Twisted bilayer graphene

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1 Introduction

The mechanisms of Fe- and Cu-based high-T_c superconductivity are still a open problem in condensed matter physics. Since in both types of systems, there are stacked conducting planes, a natural idea is to build monolayer materials to reproduce the behaviors observed in these high-T_c superconductors. The twisted bilayer graphene is a Moire system, in which two layers of graphene differing with a twisted angle θ are stacked together, and a Moire pattern occurs. Band-theoretic analysis has revealed that with small θ flat bands around the Fermi energy may occur: at so-called magical angles (the smallest being $\theta \approx 1.1^\circ$), the Fermi velocity drops to zero, which may induce strongly correlated states [1]. [3] experimentally observes the unconventional superconductivity in twisted bilayer graphene, with several features similar to those of cuprates.

This report reviews relevant theoretical and experimental progress in understanding twisted bilayer graphene. Section 2

2 The lattice structure

Let us begin with the easier case of twisted square lattices. Consider Fig. 1(a), and suppose $\boldsymbol{a}_1$ is the primitive lattice vector in the x direction, and $\boldsymbol{a}_2$ is the primitive lattice vector in the y direction. We choose the origin to be a point that is a lattice point of both layers. In Fig. 1(a) we can observe supercell-like patterns, and the origin point may be seen as the center of one supercell. Any other point that is a lattice point of both layers, then, has to be the center of another supercell.

Now suppose we are to calculate the distance between two nearest supercells on the x direction in Fig. 1(a). Assume the two layers of lattices are commensurate. Suppose $n\boldsymbol{a}_2$ connects the two unit cells. From the condition that the center of a supercell is a lattice point of both lattices, we have

$$n\boldsymbol{a}_2 = m\mathbf{R}\boldsymbol{a}_2 + \boldsymbol{a}_1. \tag{1}$$

Here $\mathbf{R}$ is the rotation matrix; the difference between $n\boldsymbol{a}_2$ and $m\mathbf{R}\boldsymbol{a}_2$ should be roughly in the x direction, and it should be minimal, so we take it to be $\boldsymbol{a}_1$.[1] Since the rotation angle is not very large, if $n\boldsymbol{a}$ is between two nearest supercells, we have $m \approx n$ (because in this case the lengths of $n\boldsymbol{a}_2$ and $mR\boldsymbol{a}_2$ should be approximately the same), and therefore we get

$$\text{lattice constant of supercell} = na = a/\tan\theta \approx \frac{na}{\theta}. \tag{2}$$

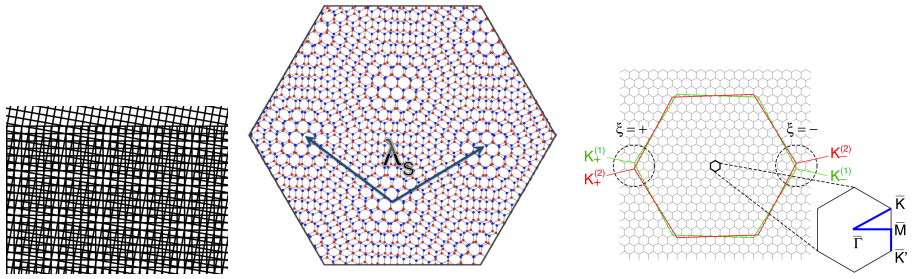
Now we move to the twisted bilayer construction of graphene (Fig. 1(b)). Following the logic of (1), we have

$$\text{lattice constant of supercell} \approx \frac{na}{\theta} \tag{3}$$

again. Note that here the lattice constants of both the honeycomb structure of each layer and the supercell are *not* the bond length: it is $\sqrt{3}$ times of the bond length. Suppose we draw a vector $\boldsymbol{\lambda}_s$ from the center of one unit cell to the unit cell directly above it, and then rotate it with the angle θ. By the definition of "center of one unit cell" above, we have $\Delta\boldsymbol{\lambda}_s$ equal to a lattice vector, but $\Delta\boldsymbol{\lambda}_s$ is roughly in the x direction and is not parallel to any bond in Fig. 1(b): the length of the shortest lattice vector in the x direction is the lattice constant of the honeycomb structure.[2]

[1] To be exact, it may not be $\boldsymbol{a}_1$, but, say, $10\boldsymbol{a}_1 + \boldsymbol{a}_2$, and if the latter value is the case, the supercell built according to (1) is just an approximate supercell; but usually this approximation is already good enough – see the discussion on incommensurability below.

[2] Recall that the graphene structure is a non-Bravais lattice. $\sqrt{3}$ times the bond length is exactly the length of a primitive lattice vector if we reconsider the graphene structure as a Bravais lattice with a two-atom basis.



(a) (b) (c)

Figure 1: Moire patterns in condensed matter physics. (a) Moire pattern of twisted bilayer square lattice. Picture taken from Wikipedia. (b) Twisted bilayer graphene in real space. Image from Fig. 1(b) in [6]. The length λ_s is the lattice constant of the hexagonal supercell. Note that λ_s is the distance between the centers of two nearest supercells, but *not* the length of each side of the supercell: it is $\sqrt{3}$ times of the length of each side of the supercell. (c) The first Brillouin zone of the two layers in (b) (red and green), and the first Brillouin zone (the black hexagon at the center) of the whole system. Image from Fig. 1(c) in [5]. The labels $\xi = \pm 1$ are valley labels (marking the two nonequivalent Dirac cones in the first Brillouin zone of graphene), and K+ and K− may alternatively be referred to as K abd K', and the labels (1) and (2) are layer labels.

With the supercell established in Fig. 1(b), we now consider the corresponding phenomenon in the reciprocal space (Fig. 1(c)). The uncertainty principle tells us that an increased unit cell in the real space means a shrunk first Brillouin zone. Under the commensurability condition imposed above, we indeed have a first Brillouin zone corresponding to the supercell (which is called the "mini Brillouin zone" in [2, 3]), which should be the "greatest common divisor" of both layers. The "common divisor" part means the two first Brillouin zones of the two layers are hexagon on the lattice points of the tessellation of the first Brillouin zone corresponding to the supercell, and the "greatest" part means the first Brillouin zone corresponding to the supercell should be as large as possible. Considering the orientation of the supercell, what we find is Fig. 1(c).

If we twist two ideal lattices with an arbitrary angle and stack them, that the two lattices are commensurate is not guaranteed, so the resulting material is not periodic, which may block electric currents. What makes this structure different from non-periodic systems like quasicrystals or amorphous is even when the two layers of lattices are not commensurate, we can still see approximate supercells, though with a varying lattice constant. However, when θ is close to zero, values of commensurate θ are highly dense, so with any θ the system is approximately periodic [7]. In practice, even prototypical crystals have spatially varying distortion of the lattice structure, and the incommensurability of the two layers seems to have nothing different from that: it can be well modeled by two commensurate layers plus small distortion. The quasi-periodic supercells may further be regularized into a truly periodic structure by lattice relaxation. Therefore, the procedure used to derive (2) is used whenever θ is close to zero enough, and the commensurate picture can always be used.[3]

3 Band theory and engineering of flat bands

A hand-waving argument about what happens after Brillouin zone folding happens according to Fig. 1(c) is given in [2], illustrated in Fig. 2. In Fig. 1(c), it can be seen that the equivalent band valleys of the upper layer and the lower layer (denoted by $K_+^{(2)}$ and $K_+^{(2)}$) are folded to the K point and K' point of the mini Brillouin zone, and the two Dirac cone cross each other. When inter-layer hopping is present, the crossings tend to be avoided, and the two intersecting Dirac cones split into four bands, the highest and the lowest being blunt cones. Since time reversal symmetry and spatial inversion symmetry are always present, the middle two bands are always connected by two Dirac points. When hybridization is strong, the gap between the highest and

[3]The incommensurability case can still be handled [4], but this is beyond the coverage of this report.

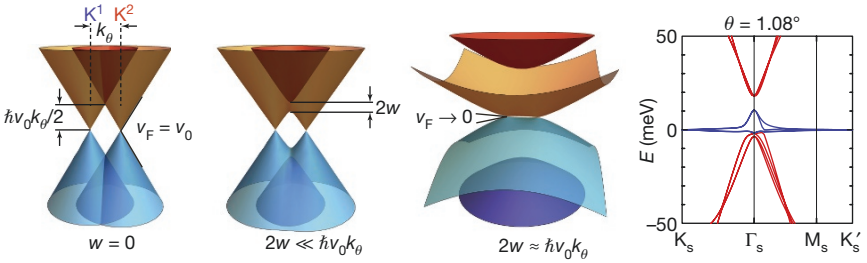


Figure 2: Flat band at the magical angle. Figure from [2]. The symbol w gives inter-band hybridization.

the lowest bands and the two bands near the Fermi level is increased, and the two Dirac points still exist, so the two bands are flattened around the Dirac points. The result band structure has almost zero Fermi velocity near the Dirac points $\mathrm{K_s}$ and $\mathrm{K_s'}$ in the mini Brillouin zone.

4 Coulomb interaction and electron correlation

5 Conclusion

References

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