

Modeling Graphene: the new and exciting material

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Circular polar form of the Schrodinger equation was used to model a particle in different potential wells. Knowledge gained from this project can be used in modelling graphene with impurities.

What is Graphene?

Graphene was first isolated experimentally in 2004 by physicists from University of Manchester and Institute for Microelectronics Technology, Chernogolovka, Russia^[1]. It is a quasi two-dimensional hexagonal lattice of carbon atoms. It is the basic structural element of graphite, carbon nanotubes, and fullerenes.

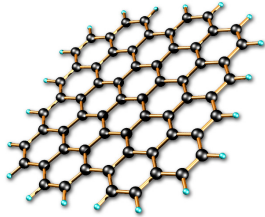


Fig. 1. One layer of Graphene. The blue spheres represent continuing bond. <http://mc2.gulf-pixels.com/wp-content/uploads/2009/07/Graphene-Sheet.jpg>

Used programs



The main modelling program used was COMSOL, version 3.2a.

Wolfram Mathematica 5.1 was used for difficult calculations.

Latex was used for word processing.



These three programs are the main programs learnt during the summer placement so far.

Schrodinger Equation

In order to model a graphene sheet, I had to familiarize myself with solving the Schrodinger equation. Because Graphene is a two dimensional crystal, the Schrodinger equation is two dimensional and is of the

$$\text{circular polar form: } \left(\frac{1}{r} \frac{d}{dr} \left(r \frac{d}{dr} \right) + \frac{1}{r^2} \frac{d^2}{d\theta^2} + V(r) \right) \Psi = E \Psi$$

Solution to Schrodinger equation

The above equation can be solved using separation of variables, with solutions^[2] $\Psi = [A J_n(\sqrt{E+V}r) + B Y_n(\sqrt{E+V}r)] e^{in\theta}$

Where J_n is the Bessel function of the first kind, Y_n is the Bessel function of the second kind, n is an integer and A and B are normalisation constants.

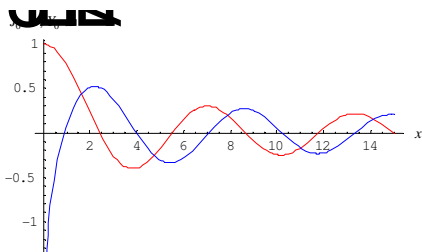


Fig. 2 Graph of Bessel functions of the first kind (red) and the second kind (blue). Both are of the zero order. The singularity at zero is mutual to Bessel functions of the second kind of any order.

Different potentials

For practice purposes, the potential was chosen to be simple. All three possibilities of infinite/finite circular potential wells (shown in Fig.3) were tried out and modelled using COMSOL.

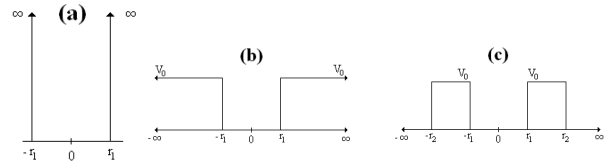


Fig. 3. (a) shows an infinite potential well (b) shows a finite potential well, with potential step of height V_0 (c) shows a finite potential step of width r_2-r_1 and height V_0

Models

Models were made in COMSOL, using PDE, coefficient form. The pictures below show the three possible potentials at their corresponding ground energy.

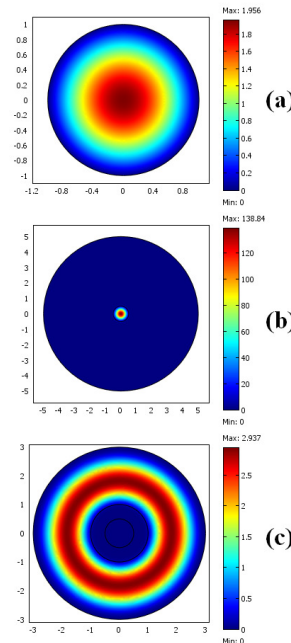


Fig.4 (a-c) This figure shows plotted wavefunctions for all the above possibilities for potential. An infinite potential well (a), finite potential well (with energy much lower than the potential) (b), and finite potential step (c).

Colours represent the value of non-normalised wavefunction. The normalisation condition is known, but since for the finite potential step, there are three equations with three unknowns (and for the finite potential well, there are five equations and five unknowns), it takes a long time to solve.

These three equations come from using the normalization condition and boundary conditions (wavefunction and its derivatives have to be continuous on the boundary).

The first two behave as expected, however, the third result is unexpected, as the wavefunction should still have the highest value around the centre. I have not found out why it behaves in this way.

What comes next?

With the experience gained from the above experiments, it will be possible to model, for example, a sheet of graphene with an impurity as an area with different potential. This could give some more insight in the properties of graphene, and their usage.

Acknowledgments

I would like to thank P. Holland for teaching me how to use the programs and explaining me the theory I needed to know. I would also like to thank F.V. Kusmartsev for allowing me to do this work and helping me with theory.

For further information

Please contact me on email m.brada-07@student.lboro.ac.uk. More information on the subject can be found everywhere, as graphene is a very hot topic nowadays.

References:

^[1] <http://en.wikipedia.org/wiki/Graphene>

^[2] Erwin Kreyszig – Advanced Engineering Mathematics, 9th Edition

