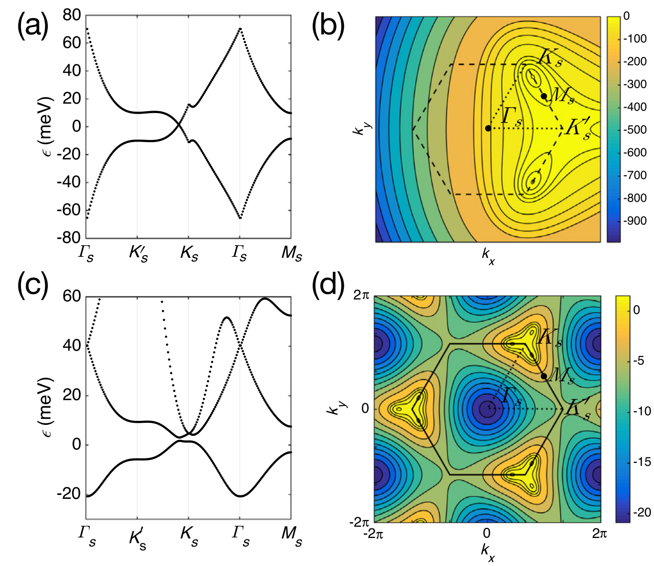

Fig. 2. Low-energy band structure and contour plot of the valence band. (a) Low-energy dispersion of the TLG without hBN is displayed in the proximity of the valley K along the high symmetry lines of the mBZ. (b) Contour plot of the corresponding valence band near the CNP. The dashed black hexagon implies the mBZ once hBN is coupled to the TLG. The Dirac points are split away from K_s' and extend to almost the vicinity of K_s. Triple van Hove points gather near K_s' instead. (c) Low-energy Moire band structure for the valley K whose Dirac points are close to K_s in the mini-BZ. The Dirac points near K_s are gapped out by the Moire potential. In obtaining this band structure, we have adopted the parameters used in Ref. [14] and the Moire potential strength 80 meV on the bottom layer of the TLG. (d) Contour plot of the corresponding valence band near the CNP in the mBZ (black hexagon). The vicinity of K_s' hosts three saddle points where the density of states diverges for this valley band. Color represents energy in unit of meV.

Using the effective two-component Hamiltonian for the TLG [14], we have calculated the band structures with the Moire scattering potential V_{M} assumed to act only on the bottom graphene layer [13]. Since the two valley bands are connected through the mirror transformation M_x, we can just focus on the K valley. In Fig. 2c, the electronic structure for the bands of valley K is displayed. The contour plot of the corresponding valence band near the CNP is also shown in Fig. 2d. The triple Dirac points originally at K_s' are separated to locate along the boundary of the mBZ towards K_s, reducing the energy dispersion and inducing the triple van Hove singularity near K_s'. When the Dirac points are further gapped out, the remaining triple van Hove points are the most remarkable fingerprint of the Moire band structure. More precisely, three van Hove points actually line along the mBZ boundary and center around the zone corner K_s'. Increasing the value of V_M pushes the three van Hove points towards K_s'. Above all, due to the Moire scattering and the Dirac physics, the kinetic energy scale is quenched from 1 to 20 meV. Because the valence band is separated from the other bands, we are able to write a one-band minimal tight-binding model with valley and spin degeneracy.

Given the Moire mini-band structure, the minimal model should satisfy all the symmetries mentioned above, and reproduce the key feature of mini-valence-band: the triple van Hove points and ultra-flat dispersion. In the triangular Moire lattice sites