CNT Bands Challenge Problem

Challenge

It is important to have a quantitative model describing how the interaction of a CNT with its environment (e.g. supporting substrate, other nanotubes, polymer matrix, etc.) influences its ability to conduct current. One possible mathematical formulation of this physical problem can be stated as follows.

Given:

In a first nearest neighbor pi-orbital tight-binding approximation, let us assume that random distortion is described by random shifts $?_{ii}$ of on-site Hamiltonian matrix elements h_{ii}. The dispersion ? of on-site shifts is defined in its usual way:

$$\sigma^2 = < \Delta_{ii}^2 > - < \Delta_{ii} >^2$$

,

where angular brackets denote averaging over all atoms *i*.

For each given energy the localization length of a randomly distorted CNT is defined as CNT length, for which the logarithm of the ratio of ideal transmission to the transmission in the CNT subjected to distortion equals 2.

Find:

For the given CNT indexes (n_1, n_2) and dispersion ?, find the localization length as function of electron energy.

The article contains detailed and self-contained explanation of quantum transmission calculations. As an example providing insight on the properties of Green's functions and contact self-energies, analytical expression for localization length in randomly distorted CNT is derived (Section VIII, Eqs.(41-43)). Download: Real-Life-Problem_CNT.pdf (825 KB, uploaded by 9 months 2 weeks ago)

The figure below plots analytical expression for localization length (blue line) along with the simulated localization length, which has been statistically averaged over an ensemble of 750 randomly distorted CNTs (green line). Localization length is measured in numbers of CNT's unit cells. The unit cell is defined as a minimum size unit cell, which interacts only with its nearest neighbors. Red line is the transmission of the ideal (undistorted) CNT in arbitrary units.