The effect of a third nearest neighbor tight binding model on the pseudo-magnetic field in graphene

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Abstract

The lattice structure of graphene consists of two Bravais sub-lattices. The electronic bands of the two sub-lattice sites are degenerate. However, when the surrounding structure of each of these two sites differ, as when non-uniform strain is applied, this degeneracy is broken. The impact of strain in graphene when described using a Dirac Hamiltonian in the continuum approximation mimics that of a magnetic field for the spin degree of freedom [1]. Consequently, the lattice degree of freedom has been termed pseudo-spin, and the effect of strain can be related to a pseudo-magnetic field. One of the most striking consequences of this effect, is the appearence of Landau-like levels [1]. Landau quantization usually arises from the cyclotron motion of electrons (charged particles) in *real* magnetic fields, where electrons can only occupy orbits with discrete energy values, called Landau levels. These Landau levels are reflected in the density of states (DOS).

Landau-like levels consequence of lattice deformation were first observed using scanning tunneling spectroscopy on an accidentally produced bubble in graphene [2]. The experimental confirmation of such a peculiar phenomena opens two main questions. The first one is related to the validation of the continuum approach, in which an analytical expression for the strain field is introduced, from which the value of the psedo-magnetic field and the DOS with the corresponding Landau-like signatures are derived. A first challenge to such a model was presented using a semi-empirical single-orbital and distance-dependent tight binding model (TBM) [3,4] up to first nearest neighbors. Within this model, the strain field was explicitly included in the coordinates of toy models (e.g. an hexagonal flake) subject to relaxation using classical molecular dynamics. The value of the pseudo-magnetic field was extracted from the numerical computation of the DOS, finding that the discrepancy between the two models is important.

The simplest TBM to describe the electronic properties of graphene consists in a one orbital model, and is sufficient to describe the band structure close to the Fermi level. This approximation can be done because the π orbitals in graphene are effectively decoupled from the σ orbitals. This simple model, that usually includes only nearest-neighbor interactions, is very successful in describing the properties of graphene at low energies. However, Mintmire et al. showed that for an accurate description of the properties of graphene and graphene nanoribbons, particularly the ones with armchair edges, third nearest neighbor interactions must be included [5]. It has been predicted that the effect of the strain in hexagonal graphene depends on the edge shape [3]. This work addresses the impact on the pseudomagnetic field of a third nearest neighbor model of graphene.

References

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