Physics 440, Fall 2008
Problem Set #10
Due: Friday, November 7

Hour Test II: Chapters 4-5, Monday November 10th

1. *K* Chapter 6 Problems 1-2. For its possible entertainment value, note in Problem 2 part (c) that the *observed* value for the (low-temperature) bulk modulus for K is $B_{obs} \simeq 2.81 \text{ x } 10^{10}$ dynes/cm^2. For this, and many other reasons, the alkalis were a perennial favorite among theoretical physicists in the early phases of solid state physicists.

2. *Chemical potential in two dimensions* [Replaces *K* problem 3]
   The two-dimensional free electron gas is more important than you might imagine, given the two-dimensional quantized Hall effect and the existence of such an electron gas in certain MOSFET's.

   (a) Show that the energy density of states per unit area $g(E) = \frac{m}{\pi\hbar^2}$; don't forget the spin degeneracy.

   (b) What is the (simple!) connection between the Fermi energy ε_F and (two dimensional) number density $n \equiv \frac{N}{A}$ at $T = 0$? Remember that at $T = 0$ $\mu = \varepsilon_F$.

   (c) Show that the equation used to find the chemical potential is

   $$n = g(E) k_B T \ln\left(1 + \exp\frac{\mu}{k_B T}\right).$$

   Since $g(E)$ is a constant, using the fact that

   $$\ln(1 + \exp x) = \ln(\exp x\,[1 + \exp(-x)])$$

   and the results of parts (a) and (b), show that

   $$\varepsilon_F = \mu + k_B T \ln[1 + \exp\left(-\frac{\mu}{k_B T}\right)]$$

   (d) Show that

   $$\frac{\varepsilon_F - \mu}{\varepsilon_F} = -\left(\frac{T}{T_F}\right) \ln\left[1 - \exp\frac{-1}{(T/T_F)}\right],$$

   where T_F is the Fermi temperature. [*Hint:* You may find it convenient to define $x = \varepsilon_F - \mu$ and solve for x.]

   (e) For $T/T_F = .01, .1, 1$, calculate $\frac{\varepsilon_F - \mu}{\varepsilon_F}$. Plot the function and compare your results with what you see in Kittel's Figure 8, Chapter 6 for 1 and 3 dimensions and comment.

   (f) What is the Taylor series for $\frac{\varepsilon_F - \mu}{\varepsilon_F}$ about $T = 0$?

3. *Free electron density near a surface*
   Periodic boundary conditions naturally prevent examining properties of a system with a *surface*. The requirements of the Fermi exclusion principle impose characteristic oscillations (known as *Friedel* or *RKKY* oscillations in the electron density around a perturbation, *e.g.*, a charged impurity, or the surface of a metal. This problem acquaints you with this effect and with a naive but suggestive choice of wavefunction for free electrons confined to a finite slab.

   Consider a slab of metal [see Fig. 1] inside which otherwise free electrons are confined by an infinitely high barrier at the surfaces. (This buffoonish parody of reality used to be taken as a legitimate model, called the 'infinite barrier model'.)

   (a) In this geometry verify that as $a \to \infty$

   $$\psi_{k_\perp,k_z}(\vec{r}) = \frac{1}{\sqrt{A}} e^{i\mathbf{k}_\perp \cdot \mathbf{r}_\perp} \sqrt{\frac{2}{L}} \sin k_z z \tag{1}$$

   [where $\mathbf{k}_\perp = (k_x, k_y)$ and $A = a^2$ is the slab area] is a normalized eigenfunction for an electron-in-a-slab, with energy

   $$E_{k_\perp,k_z} = \frac{\hbar^2}{2m}(k_\perp^2 + k_z^2), \quad k_z = \frac{\pi\ell}{L}, \ \ell = 1, 2, 3, \ldots \tag{2}$$

   [*Verify* means simply confirm that this wavefunction (i) obeys the (three-dimensional) Schrödinger equation for a free particle with the energy given, and (ii), $\int_{\text{all space}} d^3r\, |\psi_{k_\perp,k_z}(\vec{r})|^2 = 1$, so that $|\psi_{k_\perp,k_z}(\vec{r})|^2$ can be interpreted as a probability density.

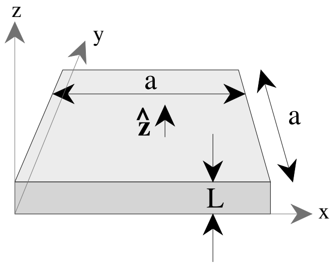

Figure 1: Metal slab: a is very large and as $L \to \infty$ the slab has *one* surface, the plane $z = 0$.

At T=0 the ground state electron number density may be written

$$\begin{aligned} n(\mathbf{r}) &= 2 \sum_{\mathbf{k}\,\text{occupied}} |\psi_{\mathbf{k}}(\mathbf{r})|^2 \\ &= 2 \sum_{\mathbf{k}_\perp} \sum_{\mathbf{k}_z} \theta(E_F - E_{\mathbf{k}_\perp, k_z})\, |\psi_{\mathbf{k}_\perp, k_z}(\mathbf{r})|^2, \end{aligned} \tag{3}$$

where $E_F = \frac{\hbar^2}{2m} k_F^2$ is the Fermi energy; the factor of two reflects the fact that spin up and spin down electrons have the same energy. The θ (or Heaviside) function

$$\theta(x - a) \equiv \begin{cases} 0, & x < a \\ 1, & x > a \end{cases} \tag{4}$$

is just the 'step' function which the Fermi-Dirac distribution becomes for temperature $T = 0$. In the limit of large A and $L \to \infty$, the sums naturally become integrals, as we (like Carl Sagan) have done billions and billions of times.

(b) Show that as $L \to \infty$ [giving a *semi-infinite* slab, a system with *one* surface],

$$n(z) = n_0 [1 - \frac{3 j_1(u)}{u}] \tag{5}$$

where n_0 is the 'bulk' electron number density, $u = 2k_F z$, and $j_1(x) \equiv \frac{\sin x}{x^2} - \frac{\cos x}{x}$ is a spherical Bessel function. Thus, as advertised, electron number densities typically oscillate with a 'spatial frequency' $2k_F$ in response to a perturbation (here, the abrupt, infinitely high potential at the surface).

[**Hint**: Do the $\mathbf{k}_\perp$ integral first. For fixed k_z the effect of the step function is then to restrict $|\mathbf{k}_\perp|$ to the range 0 to $\sqrt{k_F^2 - k_z^2}$. After this integral is done, the permissible range of k_z is 0 to k_F.]

(c) Plot $n(z)$ *carefully* and comment on any notable features.