Theory of moiré Hofstadter's butterfly in magic-angle graphene

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In the following work, we present our recent theoretical results on the electronic structure and correlations in the twisted bilayer graphene system [1]. We provide a Hofstadter's butterfly spectrum for the magic-angle twisted bilayer graphene, obtained using an ab initio-based multimillion-atom tight-binding model. Incorporating a hexagonal boron nitride substrate and out-of-plane atomic relaxation, we introduce the effects of a magnetic field via the Peierls modification of the long-range tight-binding matrix elements and the Zeeman spin splitting effects. We study a nanoribbon geometry and analyze the quantum size effects for sample widths up to 1 μm, both for a large energy window and for the flat band around the Fermi level. For sufficiently wide ribbons, where the role of the finite geometry is minimized, we obtain and plot the Hofstadter spectrum and identify the in-gap Chern numbers by counting the total number of chiral edge states crossing these gaps. Subsequently, we examine the Wannier diagrams to identify the insulating states at charge neutrality. We establish the presence of three types of electronic states: moiré, mixed, and conventional. Additionally, we discuss the role of electron-electron interactions on the mean field level.

[1] Alina Wania Rodrigues, Maciej Bieniek, Paweł Potasz, Daniel Miravet, Ronny Thomale, Marek Korkusiński, and Paweł Hawrylak, Atomistic theory of the moiré Hofstadter butterfly in magic-angle graphene, Phys. Rev. B 109, 075166 (2024)