Use of the tight-binding approach to investigate the Wannier functions of graphene

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Abstract

At the very frontier of science for several years [1], graphene has been studied because of its unique transport properties and relative ease of manufacturing. It is one of the most promising materials for a wide range of applications in nano-electronics, opto-electronics and photodetectors [2, 3]. Recent work has shown that a tight-binding approximation [4] associated with generalized Wannier functions provides a physically intuitive picture of the electronic bands of graphene [5-7]. The crystalline structure of graphene is a planar honeycomb atomic array with covalent bonds between sp^2 hybrid orbitals. In the present work, the symmetry and the localization properties of the Wannier functions of graphene are investigated. The Bloch functions, which depend on the three spatial coordinates and on the two-dimensional wave vector, are obtained through the tight-binding method. Only the on-site and the nearest-neighbor matrix elements of the Hamiltonian are taken into account. Due to symmetry, the band structure is split into six s-p_x-p_y bands and two p_z bands. The phase of the Bloch functions of each band is appropriately chosen, in order to produce Wannier functions of maximal localization. The calculated Wannier functions are shown to resemble either bonding or anti-bonding molecular orbitals, whose relation with the sp^2 hybrid orbitals is discussed. The numerical code gives Bloch functions that depend smoothly on the wave vector, and this leads to well localized Wannier functions. They also show rotational and mirror symmetries. Nevertheless, the phase of the Bloch functions is further improved in order to minimize the spread of the Wannier functions. Such functions are compared with the available multi-band Wannier functions [7]. The present approach sheds further light on the physical properties of graphene and provides a simple mathematical treatment of Wannier functions in two-dimensional materials.

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References

[1] K. S. Novoselov et al. **Science** 306, 666, (2004).
[2] A. H. Castro Neto *et al*., **Rev. Mod. Phys**. 81, 109 (2009).
[3] C. H. Liu et al. **Nature Nanotechnology** 9, 273 (2014).
[4] R. Kundu, **Modern Physics Letters B** 25 (3), 163 (2011).
[5] J. Jung and A. H. MacDonald, **Phys. Rev. B**, 87, 195450 (2013).
[6] J. Jung and A. H. MacDonald, **Phys. Rev. B** 89, 035405 (2014)
[7] N. Marzari et al, **Rev. Mod. Phys**. 84, 1419 (2012).