Graphene structures with circular shape: a study of the influence of topological defects in transport properties

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Abstract

We investigate the transport properties of graphene layers with circular shapes (quantum dots) and several kind of topological defects. An example is drawn in the Figure 1, which shows a pentagonal defect. For dynamical relaxation we use a Tersoff-Brenner potential in order to get their 3D arrangement. We check that variations in bond lengths are lower than 5%. We calculate the density of states of these structures and check that it shows several peaks associated with quasi-bound states. Other authors have made similar studies but considering different geometries: Zhang *et al.* [1, 2] worked on transport with narrow ballistic ribbon of graphene with zigzag edges including topological defects. Carpio *et al.* [3] studied just electronic properties in a similar structure but with dislocations consisting of heptagon–pentagon pairs in an hexagon lattice.

In our calculations we employ a tight-binding model which only takes into account one π-orbital per atom. The overlap energy between nearest neighbors is taken as $t = -2.66$ eV where second-neighbor interactions are neglected. Interactions with media sorrounding the graphene layer are not considered. We calculate electronic properties of our graphene structures, as density of states and transmission function using the Green's function method [4], using the standard expression $\hat{G}(E) = \left(E\hat{I} - \hat{H}_n - \hat{\Sigma}_L - \hat{\Sigma}_R\right)^{-1}$, and the formalism developed by López Sancho *et al.* [5]. The latter has the advantage that converges very fast and has been applied to graphene layers by other authors (see. e. g. [6]). We also calculate the eigen-energies E_n and eigen-functions Ψ_n, in order to obtain the participation number P_n: $P_n^{-1} = \sum_m |\Psi_n(m)|^4$, which gives a measure of the wavefunction extension and help to find out the localized or extended nature of an electronic state.

With the formalism developed above we show that density of states shows several peaks associated with both the pressence of quasi-bound states (due to the circular confinement) and localized edge states due to circular boundaries of the finite lattice. These results are manifested in the peak structure in the transmission function and are checked calculating the local density of states and participation number obtained directly from the eigenstates. We observe a change in the available quasi-bound states due to the defects presence and new peak of the transmission function.

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Figures

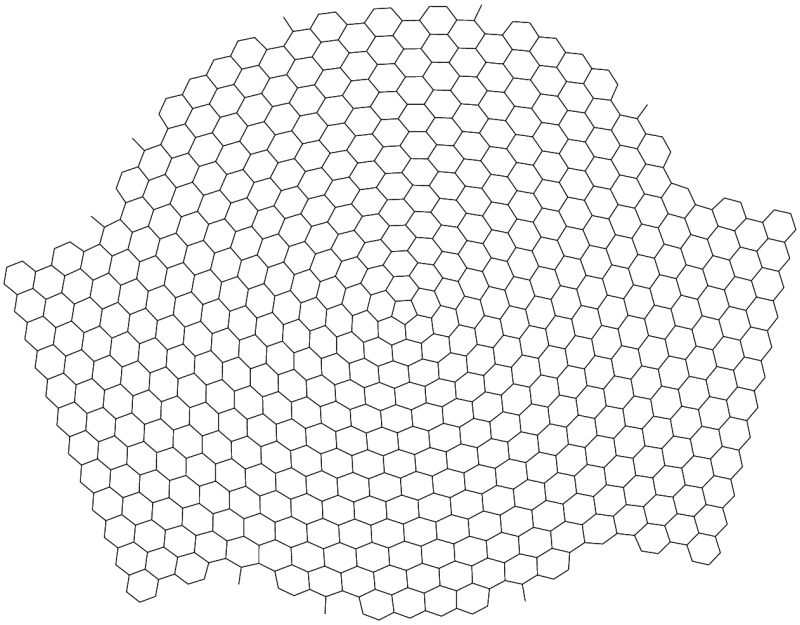

Figure 1: Geometry of the graphene sheet studied in this work. Note the pentagonal defect placed at its centre. This structure is connected to 2 semi-infinite graphene leads, which are partially shown in the figure.