GRAPHENE AND 2DM VIRTUAL CONFERENCE & EXPO

Graphene online 2020 October 19-23

Topology of Twisted Graphene-hBN Heterostructures

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Abstract

We characterize the topology and simulate the longitudinal and Hall conductivity of multilayers of graphene encapsulated with hexagonal boron-nitride [1-3]. Our model is based on DFT and captures the coupling between layers in a heterostructure. For graphene sitting on an hBN substrate, we can continuously tune the twist angle of each layer, and realize multiple moire patterns with different spatial ranges. We can further simulate two layers of hBN encapuslating one of graphene, with two moire patterns formed by lattice mismatch and relative twist angles. We develop linear scaling algorithms to be able to simulate the longitudinal conductivity as well as the Hall conductivity. Furthermore, when placed under a magnetic field, the system develops topologically non-trivial gaps. We are able to characterize the topology by efficiently compute the Chern number [4].

Model

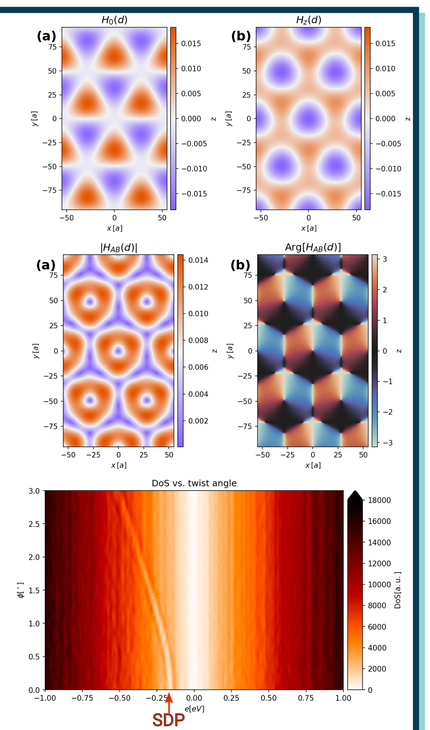
The model [1] links the short-range stacking configurations with the large-ragen moiré pattern. It takes the parameters from DFT expansions and Wannier representations of the Bloch bands at low energy.

Expanded onto a lattice, the graphene layer acquires an effective Dirac mass comming from the hBN layer, plus pseudo-magnetic field from the strain.

The Hamiltonian is

$$H(\boldsymbol{d}) = H_0(\boldsymbol{d}) + H_z(\boldsymbol{d}) + H_{AB}(\boldsymbol{d})$$

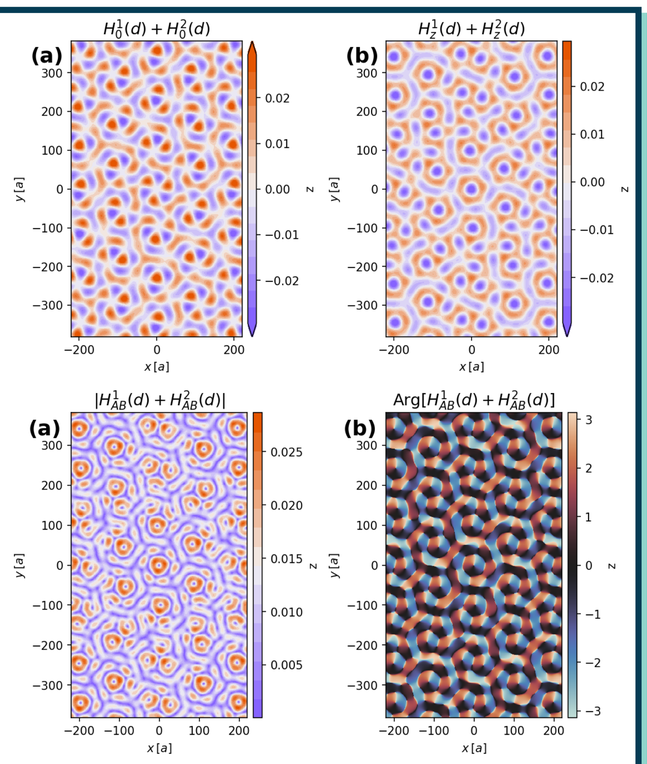
We can vary the twist angle and follow the formation of a second Dirac point gap.



Heterostructures

A graphene layer encapsulated with two layers of hBN will effectively have the contributions from both potentials, realizing a complex supermoiré pattern, which is under intensive study [2].

The size needed to reproduce the low-energy features of these supermoiré structures is very large, and the supermoiré patterns themselves are generally incommensurate [3].



KPM expansion

The Kernel Polynomial Method expands any operator function [5] that depends on the Hamiltonian and other parameters.

$$\hat{f}(\lambda, H)\,|v\rangle = \sum_{m=0}^{M} g_m \mu_m(\lambda) T_m(H)\,|v\rangle$$

$$\mu_m(\lambda) = \frac{2}{\pi}\int_{-1}^{1} \frac{\hat{f}(\lambda, e) T_m(e)}{\sqrt{1-e^2}}\mathrm{d}e.$$

The recursion relation makes it very efficient, with linear scaling.

$$|v_m\rangle = T_m(H)\,|v\rangle$$
$$|v_{m+1}\rangle = 2H\,|v_m\rangle - |v_{m-1}\rangle$$

Typical operators are:

* the density states

$$\rho(e_F, H) = \delta(e_F - H)$$

* the Green's functions (A and R)

$$G^{-}(e_F, H) = \frac{1}{e_F - H + i0^{+}}$$

* the projector over occupied bands.

$$\hat{P}(e_F, H) = \Theta(e_F - H)$$

With these tools we efficiently compute the Kubo conductivity [7]

$$\sigma_{\alpha,\beta} = \frac{ie^2\hbar}{\Omega}\int \mathrm{d}e\, f(e) \times \mathrm{Tr}\left[\, v_\alpha \delta(e-H) v_\beta \frac{\mathrm{d}G^{+}(e,H)}{\mathrm{d}e} - v_\alpha \frac{\mathrm{d}G^{-}(e,H)}{\mathrm{d}e} v_\beta \delta(e-H)\,\right]$$

and the local Chern marker [4, 6].

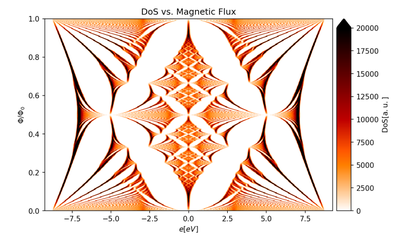
$$C(e) = 2\pi i \mathrm{Tr}_{uc}\left[[Q(e,H)\hat{x}, P(e,H)\hat{y}]\right]$$

The Chern marker describes the topology for non-periodic systems.

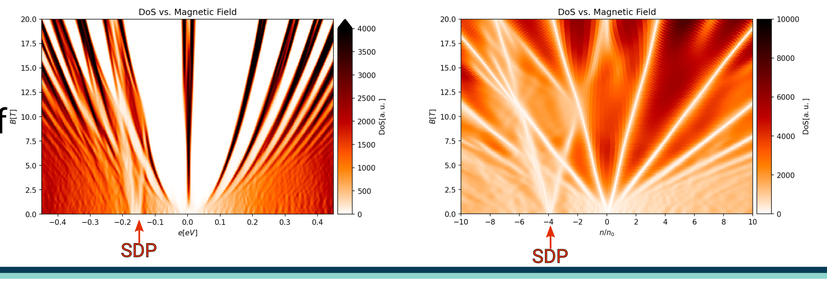
Topology

We can compute the Kubo Hall conductivity and the Chern number on large moiré and supermoiré patterns.

The Chern number characterizes the topology of the gaps. These gaps come from Landau levels induced by magnetic fields, and also from secondary Dirac points (SDP) from the moiré pattern.



Landau fan plot shows the influence of the SDP in a measure vs. electronic density.



Conclusions

* We have developed and composed very powerful methods to simulate very large moiré patterns that allows us to describe the physics at low energies.
* The effective model [1, 3] can succesfully capture the most relevant features of low angle twisted graphene heterostructures.
* The application of the KPM expansion to the computation of the Chern number [4] is efficient enough to characterize the topology of large, complex moiré patterns, even in the incommensurate limit.

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Graphene online 2020