EFFECTS OF DISORDER ON THE DENSITY OF STATES IN MAGIC ANGLE TWISTED BILAYER GRAPHENE*

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This work presents results of numerical simulations of the density of states of a finite twisted bilayer graphene system twisted by different angles, and shows the relation between the twist angle and the position of the peaks in the density of states. Further analysis considers how adding the Anderson-like disorder affects this system. Demonstrated results correspond to disorder strengths in the range of 100 meV–500 meV and their influence on the peaks in the density of states.

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1. Introduction

Graphene, a 2D carbon material with low-energy electronic properties governed by massless Dirac fermions [1–3] has established its position as one of the most fascinating materials due to its superior mechanical, electronic and optical properties [4–10]. Soon after its mechanical exfoliation and transport measurements, a few-layer graphene (FLG) has also become a point of interest [11–15]. The energy dispersion of an AB stacked bilayer is parabolic, and the carriers are massive chiral fermions [16]. Both mono- and bi-layer samples are gapless, however, in the bilayer case, the energy gap can be opened by the application of an external electric field [17]. Even more interesting structure is created when two layers of graphene are twisted against each other [18]. Once we start rotating one of the sheets, the Fermi velocity renormalization is predicted [18], and the valence and conduction bands begin to flatten [19]. At what is called a magic angle [20], $\theta = 1.05°$, the velocity almost vanishes [21]. At this specific twist angle, the system is expected to exhibit strong electron–electron correlations that are currently

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vigorously studied [22–35], especially since the experiments have shown that they can be a source of magnetic and superconducting properties in the magic angle twisted bilayer graphene (MATBG) [36, 37].

To gain insight into electronic properties of a material beyond transport experiments, usually probing states only very close to the Fermi level, scanning tunneling microscopy (STM) measurements have to be performed. Recently, they demonstrated that for specific twist angles (so-called commensurate angles [18]), a new periodic moiré lattice is formed [38]. In theoretical models [20], the density of states (DOS) of the MATBG system exhibits a large, isolated peak around zero. Recent experiments have confirmed these predictions [38] and showed that the position of the peaks can be precisely controlled by the twist angle [39, 40]. Previously mentioned correlations are related to narrow bands that result from high DOS. Despite its importance, little is known about how perturbations affect this feature [41–43]. Even though disorder in samples (*e.g.* impurities or defects) is predicted to be rather small, there is a large, inhomogeneous contribution from randomly distributed variations in twist angle. A question how these irregularities influence the electronic states and correlations is challenging, due to the intrinsically large scale of the problem, caused by a large number of atoms in the moiré unit cell for small twist angles. The effect of this "twisting disorder" has been studied in Ref. [43]. In that work, it was shown that the Fermi velocity is almost completely independent from the randomness in the twist angle, while the miniband width is affected strongly. One of possible implications is that the "twisting disorder" is responsible for changes in MATBG physics, *e.g.* varied strength of insulating phases in seemingly identical samples.

In the following work, we adopt a simpler approach to study the effects of disorder on the van Hove singularity peaks in a MATBG system. DOS of a MATBG system exhibits three van Hove singularities — the centre one corresponding to the zero energy flat band, and two smaller satellite peaks that are a consequence of an overlap of the Dirac cones of two graphene layers. The position of the two satellite peaks can be used to determine the twist angle of the sample [44], and as such their behaviour in a disordered system poses an interesting question. We conduct a study on a real space model examining the influence of an Anderson-like disorder on the DOS of finite-size systems. First, we establish a procedure that allows to separate edge-states contributions, naturally dominating low-energy spectrum in finite graphene flakes, from more experimentally relevant bulk states, usually measured in large scale samples via the STM technique. Then, we show that in a large system, reaching 10^6 atoms, one can reproduce peaks in DOS for the MATBG. In the next step, we study how the position of these peaks changes in relation to the twist angle and how they are affected by

the Anderson-like disorder in a MATBG system. The paper is organized as follows: in Section 2, we describe the theoretical model and the procedure of the analysis of edge/bulk contributions to the DOS. In Section 3, we describe the numerical results of large scale simulations for clean and disordered systems, and then we present our conclusions in Section 4.

2. The model

We consider a model demonstrated in Fig. 1, consisting of two graphene sheets, one on top of the other in AB stacking, separated by a distance $c = 3.35\,\text{Å}$ and twisted by an angle θ against each other. Figure 1 (a) shows the top and side view of a non-twisted bilayer, while Fig. 1 (b) shows the same system after rotating the bottom layer by a given angle θ. Top view of a larger sample is demonstrated in Fig. 1 (c), where one can notice the periodicity of the superlattice being formed, making the moiré pattern clearly visible.

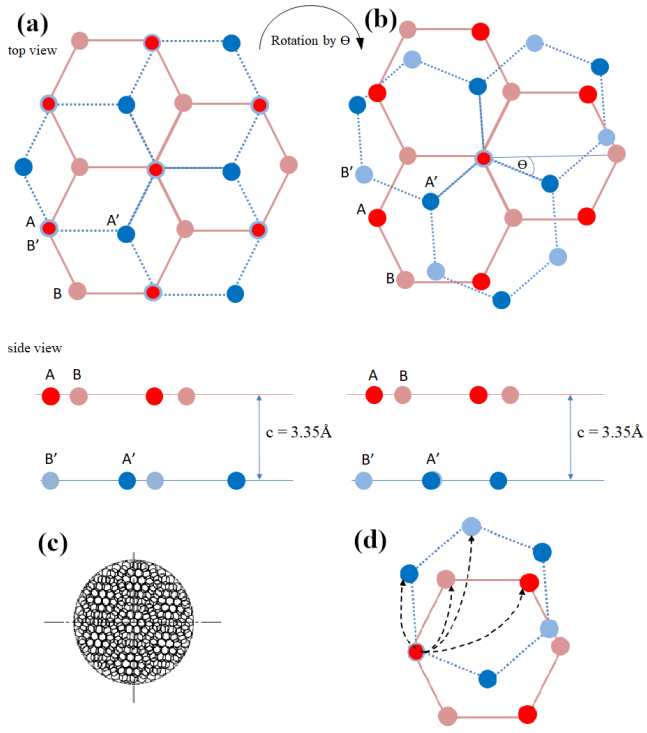

Fig. 1. Two graphene sheets in AB stacking viewed from above and from the side before (a) and after (b) the twist by θ. (c) Two graphene sheets twisted against each other with an emerging moiré pattern. (d) Example of various hoppings between atoms included in Eq. (1).

We study electronic structure using tight-binding approximation. The Hamiltonian has the form of [45]

$$H = \sum_{i,j} t_{i,j} \left|i\right\rangle \left\langle j\right| . \tag{1}$$

Hopping parameters, describing both inter- and intra-layers tunneling processes (shown schematically in Fig. 1 (d)) are given by

$$\begin{aligned} t_{i,j} \;=\; & n^2 \gamma_0 \exp\left[\lambda_1 \left(1 - \frac{|r_i - r_j|}{a}\right)\right] \\ & + \left(1 - n^2\right) \gamma_1 \exp\left[\lambda_2 \left(1 - \frac{|r_i - r_j|}{c}\right)\right] , \end{aligned} \tag{2}$$

where $r_{i,j}$ are the positions of lattice sites and n is the direction cosine of the twist angle of $r_i - r_j$ along the out-of-plane axis (z-axis). γ_0 and γ_1 are the intra- and inter-layer hopping parameters, respectively. $\lambda_{1,2}$ are corresponding hopping decay constants. The values of these parameters were taken from Ref. [45].

We have started the analysis from examining the bilayer graphene without a twist ($\theta = 0°$). Contrary to predictions, a large peak around energy $E = 0$ was observed. We have identified this peak to be a consequence of the edge states present in the finite system. To exclude those from future calculations, we have set a cut-off radius for the atoms taken into consideration (at 95% of the radius of the whole system). Each atom is then examined by its wave function's contribution to the bulk and the edge. Wave functions localized mostly at the edges are then excluded from DOS. Applying these procedures to our model, we have obtained DOS that reaches its minimum at energy $E = 0$, which corresponds to the experiment and other theoretical predictions. After twisting the bilayer by a magic angle equal to $\theta = 1.05°$, the DOS changes, however, a clear structure of three van Hove peaks may be observed only in systems consisting of at least 200 000 atoms. As such, in our further calculations, we have used systems larger than that, reaching a computational limit with 1.2×10^6 atoms.

In the next step, we consider the Anderson disorder, simulated by adding a random number from a given range $(-W/2, W/2)$ to the diagonal in the Hamiltonian, representing on-site energy of A(B) and A'(B') atoms from lower and upper graphene layer, respectively. Calculations of DOS are repeated over 10 disorder configurations in order to get more reliable results. Small number of disorder configurations is restricted by large computational effort related to large number of atoms and long-range nature of the tight-binding model.

3. Results

The position of the satellite peaks is an important feature of the system as it allows for determining its twist angle. As such, we have compared the results obtained in our simulations for different twist angles with best fit to experimental data extracted from Ref. [44]. As one can see in Fig. 2, the position of the satellite peaks changes linearly with the twist angle with the exception of the magic angle ($\theta = 1.05°$). The small discrepancy between the simulation and the experiment can be a matter of parametrization.

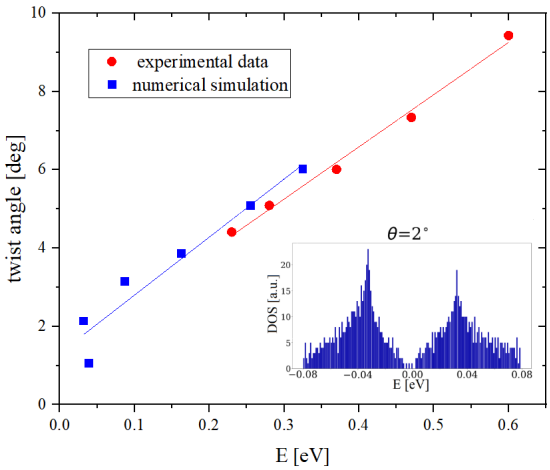

Fig. 2. (Colour on-line) Comparison of the positions of satelite peaks — red dots refer to experimental data extracted from Ref. [44], blue squares refer to our numerical simulations. Inset: DOS of a graphene bilayer twisted by $\theta = 2°$ consisting of 725 716 atoms.

Figure 3 shows the results for different strengths of the disorder applied in a MATBG system consisting of 0.25×10^6 atoms. One can notice that the disorder has a strong effect on the peak and relatively small effect on the rest of the DOS. What is interesting, it does not change the position of the satellite peaks on the energy scale, consistently with results for twisting disorder [43].

Analysing the disorder strength as a function of the peak magnitude, one can notice that the relation is linearly decreasing as the disorder strength grows, as demonstrated in the inset of Fig. 3 (blue line). For the disorder strength in the range of 500 meV, the peak has decreased by over 45% which leads to the DOS being spread more evenly. One can also notice that the average magnitude of two satelite peaks remains quite stable regardless the disorder strength (inset of Fig. 3 (red line)).

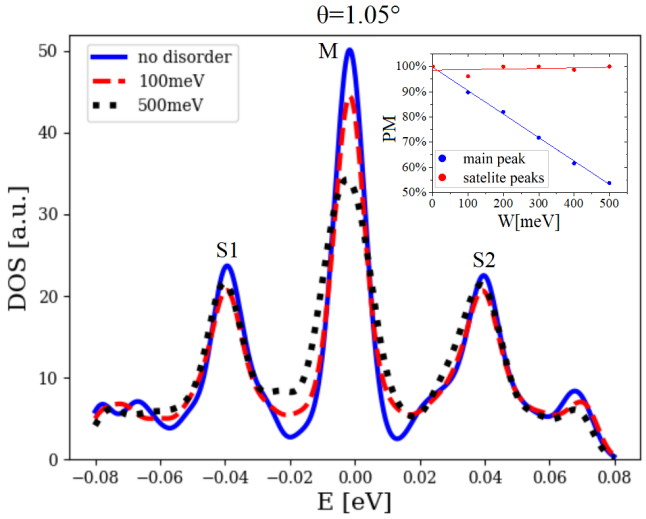

Fig. 3. (Colour on-line) A difference between the DOS of a clean system (blue, solid line) and one with disorder of 100 meV (red, dashed line) and 500 meV (black, dotted line). Inset: relation of disorder strength W and the peak magnitude (PM) at $E = 0$ meV (blue line — decreasing from 100% to almost 50%) and the averaged two satellite peaks around the energies $E = \pm 0.04$ meV (red line — keeping steady around 100%).

4. Discussion

In this work, we conducted a series of numerical simulations for large MATBG samples within real-space tight-binding approximation. We have observed that only for systems large enough, properties of DOS predicted by the continuum models can be obtained. Focusing on density of states near the Fermi level, addition of Anderson-like disorder influences mainly the central DOS peak, weakly affecting the satellite ones. Interestingly, we observe linear behaviour between height of the central peak in DOS and disorder strength W.

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REFERENCES

[1] K.S. Novoselov *et al.*, *Science* **306**, 666 (2004).

[2] K.S. Novoselov *et al.*, *Nature* **438**, 197 (2005).

[3] Y. Zhang, Y.-W. Tan, H.L. Stormer, P. Kim, *Nature* **438**, 201 (2005).

[4] A.D. Guclu, P. Potasz, M. Korkusinski, P. Hawrylak, «Graphene Quantum Dots», *Springer*, 2014, First edition.

[5] H. Aoki, M.S. Dresselhaus, «Physics of Graphene», *Springer*, 2014, First edition.

[6] A.H. Castro Neto *et al.*, *Rev. Mod. Phys.* **81**, 109 (2009).

[7] V.N. Kotov *et al.*, *Rev. Mod. Phys.* **84**, 1067 (2012).

[8] M.O. Goerbig, *Rev. Mod. Phys.* **83**, 1193 (2011).

[9] S. Das Sarma, S. Adam, E.H. Hwang, E. Rossi, *Rev. Mod. Phys.* **83**, 407 (2011).

[10] N.M.R. Peres, *Rev. Mod. Phys.* **82**, 2673 (2010).

[11] E. McCann, M. Koshino, *Rep. Prog. Phys.* **76**, 056503 (2013).

[12] D. Graf *et al.*, *Nano Lett.* **7**, 238 (2007).

[13] A. Reina *et al.*, *Nano Lett.* **9**, 30 (2009).

[14] A.C. Ferrari *et al.*, *Phys. Rev. Lett.* **97**, 187401 (2006).

[15] K.R. Paton *et al.*, *Nature Mater.* **13**, 624 (2014).

[16] E. McCann, V.I. Fal'ko, *Phys. Rev. Lett.* **96**, 086805 (2006).

[17] E. McCann, *Phys. Rev. B* **74**, 161403 (2006).

[18] J.M.B. Lopes dos Santos, N.M.R. Peres, A.H. Castro Neto, *Phys. Rev. Lett.* **99**, 256802 (2007).

[19] E. Suárez Morell *et al.*, *Phys. Rev. B* **82**, 121407 (2010).

[20] R. Bistritzer, A.H. MacDonald, *Proc. Natl. Acad. Sci.* **108**, 12233 (2011).

[21] B. Lian, F. Xie, B.A. Bernevig, arXiv:1811.11786 [cond-mat.mes-hall].

[22] N.F.Q. Yuan, L. Fu, *Phys. Rev. B* **98**, 045103 (2018).

[23] A. Thomson, S. Chatterjee, S. Sachdev, M.S. Scheurer, *Phys. Rev. B* **98**, 075109 (2018).

[24] T. Huang, L. Zhang, T. Ma, *Sci. Bull.* **64**, 310–314 (2019).

[25] H.C. Po, L. Zou, A. Vishwanath, T. Senthil, *Phys. Rev. X* **8**, 031089 (2018).

[26] H. Isobe, N.F.Q. Yuan, L. Fu, *Phys. Rev. X* **8**, 041041 (2018).

[27] J.F. Dodaro *et al.*, *Phys. Rev. B* **98**, 075154 (2018).

[28] H. Guo, X. Zhu, S. Feng, R.T. Scalettar, *Phys. Rev. B* **97**, 235453 (2018).

[29] M. Ochi, M. Koshino, K. Kuroki, *Phys. Rev. B* **98**, 081102 (2018).

[30] C.-C. Liu, L.-D. Zhang, W.-Q. Chen, F. Yang, *Phys. Rev. Lett.* **121**, 217001 (2018).

[31] B. Padhi, C. Setty, P.W. Phillips, *Nano Lett.* **18**, 6175 (2018).

[32] V.Y. Irkhin, Y.N. Skryabin, *JETP Lett.* **107**, 651 (2018).
[33] X.Y. Xu, K.T. Law, P.A. Lee, *Phys. Rev. B* **98**, 121406 (2018).
[34] J. Kang, O. Vafek, *Phys. Rev. X* **8**, 031088 (2018).
[35] M. Koshino *et al.*, *Phys. Rev. X* **8**, 031087 (2018).
[36] Y. Cao *et al.*, *Nature* **556**, 80 (2018).
[37] Y. Cao *et al.*, *Nature* **556**, 43 (2018).
[38] G. Li *et al.*, *Nature Phys.* **6**, 109 (2010).
[39] M. Yankowitz *et al.*, *Science* **363**, 1059 (2019).
[40] K. Kim *et al.*, *Proc. Natl. Acad. Sci.* **114**, 3364 (2017).
[41] M. Andelkovic, L. Covaci, F.M. Peeters, *Phys. Rev. Materials* **2**, 034004 (2018).
[42] A. Thomson, J. Alicea, arXiv:1910.11348 [cond-mat.str-el].
[43] J.H. Wilson, Y. Fu, S.D. Sarma, J.H. Pixley, arXiv:1908.02753 [cond-mat.dis-nn].
[44] I. Brihuega *et al.*, *Phys. Rev. Lett.* **109**, 196802 (2012).
[45] A. Kerelsky *et al.*, *Nature* **572**, 95 (2019).