598SCM Fall 2004 Homework 1

Handed out Tuesday, August 31, 2004
Due Tuesday, September 14, 2004

1. Exercise 3.1

2. Exercise 3.7. Hint: The solution can lengthy or it can be be short when done the easy way as follows. First consider case in which the number of fermions is not conserved. Then the occupation of each state is zero or one weighted by the Boltzmann factor, independent of the occupation of all other states. It immediately follows that the probability of occupation of each state given by

$$f_i^\sigma = \frac{1}{e^{\beta \epsilon_i^\sigma} + 1}. \tag{1}$$

   The final expression follows using the fact that the chemical potential μ represents the energy of particles in a reservoir that can supply arbitrary numbers of particles.

3. Exercise 3.11

4. Exercise 3.12

5. Exercise 3.13

6. Exercise 3.15. (An example of the negative exchange hole is given in Fig. 5.3.) Note that for non-interacting fermions (bosons) this means that the probability of finding two particles near one another is always reduced (increased) compared to non-interacting distinguishable particles.

7. Exercise 3.19

8. Exercise 4.3. NOTE THERE IS A MISPRINT IN THE BOOK. The value of 60° is not correct. Find the correct angle of rotation.

9. Exercise 4.7 and 4.9. These are useful later for examples treated the class. Also exercise 4.16 ONLY for the X and the L points of an fcc crystal. (The other points are straightforward but tedious.)

10. Exercise 5.1.

11. Exercise 5.13. This analytic form illustrates the nature of the exchange hole in typical solids.

Optional Problems

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

12. Exercise 3.4. Hint: Use the requirement that the wave function remains normalized when an atom is displaced.

13. Exercise 3.24. This is straightforward and is an example of the “2n+1” theorem that is not widely known.

14. Exercise 4.21. This is a very widely used definition of points for integrals in the Brillouin Zone. The theory of integration using these points is related to Gaussian quadrature and could form the basis for a project.

15. Exercise 5.9, 10, 11. These are important relations that illustrate the basic features of bands in metals in the Hartree-Fock approximation. The integrals are somewhat tedious.

16. Exercise 5.14. The Thomas-fermi approximation for the screening leads to this simple form that illustrates the typical spatial extent of the correlation among electrons.