561 Fall 2005 Homework 1 — Due Thursday, September 8

1. Estimate of magnitudes of physical quantities

This problem asks you to use knowledge of elementary solid state physics to estimate the values of important quantities. You do not need to derive the formulas used; you may give a reference to a standard textbook (such as Ashcroft and Mermin or Kittel, etc.) and quote the formulas.

Diamond carbon is the hardest material known; it is also a dense electron system with 8 atoms (32 valence electrons) per cubic cell of volume $(3.567\ \text{Å})^3$ (Kittel, 6th Ed., Table 3). Theoretical calculations predict that diamond will transform to a metal at extremely high pressures (not accessible by present-day experiments) so that the density is increased to twice the density of diamond at zero pressure. Compute the electronic density parameter r_s in atomic units (a_0 or Bohr) for metallic carbon at this high density. Consider this metal to be a homogeneous electron gas and estimate values for the following quantities:

- a. Fermi Energy of the valence electrons
- b. Thomas-Fermi screening length
- c. Fermi velocity
- d. Longitudinal sound velocity
- e. Electron plasma frequency

Problems 2-5 lead you through second quantization and statistics. Try to work them without looking at textbooks if you can. The answers are given in many texts including Mahan.

2. Harmonic Oscillator

For the harmonic oscillator $H = \hat{p}^2/2m + m\omega^2\hat{q}^2/2$, and $[\hat{p}, \hat{q}] = -i\hbar$. We can define $a = (2m\hbar\omega)^{-1/2}(\hat{p} - im\omega\hat{q})$ and $a^\dagger = (2m\hbar\omega)^{-1/2}(\hat{p} + im\omega\hat{q})$.

Show that:

- a. $[a, a^\dagger] = 1$; $[a, a] = [a^\dagger, a^\dagger] = 0$.
- b. $H = \hbar\omega(a^\dagger a + 1/2)$
- c. $[H, a^\dagger] = \hbar\omega a^\dagger; [H, a] = -\hbar\omega a$
- d. $|n\rangle = (n!)^{-1/2}(a^\dagger)^n|0\rangle$ is a normalized state with occupation n

3. Bosons

Bosons are particles of integer spin with any number of identical particles allowed to be in any state. Suppose we have non-interacting Bosons which can be in states $0, 1, 2, \ldots$ with energies $\epsilon_0, \epsilon_1, \epsilon_2, \ldots$

The eigenstate with n_0 particles in state 0, n_1 particles in state 1, etc. can be written $|n_0, n_1, \ldots\rangle$. This is the occupation number representation which forms a complete orthonormal set.

Creation and annihilation operators have the effects:
$a_k^\dagger|n_0, n_1, \cdots, n_k, \cdots\rangle = \sqrt{n_k+1}|n_0, n_1, \cdots, n_k+1, \cdots\rangle$, and
$a_k|n_0, n_1, \cdots, n_k, \cdots\rangle = \sqrt{n_k}|n_0, n_1, \cdots, n_k-1, \cdots\rangle$.
Show that for any system of bosons, independent of whether there are interactions or not:

- a. $[a_k, a_{k'}^\dagger] = \delta_{k,k'}$, and, $[a_k, a_{k'}] = [a_k^\dagger, a_{k'}^\dagger] = 0$.
- b. $a_k^\dagger a_k|n_0, n_1, \cdots, n_k, \cdots\rangle = n_k|n_0, n_1, \cdots, n_k, \cdots\rangle$.
- c. The total number operator N is given by $\sum_k a_k^\dagger a_k$.

Show that for non-interacting bosons:

- d. $\hat{H} = \sum_k \epsilon_k a_k^\dagger a_k$
- e. $[\hat{H}, a_k^\dagger] = \epsilon_k a_k^\dagger$ and $[\hat{H}, a_k] = -\epsilon_k a_k$
- f. $\exp(-\beta H) a_k^\dagger \exp(+\beta H) = \exp(-\beta\epsilon_k) a_k^\dagger$

4. Fermions

Fermions are particles with half integer spin with a possible occupation of 0 or 1 in a given state. Just as for bosons, except for the sign factors, we can define creation and annihilation operators by:
$c_k^\dagger|n_0, n_1, \cdots, n_k, \cdots\rangle = (-1)^S \delta_{n_k,0}|n_0, n_1, \cdots, n_k+1, \cdots\rangle$, $S = \sum_{j<k} n_j$, and
$c_k|n_0, n_1, \cdots, n_k, \cdots\rangle = (-1)^S \delta_{n_k,1}|n_0, n_1, \cdots, n_k-1, \cdots\rangle$, $S = \sum_{j<k} n_j$.
Show that for any system of fermions, all the relations shown above for bosons carry over with the only change that the commutation relations are replaced by anticommutation relations:
a. $[c_k, c_{k'}^\dagger]_+ = \delta_{k,k'}$, and, $[c_k, c_{k'}]_+ = [c_k^\dagger, c_{k'}^\dagger]_+ = 0$, where $[a, b]_+ = ab + ba$.
b-f are the same with $a \to c$.

5. Independent particle statistics

Using the above relations derive the well-known expectation values for the occupation numbers for non-interacting bosons and fermions at temperature $k_B T = \frac{1}{\beta}$ and chemical potential μ:
Fermions:

$$f_k = \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1}, \tag{1}$$

Bosons:

$$f_k = \frac{1}{e^{\beta(\epsilon_k - \mu)} - 1}, \tag{2}$$

6. Two-body interactions in second quantization

Phillips Problem 3.2. [Note that there is an error in the statement of this problem: the reference to Eq. (6.47) should be to Eq. (3.37).]

7. Hartree-Fock approximation for the homogeneous electron gas

The formula for the eigenvalues in the Hartree-Fock approximation are given in Pines, "Elementary Excitations in Solids", Eq. 3-46, and Phillips in Chapter 5. Find the band width for the occupied states (the Fermi energy minus the energy of lowest eigenvalue) in the Hartree-Fock approximation for the example of the dense carbon metal in Exercise 1. Compare the width to the free-electron band width in Exercise 1a. What is the Fermi velocity in the Hartree-Fock approximation compared to the Fermi velocity for free electrons given in Exercise 1a?

8. Exchange Hole

In the Hartree-Fock approximation, the pair distribution function for electrons $g(\mathbf{r}, \mathbf{r}')$ can be expressed in a simple form involving the Hartree-Fock orbitals. This is valid for any system of fermions within the Hartree-Fock approximation. Show directly from the definition of $g(\mathbf{r}, \mathbf{r}')$ that the integral of the exchange hole $g(\mathbf{r}, \mathbf{r}')$ satisfies the sum rule

$$\int d^3r'[g(\mathbf{r}, \mathbf{r}') - 1]n(\mathbf{r}') = -1. \tag{3}$$

Thus the exchange hole always denotes one missing electron around an electron at any point $\mathbf{r}$.