Transport Properties of Graphene Doped with Adatoms

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1) Abstract

The aim of the work is to investigate the effects of adatoms on the **localisation** of electrons in graphene. A numerical model was produced, modelling the conductance of graphene samples. **Delocalised states** near zero energy were observed in the doped samples, and the application of magnetic field was found to destroy localisation.

2) Introduction

Since the micro-mechanical cleavage technique for producing graphene from bulk graphite was developed by Geim and Novoselov, there has been a huge volume of scientific interest in graphene. The effects of disorder and magnetic fields on the localisation of states in graphene are important for determining the **dominant transport regime** [1].

This work has important applications for the development of graphene-based electronic devices, because the addition of adatoms can create a tuneable band gap.

3) Details of the method

The program calculates the net conductance across a sample using the nearest neighbour **tight binding approximation**. Vacancies were introduced by setting the potential of the sites to a large, finite value. The size of the sample, vacancy concentration, direction of the current and magnetic field are parameters.

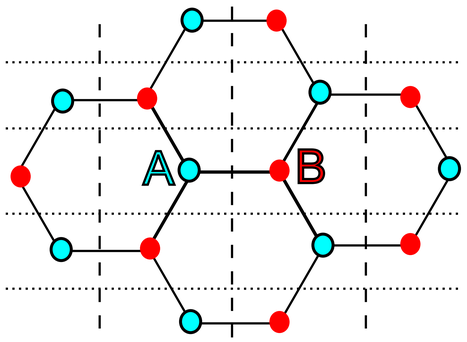

Figure 1: A diagram of the hexagonal structure of graphene. The A and B sublattices are marked separately. The dividing lines show how the structure is divided in to planes for the scattering matrix approach, the dotted lines for Y conductance, and the dashed lines for X conductance.

The method is as follows:

1. Split the sample in to blocks as described by **Figure 1**.
2. Solve for the **transmission** through a block by applying Schrödinger's equation.
3. Combine these transmission values to obtain the **net conductance** through the sample.
4. Increment the energy values used to find the dependence of the net conductance on energy.
5. Repeat and average the previous steps over a number of lattices with **randomised vacancies**.
6. Repeat this process, incrementing the magnetic field and changing the **wrapping** of the sample, so phase diagrams can be created.

4) Localisation - Results

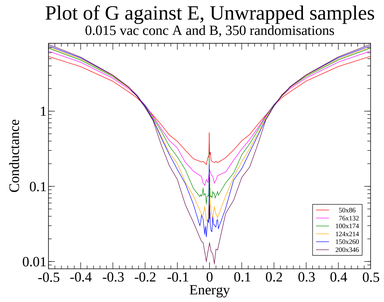

Figure 2: Conductance for various sizes of square samples, showing the transition from the delocalised to the localised regime near E = $\pm$ 0.2

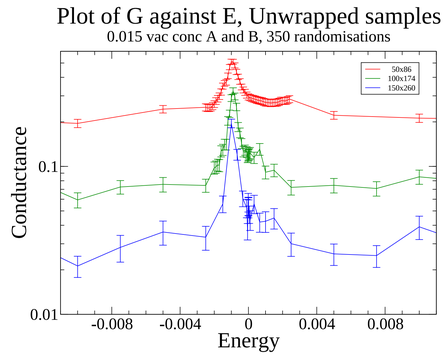

Figure 3: A zoomed plot of the central, low energy region of **Figure 2** showing the conductance peak at E= -10^{-3} .

5) Analysis

Figure 2 shows that at energies greater than $\pm$0.2 all states are **delocalised** and contribute ballistically to conductance. **Figure 3** shows direct evidence for **delocalised states** close to zero energy. The localisation length of these states has been found to be limited by the sample size.

Applying a magnetic field was found to destroy localisation. With an applied magnetic field, the Landau levels are predicted by:

$$E_n = \pm v_f \sqrt{2e\hbar Bn} \tag{1}$$

Figure 4 shows close agreement with the theory at high magnetic field. At low fields the phase diagram shows the transition between localised and delocalised states. Since this transition must be continuous the energy levels "float" up as $B \to 0$ [2]. This is visible in **Figure 4** for magnetic fields below 0.01.

Figure 5 shows the behaviour of the zeroth Landau level, which is suggestive of delocalised states at low energies, produced by the applied magnetic field.

These states are a relatively unexplored feature in the literature and rely heavily on the two dimensional and relativistic form of the electron transport equations in graphene.

6) Magnetic field - Results

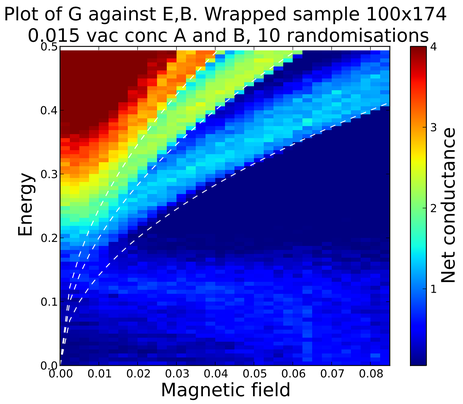

Figure 4: Unwrapped sample with the theoretical position of the 1st, 2nd and 3rd Landau level plotted in the dashed white lines, see Equation (1).

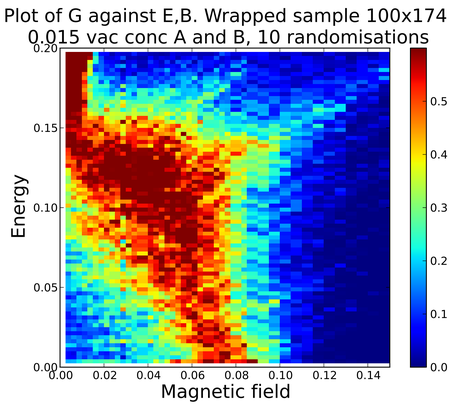

Figure 5: A zoom of **Figure 4** at low energy, showing delocalised states produced by the applied magnetic field.

7) Future work

- Investigate the effect of approximating vacancies with a **finite on-site potential** This is the origin on the offset of the central peak in **Figure 3**. The behaviour of **localisation length** at low energies will also be investigated.
- Explore the effect of **lattice size** and **disorder concentration** on the overall conductance. The expected scaling with N_0 ,the impurity concentration, is $E \propto \sqrt{N_0}$ and $B \propto N_0$.
- The model presented is a single electron system. A more physical description is provided by the **variable range hopping** model.

8) References

[1] J.L. Pichard, *et al*, *Broken symmetries and localisation lengths in Anderson insulators: Theory and experiment* Phys. Rev. Lett. 65, 1812 (1990)

[2] B.I. Halperin *et al.*, *Quantised Hall conductance, current carrying edge states and the existence of extended states in a two-dimensional disordered potential*, Phys Rev B 25, 2185-2190 (1982)

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