Electronic structure of monolayer and bilayer graphene on hexagonal substrates

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The overlaying of two two-dimensional crystals with different periodicity leads to the creation of a moiré pattern, an ideal example being a heterostructure of graphene and hexagonal boron nitride (hBN) [1, 2, 3]. Due to the honeycomb lattice of graphene and hBN, the moiré pattern in this case has the form of a hexagonal lattice with a longer period for a perfect alignment of the two crystalline lattices. Outstanding quality and atomic-scale flatness of such layered structures make it possible for electrons in graphene to undergo coherent Bragg scattering on the moiré potential created by the hBN layer thus imposing a miniband structure on the electronic spectrum.

We develop a phenomenological, symmetry-based theory of monolayer [4] and bilayer [5] graphene placed on substrates with hexagonal Bravais symmetry, such as hBN, and investigate electronic spectra of such structures as a function of symmetry-allowed perturbation parameters. For monolayer graphene, we identify conditions at which the first moiré miniband is separated from the rest of the spectrum by either one or a group of three isolated mini Dirac points and is not obscured by dispersion surfaces coming from other minibands. In such cases the Hall coefficient exhibits two distinct alternations of its sign as a function of charge carrier density. We also show that for bilayer graphene the interplay between the directions of the supercell Brillouin zone and trigonal warping of the electronic spectrum plays an important role in forming the global features of the miniband spectrum. For no lattice misalignment between BLG and hBN, $\theta = 0$, trigonal warping leads to overlapping of different minibands for a considerable part of the perturbation parameter space. At the same time, for small misalignment angles $\theta \approx 0.5°$, the electronic spectrum of BLG on hBN is most likely to exhibit global gaps or secondary isolated Dirac points at the edge of the first moiré miniband. For the case of large misalignment angles, $\theta \gtrsim 1.2°$, the folded chiral bands cross the high-energy bands.

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[4] J. R. Wallbank, A. A. Patel, M. Mucha-Kruczynski, A. K. Geim, and V. I. Fal'ko, arXiv:1211.4711 (2012).
[5] M. Mucha-Kruczynski, J. R. Wallbank, and V. I. Fal'ko, in preparation.