Physics 361 Solutions to Problem Set 8

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1 Effective Masses

Electrons near a band minimum have a dispersion of the form

$$\mathcal{E}(\mathbf{k}) = \mathcal{E}_0 + \frac{1}{2}\hbar^2(\mathbf{k}-\mathbf{k}_0)\cdot\mathbf{M}^{-1}\cdot(\mathbf{k}-\mathbf{k}_0)$$

For convenience, we define the matrix $\mathbf{Q} = \frac{1}{2}\hbar^2\mathbf{M}^{-1}$. We may assume that $\mathbf{Q}$ is symmetric and positive-definite (or negative definite in the case of a band maximum.) A matrix $\mathbf{Q}$ is positive definite if $\mathbf{k}\cdot\mathbf{Q}\cdot\mathbf{k} > 0$ for any nonzero vector $\mathbf{k}$. Later we will use the fact that for a positive-definite symmetric matrix $\mathbf{Q}$, there always exists another matrix $\mathbf{L}$ such that $\mathbf{Q} = \mathbf{L}^{\mathrm{T}}\cdot\mathbf{L}$.

The cyclotron effective mass can be determined from the function $A(E, k_z)$, defined as

$$A(E,k_z) \equiv \int dk_x\, dk_y \Theta[E - \mathcal{E}(\mathbf{k})]$$

This is the area enclosed by the orbit of constant k_z and energy E. Note that in a plane of fixed k_z, we may regard $\mathcal{E}(\mathbf{k})$ as a quadratic polynomial in k_x, k_y. The constant energy curves of this polynomial in the fixed k_z plane are ellipses with a common (k_z-dependent) center. Let $\mathbf{k}^c = (k_x^c, k_y^c, k_z)$ denote this center. We use the fact that the xy-plane component of $\nabla\mathcal{E}$ must vanish at $\mathbf{k}^c$:

$$\begin{aligned}
\nabla\mathcal{E}(\mathbf{k}) &= (\mathbf{k}-\mathbf{k}_0)\cdot\mathbf{Q} + \mathbf{Q}\cdot(\mathbf{k}-\mathbf{k}_0) = 2\mathbf{Q}\cdot(\mathbf{k}-\mathbf{k}_0) \\
(\mathbf{k}^c-\mathbf{k}_0)\cdot\mathbf{Q} &= [\mathbf{Q}\cdot(\mathbf{k}^c-\mathbf{k}_0)\cdot\hat{\mathbf{z}}]\;\hat{\mathbf{z}} \\
\mathcal{E}(\mathbf{k}) &= \mathcal{E}_0 + [(\mathbf{k}^c-\mathbf{k}_0) + (\mathbf{k}-\mathbf{k}^c)]\cdot\mathbf{Q}\cdot[(\mathbf{k}^c-\mathbf{k}_0) + (\mathbf{k}-\mathbf{k}^c)] \\
&= \mathcal{E}_0 + (\mathbf{k}^c-\mathbf{k}_0)\cdot\mathbf{Q}\cdot(\mathbf{k}^c-\mathbf{k}_0) + (\mathbf{k}-\mathbf{k}^c)\cdot\mathbf{Q}\cdot(\mathbf{k}-\mathbf{k}^c) \\
&= \mathcal{E}_1(k_z) + (\mathbf{k}-\mathbf{k}^c)\cdot\mathbf{Q}^{(2)}\cdot(\mathbf{k}-\mathbf{k}^c)
\end{aligned}$$

In the second to last step, two terms have been eliminated by noting that the action of $\mathbf{Q}$ on $(\mathbf{k}_c - \mathbf{k}_0)$ leaves a vector parallel to $\hat{\mathbf{z}}$ while $(\mathbf{k}-\mathbf{k}^c)$ lies in the xy-plane (since $k_z^c = k_z$). In the last step, we have defined $\mathcal{E}_1 \equiv \mathcal{E}_0 + (\mathbf{k}^c-\mathbf{k}_0)\cdot\mathbf{Q}\cdot(\mathbf{k}^c-\mathbf{k}_0)$ which depends only on

k_z through $\mathbf{k}^c(k_z)$. Since $(\mathbf{k}-\mathbf{k}^c)$ lies in the xy-plane, we may regard it as a 2-dimensional vector and replace $\mathbf{Q}$ in the last step by its 2×2 submatrix

$$\mathbf{Q}^{(2)} \equiv \begin{pmatrix} Q_{xx} & Q_{xy} \\ Q_{yx} & Q_{yy} \end{pmatrix}$$

The preceeding discussion is merely an elaborate way of showing that $Q^{(2)}$ is the effective inverse mass matrix for $\mathcal{E}(\mathbf{k})$ when k_z is held constant. Since $Q^{(2)}$ is also symmetric and positive definite, there is a 2×2 matrix $\mathbf{L}$ such that $Q^{(2)} = \mathbf{L}^{\mathrm{T}}\cdot\mathbf{L}$. We are now prepared to compute the area function:

$$\begin{aligned} A(E,k_z) &= \int dk_x\, dk_y\, \Theta[E-(\mathbf{k}-\mathbf{k}^c)\cdot\mathbf{L}^{\mathrm{T}}\cdot\mathbf{L}\cdot(\mathbf{k}-\mathbf{k}^c)-\mathcal{E}_1(k_z)] \\ &= J^{-1}\int dp_x\, dp_y\, \Theta[E-p^2-\mathcal{E}_1(k_z)] \\ &= \frac{\pi}{J}[E-\mathcal{E}_1(k_z)] \end{aligned}$$

We have used the change of variables $\mathbf{p} = \mathbf{L}\cdot(\mathbf{k}-\mathbf{k}^c)$, which introduces the Jacobian $J = |\frac{\partial\mathbf{p}}{\partial\mathbf{k}}| = |\mathbf{L}| = |\mathbf{Q}^{(2)}|^{1/2}$. Finally, for the cyclotron effective mass we have

$$\begin{aligned} m^* &= \frac{\hbar^2}{2\pi}\frac{\partial A(E,k_z)}{\partial E} \\ &= \frac{1}{2}\hbar^2 J^{-1} \\ &= |M_{xx}M_{yy}-M_{xy}^2|^{1/2} \end{aligned}$$

The formula given in the text ($m^* = |\mathbf{M}|/M_{zz}$) is valid only when z is a principal axis of the matrix $\mathbf{M}$.

Specific heat. A Sommerfeld metal as a low-temperature specific heat

$$c_v = \frac{\pi^2}{3}k_B^2 T g(\mathcal{E}_F)$$

where $g(\mathcal{E}_F)$ is the density of states at the Fermi surface. For an ideal gas this can be written

$$g(\mathcal{E}_F) = \frac{mk_F}{\hbar^2\pi^2} = \frac{1}{\hbar^2\pi^2}\sqrt{\frac{2m^3\mathcal{E}_F}{\hbar^2}}$$

In the semiconductor case, the density of states integral is performed in a similar manner as above. Define $\mathbf{L}$ as the 3×3 matrix such that $\mathbf{Q} = \mathbf{L}^{\mathrm{T}}\mathbf{L}$.

$$\begin{aligned} g(\mathcal{E}_F) &= \frac{1}{4\pi^3}\int d\mathbf{k}\,\delta[\mathcal{E}_F-(\mathbf{k}-\mathbf{k}_0)\cdot\mathbf{Q}\cdot(\mathbf{k}-\mathbf{k}_0)-\mathcal{E}_0] \\ &= \frac{1}{4\pi^3}|\mathbf{L}|^{-1}\int d\mathbf{p}\,\delta[\mathcal{E}_F-|\mathbf{p}|^2-\mathcal{E}_0] \end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{2\pi^2}|\mathbf{L}|^{-1}\mathcal{E}_F^{1/2} \\
&= \frac{1}{2\pi^2}(|\mathbf{Q}|^{-1}\mathcal{E}_F)^{1/2} \\
&= \frac{1}{2\pi^2}(|\mathbf{M}|(\frac{1}{2}\hbar^2)^{-3}\mathcal{E}_F)^{1/2} \\
&= \frac{1}{\hbar^2\pi^2}\sqrt{\frac{2|\mathbf{M}|\mathcal{E}_F}{\hbar^2}}
\end{aligned}
$$

The effective mass is therefore $m^* = |\mathbf{M}|^{1/3}$.

2 Magnetoresistance

The current and field in band n is given by

$$\mathbf{E}_n = \boldsymbol{\rho}_n \mathbf{j}_n$$

The total current is $\mathbf{j} = \sum \mathbf{j}_n$, and the electric field $\mathbf{E}_n = \mathbf{E}$ is the same for each band.

$$
\begin{aligned}
\mathbf{j} &= \sum \mathbf{j}_n = \sum \boldsymbol{\rho}_n^{-1}\mathbf{E}_n = \left(\sum \boldsymbol{\rho}_n^{-1}\right)\mathbf{E} = \boldsymbol{\rho}^{-1}\mathbf{E} \\
\boldsymbol{\rho} &= \left(\sum \boldsymbol{\rho}_n^{-1}\right)^{-1}
\end{aligned}
$$

The resistivity tensor $\boldsymbol{\rho}_n$ for each band (as well as the net resisitivity) has the form

$$\boldsymbol{\rho} = \begin{pmatrix} \rho_n & -R_n H \\ R_n H & \rho_n \end{pmatrix}$$

In the two-band case, the net Hall coefficient R and scalar resistivity ρ work out to

$$
\begin{aligned}
R &= \frac{R_1\rho_2^2 + R_2\rho_1^2 + R_1R_2(R_1+R_2)H^2}{(\rho_1+\rho_2)^2 + (R_1+R_2)^2H^2} \\
\rho &= \frac{\rho_1\rho_2(\rho_1+\rho_2) + (\rho_1R_2^2 + \rho_2R_1^2)H^2}{(\rho_1+\rho_2)^2 + (R_1+R_2)^2H^2}
\end{aligned}
$$

Suppose that in the high-field limit, the effective carrier density $n_{\text{eff}} \to 0$. This is connected to the Hall coefficient by $n_{\text{eff}} = -1/(Rec)$, so that $1/R$ must also vanish in this limit. Note that in the high-field limit, $1/R = 1/R_1 + 1/R_2$ so that $(R_1 + R_2) \to 0$ as well. The denominator is therefore bounded as $H \to \infty$, allowing $\rho = A + BH^2$, where A and B are constants, as was to be shown.