Tight binding simulations of twisted graphene multilayers

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Abstract

Twisted multilayers of graphene have gathered significant attention in recent years. These systems present a wide variety of exotic physical behaviour that differs from graphene, including quasi-crystal behavior, and superconducting states [3],[4].

Recent studies have shown the appearance of quasicrystalline superconducting states in incommensurate Moiré systems [2], arising from a Moiré length mismatch in graphene trilayers with different combinations of rotation angles. These systems frequently have gigantic unit cells, when commensurate, which thus calls for new numerical methods to explore their properties.

Here we examine a variety of different Moiré systems by making use of a real-space kernel polynomial approach to compute their electronic properties[1]. With our approach, we are able to study the physics of commensurate and incommensurate systems with sizes approaching the micron scale. We discuss the appearance of potentially exotic localized states in different multilayer configurations, and give perspectives for their further discovery.

References

Figures

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Figure 1. Left: resonant states in the dodecagonal graphene (30°) structure. Middle: Moiré quasicrystal (θ_1 =1.42°, θ_2 =-1.88°). Right: resonant edge states of dodecagonal graphene.