Twisted bilayer graphene

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1 Introduction

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 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). 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

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

If we twist two ideal lattices with an arbitrary angle and stack them, that the two lattices are commensurable 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 commensurable, we can still see approximate supercells, though with a varying lattice constant. 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. 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 even when the two layers of lattices are not, if viewed as ideal lattices, commensurable.

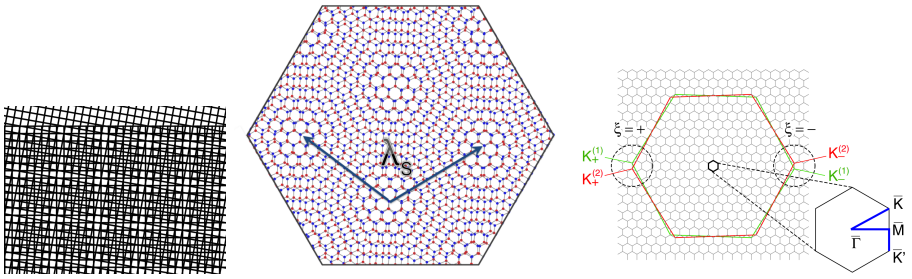
Now we move to the twisted bilayer construction of graphene (Fig. 1(b)). Following the logic of (1), we have

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

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 $\boldsymbol{\lambda}_\mathrm{s}$ 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 $\Delta\boldsymbol{\lambda}_\mathrm{s}$ equal to a lattice vector, but $\Delta\boldsymbol{\lambda}_\mathrm{s}$ is roughly in the x direction and is not parallel to any bond in Fig. 1(b): the shortest lattice vector in the x is ().[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 [2]. 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 [1].

3 Band theory and engineering of flat bands

4 Coulomb interaction and electron correlation

5 Conclusion

References

[1] Mikito Koshino. Band structure and topological properties of twisted double bilayer graphene. *Physical Review B*, 99(23):235406, 2019. Publisher: APS.

[2] Bikash Padhi, Chandan Setty, and Philip W Phillips. Doped twisted bilayer graphene near magic angles: proximity to Wigner crystallization, not Mott insulation. *Nano Letters*, 18(10):6175–6180, 2018. Publisher: ACS Publications.