Physics 240B, Spring 2008
Homework 1 Solutions

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

Problem 1)

Chapter 6 of Kittel is very helpful for this problem. Portions not worked out explicitly here appear in the recommended texts.

a)

The total number of electrons up to wavevector k is:

$$N_e = 2 \times \frac{\pi k^3}{(2\pi/L)^3} = \frac{V}{3\pi^2} k^3 \tag{1}$$

The density of states, $D(k)$ is:

$$D(k) = \frac{dN}{dk} = \frac{V}{\pi^2} k^2 \tag{2}$$

while:

$$\epsilon = \frac{\hbar^2 k^2}{2m} \tag{3}$$

Yielding

$$D(\epsilon) = \frac{dN}{d\epsilon} = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \epsilon^{1/2} \tag{4}$$

b)

The total number of electrons is:

$$N = \frac{V}{3\pi^2} \left(\frac{2m\epsilon_F}{\hbar^2}\right)^{3/2} \rightarrow \epsilon_F^{1/2} = \frac{3N}{\epsilon_F} \left[\frac{V}{\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2}\right]^{-1} \tag{5}$$

Entering this expression for $\epsilon_F^{1/2}$ into Eqn (4) gives:

$$D(\epsilon_F) = \frac{3N}{2\epsilon_F} \tag{6}$$

c)

$$C_v = \frac{\partial U}{\partial T} \tag{7}$$

The total energy of the sytem being

$$U = \int \epsilon f(\epsilon, T) D(\epsilon) d\epsilon \tag{8}$$

which depends on temperature only through the Fermi-Dirac distribution. The Sommerfield expansion [Eqn 2.70 in Ashcroft and Mermin] can be applied, or a direct following of Kittel's derivation gives:

$$C_v = \frac{\pi^2}{3} k_b^2 T D(\epsilon_F) \tag{9}$$

d)

If we associate an energy $\pm\mu H$ with spin up/down electrons, we can find the paramagnetic susceptibility of the free electron gas, defined as

$$\chi = \frac{\partial M}{\partial H} \tag{10}$$

The total magnetic moment per volume is $M = \mu(n_+ - n_-)$, arising from the difference in the number of spin up and spin down electrons.

$$M = \frac{1}{2}\mu \int \left[f(\epsilon - \mu H) - f(\epsilon + \mu H) \right] D(\epsilon) d\epsilon \tag{11}$$

The 1/2 accounts for the spin in the standard density of states formula. Taking μH to be small with respect to the electronic energies [Ziman pg.332], and the energy derivative of the Fermi-Dirac distribution to be a delta function peaked at ϵ_F:

$$M = \mu^2 H D(\epsilon_F) \tag{12}$$

or

$$\chi = \mu^2 D(\epsilon_F) \tag{13}$$

e)

The thermal conductivity is defined as the negative ratio between the temperatue gradient and the total flux of thermal energy.

$$K = -\frac{dT}{dx}\frac{1}{j_U} \tag{14}$$

From the kinetic theory of gases [Kittel pg.122] we arrive at

$$K = \frac{1}{3} cnvl = \frac{1}{3} ncv_F^2 \tau \tag{15}$$

where c is the specific heat per electron.

f)

The electrical conductivity is defined as

$$\mathbf{j} = \sigma \mathbf{E} \tag{16}$$

and is in general a tensor. Using the Drude approach, and giving breaking the current into the form

$$\mathbf{j} = \mathbf{nev} \tag{17}$$

we assume that each electron is accelerated by an electric field $\mathbf{E}$ in between collisions. The average velocity attained over a time τ, using a simple $F = ma$ model, is

$$\Delta v = \frac{-e\mathbf{E}}{m}\tau \tag{18}$$

putting 16,17,and 18 together, we find

$$\sigma = \frac{ne^2\tau}{m} \tag{19}$$

g)

The Wiedeman-Franz ratio is the ratio of the thermal conductivity to the electrical conductivity.

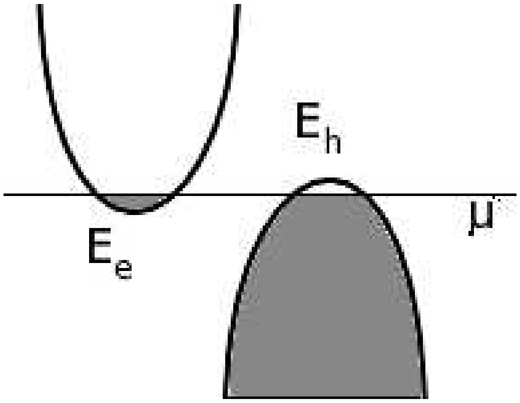
$$\frac{K}{\sigma} = \frac{v_F^2 mc}{e^2} \tag{20}$$

Inserting our forumla for heat capacity, and using $\epsilon_F = \frac{1}{2}mv_F^2$, $D(\epsilon_F) = \frac{3N}{2\epsilon_F}$:

$$\frac{K}{\sigma} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 T = LT \tag{21}$$

Problem 2)

For a semimetal at very low temperatures, we assume parabolic bands and can treat both the equal number of electrons and holes as free particles of effective mass m_e and m_h respectively.



We can use results from problem 1, except the zero is now at μ, and we have an effective mass

$$N_e = \frac{V}{3\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}(\mu - E_e)^{3/2} = \frac{V}{3\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2}(E_h - \mu)^{3/2} = N_h \tag{22}$$

From this we get the value of the chemical potential:

$$\mu = \frac{m_e E_e + m_h E_h}{m_e + m_h} \tag{23}$$

The density of states is the sum of the contributions from the electrons and the holes

$$D(\epsilon) = \frac{V}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}(\epsilon - E_e)^{1/2}\Theta(\epsilon - E_e) + \frac{V}{2\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2}(E_h - \epsilon)^{1/2}\Theta(E_h - \epsilon) \tag{24}$$

From the free electron theory $C_v = \frac{\pi^2}{3}k_B^2 T D(\mu)$, then

$$C_v = \frac{\sqrt{2}}{3}\frac{V k_B^2 T}{\hbar^3}(m_e + m_h)\left(\frac{1}{m_e} + \frac{1}{m_h}\right)^{1/2}(E_h - E_e)^{1/2} \tag{25}$$

after using the identity for μ [Eqn 23]

Problem 3)

A electron on the Fermi surface of Na acts very much like a free electron. A free electron moving in a magnetic field will have a circular orbit, balancing the forces:

$$m\frac{v^2}{r} = \frac{evH}{c} \tag{26}$$

Where the characteristic velocity is the Fermi velocity. In Na, the Fermi wavevector, $(3\pi^2 n)^{1/3}$ is related to the velocity by $v_F = \hbar k_F/m$. This gives, for a concentration $2.65 \times 10^{22}\mathrm{e/cm^3}$ [Kittel pg.139],

$$r = 6 \times 10^{-4}\mathrm{cm} \tag{27}$$

We can easily relate r to k_F.

$$r = \frac{\hbar c}{eH}k_F \tag{28}$$

which gives the relation between the areas of the real- and k-space orbits.

$$\frac{A_k}{A_{real}} = \left(\frac{eH}{\hbar c}\right)^2 \tag{29}$$

Problem 4)

Our goal is to find the rate of change of the momentum vector, which is essentially the frequency of the cyclotron oscillation in a non-circular orbit.

$$E = Ak_x^2 + Bk_y^2 \to 1 = \left(\frac{k_x}{\sqrt{E/A}}\right)^2 + \left(\frac{k_y}{\sqrt{E/B}}\right)^2 \tag{30}$$

This gives the area of the ellipse in k-space

$$S = \frac{\pi E}{\sqrt{AB}} \tag{31}$$

$$m^* = \frac{1}{2\pi}\frac{dS}{dE} = \frac{1}{2\sqrt{AB}} \tag{32}$$

Using the formula for the frequency of a cyclotron orbit given an effective mass

$$\omega_c = \frac{eH}{m^* c} = \frac{2\sqrt{AB}eH}{c} \tag{33}$$

The real space orbit will be an ellipse, just like the k-space orbit, but will be rotated 90°, and translated away from the origin to some (x_0, y_0).

Problem 5)

Ziman Sections 5.4, and 5.5 contain a very good outline of this problem.

a)

Friedel Oscillations are the induced charge density caused by an impurity. They show a space-oscillating behavior that goes as $\sim \frac{cos(2k_F r)}{r^3}$ rather than $exp{-k_s r}$. This is related to the sharp cutoff of the Fermi-Dirac distribution at k_F.

b)

Using the effective mass Hamiltonian

$$H = \frac{\hbar^2 \nabla^2}{2m^*} + V(\mathbf{r}) \tag{34}$$

and assuming a spherically symmetric potential, we have solutions of the form

$$\psi_{k,l} = \frac{1}{r}\sin(kr - \frac{l\pi}{2} + \eta_l)P_l(\cos\theta) \tag{35}$$

where η_l is the phase shift due to the impurity potential, and is zero when $V(\mathbf{r})$ is not present.

Now, we normalize to a spherical box of radius R, and impose zero charge fluctuation there.

$$\psi_{k,l}(R) = 0 \rightarrow kR - \frac{l\pi}{2} + \eta_l = n\pi \tag{36}$$

where n is an integer. This gives, for our normalized wavefunction in the presence of an impurity:

$$\psi_{k,l} = \frac{1}{\sqrt{2\pi R}}\frac{1}{r}\sin(kr - \frac{l\pi}{2} + \eta_l)P_l(\cos\theta) \tag{37}$$

Now, we would like to calculate the induced charge density. For this we subtract off the density present with zero potential ($\eta_l = 0$) from our arbitrary spherically symmetric potential.

$$\Delta\rho(r) = e\sum_l (2l+1)\int_0^{k_F} \left\{|\psi_{k,l}(\eta_l)|^2 - |\psi_{k,l}(0)|^2\right\} \frac{2R}{\pi}dk \tag{38}$$

The sum over $(2l + 1)$ is due to the degeneracy of each of these levels, while the R/π results from the density of states, and the 2 gives the spin degeneracy.

If we use, for the wavefunction integral,

$$\sin^2(x+a) - \sin^2(x) = \sin(2x+a)\sin(a) \tag{39}$$

Our integral becomes

$$\Delta\rho(r) = \frac{e}{\pi^2}\sum_l (2l+1)\int_0^{k_F} \sin(\eta_l)\sin(2kr - l\pi + \eta_l)\frac{1}{r^2}dk \tag{40}$$

If we assume η_l is a constant, then the integral has the basic form

$$\Delta\rho(r) \sim \frac{1}{r^3}\cos(2k_F r) \tag{41}$$

c)

Starting from

$$kR - \frac{l\pi}{2} + \eta_l = n\pi \tag{42}$$

The largest value of $n = N_{max}$ occurs at $k = k_F$. For $\eta_l = 0$

$$N^l_{max}(0) = \frac{k_F R}{\pi} - \frac{l}{2} \tag{43}$$

or, more generally

$$N^l_{max}(\eta_l) = \frac{k_F R}{\pi} - \frac{l}{2} + \frac{\eta_l(k_F)}{\pi} \tag{44}$$

The extra electron(s) screening the impurity potential is

$$\Delta N = \sum_l 2(2l+1)\left[N^l_{max}(\eta_l) - N^l_{max}(0)\right] = \frac{2}{\pi}\sum_l (2l+1)\eta_l(k_F) \tag{45}$$

This must be exactly equal the impurity charge to keep charge neutrality outside of R, giving the Freidel Sum Rule.

$$Z = \frac{2}{\pi}\sum_l (2l+1)\eta_l(k_F) \tag{46}$$

d)

The Kohn Effect is a "kink" in the phonon frequency dispersion at $q = 2k_F$. This is related to the singularity of $\frac{dE}{dq}$ at $2k_F$, for $\epsilon(q,0)$, which is the static case.

The phonon dispersion of a metal is approximately given by screening the ionic plasma frequency by $\epsilon(q,0)$, or more precisely

$$\omega^2(q) = \frac{\Omega_q^2}{\epsilon(q,0)} \tag{47}$$

$$2\omega\frac{d\omega}{dq} = -\frac{\Omega_q^2}{\epsilon(q,0)}\frac{d\epsilon}{dq} \tag{48}$$

hence the kink in $\omega(q)$ reflects the singularity in $\frac{d\epsilon}{dq}$.

(49)

(50)

(51)

(52)