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Efficient and extensible tight-binding model for twisted bilayer graphene

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Abstract

Atomically thin (2D) twisted materials have attracted the attention of theoretical and experimental studies that aim to understand the exotic properties of low-dimensional systems. In this sense, a comprehensive theory of 2D twisted materials is desirable to interpret ongoing and future experiments. Most novel properties of such materials are a result of out-of-plane interactions between their layers, which may lead to strong interlayer coupling and lattice reconstruction. The introduction of a twist, however, changes the periodicity formed between the layers due to their crystalline nature. These effects, together, induce the formation of Moiré superlattices with unique physical properties. In the case of twisted bilayer graphene (TBG), the Dirac cone bands are flattened as the twist angle decreases. This delocalization in momentum space - and consequent localization in real space - is associated with strongly correlated quantum states due to the predominance of electron-electron interactions over kinetic energy. For small twist angles, however, the unit cell of a Moiré superlattice may have thousands of atoms. The use of first-principles calculations alone is hence limited due to their large computational complexity, and more efficient approaches become necessary.

We developed a computer code to calculate the eigenstates of large tight-binding TBG Hamiltonian NxN matrices in momentum space. The inputs are the twist angle and the hopping energy functions. To validate our code, a small number of electronic bands in the range of low energy excitations were calculated, for carefully chosen twist angles. This was sufficient to describe the Dirac cone bands flattening of TBG with decreasing twist angle. Our approach showed to be efficient and has potential for several extensions: (i) we can compute the full spectrum of bands and wave functions of N~O(10^3) unit cells, or even O(10^4) with the help of computer clusters; (ii) the computed wave functions can be used in further investigations; and (iii) we can introduce vacancies, defects, geometric deformations, and electromagnetic fields without drastically affecting the computational cost.