598SCM Fall 2004 Homework 3 - PART II

Handed out Tuesday, October 5, 2004

Due Tuesday, October 19, 2004

There will be an "Office hour" session before the due date. Anyone is welcome to come to discuss the solutions to the problems. Time to be announced.

- 1. Exercise 14.6. The part on the density of states is optional since we have not discussed the derivation of the density of states. If you want to work this part, there is useful help in the book "Solid State Physics: Problems and Solutions", by Mihaly and Martin, Wiley (1996).
- 2. Derive the expression for the π bands in a sheet of graphene assuming only nearest neighbor interactions. Show that the bands touch at the corner of the BZ called K. The expression given in the text is Eq. (14.16); however, the definition of x and y may be different in your expression. Nevertheless, the resulting eigenvalues should be equivalent. Also there is an error in the quoted expression for the K point below Eq. (14.16). The important point is that you should derive the expression yourself for the corner of the BZ.

Optional Problems

Good for understanding - Prof. Martin will be happy to discuss the solution of these problems

3. Download the TBPW code and use it to calculate bands. There are example inputs and outputs. Ideas for problems to do: Test to see that you reproduce the bands of Si and or GaAs. Displace the atoms in the (111) direction and see the splitting of the top of the valence band. Calculate bands for C nanotubes.