Physics 555 Fall 2004
Final Exam, Friday December 17, 8:00-10:30am
Choose any 4 problems out of the 6 given here.

1. **Crystallography; answer any 2 out of 3 parts**

   a. Metallic copper has the *fcc* crystal structure, that is, an *fcc* lattice and one atom per cell. The lattice constant (not the nearest neighbor distance, but the edge of the conventional non-primitive cubic cell) is a =3.61 Å. You have a single crystal of copper and a beam of x-rays which you can tune to a desired wavelength. The (100) crystal axis faces toward the x-ray source. What is the longest wavelength that will reflect directly back toward the x-ray source? How many eV of energy do the x-ray photons have? What happens if you use a wavelength half as big?

   b. $SrTiO_3$ has the perovskite crystal structure, with 5 atoms in a primitive cell and simple cubic translational symmetry. Sr atoms lie on the corners of a cube of length a =3.905 Å, Ti atoms in the center, and oxygen atoms on the centers of the faces. What are the reciprocal lattice vectors (seen as crystal momentum transfers $\vec{G} = \vec{k}_f - \vec{k}_i$ in Bragg scattering)? Below 110K, new Bragg peaks, very weak, appear in addition to the ones seen at higher T. These have $|\vec{k}_f - \vec{k}_i|$ smaller by a factor of $\sqrt{3}/2$ than the smallest $|\vec{G}|$ normal Bragg peaks. What does that tell you?

   c. Diamond has an *fcc* lattice with a basis of two atoms in the primitive cell. It is easy to distinguish this crystal structure from a primitive *fcc* crystal like copper, because certain Bragg peaks disappear in diamond. Why is this? In terms of the *fcc* lattice constant a, what is the smallest reciprocal lattice vector whose corresponding Bragg peak disappears?

2. **Phonons – mean square momentum of an atom.** Suppose harmonic approximation works well for a crystal with one atom of mass M per unit cell. Then the vibrational Hamiltonian is

$$\mathcal{H} = \sum_Q^{\text{BZ}} \hbar\omega_q (a_Q^\dagger a_Q + 1/2),$$

where Q is short for $(\vec{Q}, \mu)$ and $\mu = 1, 2, 3$ indexes the branches. Remember that the operator for the displacement of the ℓ'th atom is

$$\vec{u}_\ell = \sum_Q^{\text{BZ}} \sqrt{\frac{\hbar}{2MN\omega_Q}} e^{i\vec{Q}\cdot\vec{\ell}} \hat{\epsilon}_Q (a_Q + a_{-Q}^\dagger),$$

where the unit polarization vectors $\hat{\epsilon}(\vec{Q}, \mu)$ for $\mu = 1, 2, 3$ are an orthonormal triad for each of the N $\vec{Q}$'s in the Brillouin zone (BZ). It is also true that the momentum $\vec{P}_\ell$ is

$$\vec{P}_\ell = \frac{1}{i} \sum_Q^{\text{BZ}} \sqrt{\frac{\hbar M\omega_Q}{2N}} e^{i\vec{Q}\cdot\vec{\ell}} \hat{\epsilon}_Q (a_Q - a_{-Q}^\dagger).$$

   a. Show that the commutation relation $[P_{\ell\alpha}, u_{\ell'\beta}] = (\hbar/i)\delta_{\ell,\ell'}\delta_{\alpha,\beta}$ is obeyed. You may use the standard commutation relations of Boson creation operators (harmonic oscillator raising operators). You may also use the orthogonality and completeness relations for the phonon eigenvectors,

$$\sum_\alpha \epsilon_\alpha(\vec{Q}, \mu)\epsilon_\alpha(-\vec{Q}, \mu') = \delta_{\mu,\mu'}$$

$$\sum_\mu \epsilon_\alpha(\vec{Q}, \mu)\epsilon_\beta(-\vec{Q}, \mu) = \delta_{\alpha,\beta}$$

b. Find the formula for $< P_\ell^2 >$ at a general temperature T in terms of $\omega_Q = \omega_{-Q}$.

c. At $T = 0$, find a formula for $\sqrt{< P_\ell^2 >< u_\ell^2 >}$ in terms of some of the moments $< \omega^n > = (1/3N) \sum_Q \omega_Q^n$.

d. What is the limiting high T value of $< P_\ell^2 >$?

3. **Pauli susceptibility of a normal metal:** The Hamiltonian for non-interacting electrons in a magnetic field B can be written as

$$\mathcal{H}_0 = \sum_{k\sigma} (\epsilon_k - \mu_B B \sigma) c_{k\sigma}^\dagger c_{k\sigma}$$

where k is short for wavevector and band index $(\vec{k}, n)$ and the spin index $\sigma = \pm 1$ is written explicitly. Note that the single particle Bloch state eigenenergies ϵ_k do not depend on the spin orientation. The Bohr magneton μ_B should not be confused with the chemical potential μ which is equal to the Fermi energy ϵ_F, plus corrections of order $(k_B T/\epsilon_F)^2$ which you can ignore by assuming that the temperature is not large, $k_B T \ll \epsilon_F$.

a. Derive Pauli's low temperature form for the magnetic susceptibility $\chi \equiv \mu_B(N_\uparrow - N_\downarrow)/BV$. Express the answer in terms of the density of electron states of single spin orientation at the Fermi energy, $\mathcal{D}_\uparrow(0)$.

b. The Bohr magneton $\mu_B = e\hbar/2m$ (SI units) has the value 9.274 $\times 10^{-24}$ J/T. How big a field gives a splitting $2\mu_B B$ equal to 1K? 1meV?

c. Estimate to within a factor of 2 or 3, the value of $\mathcal{D}_\uparrow(0)$ (use units states per eV atom) for metallic Na with one electron per atom and 2 atoms in the conventional (non-primitive) *bcc* cube of side a=4.29 Å.

4. **Quasiparticle excitatinos of a BCS superconductor:** In a BCS superconductor, the part of the Hamiltonian relevant to quasiparticle excitations is

$$\mathcal{H} = \sum_k E_k (\gamma_{k0}^\dagger \gamma_{k0} + \gamma_{k1}^\dagger \gamma_{k1})$$

where the quasiparticle energy is $E_k = \sqrt{\xi_k^2 + |\Delta|^2}$ with $\xi_k = \epsilon_k - \epsilon_F$. The quasiparticle excitations disappear in equilibrium as $T \to 0$. The BCS ground state is defined by $\gamma_{k0}|\text{BCS} >= \gamma_{k1}|\text{BCS} >= 0$). The number of thermally excited quasiparticles is

$$N_{\text{exc}} = \sum_k (< \gamma_{k0}^\dagger \gamma_{k0} > + < \gamma_{k1}^\dagger \gamma_{k1} >).$$

Explain how to derive the formula

$$N_{\text{exc}} = 2\mathcal{D}_\uparrow(0) \int_{|\Delta|}^\infty dE \frac{E}{\sqrt{E^2 - |\Delta|^2}} \frac{1}{e^{\beta E} + 1}$$

valid for all $T < T_c$. The upper limit is set to infinity only because the integrand is small enough that this does not matter. One result of this formula, which you do not have to work out, is that when $k_B T \ll |\Delta|$, the integral gives

$$N_{\text{exc}} = 2\mathcal{D}_\uparrow(0) \sqrt{\pi k_B T |\Delta|} e^{-|\Delta|/k_B T}.$$

Thus the BCS gap causes thermal effects at low T to be exponentially small. This result is derived by approximating the factor $E/\sqrt{E^2 - |\Delta|^2}$ at low T by $\sqrt{|\Delta|/2(E - |\Delta|)}$.

5. **Intrinsic (undoped) semiconductor:** Here is the simplest model of a semiconductor. Assume a "direct" gap E_g=1.0 eV, with conduction band minimum and valence band maximum both at $\vec{k} = 0$. Let the effective masses m_c and m_v both be equal to the free electron mass m. There are no donors or acceptors (it is "intrinsic.")

a. What is the formula for the chemical potential μ as a function of temperature T?

b. How many thermal holes are found at T=300K? You may use the formula

$$\int_0^\infty dx x^{1/2} e^{-x} = \sqrt{\pi}/2.$$

c. How many thermal electrons are found at T=300K?

d. What happens if donor atoms and acceptor atoms are put into the crystal in equal numbers?

e. Suppose the mass m_v is $2m$. Now what is the formula for the chemical potential as a function of T?

6. **Photoemission:** Suppose you have a lab for angle-resolved photoemission spectroscopy (ARPES) of solids. You have two systems, one in the basement of your department, and one attached to a beam line at a synchrotron light source. You can refer to either one when answering this question.

a. In order to get a big enough flux of photons, you want to use low energy photons when possible. What would be the lower limit, approximately, and why?

b. Sketch a schematic of the apparatus. Show in particular where the sample sits.

c. What kind of sample do you need to do the experiment well? Explain why you might choose graphite as a material for a first experiment for a new graduate student.

d. You obtain a good sample of graphite. What do you expect your student to do with it? What does the student try to measure? What kinds of equipment are needed to allow this sample to be measured well?

e. Your apparatus has an optimum energy resolution of 20 meV. Do you need to cool the sample? What factors might be limiting this resolution?

f. Why is the layer structure of graphite such a big advantage in data analysis?

g. What kinds of data will you publish? Sketch some representative graphs.