Physics 211B : Solution Set #1

[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.

<u>Solution:</u> We must evaluate

$$\sigma_{\alpha\beta} = 2e^2\tau \int\limits_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3}\ v^\alpha\,v^\beta\left(-\frac{\partial f}{\partial \varepsilon}\right) \ ,$$

where the dispersion is

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

The velocity is

$$\boldsymbol{v}(\boldsymbol{k}) = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \boldsymbol{k}} = \frac{2ta}{\hbar}\Big(\sin(k_x a),\ \sin(k_y a),\ \sin(k_z a) \Big) \ .$$

As a consequence of the cubic symmetry, $\sigma_{\alpha\beta} = \sigma\,\delta_{\alpha\beta}$ is diagonal, and we may write

$$\sigma = 2e^2\tau\left(\frac{2ta}{\hbar}\right)^2 \int\limits_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3}\ \sin^2(k_z a)\left(-\frac{\partial f}{\partial \varepsilon}\right) \ .$$

The monovalency condition means that there is one electron per unit cell, which in turn means the chemical potential lies at $\mu = 0$ so the s-band is half-filled. Changing variables to $u = k_x a$, *etc.*,

$$\sigma = \frac{e^2\tau\,t}{2\pi^3\hbar^2 a} \int\limits_{-\pi}^{\pi} du \int\limits_{-\pi}^{\pi} dv \int\limits_{-\pi}^{\pi} dw\ \sin^2(w)\,\delta(\cos u + \cos v + \cos w) \ .$$

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We now use

$$\mathcal{I}(\lambda) = \int\limits_{-\pi}^{\pi} du \int\limits_{-\pi}^{\pi} dv\, \delta(\cos u + \cos v + 2\lambda) \tag{1}$$

$$= 4 \int\limits_{-1}^{1-2|\lambda|} \frac{1}{\sqrt{1-x^2}} \frac{1}{\sqrt{1-\left(x+2|\lambda|\right)^2}} \tag{2}$$

$$= 4\left(1-|\lambda|\right) \int\limits_{-1}^{1} \frac{ds}{\sqrt{\left(1+|\lambda|\right)^2 - 2\left(1+|\lambda|^2\right)s^2 + \left(1-|\lambda|\right)^2 s^4}} \tag{3}$$

$$= \frac{8}{1+|\lambda|}\, \mathrm{K}\!\left(\frac{1-|\lambda|}{1+|\lambda|}\right) = 4\,\mathrm{K}\!\left(\sqrt{1-\lambda^2}\right) . \tag{4}$$

Thus,

$$\sigma = \frac{8\mathcal{C}}{\pi^3} \cdot \frac{e^2 \tau\, t}{\hbar^2 a} . \tag{5}$$

where

$$\mathcal{C} = \int\limits_{0}^{1} dx\, \sqrt{1-x^2}\, \mathrm{K}\!\left(\sqrt{1-\tfrac{1}{4}x^2}\right) .$$

Numerical integration gives $\mathcal{C} \simeq 2.59011$.

Expanding the dispersion about the zone center, we find

$$\varepsilon(\boldsymbol{k}) = -6t + ta^2 \boldsymbol{k}^2 + \mathcal{O}(k^4) , \tag{6}$$

hence the effective mass is given by

$$ta^2 \equiv \frac{\hbar^2}{2m^*} \quad \Longrightarrow \quad m^* = \frac{\hbar^2}{2ta^2} . \tag{7}$$

The Drude conductivity is then

$$\sigma = \frac{ne^2 \tau}{m^*} = ne^2 \tau \cdot \frac{2ta^2}{\hbar^2} = 2x \cdot \frac{e^2 \tau t}{\hbar^2 a} , \tag{8}$$

where $x \equiv na^3$ is the dimensionless density, equal to the average number of electrons per unit cell ($0 \le x \le 2$). For a monovalent metal, the band is half filled, and $x = 1$, and the prefactor $2x$ is 2. The exact value of the prefactor is $8\mathcal{C}/\pi^3 \simeq 0.668$.

[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 Π. 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 ?

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Solution: We begin with the Boltzmann equation,

$$\boldsymbol{v} \cdot \left[e\boldsymbol{\mathcal{E}} + \frac{\varepsilon - \mu}{T} \boldsymbol{\nabla} T \right] \left(-\frac{\partial f}{\partial \varepsilon} \right) = \frac{e}{\hbar c} \boldsymbol{v} \times \boldsymbol{B} \cdot \frac{\partial \delta f}{\partial \boldsymbol{k}} - \frac{\delta f}{\tau} \ .$$

We take $\varepsilon(\boldsymbol{k}) = \hbar^2 \boldsymbol{k}^2 / 2m^*$, and we write

$$\delta f(\boldsymbol{k}) = \boldsymbol{k} \cdot \boldsymbol{A}(\varepsilon)$$

$$\Rightarrow \quad v_x \frac{\partial \delta f}{\partial k_y} - v_y \frac{\partial \delta f}{\partial k_x} = \frac{\hbar}{m^*} \left(k_x A_y - k_y A_x \right) ,$$

from which we obtain the linear relations

$$\begin{pmatrix} 1 & +\omega_{\rm c}\tau & 0 \\ -\omega_{\rm c}\tau & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} = \frac{\hbar\tau}{m^*} \frac{\partial f^0}{\partial \varepsilon} \begin{pmatrix} e\mathcal{E}_x + \frac{\varepsilon - \mu}{T} \partial_x T \\ e\mathcal{E}_y + \frac{\varepsilon - \mu}{T} \partial_y T \\ e\mathcal{E}_z + \frac{\varepsilon - \mu}{T} \partial_z T \end{pmatrix} \ .$$

The solution is easily obtained:

$$\begin{pmatrix} A_x \\ A_y \\ A_z \end{pmatrix} = \frac{\hbar\tau/m^*}{1 + \omega_{\rm c}^2\tau^2} \frac{\partial f^0}{\partial \varepsilon} \begin{pmatrix} 1 & -\omega_{\rm c}\tau & 0 \\ +\omega_{\rm c}\tau & 1 & 0 \\ 0 & 0 & 1 + \omega_{\rm c}^2\tau^2 \end{pmatrix} \begin{pmatrix} e\mathcal{E}_x + \frac{\varepsilon - \mu}{T} \partial_x T \\ e\mathcal{E}_y + \frac{\varepsilon - \mu}{T} \partial_y T \\ e\mathcal{E}_z + \frac{\varepsilon - \mu}{T} \partial_z T \end{pmatrix} \ .$$

The electrical and thermal currents are given by

$$j_\alpha = -\frac{2e}{3\hbar} \int d\varepsilon \, g(\varepsilon) \, \varepsilon \, \mathcal{A}_\alpha$$

$$j_\alpha^q = \frac{2}{3\hbar} \int d\varepsilon \, (\varepsilon - \mu) \, g(\varepsilon) \, \varepsilon \, \mathcal{A}_\alpha \ .$$

We now read off the transport coefficients from the relations

$$\boldsymbol{j} = \rho^{-1}\boldsymbol{\mathcal{E}} - \rho^{-1} Q \boldsymbol{\nabla} T$$

$$\boldsymbol{j}_q = \Pi \rho^{-1}\boldsymbol{\mathcal{E}} - (\kappa + \Pi \rho^{-1} Q)\boldsymbol{\nabla} T \ .$$

We find

$$\rho^{-1} = \frac{2e}{3m} \int d\varepsilon \, g(\varepsilon) \, \varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) \frac{\tau}{1 + \omega_{\rm c}^2\tau^2} \begin{pmatrix} 1 & -\omega_{\rm c}\tau & 0 \\ +\omega_{\rm c}\tau & 1 & 0 \\ 0 & 0 & 1 + \omega_{\rm c}^2\tau^2 \end{pmatrix}$$

$$\rho^{-1}Q = -\frac{2e}{3m^*} \int d\varepsilon \, g(\varepsilon) \frac{\varepsilon(\varepsilon - \mu)}{T} \left(-\frac{\partial f}{\partial \varepsilon} \right) \frac{\tau}{1 + \omega_{\rm c}^2\tau^2} \begin{pmatrix} 1 & -\omega_{\rm c}\tau & 0 \\ +\omega_{\rm c}\tau & 1 & 0 \\ 0 & 0 & 1 + \omega_{\rm c}^2\tau^2 \end{pmatrix}$$

$$\Pi\rho^{-1} = -\frac{2e}{3m^*} \int d\varepsilon \, (\varepsilon - \mu) \, g(\varepsilon) \, \varepsilon \left(-\frac{\partial f}{\partial \varepsilon} \right) \frac{\tau}{1 + \omega_{\rm c}^2\tau^2} \begin{pmatrix} 1 & -\omega_{\rm c}\tau & 0 \\ +\omega_{\rm c}\tau & 1 & 0 \\ 0 & 0 & 1 + \omega_{\rm c}^2\tau^2 \end{pmatrix}$$

$$\kappa + \Pi\rho^{-1}Q = \frac{2}{3m^*} \int d\varepsilon \, g(\varepsilon) \frac{\varepsilon(\varepsilon - \mu)^2}{T} \left(-\frac{\partial f}{\partial \varepsilon} \right) \frac{\tau}{1 + \omega_{\rm c}^2\tau^2} \begin{pmatrix} 1 & -\omega_{\rm c}\tau & 0 \\ +\omega_{\rm c}\tau & 1 & 0 \\ 0 & 0 & 1 + \omega_{\rm c}^2\tau^2 \end{pmatrix} .$$

We evaluate the integrals using the Sommerfeld expansion, and invoking the density of states

$$g(\varepsilon) = \frac{\sqrt{2}\,(m^*)^{3/2}}{\pi^2 \hbar^3}\,\sqrt{\varepsilon}\;.$$

With an energy-independent relaxation time τ, we obtain

$$\varrho^{-1} = \sigma = \frac{ne^2\tau}{m^*}\,\frac{1}{1+\omega_{\mathrm{c}}^2\tau^2}\begin{pmatrix} 1 & -\omega_{\mathrm{c}}\tau & 0 \\ +\omega_{\mathrm{c}}\tau & 1 & 0 \\ 0 & 0 & 1+\omega_{\mathrm{c}}^2\tau^2 \end{pmatrix}$$

The quantity $\rho^{-1}Q$ is proportional to the same matrix as is ρ^{-1}, and one readily finds that Q is a multiple of the unit matrix,

$$Q = -\frac{\pi^2 k_{\mathrm{B}}^2 T}{2e\varepsilon_{\mathrm{F}}}\cdot\mathbb{I}\;.$$

Here we have used the results

$$\int d\varepsilon\, g(\varepsilon)\,\varepsilon\,(\varepsilon-\mu)\left(-\frac{\partial f}{\partial \varepsilon}\right) = \tfrac{1}{2}\pi^2(k_{\mathrm{B}}T)^2 g(\mu) + \mathcal{O}(T^4)$$

$$g(\varepsilon_{\mathrm{F}}) = \frac{m^* k_{\mathrm{F}}}{\pi^2\hbar^2} = \frac{3n}{2\varepsilon_{\mathrm{F}}}\;.$$

We also find

$$\Pi = T\,Q^{\mathrm{t}}(-\boldsymbol{B}) = -\frac{\pi^2(k_{\mathrm{B}}T)^2}{2e\varepsilon_{\mathrm{F}}}\cdot\mathbb{I}\;.$$

Finally, the thermal conductivity tensor is

$$\kappa = \tfrac{1}{3}\pi^2\,k_{\mathrm{B}}^2 T\,\frac{n\tau/m^*}{1+\omega_{\mathrm{c}}^2\tau^2}\begin{pmatrix} 1 & -\omega_{\mathrm{c}}\tau & 0 \\ +\omega_{\mathrm{c}}\tau & 1 & 0 \\ 0 & 0 & 1+\omega_{\mathrm{c}}^2\tau^2 \end{pmatrix}$$

Thus, the Wiedemann-Franz law,

$$\kappa = \frac{\pi^2}{3e^2}\,k_{\mathrm{B}}^2 T\,\rho^{-1}$$

holds at the matrix level as well.

[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,

$$\varepsilon_{\mathrm{v}}(\boldsymbol{k}) = \varepsilon_0^{\mathrm{v}} - \tfrac{1}{2}\hbar^2 {m_{\alpha\beta}^{\mathrm{v}}}^{-1} k^\alpha k^\beta$$

$$\varepsilon_{\mathrm{c}}(\boldsymbol{k}) = \varepsilon_0^{\mathrm{c}} + \tfrac{1}{2}\hbar^2 {m_{\alpha\beta}^{\mathrm{c}}}^{-1} k^\alpha k^\beta\;.$$

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

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

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.

<u>**Solution:**</u> This problem is essentially solved in the notes in section **1.7**. All that is left to do is to sum the contributions from the valence and conduction bands:

$$\sigma_{xx}(\omega) = \frac{n_\mathrm{c} e^2 \tau_\mathrm{c}}{m^*_{\mathrm{c},x}} \frac{1 - i\omega\tau_\mathrm{c}}{(1 - i\omega\tau_\mathrm{c})^2 + \omega^2_{\mathrm{c},\perp}\tau_\mathrm{c}^2} + \frac{p_\mathrm{v} e^2 \tau_\mathrm{v}}{m^*_{\mathrm{v},x}} \frac{1 - i\omega\tau_\mathrm{v}}{(1 - i\omega\tau_\mathrm{v})^2 + \omega^2_{\mathrm{c},\perp}\tau_\mathrm{v}^2}$$

$$\sigma_{xy}(\omega) = -\frac{n_\mathrm{c} e^2 \tau_\mathrm{c}}{\sqrt{m^*_{\mathrm{c},x} m^*_{\mathrm{c},y}}} \frac{\omega_{\mathrm{c},\perp}\tau_\mathrm{c}}{(1 - i\omega\tau_\mathrm{c})^2 + \omega^2_{\mathrm{c},\perp}\tau_\mathrm{c}^2} + \frac{p_\mathrm{v} e^2 \tau_\mathrm{v}}{\sqrt{m^*_{\mathrm{v},x} m^*_{\mathrm{v},y}}} \frac{\omega_{\mathrm{v},\perp}\tau_\mathrm{v}}{(1 - i\omega\tau_\mathrm{v})^2 + \omega^2_{\mathrm{c},\perp}\tau_\mathrm{v}^2}$$

$$\sigma_{zz}(\omega) = \frac{n_\mathrm{c} e^2 \tau_\mathrm{c}}{m^*_{\mathrm{c},z}} \frac{1}{1 - i\omega\tau_\mathrm{c}} + \frac{p_\mathrm{v} e^2 \tau_\mathrm{v}}{m^*_{\mathrm{v},z}} \frac{1}{1 - i\omega\tau_\mathrm{v}}\ .$$

[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 jth 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

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

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

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

$$p_{ij} = \frac{e^{-E_i/k_{\mathrm{B}}T}}{\sum_k e^{-E_k/k_{\mathrm{B}}T}} \cdot \frac{(E_i - E_i)/k_{\mathrm{B}}T}{1 - e^{-(E_i - E_j)/k_{\mathrm{B}}T}}$$

$$Q_{ij} = \tfrac{1}{2}\left|\langle\, i\,|\, J^+ \,|\, j\,\rangle\right|^2 + \tfrac{1}{2}\left|\langle\, i\,|\, J^- \,|\, j\,\rangle\right|^2 + \left|\langle\, i\,|\, J^z \,|\, j\,\rangle\right|^2 ,$$

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

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

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

<u>**Solution:**</u> The collision term in Boltzmann equation is, from Fermi's golden rule,

$$\mathcal{I}_{\boldsymbol{k}\sigma}[f] = \frac{2\pi}{\hbar} \sum_{ij} \sum_{\boldsymbol{k}'\sigma'} P_i \left|\langle\, j\boldsymbol{k}\sigma\,|\,\mathcal{H}_{\mathrm{imp}}\,|\, i\boldsymbol{k}'\sigma'\,\rangle\right|^2 \delta\!\left(E_j + \varepsilon_{\boldsymbol{k}} - E_i - \varepsilon_{\boldsymbol{k}'}\right) f_{\boldsymbol{k}'\sigma'}(1 - f_{\boldsymbol{k}\sigma})$$

$$- \frac{2\pi}{\hbar} \sum_{ij} \sum_{\boldsymbol{k}'\sigma'} P_i \left|\langle\, f\boldsymbol{k}'\sigma\,|\,\mathcal{H}_{\mathrm{imp}}\,|\, i\boldsymbol{k}\sigma'\,\rangle\right|^2 \delta\!\left(E_j + \varepsilon_{\boldsymbol{k}'} - E_i - \varepsilon_{\boldsymbol{k}}\right) f_{\boldsymbol{k}\sigma}(1 - f_{\boldsymbol{k}'\sigma'}) ,$$

where P_i is the Boltzmann weight for the ion in state i:

$$P_i = \frac{\exp(-E_i/k_{\mathrm{B}}T)}{\sum_n \exp(-E_n/k_{\mathrm{B}}T)} .$$

Using plane wave states $\psi_{\boldsymbol{k}}(\boldsymbol{r}) = V^{-1/2}\exp(i\boldsymbol{k}\cdot\boldsymbol{r})$, the matrix element is obtained:

$$\langle\, j\boldsymbol{k}\sigma\,|\,\mathcal{H}_{\mathrm{imp}}\,|\, i\boldsymbol{k}'\sigma'\,\rangle = -\frac{1}{V}\, A\,(g - 1)\,\hbar^{-2} \sum_{\boldsymbol{R}} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}}\,\langle\, j\sigma'\,|\,\boldsymbol{S}\cdot\boldsymbol{J}\,|\, i\sigma\,\rangle .$$

We assume the impurity positions are uncorrelated, so that

$$\overline{\left|\langle\, j\boldsymbol{k}\sigma\,|\,\mathcal{H}_{\mathrm{imp}}\,|\, i\boldsymbol{k}'\sigma'\,\rangle\right|^2} = \frac{A^2(g - 1)^2}{\hbar^2 V^2}\left|\langle\, j\sigma'\,|\,\boldsymbol{S}\cdot\boldsymbol{J}\,|\, i\sigma\,\rangle\right|^2 \overline{\sum_{\boldsymbol{R},\boldsymbol{R}'} e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot(\boldsymbol{R}-\boldsymbol{R}')}}$$

$$= \frac{N_{\mathrm{imp}}}{V^2}\frac{A^2(g - 1)^2}{\hbar^4}\left|\langle\, j\sigma'\,|\,\boldsymbol{S}\cdot\boldsymbol{J}\,|\, i\sigma\,\rangle\right|^2 \left(1 + (N_{\mathrm{imp}} - 1)\delta_{\boldsymbol{k}\boldsymbol{k}'}\right) .$$

The term proportional to $\delta_{\boldsymbol{k}\boldsymbol{k}'}$ cancels when inserted into the collision integral. We are left with

$$\mathcal{I}_{\boldsymbol{k}\sigma}[f] = \frac{2\pi}{\hbar^5} A^2(g - 1)^2 n_{\mathrm{imp}} \sum_{ij\sigma'} \int_{\hat{\Omega}} \frac{d^3k'}{(2\pi)^3}\, \delta\!\left(E_j + \varepsilon_{\boldsymbol{k}'} - E_i - \varepsilon_{\boldsymbol{k}}\right)\left|\langle\, j\sigma'\,|\,\boldsymbol{S}\cdot\boldsymbol{J}\,|\, i\sigma\,\rangle\right|^2$$

$$\times \left\{ P_j\, f_{\boldsymbol{k}'\sigma'}(1 - f_{\boldsymbol{k}\sigma}) - P_i\, f_{\boldsymbol{k}\sigma}(1 - f_{\boldsymbol{k}'\sigma'}) \right\} .$$

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Note that the Fermi-Dirac distribution $f^0_{k\sigma}$ is annihilated by $\mathcal{I}$:

$$P_j\, f^0_{k'\sigma'}(1 - f^0_{k\sigma}) = \frac{e^{-\beta E_j}}{\sum_n e^{-\beta E_n}} \frac{1}{e^{\beta(\varepsilon_{k'}-\mu)} + 1} \frac{e^{\beta(\varepsilon_k-\mu)}}{e^{\beta(\varepsilon_k-\mu)} + 1} \delta\big(E_j + \varepsilon_{k'} - E_i - \varepsilon_k\big)$$

$$= \frac{e^{-\beta E_i}}{\sum_n e^{-\beta E_n}} \frac{e^{\beta(\varepsilon_{k'}-\mu)}}{e^{\beta(\varepsilon_{k'}-\mu)} + 1} \frac{1}{e^{\beta(\varepsilon_k-\mu)} + 1} \delta\big(E_j + \varepsilon_{k'} - E_i - \varepsilon_k\big)$$

$$= P_i\, f^0_{k\sigma}(1 - f^0_{k'\sigma'})\ .$$

We therefore write

$$f_{k\sigma} = f^0_{k\sigma} + \delta f_{k\sigma} \qquad , \qquad f^0_{k\sigma} = f^0_k = \frac{1}{e^{\beta(\varepsilon_k-\mu)} + 1}$$

and find

$$P_j\,(f^0_{k'\sigma'} + \delta f_{k'\sigma'})\,(1 - f^0_{k\sigma} - \delta f_{k\sigma}) - P_i\,(f^0_{k\sigma} + \delta f_{k\sigma})\,(1 - f^0_{k'\sigma'} - \delta f_{k'\sigma'})$$

$$= \big[P_j\,(1 - f^0_{k\sigma}) + P_i f^0_{k\sigma}\big]\delta f_{k'\sigma'} - \big[P_j\, f^0_{k'\sigma'} + P_i\,1 - f^0_{k'\sigma'}\big]\delta f_{k\sigma}\ .$$

The Boltzmann equation then takes the form

$$e\boldsymbol{v_k}\cdot\boldsymbol{\mathcal{E}}\left(-\frac{\partial f}{\partial\varepsilon}\right) = \frac{2\pi}{\hbar^5}A^2(g-1)^2 n_{\text{imp}} \sum_{ij\sigma'} \big|\langle\, j\sigma'\,|\,\boldsymbol{S}\cdot\boldsymbol{J}\,|\,i\sigma\,\rangle\big|^2$$

$$\times \int_{\hat{\Omega}} \frac{d^3k'}{(2\pi)^3}\, \delta\big(E_j + \varepsilon_{k'} - E_i - \varepsilon_k\big)\bigg\{\big[P_j\,(1 - f^0_{k\sigma}) + P_i f^0_{k\sigma}\big]\delta f_{k'\sigma'}$$

$$- \big[P_j\, f^0_{k'\sigma'} + P_i\,(1 - f^0_{k'\sigma'})\big]\delta f_{k\sigma}\bigg\}\ .$$

We now sum both sides on σ and divide by two. Using

$$\sum_\sigma \big|\langle\, j\sigma'\,|\,\boldsymbol{S}\cdot\boldsymbol{J}\,|\,i\sigma\,\rangle\big|^2 = \sum_\sigma \langle\, j\,|\,J^\alpha\,|\,i\,\rangle\langle\, i\,|\,J^\beta\,|\,j\,\rangle \times \langle\,\sigma'\,|\,S^\alpha\,|\,\sigma\,\rangle\langle\,\sigma\,|\,S^\beta\,|\,\sigma'\,\rangle$$

$$= \tfrac{1}{3}\hbar^2 S(S+1)\delta^{\alpha\beta}\,\langle\, j\,|\,J^\alpha\,|\,i\,\rangle\langle\, i\,|\,J^\beta\,|\,j\,\rangle$$

$$= \tfrac{1}{4}\hbar^2\big|\langle\, j\,|\,\boldsymbol{J}\,|\,i\,\rangle\big|^2\ ,$$

we obtain

$$e\boldsymbol{v_k}\cdot\boldsymbol{\mathcal{E}}\left(-\frac{\partial f}{\partial\varepsilon}\right) = \frac{2\pi}{\hbar^5}A^2(g-1)^2 n_{\text{imp}} \sum_{ij} \big|\langle\, j\,|\,\boldsymbol{J}\,|\,i\,\rangle\big|^2 \int_{\hat{\Omega}} \frac{d^3k'}{(2\pi)^3}\, \delta\big(E_j + \varepsilon_{k'} - E_i - \varepsilon_k\big)$$

$$\times \bigg\{\big[P_j\,(1 - f^0_{k\sigma}) + P_i f^0_{k\sigma}\big]\delta f_{k'\sigma'} - \big[P_j\, f^0_{k'\sigma'} + P_i\,1 - f^0_{k'\sigma'}\big]\delta f_{k\sigma}\bigg\}\ .$$

It is convenient to define the *structure factor*

$$S(u) \equiv \sum_{ij} P_i\, \big|\langle\, j\,|\,\boldsymbol{J}\,|\,i\,\rangle\big|^2\, \delta(u - E_j + E_i)\ . \tag{9}$$

Note that $S(-u) = e^{-\beta u} S(u)$.

We assume a solution of the form

$$\delta f_{\boldsymbol{k}} = e\tau(\varepsilon_{\boldsymbol{k}}) \cdot \boldsymbol{\mathcal{E}} \frac{\partial f^0}{\partial \varepsilon}$$

and plug this into our Boltzmann equation. Further assuming an isotropic Fermi surface, the $\delta f_{\boldsymbol{k}'}$ term integrates to zero since it is proportional to $\boldsymbol{v}_{\boldsymbol{k}'}$, aside from energy-dependent (hence rotationally isotropic) factors. We then have

$$\frac{1}{\tau(\varepsilon_{\boldsymbol{k}})} = \frac{\pi}{2\hbar^3} A^2 (g-1)^2 n_{\text{imp}} \int\limits_{-\infty}^{\infty} du\, S(u) \int\limits_{\hat{\Omega}} \frac{d^3 k'}{(2\pi)^3}\, \delta(u + \varepsilon_{\boldsymbol{k}'} - \varepsilon_{\boldsymbol{k}})$$
$$\times \left[1 - f_{\boldsymbol{k}'}^0 + e^{-\beta u} f_{\boldsymbol{k}}^0 \right].$$

Furthermore, since $u = \varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}'}$, we have

$$1 - f_{\boldsymbol{k}'}^0 + e^{-\beta u} f_{\boldsymbol{k}}^0 = \frac{1 - f_{\boldsymbol{k}'}^0}{1 - f_{\boldsymbol{k}}^0},$$

giving

$$\boxed{\frac{1}{\tau(\varepsilon_{\boldsymbol{k}})} = \frac{\pi}{2\hbar^3} A^2 (g-1)^2 n_{\text{imp}} \int\limits_{-\infty}^{\infty} du\, S(u) \int\limits_{\hat{\Omega}} \frac{d^3 k'}{(2\pi)^3}\, \delta(u + \varepsilon_{\boldsymbol{k}'} - \varepsilon_{\boldsymbol{k}}) \frac{1 - f_{\boldsymbol{k}'}^0}{1 - f_{\boldsymbol{k}}^0}}$$

(a) The conductivity is determined from

$$\boldsymbol{j} = 2e \int\limits_{\hat{\Omega}} \frac{d^3 k}{(2\pi)^3}\, e\tau(\varepsilon_{\boldsymbol{k}}) \left(\boldsymbol{v}_{\boldsymbol{k}} \cdot \boldsymbol{\mathcal{E}} \right) \boldsymbol{v}_{\boldsymbol{k}} \left(-\frac{\partial f}{\partial \varepsilon} \right),$$

which, for free electrons, gives

$$\sigma = \frac{ne^2 \langle \tau \rangle}{m}$$

$$\langle \tau \rangle = \int d\varepsilon\, \varepsilon\, g(\varepsilon)\, \tau(\varepsilon) \left(-\frac{\partial f}{\partial \varepsilon} \right) \bigg/ \int d\varepsilon\, \varepsilon\, g(\varepsilon) \left(-\frac{\partial f}{\partial \varepsilon} \right).$$

Now the triangle inequality requires for any real functions $f(\varepsilon)$ and $g(\varepsilon)$

$$\left[\int d\varepsilon\, f(\varepsilon)\, h(\varepsilon) \right]^2 \leq \left[\int d\varepsilon\, f(\varepsilon) \right] \left[\int d\varepsilon\, h(\varepsilon) \right],$$

so taking

$$f(\varepsilon) \equiv \left[\varepsilon\, g(\varepsilon) \left(-\frac{\partial f}{\partial \varepsilon} \right) \tau(\varepsilon) \right]^{1/2}$$

$$h(\varepsilon) \equiv \left[\varepsilon\, g(\varepsilon) \left(-\frac{\partial f}{\partial \varepsilon} \right) \frac{1}{\tau(\varepsilon)} \right]^{1/2}$$

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we conclude

$$\langle \tau(\varepsilon)\rangle \cdot \left\langle \frac{1}{\tau(\varepsilon)}\right\rangle \geq 1$$

hence

$$\rho = \frac{m}{ne^2 \langle \tau\rangle} \leq \frac{m}{ne^2}\left\langle \frac{1}{\tau}\right\rangle .$$

(b) Let us compute $\langle \tau^{-1}\rangle$. Noting that

$$\left(-\frac{\partial f}{\partial \varepsilon}\right) = \beta f^0 \left(1 - f^0\right) ,$$

we have

$$\left\langle \frac{1}{\tau}\right\rangle = \frac{2m}{3n} \cdot \frac{\pi}{2\hbar^3} A^2 (g-1)^2 \beta n_{\text{imp}} \int\limits_{\hat{\Omega}} \frac{d^3k}{(2\pi)^3} \int\limits_{\hat{\Omega}} \frac{d^3k'}{(2\pi)^3}$$

$$\times \int du\, S(u)\, \delta(u + \varepsilon_{\mathbf{k'}} - \varepsilon_{\mathbf{k}})\, f_{\mathbf{k}}^0 \left(1 - f_{\mathbf{k'}}^0\right) \boldsymbol{v}_{\mathbf{k}}^2$$

$$= \frac{\pi m}{3\hbar n} \frac{A^2 (g-1)^2}{(2\pi)^6 \hbar^4} \beta\, n_{\text{imp}} \int du\, S(u) \int d\varepsilon \int d\varepsilon'\, \delta(u + \varepsilon' - \varepsilon)$$

$$\times f^0(\varepsilon)\left(1 - f^0(\varepsilon')\right) \int dS_\varepsilon\, |\boldsymbol{v}| \int dS_{\varepsilon'}\, |\boldsymbol{v'}|^{-1} .$$

The factor $f^0(\varepsilon)\left(1 - f^0(\varepsilon - u)\right)$ varies on a scale $k_{\text{B}}T$. If $k_{\text{B}}T \ll \mu$ and if $u \ll \mu$ then we can approximate

$$\int dS_\varepsilon\, |\boldsymbol{v}| \int dS_{\varepsilon'}\, |\boldsymbol{v'}|^{-1} \approx \left(4\pi k_{\text{F}}^2\right)^2 ,$$

and the energy integral becomes

$$\int d\varepsilon\, f^0(\varepsilon)\left(1 - f^0(\varepsilon)\right) = \frac{\omega}{e^{\beta\omega} - 1} .$$

Thus,

$$\left\langle \frac{1}{\tau}\right\rangle = \frac{m}{12\pi^3 \hbar n} A^2 (g-1)^2 (k_{\text{F}}/\hbar)^4 n_{\text{imp}} \int du\, \frac{\beta u}{e^{\beta u} - 1}\, S(u) ,$$

and

$$\rho \leq \frac{m}{ne^2}\left\langle \frac{1}{\tau}\right\rangle = \frac{3\pi}{8} \frac{mA^2 (g-1)^2}{e^2 \hbar \varepsilon_{\text{F}}}\, n_{\text{imp}} \int du\, \frac{\beta u}{e^{\beta u} - 1}\, S(u)$$

since $n = k_{\text{F}}^3 / 3\pi^2$ and $\varepsilon_{\text{F}} = \hbar k_{\text{F}}^2 / 2m$. Note that

$$\int du\, \frac{\beta u}{e^{\beta u} - 1}\, S(u) = \sum_{ij} \frac{\beta(E_j - E_i)}{e^{\beta(E_j - E_i)} - 1} \frac{e^{-\beta E_i}}{\sum_n e^{-\beta E_n}}\, |\langle j\,|\,\boldsymbol{J}\,|\,i\,\rangle|^2$$

$$\equiv \sum_{ij} p_{ij}\, Q_{ji} ,$$

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where

$$p_{ij} = \frac{\beta(E_j - E_i)}{e^{\beta(E_j - E_i)} - 1} \frac{e^{-\beta E_i}}{\sum_n e^{-\beta E_n}}$$

$$Q_{ji} = |\langle j | \boldsymbol{J} | i \rangle|^2 = \tfrac{1}{2}|\langle j | J^+ | i \rangle|^2 + \tfrac{1}{2}|\langle j | J^i | i \rangle|^2 + |\langle j | J^z | i \rangle|^2 .$$

Therefore, the upper bound on the resistivity is $\rho_+ = \rho_0 \, p_{ij} \, Q_{ji}$, with

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

(c) At high temperatures, $\beta u/(e^{\beta u} - 1) \to 1$ and therefore $p_{ij} \to P_i$, independent of j. In this limit, then,

$$\sum_{ij} p_{ij} Q_{ji} = \sum_i e^{-\beta E_i} \sum_j |\langle j | \boldsymbol{J} | i \rangle|^2 \Big/ \sum_n e^{-\beta E_n}$$

$$= \sum_i \langle i | \boldsymbol{J}^2 | i \rangle \Big/ \sum_n e^{-\beta E_n}$$

$$= J(J+1) .$$

Hence, $\rho_+ = J(J+1)\rho_0$ at high temperatures.

[5] *Cyclotron resonance in Si and Ge* – Both Si and Ge are indirect gap semiconductors with anisotropic conduction band minima and doubly degenerate valence band maxima. In Si, the conduction band minima occur along the $\langle 100 \rangle$ ($\langle \Gamma X \rangle$) directions, and are six-fold degenerate. The equal energy surfaces are cigar-shaped, and the effective mass along the $\langle \Gamma X \rangle$ principal axes (the 'longitudinal' effective mass) is $m_l^* \simeq 1.0\, m_e$, while the effective mass in the plane perpendicular to this axis (the 'transverse' effective mass) is $m_t^* \simeq 0.20\, m_e$. The valence band maximum occurs at the unique Γ point, and there are two isotropic hole branches: a 'heavy' hole with $m_{hh}^* \simeq 0.49\, m_e$, and a 'light' hole with $m_{lh}^* \simeq 0.16\, m_e$.

In Ge, the conduction band minima occur at the fourfold degenerate L point (along the eight $\langle 111 \rangle$ directions) with effective masses $m_l^* \simeq 1.6\, m_e$ and $m_t^* \simeq 0.08\, m_e$. The valence band maximum again occurs at the Γ point, where the hole masses are $m_{hh}^* \simeq 0.34\, m_e$ and $m_{lh}^* \simeq 0.044\, m_e$. Use the following figures to interpret the cyclotron resonance data shown below. Verify whether the data corroborate the quoted values of the effective masses in Si and Ge.

Solution: We found that $\sigma_{\alpha\beta} = ne^2 \, \Gamma_{\alpha\beta}^{-1}$, with

$$\Gamma_{\alpha\beta} \equiv (\tau^{-1} - i\omega)\, m_{\alpha\beta} \pm \frac{e}{c} \, \epsilon_{\alpha\beta\gamma} \, B^\gamma$$

$$= \begin{pmatrix} (\tau^{-1} - i\omega\tau)m_x^* & \pm eB_z/c & \mp eB_y/c \\ \mp eB_z/c & (\tau^{-1} - i\omega)m_y^* & \pm eB_x/c \\ \pm eB_y/c & \mp eB_x/c & (\tau^{-1} - i\omega)m_z^* \end{pmatrix} .$$
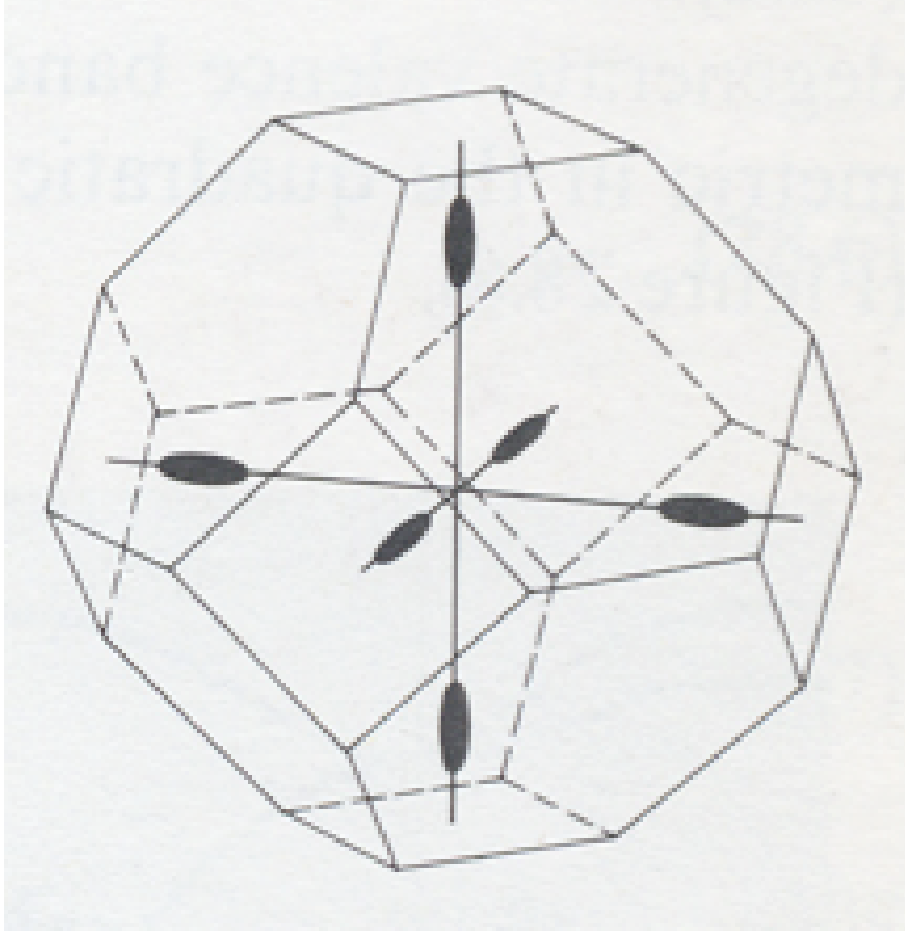
Figure 1: Constant energy surfaces near the conduction band minima in silicon. There are six symmetry-related ellipsoidal pockets whose long axes run along the $\langle 100 \rangle$ directions.

The valence band maxima are isotropic in both cases, with

$$m_{hh}^*(\text{Si}) \simeq 0.49\, m_e \qquad\qquad m_{hh}^*(\text{Ge}) \simeq 0.34\, m_e$$
$$m_{lh}^*(\text{Si}) \simeq 0.16\, m_e \qquad\qquad m_{lh}^*(\text{Ge}) \simeq 0.044\, m_e \ .$$

With isotropic bands, the absorption is peaked at $\omega = \omega_c = eB/m^*c$, assuming $\omega_c \tau \gg 1$. Writing $\omega = 2\pi f$, the resonance occurs at a field

$$
\begin{aligned}
B(f) &= 2\pi f \cdot \frac{m^* c}{e} \\
&= \frac{hc}{e} \cdot \frac{m^*}{m_e} \cdot \frac{1}{2\pi a_B^2} \cdot \frac{hf}{(e^2/a_B)} \\
&= 3.58 \times 10^{-7}\,\text{G} \cdot \frac{m^*}{m_e} \cdot f[\text{Hz}] \\
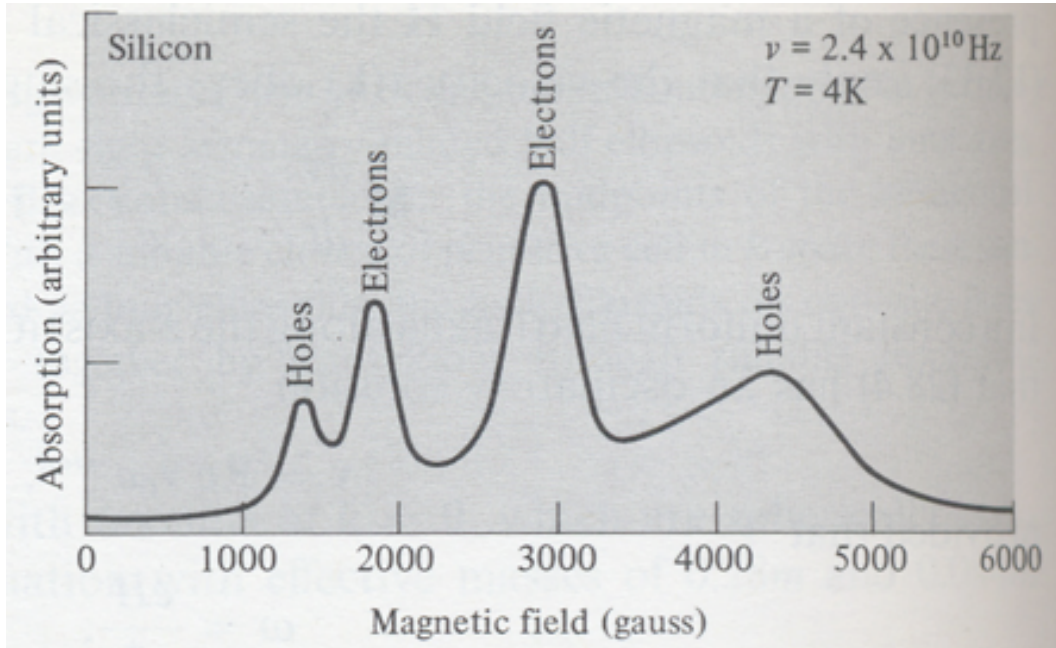&= 8590\,\text{G} \cdot \frac{m^*}{m_e} \ ,
\end{aligned}
$$

Figure 2: Cyclotron resonance data in Si (G. Dresselhaus *et al.*, *Phys, Rev,* **98**, 368 (1955).)
The field lies in a (110) plane and makes an angle of 30° with the [001] axis.

where we have used

$$\frac{hc}{e} = 4.137 \times 10^{-7}\,\mathrm{G \cdot cm^2}$$

$$a_{\mathrm{B}} = \frac{\hbar^2}{m_{\mathrm{e}}\,e^2} = 0.529\,\text{Å}$$

$$h = 4.136 \times 10^{-15}\,\mathrm{eV \cdot s}$$

$$\frac{e^2}{a_{\mathrm{B}}} = 27.2\,\mathrm{eV} = 2\,\mathrm{Ry}$$

$$f = 2.40 \times 10^{10}\,\mathrm{Hz}\ .$$

Thus, we predict

$$B_{\mathrm{hh}}(\mathrm{Si}) \simeq 4210\,\mathrm{G} \qquad B_{\mathrm{hh}}(\mathrm{Ge}) \simeq 2920\,\mathrm{G}$$
$$B_{\mathrm{lh}}(\mathrm{Si}) \simeq 1370\,\mathrm{G} \qquad B_{\mathrm{lh}}(\mathrm{Ge}) \simeq 378\,\mathrm{G}\ .$$
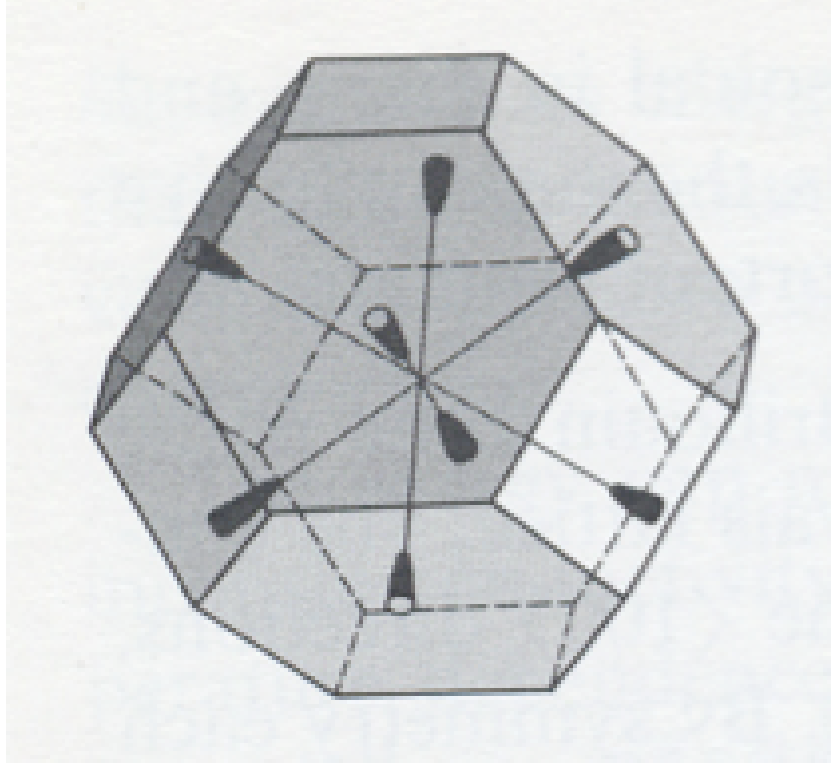
All of these look pretty good.

Figure 3: Constant energy surfaces near the conduction band minima in germanium. There are eight symmetry-related half-ellipsoids whose long axes run along the $\langle 111 \rangle$ directions, and are centered on the midpoints of the hexagonal zone faces. With a suitable choice of primitive cell in $\boldsymbol{k}$-space, these can be represented as four ellipsoids, the half-ellipsoids on opposite faces being joined together by translations through suitable reciprocal lattice vectors.

Now let us review the situation with electrons near the conduction band minima:

<div align="center">

Si: 6-fold degenerate minima along $\langle 100 \rangle$

Ge: 4-fold degenerate minima along $\langle 111 \rangle$ (at L point)

</div>

$$m_l^*(\text{Si}) \simeq 1.0\,m_{\text{e}} \qquad\qquad m_l^*(\text{Ge}) \simeq 1.6\,m_{\text{e}}$$
$$m_t^*(\text{Si}) \simeq 0.20\,m_{\text{e}} \qquad\qquad m_t^*(\text{Ge}) \simeq 0.08\,m_{\text{e}}\ .$$

The resonance condition is that $\sigma_{\alpha\beta} = \infty$, which for $\tau > 0$ occurs only at complex frequencies, *i.e.* for real frequencies there are no true divergences, only resonances. The location of the resonance is determined by $\det \Gamma = 0$. Taking the determinant, one finds

$$\det \Gamma = (\tau^{-1} - i\omega)\,m_l^* \cdot \left\{ (\tau^{-1} - i\omega)^2 m_t^{*2} + \frac{e^2}{c^2}\,B_z^2 + \frac{m_t^*}{m_l^*}\frac{e^2}{c^2}\left(B_x^2 + B_y^2\right) \right\}\ .$$
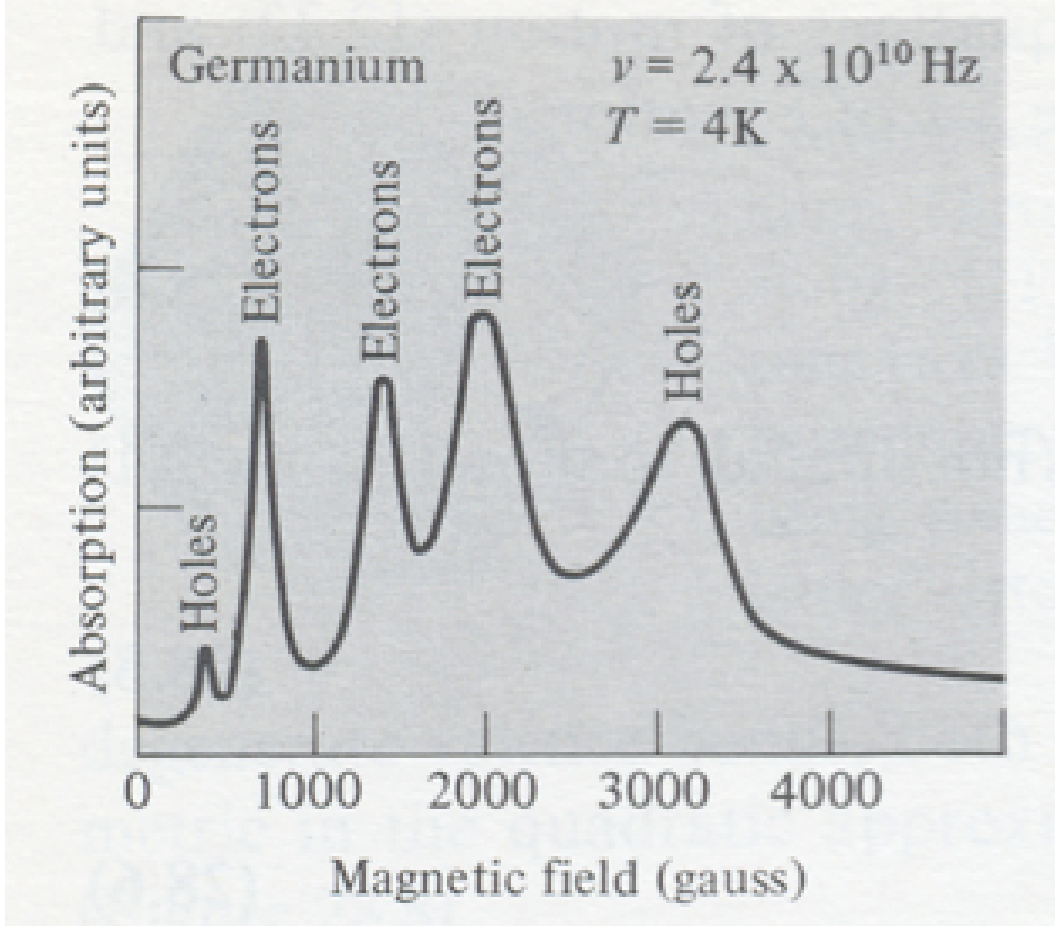
Figure 4: Cyclotron resonance data in Ge (G. Dresselhaus *et al.*, *Phys, Rev,* **98**, 368 (1955).) The field lies in a (110) plane and makes an angle of 60° with the [001] axis.

Assuming $\omega\tau \gg 1$, the location of the resonance is given by

$$\omega^2 = \left(\frac{eB_\parallel}{m_t^* c}\right)^2 + \frac{m_t^*}{m_l^*}\left(\frac{e\boldsymbol{B}_\perp}{m_t^* c}\right)^2 ,$$

where $B_\parallel \equiv B_z$ and $\boldsymbol{B}_\perp \equiv B_x\,\hat{\boldsymbol{x}} + B_y\,\hat{\boldsymbol{y}}$. Let the polar angle of $\boldsymbol{B}$ be θ, so $B_\parallel = B\cos\theta$ and $B_\perp = B\sin\theta$. We then have

$$\omega^2 = \left(\frac{eB}{m_t^* c}\right)^2\left\{\cos^2\theta + \frac{m_t^*}{m_l^*}\sin^2\theta\right\}$$

$$B(f) = 8600\,\text{G}\cdot\left(\frac{m_t^*}{m_e}\right)\Big/\sqrt{\cos^2\theta + \frac{m_t^*}{m_l^*}\sin^2\theta} ,$$

where again we take $f = \omega/2\pi = 2.4 \times 10^{10}$ Hz.

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According to the diagrams, the field lies in the (110) plane, which means we can write

$$\hat{\boldsymbol{B}} = \sqrt{\tfrac{1}{2}}\,\sin\chi\,\hat{\boldsymbol{e}}_1 - \sqrt{\tfrac{1}{2}}\,\sin\chi\,\hat{\boldsymbol{e}}_2 + \cos\chi\,\hat{\boldsymbol{e}}_3\ ,$$

where χ is the angle $\hat{\boldsymbol{B}}$ makes with $\hat{\boldsymbol{e}}_3 = [001]$.

Ge

We have

$$\frac{m_t^*}{m_e} = 0.082 \qquad \frac{m_t^*}{m_l^*} = 0.051\ ,$$

and we are told $\chi = 60°$, so

$$\hat{\boldsymbol{B}} = \sqrt{\tfrac{3}{8}}\,\hat{\boldsymbol{e}}_1 - \sqrt{\tfrac{3}{8}}\,\hat{\boldsymbol{e}}_2 + \tfrac{1}{2}\,\hat{\boldsymbol{e}}_3\ .$$

The conduction band minima lie along $\langle 111 \rangle$, which denotes a *set* of directions in real space:

$$\pm[111]\ :\ \hat{\boldsymbol{n}} = \pm\tfrac{1}{\sqrt{3}}(\hat{\boldsymbol{e}}_1 + \hat{\boldsymbol{e}}_2 + \hat{\boldsymbol{e}}_3) \quad \Rightarrow \quad \cos^2\theta = (\hat{\boldsymbol{B}}\cdot\hat{\boldsymbol{n}})^2 = \tfrac{1}{12} \quad \Rightarrow \quad B = 1950\,\text{G}$$

$$\pm[11\bar{1}]\ :\ \hat{\boldsymbol{n}} = \pm\tfrac{1}{\sqrt{3}}(\hat{\boldsymbol{e}}_1 + \hat{\boldsymbol{e}}_2 - \hat{\boldsymbol{e}}_3) \quad \Rightarrow \quad \cos^2\theta = (\hat{\boldsymbol{B}}\cdot\hat{\boldsymbol{n}})^2 = \tfrac{1}{12} \quad \Rightarrow \quad B = 1950\,\text{G}$$

$$\pm[\bar{1}11]\ :\ \hat{\boldsymbol{n}} = \pm\tfrac{1}{\sqrt{3}}(-\hat{\boldsymbol{e}}_1 + \hat{\boldsymbol{e}}_2 + \hat{\boldsymbol{e}}_3) \quad \Rightarrow \quad \cos^2\theta = (\hat{\boldsymbol{B}}\cdot\hat{\boldsymbol{n}})^2 = \tfrac{7-2\sqrt{6}}{12} \quad \Rightarrow \quad B = 1510\,\text{G}$$

$$\pm[1\bar{1}1]\ :\ \hat{\boldsymbol{n}} = \pm\tfrac{1}{\sqrt{3}}(\hat{\boldsymbol{e}}_1 - \hat{\boldsymbol{e}}_2 + \hat{\boldsymbol{e}}_3) \quad \Rightarrow \quad \cos^2\theta = (\hat{\boldsymbol{B}}\cdot\hat{\boldsymbol{n}})^2 = \tfrac{7+2\sqrt{6}}{12} \quad \Rightarrow \quad B = 710\,\text{G}\ .$$

All OK!

Si

Again, $\boldsymbol{B}$ lies in the (110) plane, this time with $\chi = 30°$, so

$$\hat{\boldsymbol{B}} = \sqrt{\tfrac{1}{8}}\,\hat{\boldsymbol{e}}_1 - \sqrt{\tfrac{1}{8}}\,\hat{\boldsymbol{e}}_2 + \sqrt{\tfrac{3}{4}}\,\hat{\boldsymbol{e}}_3\ .$$

The conduction band minima lie along $\langle 100 \rangle$, so

$$\pm[001]\ :\ \hat{\boldsymbol{n}} = \pm\hat{\boldsymbol{e}}_3 \quad \Rightarrow \quad \cos^2\theta = (\hat{\boldsymbol{B}}\cdot\hat{\boldsymbol{n}})^2 = \tfrac{3}{4} \quad \Rightarrow \quad B = 1820\,\text{G}$$

$$\pm[010]\ :\ \hat{\boldsymbol{n}} = \pm\hat{\boldsymbol{e}}_2 \quad \Rightarrow \quad \cos^2\theta = (\hat{\boldsymbol{B}}\cdot\hat{\boldsymbol{n}})^2 = \tfrac{1}{8} \quad \Rightarrow \quad B = 2980\,\text{G}$$

$$\pm[100]\ :\ \hat{\boldsymbol{n}} = \pm\hat{\boldsymbol{e}}_1 \quad \Rightarrow \quad \cos^2\theta = (\hat{\boldsymbol{B}}\cdot\hat{\boldsymbol{n}})^2 = \tfrac{1}{8} \quad \Rightarrow \quad B = 2980\,\text{G}\ .$$

These also look pretty good.