QMC-HAMM P4: Moiré scale effective interaction in twisted bilayer graphene

Run Hou, Scott Jensen, Yueqing Chang, Lucas K. Wagner, Andriy H. Nevidomskyy

Calculating the effective interaction

We provide functions for generating effective interactions for the user defined lattice positions, tight binding models and atomistic interactions

- We project the atomistic interactions onto active bands to obtain effective Moiré-scale interactions
- The nearly flat bands at a magic small twist angle lead to correlated electronic states. It is important to obtain accurate low energy effective models for studying the rich phase diagram of the system.

Methods

- Lattice relaxation
  - Atomic positions

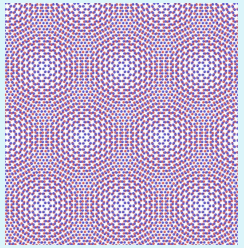
  Rigid lattice, MD relaxed lattice
- Tight-binding models

  E.g., MK [1], LETB [2]
  - Result in TB bands or HF bands and orbitals
- Downfolding interaction onto active bands
  - Full data of effective interaction

Workflow

Input

Lattice structure + Tight-binding model

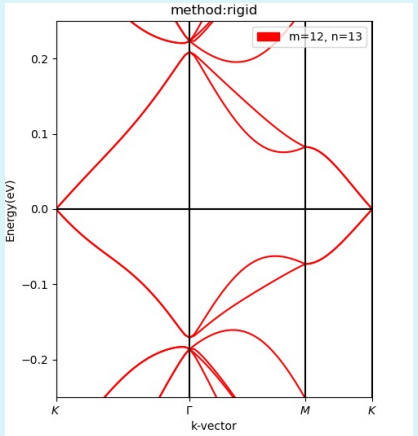


$t_{ij}(r)$

Diagonalization

Tight binding bands

TB bands $\theta = 2.65°$



+

Microscopic interaction

- On-site interaction

$$U_0$$

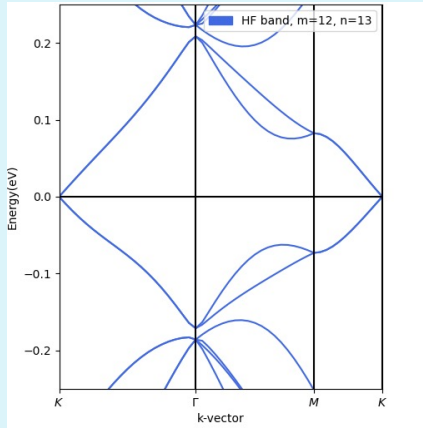
- Long-range interaction

$$V(q) = V_0 \frac{tanh(dq)}{q}$$

Atomistic Hartree-Fock calculation

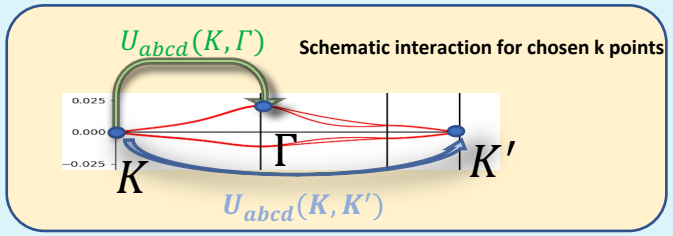
Hartree-Fock bands

HF bands with on-site interaction $U_0 = 4\text{eV}, \theta = 2.65°$



Output

Projected interaction U_{abcd} for 4 bands per spin in the low energy Moiré -scale model of TBLG



Examples of effective interactions for several twist angles

(m,n) (k_1,k_2)	(3,4) (K_M,Γ)	(12,13) (K_M,Γ)	(27,28) (K_M,Γ)	(31,32) (K_M,Γ)
U_0(eV)	4.00			
U_{1111}(meV)	9.43	0.66	0.23	0.16
U_{1221}(meV)	8.49	0.70	0.30	0.16
U_{2121}(meV)	8.58	0.66	0.28	0.16

The effective interactions can be further used to study the phase diagram of TBLG by highly accurate many-body methods such as DQMC

Reference

1] Moon, Pilkyung, and Mikito Koshino. "Energy spectrum and quantum Hall effect in twisted bilayer graphene." *Physical Review B* 85.19 (2012): 195458.

[2] See QMC-HAMM P2. "An accurate tight binding model for twisted bilayer graphene".

Acknowledgements

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