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Moiré patterns in twisted bilayer graphene

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Introduction

Graphene has been in the spotlight due to its extraordinary physical and chemical properties. In 2018, unconventional superconductivity was found in bilayer graphene with a twist angle of 1.1° (magic angle) [1], which is a consequence of the appearance of a new periodicity in the lattice (known as Moiré pattern). Thus, motivated by this unconventional property, in this work we explore the new electronic phases triggered by the Moiré patterns in twisted bilayer graphene.

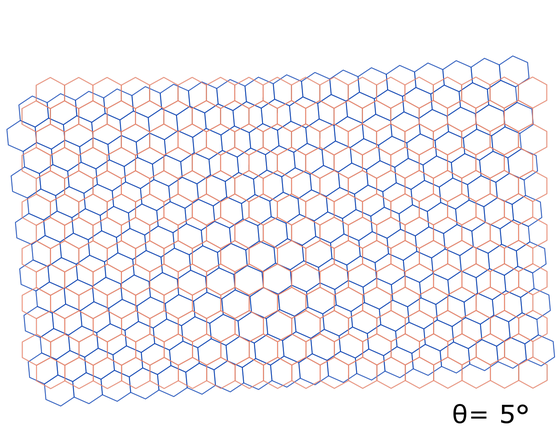


Fig. 1: Schematic view of twisted bilayer graphene.

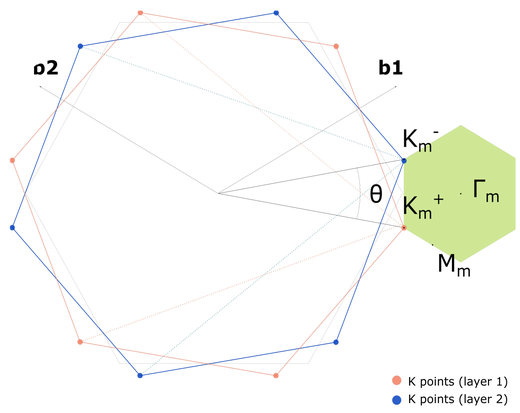


Fig. 2: Momentum-space geometry of a twisted bilayer. (Orange and blue) First Brillouin zone of each rotated layer. (Green) Frist Brillouin zone of twisted bilayer

Methodology

The stacking and rotating two layers are modeled using a continuum low-energy Hamiltonian[2] (Fig. 4). This Hamiltonian only considered the interlayer hopping between close Dirac points. Diagonalizing this Hamiltonian, we plotted the band structure and density of states (DOS) using home-made Python codes.

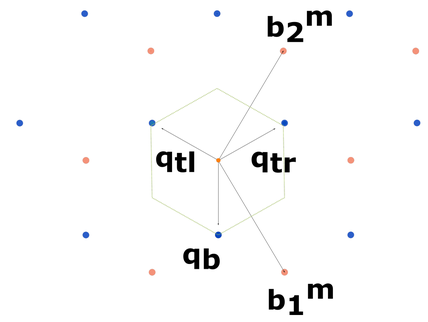


Fig. 3: Closer look of the momentum-space geometry. Reciprocal lattice. (Green) First Brillouin zone of twisted bilayer graphene. At the corner of this zone are the three equivalent Dirac points of layer 2.

$$H^K_{4,tBLG}(\mathbf{q}) = \begin{bmatrix} H_1^K(\mathbf{q}) & T_{\mathbf{qb}} & T_{\mathbf{qtr}} & T_{\mathbf{qtl}} \\ T^\dagger_{\mathbf{qb}} & H_2^K(\mathbf{q}+\mathbf{qb}) & 0 & 0 \\ T^\dagger_{\mathbf{qtr}} & 0 & H_3^K(\mathbf{q}+\mathbf{qtr}) & 0 \\ T^\dagger_{\mathbf{qtl}} & 0 & 0 & H_2^K(\mathbf{q}+\mathbf{qtl}) \end{bmatrix}$$

Fig. 4: Truncated Bloch-Hamiltonian which considers a state in layer 1 (K1+**q**) coupled with states in layer 2 (K2+**qb**, K2+**qtr** and K2+**qtl**).

Results & discussion

We plotted the band structure and DOS for single-layer graphene (Fig. 5) and twisted bilayer graphene an angle θ=5° (Fig. 6). With a twist angle of 5°, electron-hole symmetry is preserved and the linear dispersion still appears near K, K' points; however, the Fermi velocity is renormalized. Also, in twisted bilayer graphene DOS, Van Hove singularities are seen at lower energies [4].

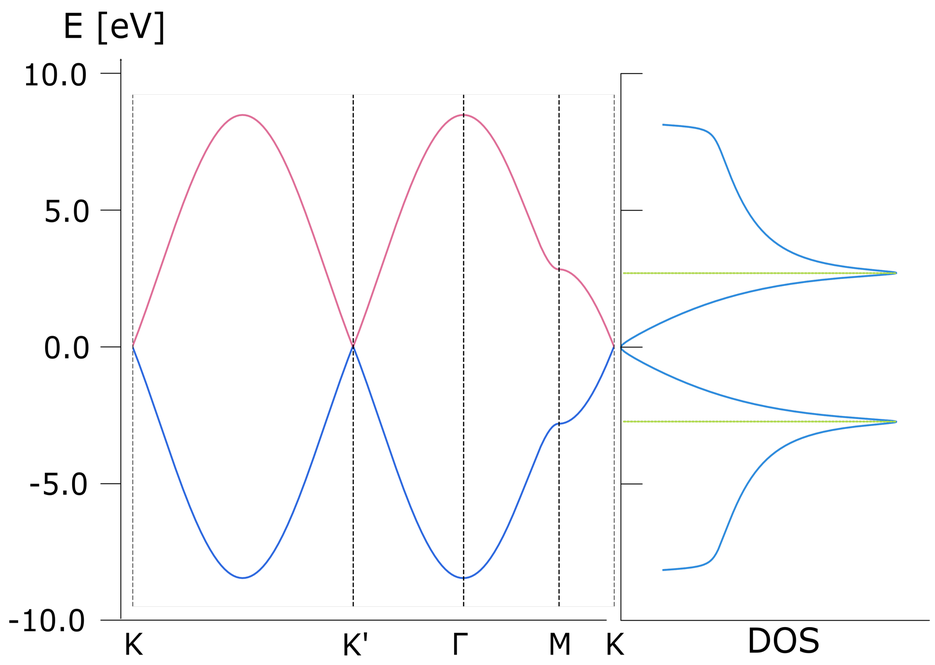


Fig. 5: Band structure and DOS of single layer graphene.

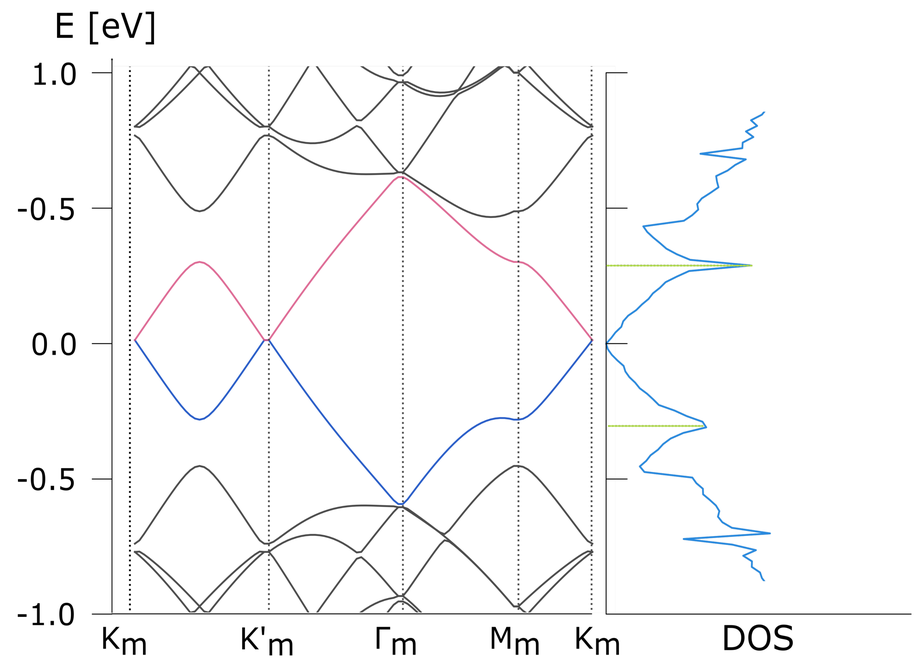


Fig. 6: Band structure and DOS of twisted bilayer graphene.

Conclusions

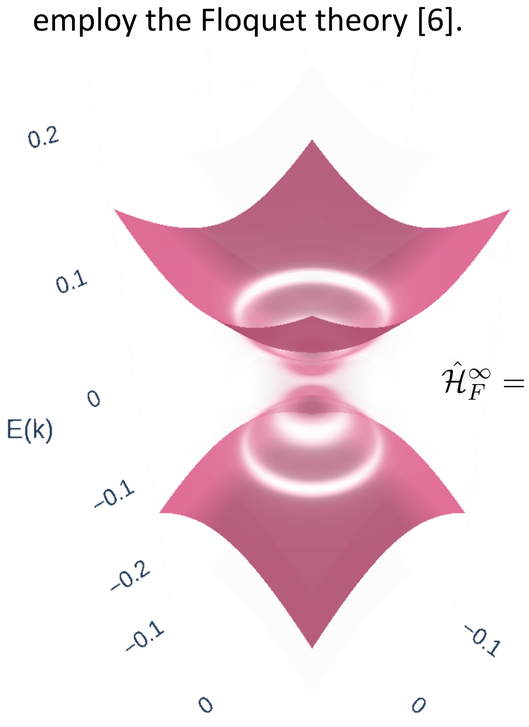
Through the stacking and relative rotation of two graphene layers, it is possible to generate a new periodicity and tune new electronic properties on the material. An effective description can be performed for small angles (10°) if the continuum low-energy Hamiltonian is truncated at a reasonable size.

For more information about this work, please visit:

https://monx-ne.github.io/graf-ge/

Prospects

To enrich the electronic properties of the material, light interaction will be included through a periodic vector potential in time, as done before for the graphene monolayer [5]. To solve this problem we will employ the Floquet theory [6].



$$\hat{\mathcal{H}}_F^\infty = \begin{bmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \iddots \\ \cdots & v_F\mathbf{p}\cdot\boldsymbol{\sigma} + 2\hbar\Omega\mathbf{I} & \frac{v_F e}{2}A_0\sigma_- & \mathbf{0} & \mathbf{0} & \cdots \\ \cdots & \frac{v_F e}{2}A_0\sigma_+ & v_F\mathbf{p}\cdot\boldsymbol{\sigma} + \hbar\Omega\mathbf{I} & \frac{v_F e}{2}A_0\sigma_- & \mathbf{0} & \cdots \\ \cdots & \mathbf{0} & \frac{v_F e}{2}A_0\sigma_+ & v_F\mathbf{p}\cdot\boldsymbol{\sigma} & \frac{v_F e}{2}A_0\sigma_- & \cdots \\ \cdots & \mathbf{0} & \mathbf{0} & \frac{v_F e}{2}A_0\sigma_+ & v_F\mathbf{p}\cdot\boldsymbol{\sigma} - \hbar\Omega\mathbf{I} & \cdots \\ \iddots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Fig. 7: Floquet-Hamiltonian of single layer graphene with periodic vector potential.

Fig. 8: Band structure of single layer graphene with periodic vector potential.

Acknowledgments

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