Tight binding and Anderson models for Graphene band structure

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I. TIGHT BINDING MODEL

Using the tight binding model from [3], I plotted the energy levels of graphene in figure 1 with Numpy[**?**] and Gnuplot[**?**].

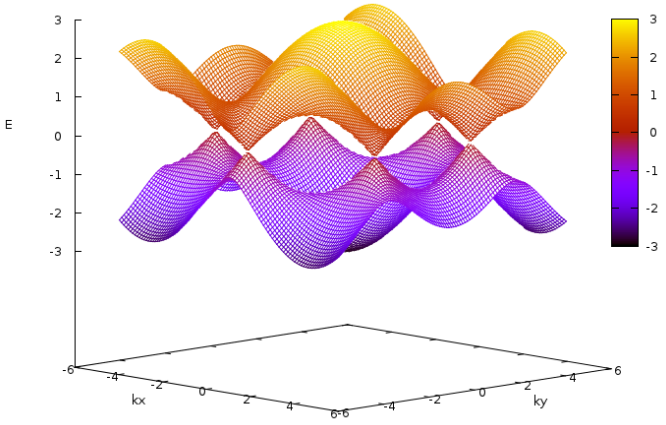

FIG. 1: Energy levels of graphene. Energy (z axis) in units of eV.

In figure 2, I plotted the density of states for graphene (frequency distribution of energies) using the same tight binding model.

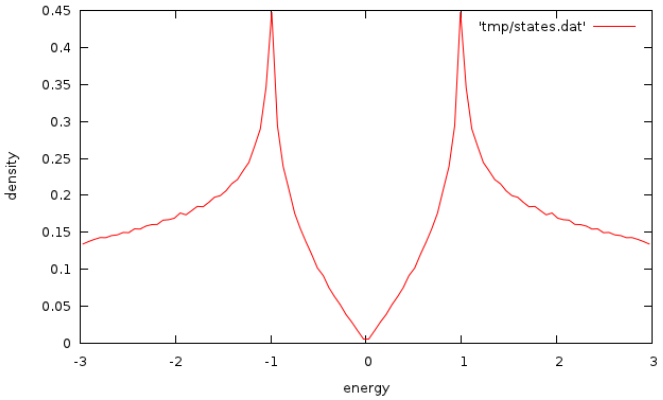

FIG. 2: Density of states for graphene. Energy in units of eV.

II. ANDERSON MODEL

A. Introduction

The Anderson model [1] consists of a Hamiltonian in the form of an adjacency matrix with random diagonal elements, which is solved for the energy levels (eigenvalues) and wave functions (eigenvectors).

Consider the graphene system shown in figure 3. The Hamiltonian for this system could, for example, be that of figure 4. The diagonal elements are randomly uniformly selected from $(-W/2, W/2)$, where W is the *disorder width*.

The i-j element is 1 if sites i and j are neighbors and 0 otherwise.

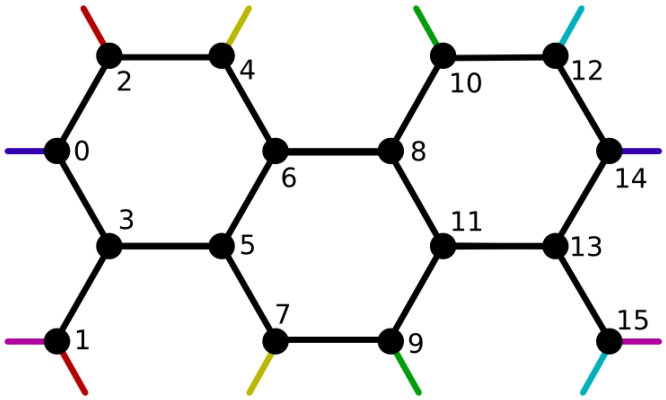

FIG. 3: Example graphene system with 16 sites. Note: same-colored edges are connected via periodic boundary conditions.

$$\begin{bmatrix}
-.17 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & .47 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
1 & 1 & -.44 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & -.12 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & -.03 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & .15 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 1 & .36 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 1 & 0 & .46 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -.08 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & .17 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & .33 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & .41 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -.49 & 0 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -.48 & 1 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & -.38 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & .05
\end{bmatrix}$$

FIG. 4: Example Hamiltonian in the Anderson model.

B. Density of states

To find the energy levels ε_i, we need to solve for the eigenvalues ε_i in the Schrödinger equation $H\psi_i = \varepsilon_i\psi_i$, where H is the Hamiltonian and the eigenvectors ψ_i are the wave functions. I plotted two examples of this in figure 5 (for two different disorder widths W).

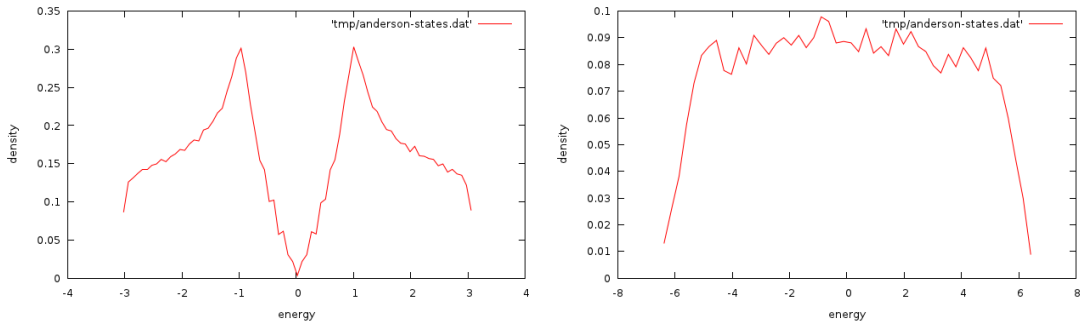

FIG. 5: Density of states using the Anderson model with disorder widths $W = 1$ and $W = 10$, respectively.

The tight binding model and the Anderson model match fairly closely, as is evident by comparison of figures 2 and 5.

C. Energy level spacing

We can also find the spacing between subsequent energy levels ε_i using this eigenvalue system. I plotted two examples of this in figure 6.

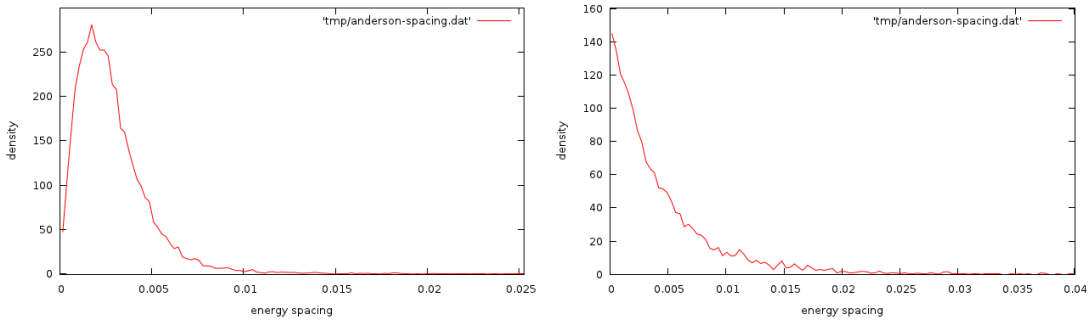

FIG. 6: Energy level spacing distribution using the Anderson model with disorder widths $W = 1$ and $W = 10$, respectively.

D. Inverse participation ratio

Following [2], we can define an *inverse participation ratio* (IPR) for each energy level ε_i using the corresponding eigenvector ψ_i:

$$\text{IPR} = \frac{\sum_j |\psi_i^{(j)}|^2}{n \sum_j |\psi_i^{(j)}|^4},$$

where n is the total number of sites in the system. Figure 7 contains two plots plots of the IPR for a graphene system.

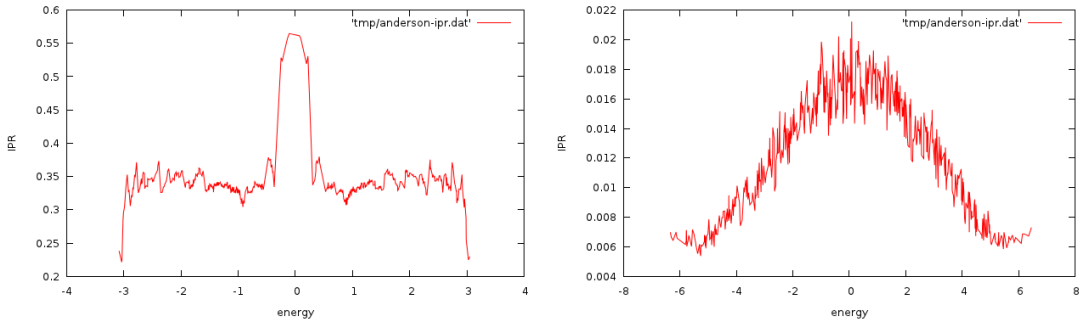

FIG. 7: Inverse participation ratio (IPR) with disorder widths $W = 1$ and $W = 10$, respectively.

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[1] P. Duxbury, *PHY480: Project 3*, `http://www.pa.msu.edu/~duxbury/courses/phy480/Project3_2011.pdf` (retrieved 2011-04-29).
[2] B. Kramer and A. MacKinnon, *Localization: theory and experiment*, Reports on Progress in Physics 56, 1469 (1993).
[3] S. Reich, J. Maultzsch, and C. Thomsen, *Tight-binding description of graphene*, Phys. Rev. B66, 035412 (2002).
[4] `http://numpy.scipy.org/`, a numeric computing library for Python.
[5] `http://www.gnuplot.info/`, a graphing program.