Topological Band Unfolding and Flat Bands in Twisted Bilayer Graphene (Poster)

A. Mckenna[1,2] and M. Hilke[1]

[1]*Department of Physics, McGill University, Montreal, Canada*

[2]andrew.mckenna@mail.mcgill.ca

In Twisted Bilayer Graphene (TBG) certain twist angles produce commensurate lattices called Moiré patterns. Remarkably, for certain small twist angles, commonly called magic angles, such as $\theta \simeq 1.08°$, flat bands are observed [1]. The different twist angles of all the Moiré patterns can be classified using techniques that stem from number theory. In general, Moiré patterns will have much larger lattice constants, Ta $(T > 1)$, than the native Single Layer Graphene (SLG) lattice constant, a, which leads to a large number of bands within the Brillouin zone of the Moiré periodicity. However, optical experiments, such as ARPES and Raman spectroscopy are much easier to interpret in graphene's native Brillouin zone [2], which requires the unfolding of the multiple Moiré bands (illustrated in Figure 1).

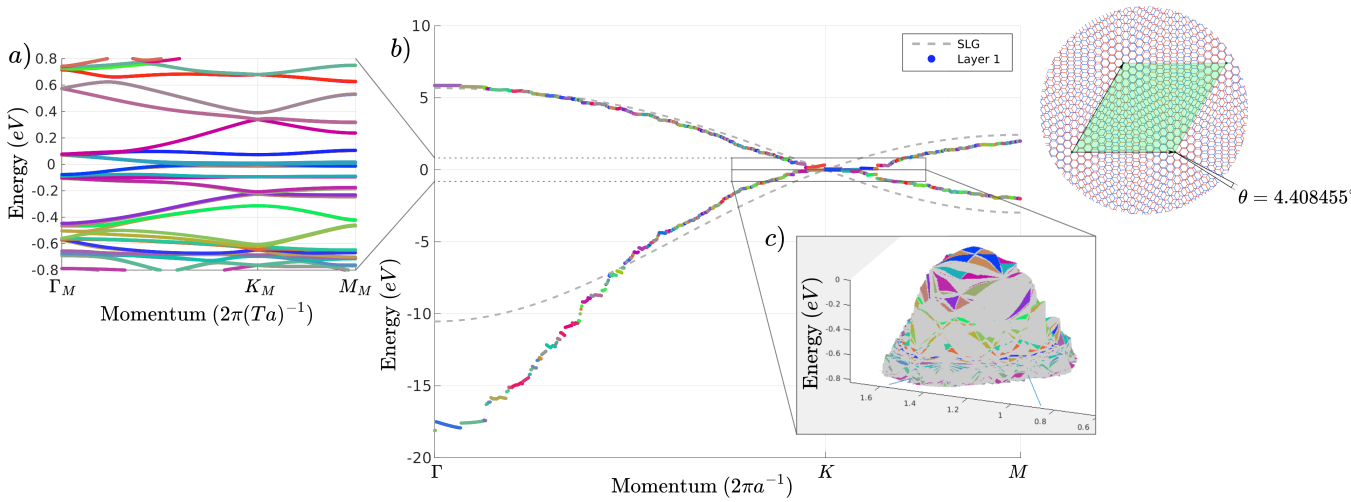

Figure 1: The band structures for SLG and TBG, where $a)$ is the folded plot (each folded band is assigned a color), $b)$ is unfolded using TBU, notice the discontinuities, and in $c)$ is an inset of the flat band at Dirac point of the bottom band.

Unlike previous works that rely on the spectral function to unfold the Moiré bands [3], here we introduce a method based on Topological Band Unfolding (TBU). TBU works by applying topological invariants to each band which don't change as the inter-layer coupling is increased from zero to a finite value. These invariants allow folded and unfolded bands to be mapped to each other in a systematic way. A particularly interesting consequence of increasing the interlayer coupling, is the increase of the magic angles (angles at which flat bands can be observed). To illustrate this point, we considered in Figure 1, a factor 4.5 increase in the interlayer coupling compared to the parameters used in ref. [1]. The increased coupling leads to a flat band at the increased magic angle of $\theta \simeq 4.41°$, similar to what is observed in experiments when pressure is applied [4]. More generally, our results show that the overall features of the band structure are largely unchanged except in the vicinity of the Dirac points, where the bands become flat and outside, where gaps appear (see Figure 1).

References

[1] G. Trambly de Laissardière, D. Mayou, and L. Magaud, Nano letters **10**, 804 (2010).

[2] K. Wei, T. Berlijn, and C.-C. Lee. Physical Review Letters **104**, 216401 (2010).

[3] H. Nishi, Y.I. Matsushita, Y. I., and A. Oshiyama, Physical Review B, **95**, 085420 (2017); F Sánchez-Ochoa *et al.* J. Phys.: Condens. Matter **32**, 025501 (2020).

[4] M. Yankowitz *et al.*, Science, **363**, 1059 (2019).