Homework 4, due February 22, 1999

Problem 1. Ashcroft-Mermin 12.2

(a) We have

$\epsilon(\vec{k}) = \frac{\hbar^2}{2}\vec{k}^T \cdot \mathbf{M}^{-1} \cdot \vec{k}$

where we have taken the minimum energy to be zero and the minimum at the origin. This does not change the results.

The area $\mathcal{A}(\epsilon, k_z)$ is the area inside the curve given by k_x and k_y obeying

$\frac{2\epsilon}{\hbar^2} = \left(\mathbf{M}^{-1}\right)_{xx} k_x^2 + 2\left(\mathbf{M}^{-1}\right)_{xy} k_x k_y + \left(\mathbf{M}^{-1}\right)_{yy} k_y^2 +$

$2\left(\mathbf{M}^{-1}\right)_{xz} k_x k_z + 2\left(\mathbf{M}^{-1}\right)_{yz} k_y k_z + \left(\mathbf{M}^{-1}\right)_{zz} k_z^2$

We can write this in the form

$A(k_x - k_x^0)^2 + 2B(k_x - k_x^0)(k_y - k_y^0) + C(k_y - k_y^0) = D$

with

$A = \left(\mathbf{M}^{-1}\right)_{xx}$, $B = \left(\mathbf{M}^{-1}\right)_{xy}$, $C = \left(\mathbf{M}^{-1}\right)_{yy}$

and

$k_x^0 = -\frac{\left(\mathbf{M}^{-1}\right)_{xz}}{\left(\mathbf{M}^{-1}\right)_{xx}} k_z$, $k_y^0 = -\frac{\left(\mathbf{M}^{-1}\right)_{yz}}{\left(\mathbf{M}^{-1}\right)_{xx}} k_z$

and

$D = \frac{2\epsilon}{\hbar^2} - \left(\mathbf{M}^{-1}\right)_{zz} k_z^2 - A(k_x^0)^2 - 2Bk_x^0 k_y^0 - C(k_y^0)^2$

The area of the ellipse is $\mathcal{A}(\epsilon, k_z) = \pi D \frac{1}{\sqrt{AC - B^2}}$

which is linear in ϵ. Therefore we have

$m^* = \frac{\hbar^2}{2\pi}\frac{\partial \mathcal{A}(\epsilon, k_z)}{\partial \epsilon} = \frac{1}{\sqrt{AC - B^2}}$

Next we use

$\left((\mathbf{M}^{-1})^{-1}\right)_{zz} = \frac{1}{\det(\mathbf{M}^{-1})}(\left(\mathbf{M}^{-1}\right)_{xx}\left(\mathbf{M}^{-1}\right)_{yy} - \left(\mathbf{M}^{-1}\right)_{xy}\left(\mathbf{M}^{-1}\right)_{yx})$

or

$(\mathbf{M})_{zz} = \det(\mathbf{M})(AC - B^2)$

from which the formula follows.

(b) The density of states follows from

$g(\epsilon) = \frac{1}{4\pi^3}\int d^3k\delta(\epsilon - \frac{\hbar^2}{2}\vec{k}^T \cdot \mathbf{M}^{-1} \cdot \vec{k})$

This can be rotated to principal axes

$g(\epsilon) = \frac{1}{4\pi^3}\int d^3q\delta(\epsilon - \frac{\hbar^2}{2}\vec{q}^T \cdot \mathbf{D}^{-1} \cdot \vec{q})$

where the matrix $\mathbf{D}$ is diagonal and $\det(\mathbf{D}) = \det(\mathbf{M})$

We now transfer to scaled coordinates and obtain

$g(\epsilon) = \frac{1}{4\pi^3} \int d^3 s \sqrt{\det(\mathbf{D})} \delta(\epsilon - \frac{\hbar^2 s^2}{2}) = \sqrt{\det(\mathbf{D})} \frac{1}{\hbar^2 \pi^2} \sqrt{\frac{2\epsilon}{\hbar^2}}$
comparing with
$g(\epsilon) = (m^*)^{\frac{3}{2}} \frac{1}{\hbar^2 \pi^2} \sqrt{\frac{2\epsilon}{\hbar^2}}$
gives the required answer.

Problem 2. Ashcroft-Mermin 12.4

(a) $\vec{j}_{total} = \sum_n \vec{j}_n = \sum_n \tilde{\rho}_n^{-1} \vec{E} \equiv \tilde{\rho}^{-1} \vec{E}$
which gives
$\tilde{\rho}^{-1} = \sum_n \tilde{\rho}_n^{-1}$

(b) From
$\tilde{\rho}_n = \begin{pmatrix} \rho_n & -R_n H \\ R_n H & \rho_n \end{pmatrix}$
we find
$\tilde{\rho}_n^{-1} = \frac{1}{\rho_n^2 + R_n^2 H^2} \begin{pmatrix} \rho_n & R_n H \\ -R_n H & \rho_n \end{pmatrix}$
and therefore
$\frac{1}{\rho^2 + R^2 H^2} \begin{pmatrix} \rho & RH \\ -RH & \rho \end{pmatrix} =$
$\frac{1}{\rho_1^2 + R_1^2 H^2} \begin{pmatrix} \rho_1 & R_1 H \\ -R_1 H & \rho_1 \end{pmatrix} + \frac{1}{\rho_2^2 + R_2^2 H^2} \begin{pmatrix} \rho_2 & R_2 H \\ -R_2 H & \rho_2 \end{pmatrix}$
This leads to the equations
$\frac{\rho}{\rho^2 + R^2 H^2} = \frac{\rho_1}{\rho_1^2 + R_1^2 H^2} + \frac{\rho_2}{\rho_2^2 + R_2^2 H^2}$
$\frac{R}{\rho^2 + R^2 H^2} = \frac{R_1}{\rho_1^2 + R_1^2 H^2} + \frac{R_2}{\rho_2^2 + R_2^2 H^2}$
Combine these using complex arithmetic:
$\frac{\rho - iRH}{\rho^2 + R^2 H^2} = \frac{\rho_1 - iR_1 H}{\rho_1^2 + R_1^2 H^2} + \frac{\rho_2 - iR_2 H}{\rho_2^2 + R_2^2 H^2}$
or
$\frac{1}{\rho + iRH} = \frac{1}{\rho_1 + iR_1 H} + \frac{1}{\rho_2 + iR_2 H}$
or
$\frac{1}{\rho + iRH} = \frac{\rho_1 + \rho_2 + iH(R_1 + R_2)}{(\rho_1 + iR_1 H)(\rho_2 + iR_2 H)} = \frac{(\rho_1 + \rho_2)^2 + H^2 (R_1 + R_2)^2}{(\rho_1 + iR_1 H)(\rho_2 + iR_2 H)(\rho_1 + \rho_2 - iH(R_1 + R_2))}$
From this we get
$\rho + iRH = \frac{(\rho_1 + iR_1 H)(\rho_2 + iR_2 H)(\rho_1 + \rho_2 - iH(R_1 + R_2))}{(\rho_1 + \rho_2)^2 + H^2 (R_1 + R_2)^2}$
which has the correct denominator. The real part of the enumerator (which is the enumerator of ρ) is

$\rho_1\rho_2(\rho_1+\rho_2) - R_1 H R_2 H(\rho_1+\rho_2) + H^2(R_1+R_2)(\rho_1 R_2+\rho_2 R_1)$

which is equal to

$\rho_1\rho_2(\rho_1+\rho_2) + H^2(\rho_1 R_2^2+\rho_2 R_1^2)$

In the same way, the imaginary part gives

$-\rho_1\rho_2 H(R_1+R_2) + (\rho_1+\rho_2)H(R_2\rho_1+R_1\rho_2) + H^3 R_1 R_2(R_1+R_2)$

which is

$H(R_2\rho_1^2+R_1\rho_2^2) + H^3 R_1 R_2(R_1+R_2)$

and this gives the correct result for R.

(c) From the equation for the Hall coefficient we have $\lim_{H\to\infty} R = \frac{R_1 R_2}{R_1+R_2}$ If the high field Hall coefficient has $n_{eff}=0$ this means that $\lim_{H\to\infty} R = \infty$ and hence $R_1+R_2=0$, compensating bands. This gives

$\rho = \frac{\rho_1\rho_2(\rho_1+\rho_2)+H^2R_1^2(\rho_1+\rho_2)}{(\rho_1+\rho_2)^2} = \frac{\rho_1\rho_2+H^2R_1^2}{(\rho_1+\rho_2)}$

Problem 3. Ashcroft-Mermin 12.6

Take a single band and consider a state with
$\psi(\vec{r}+\vec{R},t=0) = e^{i\vec{k}\cdot\vec{R}}\psi(\vec{r},t=0)$
if we can show the result for this wave function, it will also hold for a linear combination.
$H(\vec{r}+\vec{R}) = -\frac{\hbar^2}{2m}\frac{\partial}{\partial(\vec{r}+\vec{R})}\cdot\frac{\partial}{\partial(\vec{r}+\vec{R})} + U(\vec{r}+\vec{R}) + e\vec{E}\cdot(\vec{r}+\vec{R}) = H(\vec{r}) + e\vec{E}\cdot\vec{R}$
since derivatives are invariant and the potential is periodic. Therefore
$\psi(\vec{r}+\vec{R},t) = e^{-i\frac{H(\vec{r}+\vec{R})t}{\hbar}}\psi(\vec{r}+\vec{R},t=0) = e^{-i\frac{H(\vec{r})t}{\hbar}}e^{-i\frac{e\vec{E}\cdot\vec{R}t}{\hbar}}e^{i\vec{k}\cdot\vec{R}}\psi(\vec{r},t=0)$
which gives
$\psi(\vec{r}+\vec{R},t) = e^{-i\frac{e\vec{E}\cdot\vec{R}t}{\hbar}+i\vec{k}\cdot\vec{R}}e^{-i\frac{H(\vec{r})t}{\hbar}}\psi(\vec{r},t=0)$
where we could move and break up exponents since only the one with H depends on position, the other two are just numbers. Hence we have
$\psi(\vec{r}+\vec{R},t) = e^{+i(\vec{k}-\frac{e\vec{E}t}{\hbar})\cdot\vec{R}}\psi(\vec{r},t)$
which is the required result. In this case we are able to derive the result of the semi-classical equation of motion directly from quantum mechanics!