Graphene Stacks: a small rotation makes the difference

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Abstract

Graphene bilayers, with either AA or AB (Bernal) stacking have been known for years [1] but surprisingly, graphenic systems offer a much wider range of configurations. Indeed it has been shown from experiments that graphene planes can be rotated on some substrates – e.g. C face of SiC [2], graphite [3], Ni[4]- with an angle between successive layers that ranges from 0° -AA stacking- to 60° -AB stacking-. These rotations create in moiré patterns that are observed on STM images [2]. Here we show that these rotated (twisted) bilayers differ both from graphene and graphite and that their electronic structure is governed by the rotation angle. While a large rotation angle (close to 30°) results in two decoupled graphene layers [5-12], carriers in a twisted graphene bilayer evolve from Dirac fermions to strongly localized electrons or holes when the rotation angle is decreased toward very small angles (or increased toward 60°, the system is symmetric with respect to θ=30°, Figure 1).

We have investigated the electronic structure of graphene bilayers as a function of θ by a coupled ab initio – tight binding (TB) approach and we will compare our theoretical results to experimental data when available. When θ decreases, the velocity of the bilayer is first reduced with respect to the velocity of the monolayer and follows the law proposed first by Lopes dos Santos et al [8,9] (blue line in figure 1). At the intersection between two Dirac cones originating from two different layers, interaction between the states opens gaps and saddle points appear (Figure 2). At 2D such saddle points give rise to van Hove singularities (named E_+ and E_- in Figure 2) characterized by sharp peaks in the density of states (DOS). As θ is brought closer to 0°, the two van Hove singularities fall closer and closer to the Dirac point and eventually merge for θ close to 2°. While velocity renormalization remains controversial [13], van Hove singularities have indeed been observed in different systems : graphene on SiC [14], on Ni[4] confirming the theoretical predictions.

Here we will focus on the very small angle limit that have not yet been probed experimentally. When the two van Hove singularities merge, the DOS shows a sharp peak at the Dirac point. States belonging to this peak are localized in the AA region of the moiré pattern. When the angle is further reduced, velocity alternatively increases and decreases (insert Figure 2) and it is equal to zero for magic angles θ_n that follow a 1/n law [12,7]. We will show that this behavior comes from the confinement of the carriers in the AA regions of the moiré and that beyond sharp peak at the Dirac point, the confinement also leads to the appearance of sharp peaks for energies different from zero.

Eventually robustness of the theoretical predictions is tested for intermediate rotation angles with respect to different perturbations such as constrain, corrugation, point defects and pecular electronic properties are searched. A parallel with the effect of a superpotential on monolayer graphene will be made.

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Figures

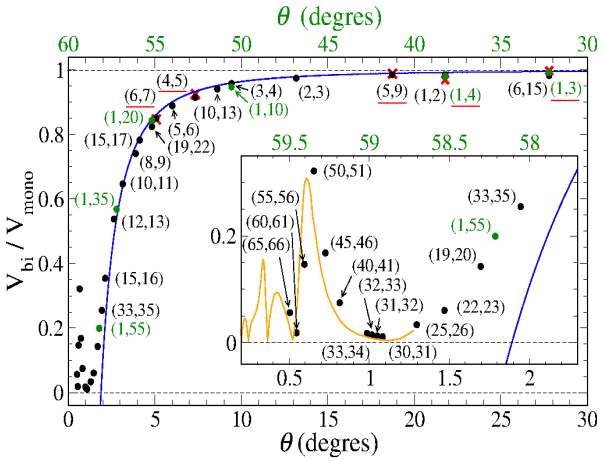

Figure 1 : Ratio between the velocities of the bilayer and of the monolayer as a function of the rotation angle. Red crosses: ab initio calculations, black and green dots: TB calculations, blue line: law by Lopes Dos Santos et al. Insert: very small angle behavior. Black dot: TB calculation, yellow line: magic angles by Bistritzer and MacDonalds.

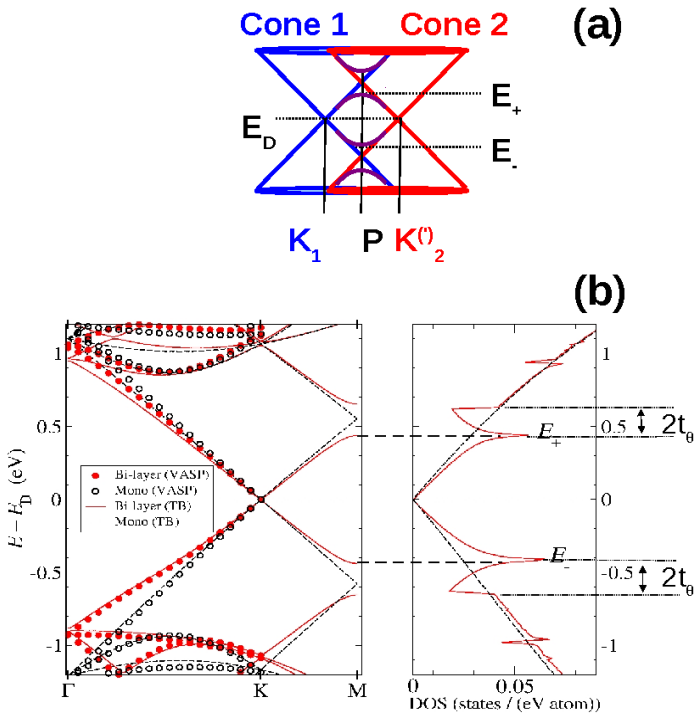

Figure 2 : Van Hove singularities and velocity renormalization. (a) scheme, (b)- left: Band structure of the (6,7) bilayer (red) compared to the free monolayer graphene one (black) , (b)-right DOS and van Hove singularities.