Physics 240B, Spring 2008
Homework 2 Solutions

Jesse Noffsinger

April 6, 2008

Solutions are in general not the original work of the author.

Problem 1)

The Hamiltonian is given by

$$H = \frac{1}{2m}\left\{\left(p_x + \frac{eH}{2c}y\right)^2 + \left(p_y + \frac{eH}{2c}x\right)^2 + p_z^2\right\} \tag{1}$$

In the Heisenberg picture, the time evolution of the operators is given by:

$$\dot{x} = \frac{i}{\hbar}[H,x] = \frac{1}{m}\left(p_x + \frac{eH}{2c}y\right) \tag{2}$$

$$\dot{y} = \frac{i}{\hbar}[H,y] = \frac{1}{m}\left(p_y - \frac{eH}{2c}x\right) \tag{3}$$

$$\dot{z} = \frac{i}{\hbar}[H,z] = \frac{p_z}{m} \tag{4}$$

$$\dot{p_x} = \frac{i}{\hbar}[H,p_x] = \frac{eH}{2mc}\left(p_y - \frac{eH}{2c}x\right) \tag{5}$$

$$\dot{p_y} = \frac{i}{\hbar}[H,p_y] = -\frac{eH}{2mc}\left(p_x + \frac{eH}{2c}y\right) \tag{6}$$

$$\dot{p_z} = \frac{i}{\hbar}[H,p_z] = 0 \tag{7}$$

Introduce the cyclotron frequency $\omega_c = \frac{|e|H}{mc}$,then,

$$\ddot{x} = -\omega_c\frac{p_y}{2m} + \frac{\omega_c^2}{4}x - \frac{\omega_c}{2}\dot{y} = -\omega_c\dot{y} \tag{8}$$

$$\ddot{y} = \omega_c\frac{p_x}{2m} + \frac{\omega_c^2}{4}y + \frac{\omega_c}{2}\dot{x} = \omega_c\dot{x} \tag{9}$$

$$\ddot{z} = 0 \tag{10}$$

The solutions of these equations are:

$$x = r_0 \cos\left(t + \phi_0\right) \tag{11}$$

$$y = r_0 \sin\left(\omega_c t + \phi_0\right) \tag{12}$$

$$z = z_0 + p_z t \tag{13}$$

Problem 2)

The Hamiltonian in a magnetic field is given by:

$$H = \frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 \tag{14}$$

Therefore the operator $\mathbf{k}$ is given by:

$$\mathbf{k} = \frac{1}{\hbar}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right) \tag{15}$$

Then

$$\mathbf{k} \times \mathbf{k} = \frac{1}{\hbar^2}\left(\mathbf{p} \times \mathbf{p} - \frac{e}{c}\mathbf{p} \times \mathbf{A} - \frac{e}{c}\mathbf{A} \times \mathbf{p} + \frac{e^2}{c^2}\mathbf{A} \times \mathbf{A}\right) \tag{16}$$

The first and last terms vanish, leaving

$$\mathbf{k} \times \mathbf{k} = -\frac{e}{\hbar^2 c}(\mathbf{p} \times \mathbf{A} + \mathbf{A} \times \mathbf{p}) \tag{17}$$

Now use $\mathbf{p} = -i\hbar\nabla_r$ and the relation

$$\nabla_r \times (\mathbf{A}\psi) = (\nabla_r \psi) \times \mathbf{A} + \psi(\nabla_r \times \mathbf{A}) \tag{18}$$

and we arrive at

$$\mathbf{k} \times \mathbf{k}\psi = -\frac{e}{i\hbar c}(\nabla_r \times \mathbf{A})\psi \tag{19}$$

Or

$$\mathbf{k} \times \mathbf{k} = \frac{ie}{\hbar c}\mathbf{H} \tag{20}$$

Problem 3)

We give a semiclassical derivatino of the de Haas-van Alphen effect starting with the equation of motion of the conduction electrons in a magnetic field $\mathbf{H}$.

$$\hbar\dot{\mathbf{k}} = \frac{e}{c}\mathbf{v} \times \mathbf{H} \tag{21}$$

This gives, assuming a common origin

$$\hbar\mathbf{k} = \frac{e}{c}\mathbf{r} \times \mathbf{H} \tag{22}$$

Now use (see problem 2)

$$\hbar\mathbf{k} = \mathbf{p} - \frac{e}{c}\mathbf{A} \tag{23}$$

and the Bohr-Sommerfield quantization rule

$$\oint \mathbf{p}\cdot d\mathbf{r} = (n+\gamma)2\pi\hbar \tag{24}$$

where γ is a constant between 0 and 1. Then,

$$(n+\gamma)2\pi\hbar = \oint \hbar\mathbf{k}\cdot d\mathbf{r} + \oint \frac{e}{c}\mathbf{A}\cdot d\mathbf{r} = \frac{e}{c}\left\{\oint \mathbf{r}\times\mathbf{H}\cdot d\mathbf{r} + \oint \mathbf{A}\cdot d\mathbf{r}\right\} \tag{25}$$

Now

$$\oint \mathbf{r}\times\mathbf{H}\cdot d\mathbf{r} = -\oint \mathbf{r}\times d\mathbf{r}\cdot\mathbf{H} = -2\mathbf{S_r}\cdot\mathbf{H} \tag{26}$$

$$\oint \mathbf{A}\cdot d\mathbf{r} = \int \nabla\times\mathbf{A}\cdot d\mathbf{S} = \mathbf{H}\cdot\mathbf{S_r} \tag{27}$$

where S_r is the area of the orbit. Thus we conclude that

$$\Phi = \mathbf{H}\cdot\mathbf{S_r} = (n+\gamma)\frac{2\pi\hbar c}{|e|} \tag{28}$$

i.e. Flux through the orbit is quantized. Alternatively, the area of the orbit is quantized

$$S_{r,n} = \frac{2\pi\hbar c}{|e|H}(n+\gamma) \tag{29}$$

Corresponding to and area in k-space

$$S_{k,n} = \left(\frac{|e|H}{\hbar c}\right)^2 S_{r,n} = 2\pi\frac{|e|H}{\hbar c}(n+\gamma) \tag{30}$$

For more detail and figures, refer to:
Kittel, *Introduction to Solid State Physics* Ch. 9
Ziman, *Theory of Solids*, Ch 9.7.

Problem 4)

a)

$f(k,r,t)$ is the distribution function

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \int dk'[f_{k'}(1-f_k)w_{kk'} - f_k(1-f'_k)w_{k'k}] \tag{31}$$

$$= \int dk' w_{kk'}(f'_k - f_k) \tag{32}$$

Due to the symmetry of the matrix element w.

For elastic collisions $\epsilon'_k = \epsilon_k$ and f is a function of the energy only. Therefore $f^0_k = f^0_{k'}$ and

$$\left(\frac{\partial f^0_k}{\partial t}\right)_{coll} = 0 \tag{33}$$

For the case of local equilibrium, $f^{le}(k,r) = f^{le}(k',r)$ and

$$\left(\frac{\partial f_k^{le}}{\partial t}\right)_{coll} = 0 \tag{34}$$

The electric current is given as:

$$\mathbf{J}(\mathbf{r}) = \frac{e}{4\pi^3}\int d\mathbf{k}(\mathbf{v})f(\mathbf{k},\mathbf{r}) \tag{35}$$

$$= \frac{e}{4\pi^3\hbar}\int d\mathbf{k}(\nabla_k\epsilon)f(\mathbf{k},\mathbf{r}) \tag{36}$$

We know that the energy is an even function of k, so then the distribution (which depends only on k through the energy) is even as well. Converseley, the gradient of an even function (the energy) is odd (the velocity). Therefore this is an odd integral over symmetric limits, giving a null result for the current when either $f = f^0$ or $f = f^{le}$.

b)

Liouville's theorem states that for a conservative ensemble the magnitude of hte area occupied by the ensemble in phase space is unchanged as a function of time.

$$\frac{d}{dt}\rho(q_1, \ldots.., q_N, p_1, \ldots..p_N, t) = 0 \tag{37}$$

where

$$\rho(q_1, \ldots.., q_N, p_1, \ldots..p_N, t)dq_1 \ldots.dq_N dp_1 \ldots..dp_N \tag{38}$$

is the probability of occupying the small volume, $dq_1 \ldots.dq_N dp_1 \ldots..dp_N$ in phase space at time t

Ashcroft and Mermin, Appendix H gives a semiclassical proof of this theorem, outlined below

$$H(r,p) = \frac{\epsilon_n}{\hbar}\left(p - \frac{e}{c}A(r,t)\right) - e\phi(r,t) \tag{39}$$

$$\dot{\mathbf{r}} = \frac{\partial H}{\partial \mathbf{p}} \tag{40}$$

$$\dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{r}} \tag{41}$$

$$\mathbf{H} = \nabla \times \mathbf{A} \tag{42}$$

so the semi-classical eqns are

$$\dot{\mathbf{r}} = \nabla(k) = \frac{1}{\hbar}\frac{\partial \epsilon}{\partial k} \tag{43}$$

since $\nabla_k\phi = \nabla_k A = 0$ and

$$\hbar\dot{\mathbf{k}} = -e[\mathbf{E}(r,t) + \frac{1}{c}\mathbf{v} \times \mathbf{H}(r,t) \tag{44}$$

Since the semiclassical equations have the same canonical Hamiltonian form for each band, the regions of 6D $\mathbf{r}-\mathbf{p}$ space should evolve in a way to preserve their volume. Also, since $\mathbf{k}=\mathbf{p}/\hbar-\frac{e}{\hbar c}\mathbf{A}$ a volume in $\mathbf{r}-\mathbf{p}$ space will have the same volume as the corresponding region in $\mathbf{r}-\mathbf{k}$ space.

So for a semiclassical system, Liouville's theorem holds.

Problem 5)

a)

The reason that the classical results come close to the quantum ones is that the electron wavepacket can be labeled with a position and momentum simultaneously and hence the Boltzmann equation can be written. In fact, the uncertanties Δk and Δx have to be much smaller than the dimensions of the cell in which $f(k,r,t)$ are defined and Δx has also to be smaller than the average distance between the scattering centers or the mean free path, i.e., the relaxation time approximatino must be possible.

In the electrical conductivity calculation we have the distribution function:

$$f=f^0-\frac{\partial f^0}{\partial\epsilon}e\tau E\cdot v \tag{45}$$

$$=f^0-\frac{\partial f^0}{\partial\epsilon}\nabla_k\epsilon\cdot E\frac{e\tau}{\hbar} \tag{46}$$

$$=f^0-\nabla_k f^0\cdot\frac{e\tau}{\hbar}E=f^0(k-\frac{e\tau}{\hbar}E) \tag{47}$$

This means that the Fermi surface is displaced by $\frac{e\tau}{\hbar}E$ in k-space (if it is a free electron gas then the displacement is rigid).

An equivalent picture is the electron in state k that gains energy $e\tau v\cdot E$, like a classical electron which travels a distance $v\tau$ through the E field. This is why the classical picture seems to work in general.

Similarly, the thermal conductivity calculation:

$$f=f^0-\frac{\partial f^0}{\partial T}\tau v\cdot\nabla T=f^0(T-\tau v\cdot\nabla T) \tag{48}$$

So, electrons traveling from hot to cold regions lose an energy $\tau v\cdot\nabla T$, and electrons traveling from cold to hot regions gain an energy $\tau v\dot{\nabla}T$. This result is equal to the classical calculation.

b)

If the impurities are dilute and the potential $U(r)$ describing the interaction between an electron and a single impurity at the origin is sufficiently weak, on can use the Golden Rule:

$$w_{k\to k'}=\frac{2\pi}{\hbar}n_i\delta(\epsilon_k-\epsilon_k')|\langle k'|U|k\rangle|^2 \tag{49}$$

where the n_i is the density of impurities. Since $\frac{1}{\tau}\propto\left(\frac{\partial f}{\partial t}\right)_{coll}=w_{kk'}$, σ is proportional to n_i. If there is no scattering at all, the periodicity of $\epsilon(k)$ will cause oscillatory rather than DC current if a DC field is applied. What happens is that, even at $T \to 0$, it is difficult to get rid of other scattering processes (like phonon *emission* and scattering by other kinds of defects), so :

$$\rho_{tot} = \rho_{Defects} + \rho_{impurities} \rightarrow \sigma_T \propto \frac{1}{\rho_D + \alpha n_i} \tag{50}$$