Graphene on Hexagonal Substrates: Moiré Patterns and Electronic Properties

J. R. Wallbank[1], M. Mucha-Kruczyński[1,2], A. A. Patel[1,3], and V. I. Fal'ko[1]
[1]Department of Physics, Lancaster University, Lancaster, LA1 4YB, UK
[2]Department of Physics, University of Bath, Bath, BA2 7AY, UK
[3]Department of Physics, Indian Institute of Technology Kanpur, Kanpur 208016, India
j.wallbank@lancaster.ac.uk

Abstract

The electronic properties of graphene-based devices can be dramatically improved by placing graphene on an atomically flat hexagonal crystal surface. At the same time, a small lattice mismatch or misalignment angle results in the formation of the large, quasi-periodic structure known as a moiré pattern. This pattern is interesting for geometrical reasons, it acts like a magnifying glass, increasing the visibility of various types of defects. Moreover, it's effect on the graphene electrons can be described in terms of scattering using the simplest harmonics of the moiré pattern, which, when combined with the symmetry of the system, allows the Hamiltonian to be written in terms of a small number of phenomenological, substrate dependent, parameters. When the substrate in question has the lattice constant similar to graphene, such as hexagonal boron nitride, it is the intravalley scattering terms that will dominate [1]. Additionally, there are many substrates, including certain transition metal dichalcogenides, with a unit cell area approximately three times larger than that of graphene. In this case, the intervalley scattering terms will dominate.

We investigate the characteristic features that appear in the graphene miniband spectrum, systematically exploring the space of phenomenological substrate parameters, and show that the zero-energy Dirac spectrum always remains intact. For a large parametric regime of the intravalley substrate scattering, we find additional mini Dirac points (mDPs), isolated on the energy axis, between the top of the first moiré miniband and the bottom of the second. This contrasts with the intervalley scattering, which can open a band gap between the two minibands.

Experimental consequences of the moiré minibands, and in particular the isolated mDPs, can be seen upon the application of an intermediate magnetic field: Both the Landau level spectra around the mDP and the sign change behaviour of the Hall coefficient upon doping through the mDP, mimic that of the main Dirac point at the conduction-valence band edge.

In stronger magnetic fields, the large size of the moiré supercell makes this an ideal system to observe the effects of the Hofstadter butterfly. When the magnetic flux per moiré supercell, $\Phi=\Phi_0\ p/q$, is increased to a significant rational fraction of the flux quanta, Φ_0, each Landau level is split into q magnetic minibands resulting in an interesting fractal pattern of energy bands with experimentally observable consequences [2].

References

[1] J. R. Wallbank, A. A. Patel, M. Mucha-Kruczyński, A.K. Geim, V. I. Fal'ko, arXiv:1211.4711 (2012)
[2] L. A. Ponomarenko, R. V. Gorbachev, D. C. Elias, G. L. Yu, A. S. Mayorov, J. R. Wallbank, M. Mucha-Kruczynski, A. A. Patel, B. A. Piot, M. Potemski, I. V. Grigorieva, K. S. Novoselov, F. Guinea, V. I. Fal'ko, A. K. Geim, arXiv:1212.5012 (2012)

Figures

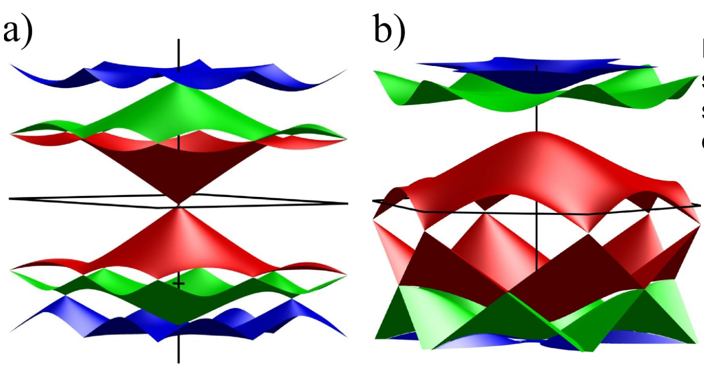

Fig1: Examples of the moiré miniband structure for graphene on a hexagonal substrate subject to intravalley scattering (a), or intervalley scattering (b).