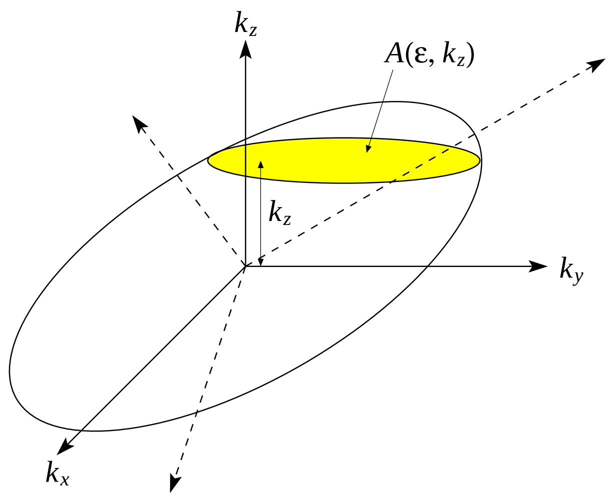
# PHYS 635 Condensed Matter Physics
## Assignment 4 (Nov 9, 2004)
## Solutions

1. **A&M Problem 12.2.** For electrons near a band minimum or maximum, we have

$$\epsilon(\mathbf{k}) = \epsilon_0 + \frac{\hbar^2}{2}(\mathbf{k}-\mathbf{k}_0)^T \mathsf{M}^{-1}(\mathbf{k}-\mathbf{k}_0), \tag{1.1}$$

where $\mathsf{M}^{-1}$ is the reciprocal effective mass tensor. As can be seen from its definition in Eq. (12.29) in A&M, the reciprocal effective mass tensor is symmetric. Near a band minimum or maximum, the eigenvalues $1/m_i^*$ of $\mathsf{M}^{-1}$ have the same sign, which means that the surfaces of constant energy as defined by (1.1) are ellipsoids.

(a) In the absence of a magnetic field we are free to choose the Cartesian axes to coincide with the principal axes of these ellipsoid. However, when a magnetic field is present, the direction of the magnetic field will usually be taken as the $z$-axis, following which the $xy$-plane will also be fixed. Therefore, for cyclotron motion, we would in general need to find an area $A(\epsilon, k_z)$ like the one shown below:




To go about calculating this area, let us get ready some useful mathematical machinery.

First, consider the integral

$$I = \iiint\limits_{x^2+y^2+z^2 \leq R^2} dx\, dy\, dz\, \delta(z-z_0). \tag{1.2}$$

By dimensional arguments, $[dx] = [dy] = [dz] =$ length, while $[\delta(z-z_0)] = 1/$length, the integral has dimensions of length$^2$, i.e. it has the dimensions of an area. Going to cylindrical coordinates, we can write the integral as

$$I = \int dz \left( \int_0^{(R^2-z^2)^{1/2}} \rho\, d\rho \int_0^{2\pi} d\phi \right) \delta(z-z_0)\, dz. \tag{1.3}$$

Performing the integration over $z$, and noting that this partial integration of the delta function modifies the limits of the remaining integration over $\rho$ and $\phi$, we find that

$$I = 2\pi \int_0^{(R^2-z_0^2)^{1/2}} \rho\, d\rho = 2\pi \left[\frac{\rho^2}{2}\right]_0^{(R^2-z_0^2)^{1/2}} = \pi(R^2 - z_0^2), \tag{1.4}$$

which is none other than the area of the (circular) section of the sphere $x^2 + y^2 + z^2 = R^2$ at a fixed $z = z_0$.

Next suppose that the set of unprimed coordinates $(x, y, z)$ are related to another set of primed coordinates $(x', y', z')$ by a linear transformation $\mathbf{r}' = \mathsf{A}\mathbf{r}$, such that

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} A_{xx} & A_{xy} & A_{xz} \\ A_{yx} & A_{yy} & A_{yz} \\ A_{zx} & A_{zy} & A_{zz} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} A_{xx}x + A_{xy}y + A_{xz}z \\ A_{yx}x + A_{yy}y + A_{yz}z \\ A_{zx}x + A_{zy}y + A_{zz}z \end{pmatrix}. \tag{1.5}$$

Then the volume element $dx'\, dy'\, dz'$ is related to the volume element $dx\, dy\, dz$ by

$$dx'\, dy'\, dz' = \begin{vmatrix} \partial x'/\partial x & \partial x'/\partial y & \partial x'/\partial z \\ \partial y'/\partial x & \partial y'/\partial y & \partial y'/\partial z \\ \partial z'/\partial x & \partial z'/\partial y & \partial z'/\partial z \end{vmatrix} dx\, dy\, dz = |\mathsf{A}|\, dx\, dy\, dz, \tag{1.6}$$

where $|\mathsf{A}|$ is the determinant of the matrix $\mathsf{A}$.

Finally, let us write the equation of a sphere in a vectorial form, i.e. instead of the usual

$$r^2 = x^2 + y^2 + z^2 = R^2, \tag{1.7}$$

we write it as

$$\mathbf{r}^T\mathbf{r} = \begin{pmatrix} x & y & z \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = R^2. \tag{1.8}$$

Now if the primed coordinates $\mathbf{r}'$ is related to the unprimed coordinates $\mathbf{r}$ by the linear transformation $\mathbf{r}' = \mathsf{A}\mathbf{r}$, and if the singular values of $\mathsf{A}$ are all nonzero, and have the same sign, then in general the primed coordinate axes are rotated and scaled with respect to the unprimed coordinate axes. If we have a sphere in the unprimed coordinates, under the linear transformation $\mathsf{A}$ we would end up with an ellipsoid in the primed coordinates. Thus

$$\mathbf{r}'^T \mathsf{A}^{-1^T} \mathsf{A}^{-1} \mathbf{r}' = R^2 \tag{1.9}$$

is the vectorial form of the equation describing an ellipsoid in the primed coordinates.

Comparing (1.9) with

$$(\mathbf{k} - \mathbf{k}_0)^T \mathsf{M}^{-1} (\mathbf{k} - \mathbf{k}_0) = 2(\epsilon - \epsilon_0)/\hbar^2, \tag{1.10}$$

we see that the surfaces of constant energy are indeed ellipsoids, as we have stated without proof earlier. Furthermore, if we think of $(\mathbf{k} - \mathbf{k}_0)$ as a vector in the 'primed' coordinates, then we may define a vector $\mathbf{q} = (q_x, q_y, q_z)$ in an 'unprimed' coordinates, such that $(\mathbf{k} - \mathbf{k}_0) = \mathsf{A}\mathbf{q}$, in which the surfaces of constant energy are spheres, given by

$$\mathbf{q}^T\mathbf{q} = 2(\epsilon - \epsilon_0)/\hbar^2 = 2E/\hbar^2, \tag{1.11}$$

where $E = \epsilon - \epsilon_0$. From (1.10) and (1.9), we see that

$$\mathsf{M}^{-1} = \mathsf{A}^{-1^T} \mathsf{A}^{-1}, \tag{1.12}$$

or equivalently,

$$\mathsf{M} = \mathsf{A}\mathsf{A}^T. \tag{1.13}$$

Now, we are ready to evaluate $A(\epsilon, k_z)$ as shown in the figure. Our analysis in (1.2) through (1.4) tells us that this is given by

$$A(\epsilon, k_z) = \iiint\limits_{\Delta\mathbf{k}'^T \mathsf{M}^{-1} \Delta\mathbf{k}' \le 2E/\hbar^2} d^3\mathbf{k}'\ \delta(k_z' - k_z), \tag{1.14}$$

where $\Delta\mathbf{k}' = (\mathbf{k}' - \mathbf{k}_0)$, and we have written the constraint to the volume of an ellipsoid in the vectorial form given in (1.9).

Next, we change integration variables to the 'unprimed' coordinates $\mathbf{q} = \mathsf{A}^{-1}(\mathbf{k}' - \mathbf{k}_0)$, so that the integration volume becomes a sphere. Since the 'primed' integration variable $k_z'$ appears in the delta-function, we need to write the arguments of $\delta(k_z' - k_z)$ in terms of $q_x$, $q_y$ and $q_z$. Using $(\mathbf{k}' - \mathbf{k}_0) = \mathsf{A}\mathbf{q}$. we know that

$$k_z' - k_{0z} = A_{zx}q_x + A_{zy}q_y + A_{zz}q_z, \tag{1.15}$$

and so

$$A(\epsilon, k_z) = \iiint\limits_{\mathbf{q}^T\mathbf{q} \leq 2E/\hbar^2} |\mathsf{A}|\, d^3\mathbf{q}\; \delta(A_{zx}q_x + A_{zy}q_y + A_{zz}q_z - (k_z - k_{0z})), \tag{1.16}$$

where we have made use of (1.6) relating the volume elements in the 'primed' and 'unprimed' coordinates.

The argument of the delta-function in the above integral looks formidable, but its geometric interpretation is actually quite simple:

$$A_{zx}q_x + A_{zy}q_y + A_{zz}q_z = (k_z - k_{0z}) \tag{1.17}$$

is the Cartesian equation for a plane in $q$-space. If we denote the perpendicular distance of this plane from the origin of $q$-space as $\lambda$, then clearly the area of the intersection between this plane and the sphere of radius $q = (2E/\hbar^2)^{1/2}$ is given by $\pi[(2E/\hbar^2) - \lambda^2]$. With this result, we might naively conclude that

$$A(\epsilon, k_z) = \pi|\mathsf{A}|\left[\frac{2E}{\hbar^2} - \lambda^2\right], \tag{1.18}$$

but this is not the case: to obtain the above result, we need the constraining delta-function to have the form $\delta(\mathbf{q}\cdot\mathbf{n} - \lambda)$, whereas the delta-function in (1.16) can at most be massaged to a form like $\delta(\alpha(\mathbf{q}\cdot\mathbf{n} - \lambda))$. To get the correct answer for $A(\epsilon, k_z)$, we need to find not just $\lambda$, but also the scaling factor $\alpha$.

To do so, let us assume the form $\alpha(\mathbf{q}\cdot\mathbf{n} - \lambda)$ for the argument of the delta-function, and compare it against that in (1.16):

$$\alpha(\mathbf{q}\cdot\mathbf{n} - \lambda) = \alpha n_x q_x + \alpha n_y q_y + \alpha n_z q_z - \alpha\lambda = A_{zx}q_x + A_{zy}q_y + A_{zz}q_z - (k_z - k_{0z}), \tag{1.19}$$

which tells us that

$$\alpha n_x = A_{zx}, \quad \alpha n_y = A_{zy}, \quad \alpha n_z = A_{zz}, \quad \alpha\lambda = (k_z - k_{0z}). \tag{1.20}$$

Using the fact that $n_x^2 + n_y^2 + n_z^2 = 1$, we find then that

$$\alpha = (A_{zx}^2 + A_{zy}^2 + A_{zz}^2)^{1/2}. \tag{1.21}$$

Finally, using $\delta(\alpha(x - x_0)) = \alpha^{-1}\delta(x - x_0)$, we can at long last perform the integration to get

$$A(\epsilon, k_z) = \frac{\pi|\mathsf{A}|}{\alpha}\left[\frac{2(\epsilon - \epsilon_0)}{\hbar^2} - \frac{(k_z - k_{0z})^2}{\alpha^2}\right]. \tag{1.22}$$

At this point, let us note that we can actually write $|\mathsf{A}|$ and $\alpha$ in terms of matrix elements of $\mathsf{M}$. First, we see from $\mathsf{M} = \mathsf{A}\mathsf{A}^T$ that

$$|\mathsf{M}| = |\mathsf{A}||\mathsf{A}^T|. \tag{1.23}$$

But $|\mathsf{A}^T| = |\mathsf{A}|$, therefore

$$|\mathsf{M}| = |\mathsf{A}|^2, \tag{1.24}$$

and we may write $|\mathbf{A}| = |\mathbf{M}|^{1/2}$. Secondly, writing out the matrix elements of $\mathbf{M}$ and $\mathbf{A}$ explicitly as

$$\begin{pmatrix} M_{xx} & M_{xy} & M_{xz} \\ M_{yx} & M_{yy} & M_{yz} \\ M_{zx} & M_{zy} & M_{zz} \end{pmatrix} = \begin{pmatrix} A_{xx} & A_{xy} & A_{xz} \\ A_{yx} & A_{yy} & A_{yz} \\ A_{zx} & A_{zy} & A_{zz} \end{pmatrix} \begin{pmatrix} A_{xx} & A_{yx} & A_{zx} \\ A_{xy} & A_{yy} & A_{zy} \\ A_{xz} & A_{yz} & A_{zz} \end{pmatrix}, \tag{1.25}$$

we find that

$$M_{zz} = A_{zx}^2 + A_{zy}^2 + A_{zz}^2 = \alpha^2, \tag{1.26}$$

allowing us to write $\alpha = M_{zz}^{1/2}$.

Putting all this together, we find that

$$A(\epsilon, k_z) = \pi \left( \frac{|\mathbf{M}|}{M_{zz}} \right)^{1/2} \left[ \frac{2(\epsilon - \epsilon_0)}{\hbar^2} - \frac{(k_z - k_{0z})^2}{M_{zz}} \right], \tag{1.27}$$

from which we obtain the cyclotron effective mass as

$$m_c^* = \frac{\hbar^2}{2\pi} \frac{\partial A}{\partial \epsilon} = \left( \frac{|\mathbf{M}|}{M_{zz}} \right)^{1/2}, \tag{1.28}$$

where we have made use of the given information that matrix elements of $\mathbf{M}$ do not depend on $\mathbf{k}$ (and hence have no dependence on $\epsilon$). (Shown)

***Alternative Method.*** Alternatively, you can also derive this result by brute force, by first writing out the dispersion relation

$$\frac{2E}{\hbar^2} = M_{xx}^{-1}\Delta k_x^2 + M_{yy}^{-1}\Delta k_y^2 + M_{zz}^{-1}\Delta k_z^2 + 2M_{xy}^{-1}\Delta k_x \Delta k_y + 2M_{xz}^{-1}\Delta k_x \Delta k_z + 2M_{yz}^{-1}\Delta k_y \Delta k_z \tag{1.29}$$

explicitly. For a fixed $k_z$ (fixed $\Delta k_z$), this equation can be put into the form

$$M_{xx}^{-1}(\Delta k_x - \Delta k_{1x})^2 + M_{yy}^{-1}(\Delta k_y - \Delta k_{1y})^2 + 2M_{xy}^{-1}(\Delta k_x - \Delta k_{1x})(\Delta k_y - \Delta k_{1y}) = \frac{2E}{\hbar^2} - F(\Delta k_z), \tag{1.30}$$

where

$$\Delta k_{1x} = \frac{M_{xz}^{-1} M_{yy}^{-1} - M_{xy}^{-1} M_{yz}^{-1}}{M_{xx}^{-1} M_{yy}^{-1} - M_{xy}^{-1} M_{xy}^{-1}} \Delta k_z, \qquad \Delta k_{1y} = \frac{M_{xx}^{-1} M_{yz}^{-1} - M_{xy}^{-1} M_{xz}^{-1}}{M_{xx}^{-1} M_{yy}^{-1} - M_{xy}^{-1} M_{xy}^{-1}} \Delta k_z, \tag{1.31}$$

and

$$\begin{aligned} F(\Delta k_z) = M_{zz}^{-1}\Delta k_z^2 - M_{xx}^{-1} &\left( \frac{M_{xz}^{-1} M_{yy}^{-1} - M_{xy}^{-1} M_{yz}^{-1}}{M_{xx}^{-1} M_{yy}^{-1} - M_{xy}^{-1} M_{xy}^{-1}} \right)^2 \Delta k_z^2 - \\ M_{yy}^{-1} &\left( \frac{M_{xx}^{-1} M_{yz}^{-1} - M_{xy}^{-1} M_{xz}^{-1}}{M_{xx}^{-1} M_{yy}^{-1} - M_{xy}^{-1} M_{xy}^{-1}} \right)^2 \Delta k_z^2 - \\ 2M_{xy}^{-1} &\left( \frac{M_{xz}^{-1} M_{yy}^{-1} - M_{xy}^{-1} M_{yz}^{-1}}{M_{xx}^{-1} M_{yy}^{-1} - M_{xy}^{-1} M_{xy}^{-1}} \right) \left( \frac{M_{xx}^{-1} M_{yz}^{-1} - M_{xy}^{-1} M_{xz}^{-1}}{M_{xx}^{-1} M_{yy}^{-1} - M_{xy}^{-1} M_{xy}^{-1}} \right) \Delta k_z^2. \end{aligned} \tag{1.32}$$

This is the equation of an ellipse, centered at $(\Delta k_{1x}, \Delta k_{1y})$ and rotated with respect to the $\Delta k_x$- and $\Delta k_y$-axes. To find the semi-major and semi-minor axes, we diagonalize the matrix

$$\begin{pmatrix} M_{xx}^{-1} & M_{xy}^{-1} \\ M_{xy}^{-1} & M_{yy}^{-1} \end{pmatrix} \tag{1.33}$$

to find the eigenvalues as

$$\lambda_+ = \frac{M^{-1}_{xx} + M^{-1}_{yy}}{2} + \frac{1}{2}\left[\left(M^{-1}_{xx} + M^{-1}_{yy}\right)^2 - 4\left(M^{-1}_{xx}M^{-1}_{yy} - M^{-1}_{xy}M^{-1}_{xy}\right)\right]^{1/2}$$
$$\frac{M^{-1}_{xx} + M^{-1}_{xy}}{2} + \frac{1}{2}\left[\left(M^{-1}_{xx} - M^{-1}_{yy}\right)^2 + 4M^{-1}_{xy}M^{-1}_{xy}\right]^{1/2} = \alpha + \beta, \tag{1.34}$$
$$\lambda_- = \frac{M^{-1}_{xx} + M^{-1}_{xy}}{2} - \frac{1}{2}\left[\left(M^{-1}_{xx} - M^{-1}_{yy}\right)^2 + 4M^{-1}_{xy}M^{-1}_{xy}\right]^{1/2} = \alpha - \beta.$$

The semi-major and semi-minor axes of the ellipse are thus

$$a = \lambda_+^{-1/2}\left[\frac{2E}{\hbar^2} - F(\Delta k_z)\right]^{1/2},$$
$$b = \lambda_-^{-1/2}\left[\frac{2E}{\hbar^2} - F(\Delta k_z)\right]^{1/2}, \tag{1.35}$$

and so the area of the ellipse is

$$A(\epsilon, k_z) = \pi ab = \pi\frac{2E/\hbar^2 - F(\Delta k_z)}{(\alpha+\beta)^{1/2}(\alpha-\beta)^{1/2}} = \pi\frac{2E/\hbar^2 - F(\Delta k_z)}{(\alpha^2-\beta^2)^{1/2}}, \tag{1.36}$$

where

$$\alpha^2 - \beta^2 = \left(\frac{M^{-1}_{xx} + M^{-1}_{yy}}{2}\right)^2 - \frac{1}{4}\left[\left(M^{-1}_{xx} - M^{-1}_{yy}\right)^2 + 4M^{-1}_{xy}M^{-1}_{xy}\right] = M^{-1}_{xx}M^{-1}_{yy} - M^{-1}_{xy}M^{-1}_{xy}. \tag{1.37}$$

Next, we make use of the fact (see for example, in G. Arfken, *Mathematical Methods for Physicists*) that

$$M_{ij} = \frac{C_{ji}}{|\mathbf{M}^{-1}|}, \tag{1.38}$$

where $C_{ji}$ is the cofactor of $\mathbf{M}^{-1}$ associated with the indices $i$ and $j$. For $i = j = z$, we have

$$M_{zz} = \frac{\begin{vmatrix} M^{-1}_{xx} & M^{-1}_{xy} \\ M^{-1}_{xy} & M^{-1}_{yy} \end{vmatrix}}{|\mathbf{M}^{-1}|} = \frac{M^{-1}_{xx}M^{-1}_{yy} - M^{-1}_{xy}M^{-1}_{xy}}{|\mathbf{M}^{-1}|}. \tag{1.39}$$

This let us write

$$M^{-1}_{xx}M^{-1}_{yy} - M^{-1}_{xy}M^{-1}_{xy} = M_{zz}|\mathbf{M}^{-1}| = \frac{M_{zz}}{|\mathbf{M}|}, \tag{1.40}$$

which in turn gives us

$$A(\epsilon, k_z) = \pi\left(\frac{|\mathbf{M}|}{M_{zz}}\right)^{1/2}\left[\frac{2E}{\hbar^2} - F(\Delta k_z)\right]. \tag{1.41}$$

Finally, noting that $F(\Delta k_z)$ contains only $\Delta k_z$ and matrix elements of $\mathbf{M}^{-1}$, which do not depend on $\epsilon$, we can take the derivative of $A(\epsilon, k_z)$ with respect to $\epsilon$ to find that

$$\frac{\partial A}{\partial \epsilon} = \frac{2\pi}{\hbar^2}\left(\frac{|\mathbf{M}|}{M_{zz}}\right)^{1/2}. \tag{1.42}$$

The cyclotron effective mass is therefore

$$m_c^* = \frac{\hbar^2}{2\pi}\frac{\partial A}{\partial \epsilon} = \left(\frac{|\mathbf{M}|}{M_{zz}}\right)^{1/2}. \qquad \text{(Shown)} \tag{1.43}$$

(b) For the band structure given in (1.1), the density of states is given by

$$g(\epsilon) = \int \frac{d^3\mathbf{k}}{4\pi^3}\,\delta\left(\epsilon - \epsilon_0 - \frac{\hbar^2}{2}(\mathbf{k}-\mathbf{k}_0)^T\mathbf{M}^{-1}(\mathbf{k}-\mathbf{k}_0)\right). \tag{1.44}$$

As done in part (a) of the problem, let us go to $q$-space to get rid of the matrix $\mathbf{M}^{-1}$. While we are at it, we might as well scale $\mathbf{q}$ further by $(2/\hbar^2)^{1/2}$ so that the argument of the delta-function becomes $(\epsilon - \epsilon_0 - \mathbf{q}^T\mathbf{q}) = (\epsilon - \epsilon_0 - q^2)$.

As in part (a) of the problem, we pick up a factor of $|\mathbf{A}| = |\mathbf{M}|^{1/2}$ with the change from integration over $\mathbf{k}$ to integration over $\mathbf{q}$, as well as a factor of $(2/\hbar^2)^{3/2}$ from the additional scaling we are introducing here. We thus have

$$\begin{aligned} g(\epsilon) &= \frac{1}{\pi^2\hbar^3}(2|\mathbf{M}|)^{1/2}\int_0^\infty q^2\,dq\;\delta(\epsilon - \epsilon_0 - q^2) \\ &= \frac{1}{\pi^2\hbar^3}(2|\mathbf{M}|)^{1/2}\int_0^\infty q^2\,dq\;\left[\frac{\delta(q - \sqrt{\epsilon-\epsilon_0})}{\sqrt{\epsilon-\epsilon_0}} + \frac{\delta(q + \sqrt{\epsilon-\epsilon_0})}{\sqrt{\epsilon-\epsilon_0}}\right] \\ &= \frac{1}{\pi^2\hbar^3}(2|\mathbf{M}|)^{1/2}\sqrt{\epsilon-\epsilon_0}. \end{aligned} \tag{1.45}$$

With this result, the electronic specific heat is therefore given by

$$c_v = \frac{\pi^2}{3}k_B^2 T g(\epsilon_F) = \frac{k_B^2 T}{3\hbar^3}(2|\mathbf{M}|)^{1/2}(\epsilon_F - \epsilon_0)^{1/2}. \tag{1.46}$$

Now, in the case of free electrons, the density of state is given by

$$g(\epsilon) = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\epsilon^{1/2}, \tag{1.47}$$

with the bare mass $m$ of the electron appearing cubed in the expression. If we want to define an effective mass $m^*$ so that (1.45) can be written as

$$g(\epsilon) = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}(\epsilon - \epsilon_0)^{1/2}, \tag{1.48}$$

then it is clear that we must have $m^{*3} = |\mathbf{M}|$, i.e. the (specific heat) effective mass is $m^* = |\mathbf{M}|^{1/3}$. (Shown)

2. **A&M Problem 13.5.** For a metal subject simultaneously to a nonzero electric field $\mathbf{E} \neq \mathbf{0}$ and nonzero thermal gradient $\nabla T \neq \mathbf{0}$, the heat production per unit volume $dq/dt$ is given by

$$\frac{dq}{dt} = \frac{du}{dt} - \mu\frac{dn}{dt}, \tag{2.1}$$

where $u$ is the energy per unit volume, $\mu$ the chemical potential, and $n$ the number of electrons per unit volume. The number density $n$ satisfies the continuity equation

$$\frac{dn}{dt} = -\nabla \cdot \mathbf{j}^n, \tag{2.2}$$

where $\mathbf{j}^n$ is the number current density. The rate of change of the energy density is

$$\frac{du}{dt} = -\nabla \cdot \mathbf{j}^\epsilon + \mathbf{E} \cdot \mathbf{j}, \tag{2.3}$$

where $\mathbf{j} = -e\mathbf{j}^n$ is the charge current density, $\mathbf{j}^\epsilon$ is the energy current density, and $\mathbf{E}$ is the electric field. Substituting (2.2) and (2.3) into (2.1), we obtain

$$\frac{dq}{dt} = -\nabla \cdot \mathbf{j}^\epsilon + \mathbf{E} \cdot \mathbf{j} + \mu\nabla \cdot \mathbf{j}^n. \tag{2.4}$$

To express the rate of heat production $dq/dt$ to the heat current density $\mathbf{j}^q$ and the charge current density $\mathbf{j}$, we use Eq. (13.40) in A&M, which tells us that

$$\mathbf{j}^q = \mathbf{j}^\epsilon - \mu\mathbf{j}^n. \tag{2.5}$$

Taking the divergence of this equation, we find that

$$\nabla \cdot \mathbf{j}^q = \nabla \cdot [\mathbf{j}^\epsilon - \mu\mathbf{j}^n] = \nabla \cdot \mathbf{j}^\epsilon - \nabla\mu \cdot \mathbf{j}^n - \mu\nabla \cdot \mathbf{j}^n, \tag{2.6}$$

or, equivalently,

$$\nabla \cdot \mathbf{j}^n = \nabla \cdot \mathbf{j}^\epsilon + \nabla\mu \cdot \mathbf{j}^n + \mu\nabla \cdot \mathbf{j}^n. \tag{2.7}$$

Substituting this into (2.4), we then find

$$\frac{dq}{dt} = -\nabla \cdot \mathbf{j}^q - \nabla\mu \cdot \mathbf{j}^n - \mu\nabla \cdot \mathbf{j}^n + \mathbf{E} \cdot \mathbf{j} + \mu\nabla \cdot \mathbf{j}^n = -\nabla \cdot \mathbf{j}^q + \frac{1}{e}\nabla\mu \cdot \mathbf{j} + \mathbf{E} \cdot \mathbf{j} = -\nabla \cdot \mathbf{j}^q + \boldsymbol{\mathcal{E}} \cdot \mathbf{j}, \tag{2.8}$$

where $\boldsymbol{\mathcal{E}} = \mathbf{E} + \frac{1}{e}\nabla\mu$ is the field associated with the electrochemical potential. (Shown)

Next, we want to write $dq/dt$ in terms of the physically measurable resistivity $\boldsymbol{\rho}$, thermal conductivity $\mathsf{K}$ and thermoelectric power $\mathsf{Q}$. To do this, let us first write down Eq. (13.45) of A&M,

$$\begin{aligned} \mathbf{j} &= \mathsf{L}^{11}\boldsymbol{\mathcal{E}} - \mathsf{L}^{12}\nabla T, \\ \mathbf{j}^q &= \mathsf{L}^{21}\boldsymbol{\mathcal{E}} - \mathsf{L}^{22}\nabla T, \end{aligned} \tag{2.9}$$

and the relations between $\boldsymbol{\rho}$, $\mathsf{K}$, $\mathsf{Q}$ and the tensors $\mathsf{L}^{ij}$,

$$\begin{aligned} \boldsymbol{\rho}^{-1} &= \boldsymbol{\sigma} = \mathsf{L}^{11}, \\ \mathsf{K} &= \mathsf{L}^{22} - \mathsf{L}^{21}\left(\mathsf{L}^{11}\right)^{-1}\mathsf{L}^{12}, \\ \mathsf{Q} &= \mathsf{L}^{12}\left(\mathsf{L}^{11}\right)^{-1}. \end{aligned} \tag{2.10}$$

When we have cubic symmetry, the tensors $\mathbf{L}^{ij}$ are diagonal and of the form

$$\mathbf{L}^{ij} = \begin{bmatrix} L^{ij} & 0 & 0 \\ 0 & L^{ij} & 0 \\ 0 & 0 & L^{ij} \end{bmatrix}, \tag{2.11}$$

and thus $\mathbf{L}^{ij}$, $\boldsymbol{\rho}$, $\mathbf{K}$ and $\mathbf{Q}$ can all be treated as scalars. With this simplification, we have

$$\begin{aligned} \mathbf{j} &= L^{11}\mathcal{E} - L^{12}\nabla T, \\ \mathbf{j}^q &= L^{21}\mathcal{E} - L^{22}\nabla T, \end{aligned} \tag{2.12}$$

and

$$\begin{aligned} \frac{1}{\rho} &= \sigma = L^{11}, \\ K &= L^{22} - \frac{L^{21}L^{12}}{L^{11}}, \\ Q &= \frac{L^{12}}{L^{11}}. \end{aligned} \tag{2.13}$$

Furthermore, from the definition of $\mathbf{L}^{ij}$ in Eq. (13.47) in A&M, we see in Eq. (13.51) of A&M that

$$L^{21} = TL^{12}. \tag{2.14}$$

With these results at hand, we write $\mathcal{E}$ in terms of $\mathbf{j}$ and $\nabla T$ as

$$\mathcal{E} = \frac{1}{L^{11}}\mathbf{j} + \frac{L^{12}}{L^{11}}\nabla T = \rho\mathbf{j} + Q\nabla T, \tag{2.15}$$

and simplify the second term of $dq/dt$ in (2.8) as

$$\mathcal{E} \cdot \mathbf{j} = \rho\mathbf{j}^2 + Q\nabla T \cdot \mathbf{j}. \tag{2.16}$$

To simplify the first term of $dq/dt$ in (2.8), let us substitute $\mathcal{E}$ into $\mathbf{j}^q$ to write

$$\mathbf{j}^q = \frac{L^{21}}{L^{11}}\mathbf{j} + \frac{L^{21}L^{12}}{L^{11}}\nabla T - \left(K + \frac{L^{21}L^{12}}{L^{11}}\right)\nabla T = TQ\mathbf{j} - K\nabla T. \tag{2.17}$$

Taking the divergence of this equation, we then find

$$\nabla \cdot \mathbf{j}^q = Q\nabla T \cdot \mathbf{j} + T\nabla Q \cdot \mathbf{j} + TQ\nabla \cdot \mathbf{j} - \nabla K \cdot \nabla T - K\nabla^2 T. \tag{2.18}$$

For uniform current flow and uniform temperature gradient, we have the conditions $\nabla\cdot\mathbf{j} = 0$ and $\nabla^2 T = 0$, which means that

$$\nabla \cdot \mathbf{j}^q = Q\nabla T \cdot \mathbf{j} + T\nabla Q \cdot \mathbf{j} - \nabla K \cdot \nabla T. \tag{2.19}$$

Combining (2.19) and (2.16), we then write

$$\frac{dq}{dt} = \rho\mathbf{j}^2 + \nabla K \cdot \nabla T - T\nabla Q \cdot \mathbf{j}. \tag{2.20}$$

Now, from the definitions of $\mathbf{L}^{ij}$, we see that $K$ and $Q$ depend on $\mathbf{r}$ essentially through the local chemical potential $\mu(\mathbf{r})$. But as with the case of global thermal equilibrium, where the chemical potential is determined by the particle number constraint to be a function of the temperature $T$, i.e. $\mu = \mu(T)$, we extend this relation to the case of local equilibrium to write $\mu(\mathbf{r}) = \mu(T(\mathbf{r}))$. This means then that $K = K(\mu(\mathbf{r})) = K(T(\mathbf{r}))$ and $Q = Q(\mu(\mathbf{r})) = Q(T(\mathbf{r}))$, and we can write their gradients as

$$\nabla K = \frac{dK}{dT}\nabla T, \quad \nabla Q = \frac{dQ}{dT}\nabla T, \tag{2.21}$$

giving us

$$\frac{dq}{dt} = \rho\mathbf{j}^2 + \frac{dK}{dT}(\nabla T)^2 - T\frac{dQ}{dT}\nabla T \cdot \mathbf{j}. \qquad \text{(Shown)} \tag{2.22}$$

In the last part of this question, we are asked to compare the numerical values of the coefficient $-T(dQ/dT)$, obtained using the relaxation time approximation in a quantum-mechanical context, and the coefficient $(ne\tau\rho/m)(d\varepsilon/dT)$, obtained using the relaxation time approximation in the classical context (i.e. the Drude approximation), of $\nabla T \cdot \mathbf{j}$. For free classical electrons, the Drude relaxation time $\tau$ is determined from the measured resistivity of the metal as (Eq. (1.7) in A&M)

$$\tau = \frac{m}{ne^2\rho}, \tag{2.23}$$

which means that the coefficient of $\nabla T \cdot \mathbf{j}$ in the Drude approximation is

$$\frac{1}{e}\frac{d\varepsilon}{dT}, \tag{2.24}$$

where $\varepsilon$ is the mean thermal energy of the electrons. For a free classical electron gas in equilibrium at temperature $T$, the average thermal energy ought to be $\varepsilon = \frac{3}{2}k_BT$, which follows from the Equipartition Theorem. In the presence of a uniform electric field and electron-electron interactions, however, there is no reason to expect the Equipartition Theorem to be valid. We simply make a leap of faith in the Drude approximation by assuming that electron-electron interactions results locally in relaxation to a local thermal distribution characterized by a temperature $T(\mathbf{r})$, which varies from point to point. Within such an approximation, the average thermal energy $\varepsilon(\mathbf{r})$, which depends on where we are in the metal, should still be given locally by $\varepsilon(\mathbf{r}) = \frac{3}{2}k_BT(\mathbf{r})$, and thus

$$\frac{1}{e}\frac{d\varepsilon}{dT} = \frac{3}{2}\frac{k_B}{e}. \tag{2.25}$$

For free quantum-mechanical electrons, we have (Eq. (2.94) in A&M)

$$Q = -\frac{\pi^2}{6}\frac{k_B}{e}\left(\frac{k_BT}{\epsilon_F}\right), \tag{2.26}$$

and thus the coefficient of $\nabla T \cdot \mathbf{j}$ in the quantum-mechanical relaxation time approximation for free electrons is

$$-T\frac{dQ}{dT} = \frac{\pi^2}{6}\frac{k_B}{e}\left(\frac{k_BT}{\epsilon_F}\right). \tag{2.27}$$

The ratio of the magnitude of the Thomson effect predicted by the quantum-mechanical relaxation time approximation as compared to that predicted by the classical Drude approximation is thus

$$\frac{-T(dQ/dT)}{(1/e)(d\varepsilon/dT)} = \frac{2\pi^2}{3}\frac{k_BT}{\epsilon_F}. \tag{2.28}$$

At room temperature, $T = 300$ K, and using the typical value of $\epsilon_F = 5$ eV, we find the numerical value of this ratio to be on the order of $10^{-2}$.

.../Siew-Ann Cheong