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Quasicrystalline Electronic States in 30° rotated Twisted Bilayer Graphene

Quasicrystal is a unique form of solid matter which is ordered but not periodic. Thus, quasicrystal can provide important insights on the effects of atomic ordering at the interface between periodic crystals and amorphous. The recently realized bilayer graphene system with a twist angle of 30° offers a new type of quasicrystal (“quasicrystalline twisted bilayer graphene”) which unites the dodecagonal quasicrystalline nature and the relativistic properties of graphene [1].

In this talk, we introduce a concise theoretical framework that fully respects both the dodecagonal rotational symmetry and the massless Dirac nature, to describe the electronic states of the system [2]. We find that the electronic spectrum consists of resonant states labeled by 12-fold quantized angular momentum, together with the extended relativistic states. The resulting quasi-band structure (Fig. 1) is composed of the nearly flat bands with spiky peaks in the density of states, where the wave functions exhibit characteristic patterns which fit to the fractal inflations of the quasicrystal tiling (Fig. 2). The flat band area in k -space is approximately 14 times as large as that of the magic angle twisted bilayer graphene [3]. We also demonstrate that the 12-fold resonant states appear as spatially-localized states in a finite-size geometry, which is another hallmark of quasicrystal.

While conventional quasicrystals can be viewed as “intrinsic quasicrystals”, where all atomic sites are intrinsically arranged in quasiperiodic order, the quasicrystalline twisted bilayer graphene and related systems can be viewed as “extrinsic quasicrystals” of which quasiperiodic nature arises from the interaction between periodic layers. We will show that the flat band area as well as the quasicrystalline nature can be widely tunable by external pressure or interlayer potential asymmetry.

The theoretical method based on the k -space tight-binding approach developed in this study is applicable to any kind of extrinsic quasicrystals as well as heterostructures of two-dimensional materials having different lattice symmetries (e.g., the combination of rectangle and hexagon).

References

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- [2] P. Moon,*[†] M. Koshino,* Y.-W. Son, Phys. Rev. B 99, 165430 (2019).
- [3] Y. Cao et al., Nature 556, 43 (2018); Y. Cao et al., Nature 556, 80 (2018).

Figures

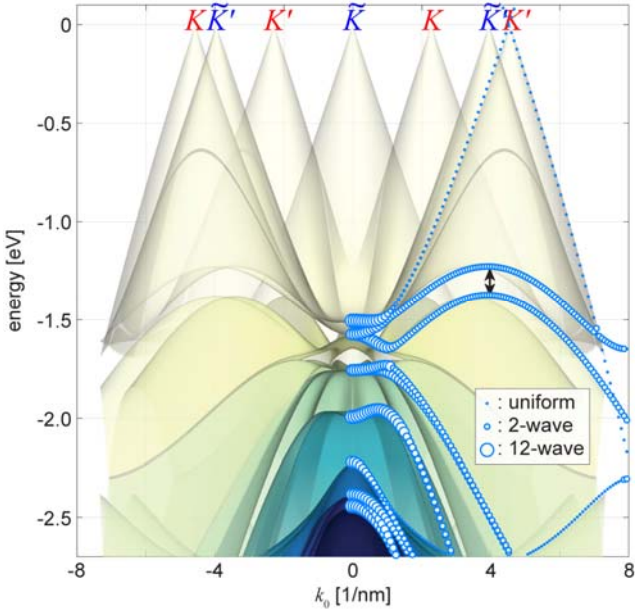


Figure 1: Electronic structures in the valence band side of quasicrystalline twisted bilayer graphene calculated by the k -space (dual) tight-binding model. Blue dots represent the degree of hybridization between the states of pristine graphene. The resonant coupling between twelve waves makes flat bands at around -1.5 and -1.8 eV.

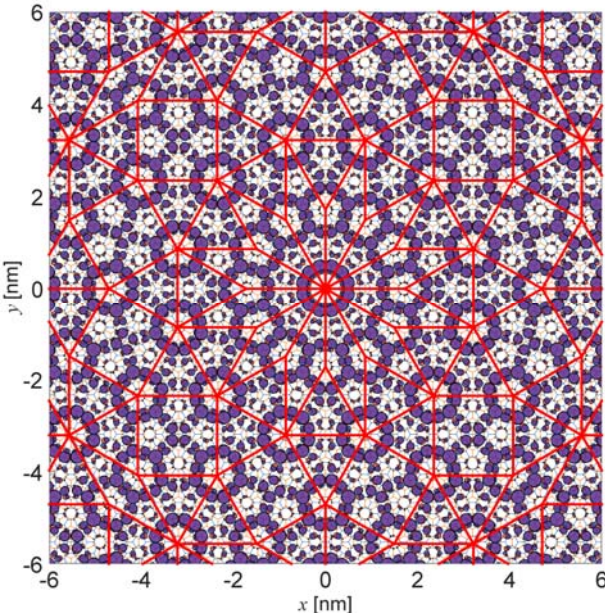


Figure 2: The valence band wave functions near the flat bands in Fig. 1. The area of each circle is proportional to the squared wave amplitude, and red and blue circles represent the states in the upper and the lower layers, respectively. Red lines represent the fourth generation of Stampfli quasicrystal tiling.