20th Brazilian Workshop on Semiconductor Physics

High-energy Landau levels in graphene beyond first nearest-hopping processes: Corrections to the effective Dirac Hamiltonian

Kevin J. U. Vidarte[1], and Caio Lewenkopf[2,3]
[1]*Instituto de Física, Universidade Federal do Rio de Janeiro, 21941-972 Rio de Janeiro – RJ, Brazil*
[2]*Instituto de Física, Universidade Federal Fluminense, 24210-346-346 Niterói – RJ, Brazil*
[3]*Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany*
kevinvidarte@pos.if.ufrj.br
caio_lewenkopf@id.uff.br

Abstract

We study the Landau level spectrum of bulk graphene monolayers beyond the Dirac Hamiltonian with linear dispersion. We consider an effective Wannier-like tight-binding model obtained from *ab initio* calculations, that includes long-range electronic hopping integral terms [1, 2]. We employ the Haydock-Heine-Kelly (HHK) recursive method [3-5] to numerically compute the Landau level spectrum of bulk graphene in the quantum Hall regime, circumventing the need of using large supercells and the corresponding restriction on the magnetic field [6], and demonstrate that this method is both accurate and computationally much faster than the standard numerical approaches used for this kind of study. The Landau level energies are also obtained analytically for an effective Hamiltonian that accounts for up to third nearest neighbor hopping processes. Our analytical approach is based, as standard, in expanding the electronic dispersion relation around the Dirac points, the K and K'-points, in powers of the canonical momentum [7]. We find an excellent agreement between both approaches. We also study the effect of disorder on the electronic spectrum. Our analysis helps to elucidate the discrepancy between the high-energy Landau levels measured using infrared transmission spectroscopy [8] and theory.

References

[1] J.-C. Charlier, J.-P. Michenaud, X. Gonze, and J.-P. Vigneron, Tight-binding model for the electronic properties of simple hexagonal graphite, Phys. Rev. B 44, 13237 (1991).
[2] A. Urban, M. Reese, M. Mrovec, C. Elsasser, and B. Meyer, Parameterization of tight-binding models from density functional theory calculations, Phys. Rev. B 84, 155119 (2011).
[3] R. Haydock, V. Heine, and M. J. Kelly, Electronic structure based on the local atomic environment for tight-binding bands, J. Phys. C: Solid State Phys. 5, 2845 (1972).
[4] R. Haydock, V. Heine, and M. J. Kelly, Electronic structure based on the local atomic environment for tight-binding bands: II, J. Phys. C: Solid State Phys. 8, 2591(1975).
[5] R. Haydock, The recursive solution of the Schrodinger equation, in Solid State Physics, Vol. 35, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic Press, 1980) pp. 215–294.
[6] R. Haydock, The recursive solution of the Schrodinger equation, Comput. Phys. Commun. 20, 11 (1980).
[7] M. O. Goerbig, Electronic properties of graphene in a strong magnetic field, Rev. Mod. Phys. 83, 1193 (2011).
[8] P. Plochocka, C. Faugeras, M. Orlita, M. L. Sadowski, G. Martinez, M. Potemski, M. O. Goerbig, J. N. Fuchs, C. Berger, and W. A. De Heer, High-energy limit massless Dirac fermions in multilayer graphene using magneto-optical transmission spectroscopy, Phys. Rev. Lett. 100, 087401 (2008).