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Disorder-induced localised gating in graphene

Thomas Aktor, Antti-Pekka Jauho and Stephen R. Power

Introduction
Gating of individual atoms in graphene would allow extremely precise control of current flow. In practice, however, this is very difficult to achieve. In this work we investigate whether doping or spatially restricted gating can be used to achieve similar control. Two systems are considered:
- Sublattice asymmetric doping within a region in a pristine graphene sheet [1,2].
- Sublattice symmetric gated region in a pristine graphene sheet [4].

Sublattice symmetric potential
The onsite potential is shifted in both sublattices, with an average change (keeping the shift times concentration constant) of: \( \varepsilon_k = \varepsilon_a = 0.1|c| \), for a varying concentration of atoms \( c \) \( = 1, 0.5, 0.2 \) within a circular region of radius 20nm. The positive energies are the most interesting.
- \( c = 1.0 \)
- \( c = 0.5 \)
- \( c = 0.2 \)

Sublattice asymmetric potential
The onsite potential is shifted in one of the sublattices, with an average change (keeping the shift times concentration constant) of: \( \varepsilon_k = 0.2|c| \), \( \varepsilon_a = 0 \), for a varying concentration of A-atoms \( c_a \) \( = 1, 0.5, 0.2 \) within a circular region of radius 20nm.
- \( c_a = 1.0 \)
- \( c_a = 0.5 \)
- \( c_a = 0.2 \)

Green’s Function of Graphene
- The 1NN tight binding model graphene pristine Hamiltonian, \( H^{(0)} = \begin{pmatrix} 0 & -t_f(k) \\ -t_f(k) & 0 \end{pmatrix} \).
- The Green’s Function, \( G^{(0)}(x, r_f) = \frac{1}{2} \int d^2k \frac{N_{xj}(k)N_{jx}(k)R_{xj}(k)}{-t_f(k)} \).
- One of the \( k \) integrals can be done analytically [4], leaving one to be calculated numerically.

Conclusions
- The key features of the DOS for the asymmetrically doped dot are largely independent of \( c_a \).
- The key features of the DOS for the uniformly gated dot are very dependent on the concentration. The peaks associated with the vortex behavior get completely smeared out.

Methods
We use:
- A 1NN tight binding model.
- The Patched Green’s Functions (PGF) method [3]
  - The PGF is explained in the right column.
  - A simple onsite energy shift for dopants.
- Sublattice density of states (shaded region is the pristine version).

Why Patched Green’s Functions?
When computing the effect of disorder, the main challenges are the "low" number of atoms that can be considered at once, and the corresponding boundary conditions, typically edges or periodicity. An alternative is to use the Patched Green’s Functions method [3], where the boundary conditions are replaced by a boundary selfenergy. This enables one to effectively imbed a region into a periodic material, as long as a simple expression for the real-space Green’s Functions is available.

Outlook
- The Patched Green’s Functions method allows for calculations for non-periodic yet infinite system, in particular in graphene.
- Using the boundary to account for lost current one can calculate, not only the transmission, but the physical current between two leads.
- Combinations of localized disorder, such as doping or vacancies can be explored.

References