Disorder-induced localised gating in graphene

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Publication date: 2017

Document Version
Publisher's PDF, also known as Version of record

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Citation (APA):
Disorder-induced localised gating in graphene

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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].

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 symmetric potential
The onsite potential is shifted in both sublattices, with an average change (keeping the shift times concentration constant) of: 
\[ \varepsilon_\text{A} = \varepsilon_\text{B} = 0.1 \varepsilon_0 \] for a varying concentration of atoms (\( c = 1.0, 0.5, 0.2 \)).

Sublattice asymmetric potential
The onsite potential is shifted in one of the sublattices, with an average change (keeping the shift times concentration constant) of: 
\[ \varepsilon_\text{A} = 0.2 \varepsilon_0 \] for a varying concentration of A-atoms (\( c_\text{A} = 1.0, 0.5, 0.2 \)) within a circular region of radius 20nm.

Density of states (shaded region is the pristine version)

Sublattice asymmetric potential

Green’s Function of Graphene

- The 1NN tight binding model graphene pristine Hamiltonian:

  \[ H(0) = \begin{pmatrix} 0 & -t_f(k) \\ -t_f(k)^* & 0 \end{pmatrix} \]

  \[ f(k) = 1 + e^{-\varepsilon_\text{A} a_1} + e^{-\varepsilon_\text{B} a_2} \]

  \[ G(0) = \frac{1}{\varepsilon_\text{A} - \varepsilon_\text{B}} \int \frac{d^2k}{(2\pi)^2} \frac{1}{f(k)} \]

  Depending on the sublattice of \( j \).

  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 \( c_\text{A} \).
- 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.

References

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. How does it work?
Step 1:
Take a pristine graphene sheet and cut a hole in it.

Step 2:
Embed a device in the cut-out region:

Step 3:
Probes for current injection and collection:

Step 4:
Apply equations:

Here \( i \) and \( j \) refers to specific sites. The \( a \) and \( r \) are the advanced and retarded GF’s respectively (of the fully connected)