Options for project 3

Option 1 - Bands and energy levels

We consider the energy levels available for an electron in periodic graphene sheets and in disordered systems. The first calculation should be quite quick and can be done using Mathematica or some other program such as Matlab. (i) Find and plot the tight binding band structure of Graphene. This calculation uses Bloch’s theorem which states that the wavefunctions of the Schrodinger equation in a periodic potential obey the relation,

$$\Psi(\vec{r} + \vec{R}) = e^{i\vec{k} \cdot \vec{R}} \Psi(\vec{r})$$

(1)

Show that near the nodal points the excitation spectrum is like that of massless relativistic particles - You can work from Eq. (6) reference [1] below. (ii) In this part, we consider the effect of disorder on the band structure and wavefunctions using the famous tight binding Anderson model. The tight binding Hamiltonian is,

$$H = \sum_{ij} t_{ij} |i><j| + \sum_i \epsilon_i |i><i| = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_i \epsilon_i n_i.$$  

(2)

This Hamiltonian can be derived starting with the simple linear combination of atomic orbitals (LCAO) wavefunction $|\Psi> = \sum_i c_i |i>$ and then using the variational principle. In periodic cases, Bloch’s theorem applies and the problem can be reduced to small matrix problems. In non-periodic cases we have to diagonalize a large matrix. In this part you first find the eigenvalues and eigenfunctions of the Anderson Hamiltonian on linear and square lattices, with the site disorder $\epsilon_i$ drawn randomly from the interval $[-W/2, W/2]$. First find all the eigenvalues and eigenvectors using Mathematica or Matlab and plot the density of states and the inverse participation ratio (IPR), $(\sum_i |\psi_i|^2)^2 / (L^d \sum_i |\psi_i|^4)$ as a function of the disorder width $W$. We will then develop a Fortran code that is much more efficient using the transfer matrix method (see pages 1500-1507 of reference [2] below). I will describe this in detail later.


Option 2 - Device model of solar cells

The most often used model of solar cells is the drift diffusion model. This model consists of solving the Poisson equation for the electrostatic potential and the drift-diffusion equations for the electrons and holes in the presence of incoming light. The electron density is \( n \), the hole density is \( p \) and the electrostatic potential is \( \psi \). Organic solar cells have the additional feature that excitons are created first and they diffuse to interfaces before that break apart into electrons and holes. In this project you will develop a Fortran program to solve the one dimensional drift diffusion model for Silicon solar cells and for Organic solar cells. Plot the electrostatic potential, the electron concentration, the hole concentration, the exciton concentration (for the organic case), the current density as a function of position in the cell. Plot the IV curves for the two cases. The equations that we use are Poisson’s equation, and a combination of the continuity equations and the drift diffusion currents, along with \( E = -\partial \psi / \partial x \): (details may be found in ref. 3), leading to:

\[
- \frac{\partial}{\partial x} n \frac{\partial \psi}{\partial x} + V_t \frac{\partial^2 n}{\partial^2 x} = \frac{g}{\mu_n},
\]

(3)

and

\[
\frac{\partial}{\partial x} p \frac{\partial \psi}{\partial x} + V_t \frac{\partial^2 p}{\partial^2 x} = \frac{g}{\mu_p}.
\]

(4)

We define reduced variables \( n' = n / N_c \) and \( \psi' = \psi / V_t \).

\[
- \frac{\partial}{\partial x} n' \frac{\partial \psi'}{\partial x} + \frac{\partial^2 n'}{\partial^2 x} = \frac{g}{\mu_n V_t'},
\]

(5)

and

\[
\frac{\partial}{\partial x} p' \frac{\partial \psi'}{\partial x} + \frac{\partial^2 p'}{\partial^2 x} = \frac{g}{\mu_p V_t'}.
\]

(6)

In reduced units, the Poisson equation becomes,

\[
\nabla^2 \psi' = \frac{qN_c}{\epsilon V_t}(n' - p'),
\]

(7)

Option 3 - Geometry and transport in disordered networks

Transport in disordered network is often treated using the percolation model [4]. In this model we consider a lattice that has either site or bonds randomly removed and study the behavior as a function of the fraction of removed sites or bonds. We will consider the case of bond dilution, where the fraction of removed bonds is $f$ and $p = 1 - f$ is the fraction of present bonds. In this project you will develop two programs. The first program is to characterize the geometry of the percolation process.

The key physical process in the percolation geometry is the fact that when enough edges in a network are removed, i.e. at the percolation threshold, the network ceases to “percolate”. The percolation process is singular in a manner similar to thermodynamic phase transitions that we studied in the melting of LJ clusters and at the Curie point in magnets. In this part of the project you will write a Fortran program to find the largest cluster in a percolating network and plot its size as a function of the fraction of bonds that are removed from the network ($f$). You will also find and plot the susceptibility as a function of bond concentration. Another nice thing to calculate is the cluster size distribution which has a power low distribution at the percolation threshold. This algorithm can be coded efficiently so that large samples may be simulated (e.g. $1000 \times 1000$ square lattices on a laptop).

To model transport in percolating networks we assign a resistance to each edge in the network. These “Random resistor networks” are used to model many different situations, ranging from transport in semiconductors to composites and porous networks in geology. Many of these cases have a non-linear response, however even in those cases the numerical methods depend on solving the linear case repeatedly. To find the resistance of the percolating network we solve Kirchoff’s laws to find the total current in the network. The Conjugate gradient method is good for this purpose and can be easily coded to take advantage of the sparseness of the problem. Find the resistance of percolating networks of size $L = 1000$ and plot it as a function of the fraction of removed bonds. Find the critical exponent $t$ describing the way in which the conductivity approaches zero at the percolation threshold. Is this critical exponent related to the geometric
exponents?