PHYSICS 211B: CONDENSED MATTER PHYSICS HW ASSIGNMENT #2

(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,

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

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:

$$\int_{-\pi}^{\pi} du \int_{-\pi}^{\pi} dv \,\delta(\cos u + \cos v + 2\lambda) = 4 \operatorname{K}(\sqrt{1 - \lambda^2}) \,\Theta(1 - \lambda^2) \quad ,$$

where 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 $\varepsilon(\mathbf{k}) = \hbar^2 \mathbf{k}^2 / 2m^*$ in the presence of a uniform magnetic field \mathbf{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 \Box . 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) Consider the currents

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Define the response coefficients ρ , Q, ω , and v by the relations

$$\boldsymbol{\mathcal{E}} = \rho \, \boldsymbol{j} + Q \, \boldsymbol{\nabla} T$$
$$\boldsymbol{J} = \omega \boldsymbol{j} - v \, \boldsymbol{\nabla} T$$

For a system with parabolic dispersion, find expressions for the transport coefficients ρ , Q, ω , and v in terms of the integrals

$$\begin{split} \mathcal{K}_n &= \frac{\tau}{12\pi^3\hbar} \int\limits_{-\infty}^{\infty} d\varepsilon \; (\varepsilon - \mu)^n \left(-\frac{\partial f^0}{\partial \varepsilon} \right) \int dS_{\varepsilon} \left| \boldsymbol{v} \right| \\ &= \frac{\sigma_0}{e^2} \, \varepsilon_{\mathrm{F}}^{-3/2} \, \mathcal{S} \left[\varepsilon^{3/2} (\varepsilon - \mu)^n \right] \Big|_{\varepsilon = \mu} \quad , \end{split}$$

where

$$S = \pi D \csc \pi D = 1 + \frac{\pi^2}{6} D^2 + \frac{7\pi^4}{360} D^4 + \dots ,$$

with $\mathcal{D} = k_{\rm B} T \, \partial_{\varepsilon}$.

(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

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

where *r* and *S* are the conduction electron position and spin operators R_j and 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

$$p_{ij} = \frac{e^{-E_i/k_{\rm B}T}}{\sum_k e^{-E_k/k_{\rm B}T}} \cdot \frac{(E_i - E_i)/k_{\rm B}T}{1 - e^{-(E_i - E_j)/k_{\rm B}T}}$$
$$Q_{ij} = \frac{1}{2} \left| \left\langle i \right| J^+ \left| j \right\rangle \right|^2 + \frac{1}{2} \left| \left\langle i \right| J^- \left| j \right\rangle \right|^2 + \left| \left\langle i \right| J^z \left| j \right\rangle \right|^2$$

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

$$\rho_0 = \frac{3\pi m \left(g - 1\right)^2 A^2 n_{\rm imp}}{8e^2 \hbar^3 \varepsilon_{\rm F}} \quad \label{eq:rho}$$

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