Physics 7440, Final Exam
(Due Thursday 12/10/09 at the beginning of lecture.)

You may use only the following references/materials while working on this exam: course notes, problem sets, and solutions; Ashcroft and Mermin; integral tables; and Mathematica, Matlab, and other similar software. You may not work together on this exam, or discuss it with anyone until the deadline has passed. To ensure no one gets an unfair advantage, I cannot answer questions, except to clarify the meaning of the problems.

Late exams: the total exam grade will be reduced by 10% of the total points for every hour the exam is late.

1. **Scattering from a crystal with substitutional disorder.**

Recall that the cross section for elastic neutron or x-ray scattering off a crystal is proportional to $|M(q)|^2$, where

$$M(q) = \sum_\alpha \int d^3 r e^{-iq \cdot r} U_\alpha(r - r_\alpha) = \sum_\alpha e^{-iq \cdot r_\alpha} U_\alpha(q).$$

Here, $\alpha$ labels the atoms of the crystal at positions $r_\alpha$, and the integral over $r$ is taken over the volume of the crystal (assuming periodic boundary conditions as usual).

Suppose we have a disordered crystal made up of two types of atoms (1 and 2). Atom 1 has a form factor $U_1(q)$, and atom 2 has form factor $U_2(q)$. We suppose that the atoms lie on the sites of a Bravais lattice, but any given site can be occupied by either atom 1 or atom 2 in a random fashion. We model this by saying, for a given site, the probability to be occupied by atom 1 (atom 2) is $p_1$ ($p_2$), and $p_1 + p_2 = 1$. Each site is independent from all others – there are no correlations in the positions of the two kinds of atoms. These probabilistic statements are meaningful when we consider taking an average of some measurable quantity over many different samples.

(a) Calculate $|M(q)|^2$, taking the average over many samples as discussed above. You will not be able to simplify the answer much at all until you take the average.

Your final answer should contain two terms that add together. One of these has a familiar form and gives the usual Bragg peaks. The other term is a new contribution that does not appear for a perfectly ordered crystal. How does the behavior of this new term as a function of $q$ compare to the term with the Bragg peaks?

(b) Give a physical argument why this calculation should still be accurate if we do a measurement on just one large sample. (I am not looking for a calculation here – just a reasonable handwaving argument will do.)

2. Consider a single band filled with a relatively small density $n$ of electrons, so that we may employ the effective mass approximation. Suppose further that this band has only a single minimum in its energy, which lies at $k = 0$. Therefore, in the effective mass approximation, we have

$$\epsilon(k) = \frac{\hbar^2}{2} k_i M_{ij}^{-1} k_j,$$

where $M$ is the effective mass tensor, which is a $3 \times 3$ symmetric and positive definite matrix.

(a) Assume that the nonequilibrium distribution function $g(r,k,t)$ does not depend on $r$ (i.e. spatial homogeneity). Starting from the Boltzmann equation in an applied electric and magnetic field, derive a first-order differential equation for the average velocity $v_{\text{avg}}$, analogous to the Drude model equation for free electrons. You should assume that it’s okay to linearize in the applied electric field. Do not assume that the applied magnetic field is small. Also, you should work in the relaxation time approximation, where the relaxation time $\tau$ is a constant independent of $\epsilon$ and $k$.

(b) For zero applied magnetic field, calculate the electrical conductivity $\sigma_{ij}$. (Recall $J_i = \sigma_{ij} E_j$.)

(c) Because $M_{ij}$ is symmetric, it can be diagonalized in an appropriate orthogonal coordinate system. Suppose we choose axes $x,y,z$ so that this happens, and we write

$$M_{ij} = \begin{pmatrix} m_x & 0 & 0 \\ 0 & m_y & 0 \\ 0 & 0 & m_z \end{pmatrix}.$$  

Suppose $B = Bz$, and the direction of $E$ is arbitrary. Find the resistivity tensor $\rho_{ij} = \sigma_{ij}^{-1}$.
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3. The kagome lattice (shown in figure) is based on the triangular Bravais lattice and has a three-site basis. The three sites in the basis can be chosen as shown in the figure.

(a) Suppose that there is a single tight-binding orbital on every lattice site, and the tight-binding Hamiltonian is

\[ H_{\text{TB}} = -t \sum_{\langle rr' \rangle} [\langle r \rangle \langle r' \rangle + \text{H.c.}] \]  \hspace{1cm} (4)

Here \( t > 0 \), the sum is over all nearest-neighbor bonds of the kagome lattice, and \( r \) labels all kagome lattice sites. Solve for the the energy bands \( \epsilon_n(k) \). You should find three non-overlapping bands – call the lowest-energy band \( \epsilon_1(k) \), the middle band \( \epsilon_2(k) \), and the highest band \( \epsilon_3(k) \). What is the energy \( \epsilon_{12} \) at which bands 1 and 2 meet? What about \( \epsilon_{23} \), the energy at which bands 2 and 3 meet?

(b) Describe how the shape of the Fermi surface changes as the Fermi energy \( \epsilon_F \) starts at \( \epsilon_{12} \) and is increased up to \( \epsilon_{23} \). You don’t need to calculate the shape of the Fermi surface – sketches are enough. As a function of \( \epsilon_F \), how many disconnected pieces of Fermi surface are there? If the number of disconnected pieces changes as a function of \( \epsilon_F \), find the values of \( \epsilon_F \) at which a change occurs.

Describe what happens at the endpoints, \( \epsilon_F = \epsilon_{12}, \epsilon_{23} \). Is the system a metal, insulator or semimetal at these points?