

## PHY480: Project 3 - Due Friday April 29th

*Energy levels in solids: Bands, density of states, energy spacing distribution*

A first approximation to the electronic energy levels in a solid is to consider effective one electron models. In these models the energy levels are found by diagonalizing an approximate Hamiltonian matrix. A compact expression for the approximate Hamiltonian of a one electron system is constructed using a set of localized wavefunctions  $u_i^l(\vec{r}_i)$  that are centered at each site of the solid. Here  $i = 1, \dots, N$  for the  $N$  sites in the solid and  $l = 1 \dots n_B$  labels the  $n_B$  basis functions that are used at each site. One approach is to use atomic wavefunctions, another is to use Gaussian local functions. The kinetic energy term in the single electron Hamiltonian promotes “hopping” between local wavefunctions, while the potential energy term promotes occupation of the lowest energy local wavefunction. In this project we will study two aspects of energy levels that are produced by this competition. The first part considers energy levels in periodic solids where bands and delocalized wavefunctions occur. The second part considers the case where the momentum is no longer a good quantum number and instead the wavefunctions can be localized. This occurs in materials such as polymers or amorphous materials such as amorphous silicon. In those cases we study the localization of the wavefunction and the distribution of energy level spacings. The latter problem has been studied a lot in nuclear physics as well and is related to an area of mathematics called random matrix theory.

(i) First we consider the energy levels available for an electron in periodic graphene sheets. The calculation can be done using Mathematica or some other program such as Matlab. By following reference [1] below and the introduction at the class [www](http://www.phy480.org) site, (i) *Find and plot the tight binding conduction and valence band dispersion relations of Graphene. This should be a 3-D plot of the energy as a function of the wavevectors.* (ii) *plot the density of states of graphene as a function of energy. This is a 2-D plot.* This calculation uses Bloch’s theorem which states that the wavefunctions of the Schrodinger equation in a periodic potential obey the relation,

$$\Psi(\vec{r} + \vec{R}) = e^{i\vec{k} \cdot \vec{R}} \Psi(\vec{r}) \quad (1)$$

In cases where there is periodicity of the potential and we use only one orbital per site and have only one orbital per unit cell of a bravais lattice,  $\phi$ , Bloch’s theorem states that the wavefunction

for an electron is,

$$\psi_{\vec{k}}(\vec{r}) = A_N \sum_j e^{i\vec{k} \cdot \vec{R}_j} \phi(\vec{r} - \vec{R}_j) \quad (2)$$

In the first part of this option you need to extend this to an important case where there are two atoms per unit cell but only one orbital per atom is used. You can work from Eq. (6) in reference [1] below and an introduction to the tight binding method is posted at the class www site.

1. S. Reich, J. Maultzsch, and C. Thomsen, "Tight-binding description of graphene", Phys. Rev. B66, 035412 (2002).

(ii) In this part, we consider the effect of disorder on the band structure and wavefunctions using the famous tight binding Anderson model (see e.g. [2] below). The Anderson model has disorder in the site energies  $\epsilon_i$  while the quantum percolation model has site energies set to zero but has the hopping elements  $t_{ij}$  set to zero with some probability,  $p$ . The tight binding Hamiltonian we use is,

$$H = \sum_{ij} t_{ij} |i\rangle \langle j| + \sum_i \epsilon_i |i\rangle \langle i| = \sum_{ij} t_{ij} c_i^\dagger c_j + \sum_i \epsilon_i n_i. \quad (3)$$

This Hamiltonian can be derived starting with the simple linear combination of atomic orbitals (LCAO) wavefunction  $|\Psi\rangle = \sum_i c_i |i\rangle$  and then using the variational principle. In periodic cases, Bloch's theorem applies and the problem can be reduced to small matrix problems, as done in part (i) above. In non-periodic cases we have to diagonalize a large matrix, that has dimension equal to  $N * n_B$ . We shall consider cases where there is only one orbital per site,  $n_B = 1$  and we consider hexagonal lattices again, so we are considering the effect of disorder on the band structure of small pieces of graphene (e.g.  $20 \times 20$  pieces). Edge effects are also important.

We consider graphene where the energy levels in Eq. (2) are random, with the values  $\epsilon_i$  drawn randomly and uniformly from the interval  $[-W/2, W/2]$ . Carry out the following calculations: **(i)** Find all of the eigenvalues and eigenvectors using Mathematica or Matlab and plot (a) the density of states (b) the inverse participation ratio (IPR),  $(\sum_i |\psi_i|^2)^2 / (L^d \sum_i |\psi|^4)$  (c) The energy level spacing distribution [3]; all as a function of the disorder width  $W$ . **(ii)** Write a fortran program to carry

out the same calculations as in (i) and import the Fortran data to the Mathematica (or Matlab) to compare with the Mathematica results.

2. B. Kramer and A. MacKinnon, "Localization: theory and experiment", Reports on Progress in Physics 56, 1469 (1993). (see e.g. Eq. (12) and Fig. 16).
3. N. Rozenzweig, "Spacing of nuclear energy levels", Phys. Rev. Lett., 1, 24 (1958).