PHYSICS 239.c : CONDENSED MATTER PHYSICS
HW ASSIGNMENT #5
Instructions: Do any two problems

(1) *Drude formula* – Consider a hypothetical monovalent s-band metal with a simple cubic crystal structure. The valence band dispersion is given by the tight binding result,

$$\varepsilon(\boldsymbol{k}) = -2t\big\{\cos(k_x a)+\cos(k_y a)+\cos(k_z a)\big\}\ .$$

Compute the DC conductivity tensor $\sigma_{\alpha\beta}$. Show that $\sigma_{\alpha\beta}=\sigma\,\delta_{\alpha\beta}$ is diagonal, and obtain an expression for σ. Numerically evaluate any integrals. The following result may prove useful:

$$\int\limits_{-\pi}^{\pi}\!du\int\limits_{-\pi}^{\pi}\!dv\,\delta(\cos u+\cos v+2\lambda) = 4\,\mathrm{K}(\sqrt{1-\lambda^2})\,\Theta(1-\lambda^2)\ ,$$

where $\mathrm{K}(x)$ is the complete elliptic integral of the second kind. Compare your result with the Drude value you would obtain by approximating the band as parabolic, based on its curvature at the zone center.

(2) *Thermal transport in a magnetic field* – Consider a metal with a parabolic band $\varepsilon(\boldsymbol{k}) = \hbar^2\boldsymbol{k}^2/2m^*$ in the presence of a uniform magnetic field $\boldsymbol{B}$. Use the Boltzmann equation* to compute **(a)** the resistivity tensor ρ, **(b)** the thermal conductivity tensor κ, **(c)** the thermopower tensor Q, and **(d)** the Peltier tensor $\sqcap$. Assume T is small, and work to lowest nontrivial order in the temperature T. Also assume a constant relaxation time τ. Does the Wiedemann-Franz law hold for the matrices κ and ρ ?

(3) *Two bands* – Calculate the frequency-dependent conductivity tensor for a direct gap semiconductor in the presence of a magnetic field $\boldsymbol{B}=B\hat{\boldsymbol{z}}$. You should begin with the Boltzmann equation in the relaxation time approximation ($f^0\to\bar f^0$, $\delta f\to\delta\bar f$ for holes),

$$\frac{\partial\,\delta f}{\partial t} - e\,\boldsymbol{v}\cdot\boldsymbol{\mathcal{E}}\,\frac{\partial f^0}{\partial\varepsilon} - \frac{e}{\hbar c}\,\boldsymbol{v}\times\boldsymbol{B}\cdot\frac{\partial\,\delta f}{\partial\boldsymbol{k}} = -\frac{\delta f}{\tau}\ ,$$

and the conduction and valence band dispersions,

$$\begin{aligned}\varepsilon_{\rm v}(\boldsymbol{k}) &= \varepsilon^{\rm v}_0 - \tfrac{1}{2}\hbar^2 {m^{\rm v}_{\alpha\beta}}^{-1}\,k^\alpha\,k^\beta\\ \varepsilon_{\rm c}(\boldsymbol{k}) &= \varepsilon^{\rm c}_0 + \tfrac{1}{2}\hbar^2 {m^{\rm c}_{\alpha\beta}}^{-1}\,k^\alpha\,k^\beta\ .\end{aligned}$$

Assume the two bands behave independently, and solve the two Boltzmann equations for the conduction electrons and valence holes. In each case, try a solution of the form

$$\delta f(\boldsymbol{k},t) = k^\mu\,A^\mu(\varepsilon(\boldsymbol{k}))\,e^{-i\omega t}\ .$$

The currents are

$$\begin{Bmatrix}\boldsymbol{j}_{\rm c}\\ \boldsymbol{j}_{\rm v}\end{Bmatrix} = 2e\int\limits_{\hat\Omega}\frac{d^3k}{(2\pi)^3}\begin{Bmatrix}-\,\boldsymbol{v}_{\rm c}\,\delta f_{\rm c}\\ +\,\boldsymbol{v}_{\rm v}\,\delta\bar f_{\rm v}\end{Bmatrix}\ .$$

Compute $\sigma_{\alpha\beta}$ along principal axes of the effective mass tensors. You may assume that m^{v} and m^{c} commute, *i.e.* they have the same eigenvectors. You should further assume that $\boldsymbol{B}$ lies along a principal axis.

(4) *Spin disorder resistivity (for the brave only!)* – Consider an isolated trivalent Tb impurity ion in a crystal field. Application of Hund's rules gives a total angular momentum $J = 6$. A cubic crystal field splits this 13-fold degenerate multiplet into six levels: two singlets, one doublet, and three triplets. The ground state is a singlet. Using the first Born approximation, calculate the temperature-dependent resistivity in a free electron model with a scattering Hamiltonian

$$\mathcal{H}_{\mathrm{imp}} = -A\,(g-1)\sum_{j=1}^{N_{\mathrm{imp}}} \delta(\boldsymbol{r} - \boldsymbol{R}_j)\,\boldsymbol{S}\cdot\boldsymbol{J}_j/\hbar^2\ ,$$

where $\boldsymbol{r}$ and $\boldsymbol{S}$ are the conduction electron position and spin operators $\boldsymbol{R}_j$ and $\boldsymbol{J}_j$ are the impurity position and angular momentum of the j^{th} Tb impurity. A is the strength of the exchange interaction, and $g = \frac{3}{2}$ is the gyromagnetic factor.

(a) In general the relaxation time is energy-dependent: $\tau = \tau(\varepsilon)$. Show that the resistivity is given by $\rho = m/ne^2\langle\tau\rangle$, where the average is with respect to the weighting function $\varepsilon\, g(\varepsilon)\,(-\partial f^0/\partial\varepsilon)$. Show also that

$$\frac{1}{\langle\tau\rangle} \le \langle\tau^{-1}\rangle,$$

which provides an upper bound for ρ which can often be computed.

(b) Use the results of **(a)** to derive an approximation to the resistivity $\rho \simeq \rho_0\, p_{ij}\, Q_{ji}$, where

$$\begin{aligned} p_{ij} &= \frac{e^{-E_i/k_{\mathrm{B}}T}}{\sum_k e^{-E_k/k_{\mathrm{B}}T}} \cdot \frac{(E_i - E_i)/k_{\mathrm{B}}T}{1 - e^{-(E_i-E_j)/k_{\mathrm{B}}T}} \\ Q_{ij} &= \tfrac{1}{2}\big|\langle\, i\,|\, J^+\,|\, j\,\rangle\big|^2 + \tfrac{1}{2}\big|\langle\, i\,|\, J^-\,|\, j\,\rangle\big|^2 + \big|\langle\, i\,|\, J^z\,|\, j\,\rangle\big|^2\ , \end{aligned}$$

where the ionic energy levels are denoted by E_i and where the summations run over the $(2J+1)$ crystal field states. Show that

$$\rho_0 = \frac{3\pi m\,(g-1)^2\,A^2\,n_{\mathrm{imp}}}{8e^2\hbar^3\varepsilon_{\mathrm{F}}}\ .$$

(c) Show that the high temperature limiting value of ρ is $J(J+1)\,\rho_0$. This is often called the spin-disorder resistivity.