PHYS 353 SOLID STATE PHYSICS STUDY GUIDE FOR PART 3

Free Electron Fermi Gas and Energy Bands

OUTLINE:

A. Quantum Theory and energy levels
   1. Schrodinger's equation
   2. quantum numbers and energy levels
   3. Fermi energy
   4. effects of temperature
   5. free electron gas

B. Heat Capacity of the electron gas

C. Electrical conductivity

D. Motion in magnetic fields
   1. review
   2. Hall effect

E. Thermal conductivity of metals

F. Nearly free electron model and the energy gap

G. Block functions

H. Kronig-Penny model

I. Wave equation of electron in a periodic potential
   1. Schrodinger's Equation
   2. The Central Equation
   3. Approximation at the zone boundary
   4. Approximation near the zone boundary

STUDY QUESTIONS: (for 3rd test - **not** for collected homework assignment)

1. a) What is meant by a free electron Fermi gas? (discuss each of the four words)
   b) What is the Schrodinger's equation for this case?
   c) What is the wavefunction, Ψ, for this case?
   d) How do energy levels come into play?
   e) What is the Fermi energy? (in words and in formula)
   f) Can any k exist? If not, why not?

2. a) How does temperature enter into the free electron Fermi gas?
   b) What is k_{Fermi} and what is T_{Fermi} ?
   c) How does ε_{Fermi} relate to N/V ? (be able to derive this)
   d) What is $D(\varepsilon)$ in words and in formula?

3. Derive $C_{electron}$ and compare to $C_{lattice}$.

4. Derive $K_{electrons}$ and compare to $K_{lattice}$ and explain the big difference.

5. Starting from Newton's 2nd Law and the current density: $\mathbf{j} = -ne\mathbf{v} = \sigma\mathbf{E}$, derive $\sigma = ne^2\tau/m$. Be sure to define each symbol used.

6. a) What is the Hall effect?
   b) Derive the Hall coefficient.
   c) Is $R_H > 0$ or $R_H < 0$ if electrons are the current carriers?

7. a) Write the wave equation (Schrodinger's Eq.) of an electron in a periodic potential.
   b) Assume appropriate solutions for the wave equation.
   c) Indicate how to get the Central equation.

8. Assuming U=0, show that #7c) gives the free electron solution.

9. Assuming all the U's = 0 except U_{-1} and U_{+1} , derive the energy gap at the zone boundary.

10. Outline the solution of the Central equation for near the zone boundary using the appropriate assumptions.

<u>COLLECTED HOMEWORK ASSIGNMENTS:</u>

21. Fermi Energy

Starting from the mass density, number of valence electrons, and the atomic mass, **show how to calculate** the electron density, Fermi energy, Fermi temperature, Fermi wavevector, and Fermi velocity for Aluminum. For Al, **given**: mass density = 2.7 gm/cm^3, valence electrons = 3, atomic mass = 27 amu = 27 gms/mole; **find:** electron density = 1.806×10^{23}/cm^3 = 1.806×10^{29}/m^3; Fermi energy = 11.63 eV; Fermi T = 13.49×10^4 K; Fermi wavevector = 1.75×10^{10}/m; Fermi velocity = 2.02×10^6 m/s. See section on Free Electron Fermi Gas, subsection 3.
Note how the Fermi velocity compares to the speed of light and to the speed of sound (phase velocity of oscillations of atoms).

22. Chemical Potential in Two Dimensions

Show that (derive) the chemical potential (μ) of a Fermi gas in **two** dimensions is given by:

$$\mu(T) = k_B T \ln[\exp\{n\pi\hbar^2/mk_BT\} - 1] \ ,$$

where n = number of electrons per unit area ($n=N/L^2$).

HINT: First show that the density of orbitals of a free electron gas in two dimensions is independent of energy: $D(\varepsilon) = L^2m/\pi\hbar^2$. HINT for showing this: $dN = D(\varepsilon)d\varepsilon = 2^*D(k_x)D(k_y)dk_xdk_y = 2D(k_x)D(k_y)2\pi kdk$ and recall $\varepsilon = \hbar^2k^2/2m$ so that $d\varepsilon = (\hbar^2/2m)2kdk$.
HINT: Start from $N = \int D(\varepsilon)\, f(\varepsilon,T)\, d\varepsilon$ (be sure to identify what N, $D(\varepsilon)$ and $f(\varepsilon,T)$ represent).
HINT: $\int (1/[e^x+1])dx = \ln(e^x/[e^x+1]) + C = x - \ln[e^x+1] + C$. Watch your limits when you substitute x for $(\varepsilon-\mu)/k_BT$, your limits will take care of the C and will include μ.
Note: for small T, $\exp\{n\pi\hbar^2/mk_BT\} >> 1$ so the 1 can be neglected; then $\ln\{e^x\} = x$ and so $\mu(T) = n\pi\hbar^2/m$ (which says μ is independent of T for small T in the 2-D case!)

23. Kinetic Energy of Electron Gas

Show that the kinetic energy of a three-dimensional gas of N electrons at 0K is: $U_O = (3/5)N\varepsilon_F$, where ε_F is the Fermi energy. [HINT: recall $U_O = N\langle\varepsilon\rangle$ where $\langle\varepsilon\rangle = \int \varepsilon f(\varepsilon,T)D(\varepsilon)d\varepsilon \ / \int f(\varepsilon,T)D(\varepsilon)d\varepsilon$, and $f(\varepsilon,0) = 1$ for $0<\varepsilon<\varepsilon_F$ and $f(\varepsilon,0) = 0$ for $\varepsilon>\varepsilon_F$.]

24. Fermi Gases in Astrophysics

(a) Given that the mass of the sun is $2x10^{30}$ kg and assuming that the sun is pure hydrogen, estimate the number of electrons in the Sun.

(b) What is the Fermi energy (in eV) for electrons assuming all the electrons are ionized in the sun? [sun's Radius = 6.96×10^8 m]

(c) In a white dwarf star this number of electrons may be ionized and contained in a sphere of radius $2x10^7$ m; find the Fermi energy of the electrons in electron volts. (The sun could become a white dwarf when it runs out of hydrogen fuel to keep it at its present size).

(d) The energy of an electron in the relativistic limit $E >\approx mc^2$ is related to the wavevector as $E = pc = \hbar kc$ (instead of $E = \hbar^2k^2/2m$). Show that the Fermi energy in this limit is $\varepsilon_F \approx 3\hbar c(N/V)^{1/3}$ [Recall from relativity that $KE = ½mv^2$ is no longer valid for any e^- with $KE >\approx m_oc^2 \approx .5$ MeV = $5x10^5$ eV.]

(e) If the above number of electrons were contained in a pulsar of radius 10 km, show that the Fermi energy would be $\approx 10^8$ eV= 100 MeV. [HINT: Consider whether part d above applies here. If it does, justify using it here.]

This value explains why pulsars are believed to be composed largely of neutrons rather than of protons and electrons, for the energy release in the reaction $n \rightarrow p + e$ is only 0.8 MeV which is not large enough to enable many electrons to form a Fermi sea. The neutron decay proceeds only until the electron concentration builds up enough to create a Fermi level of 0.8 MeV, at which point the neutron, proton, and electron concentrations are in equilibrium.

25. Frequency Dependence of the Electrical Conductivity

Use the equation:

$\Sigma\mathbf{F} = m\,\mathbf{a}$ and $\mathbf{E}(t) = \mathbf{E_o}e^{i\omega t}$,

or

$q\,\mathbf{E_o}e^{i\omega t} - m\mathbf{v}/\tau = m(d\mathbf{v}/dt)$,

and recall: $\mathbf{j} = -ne\mathbf{v} = \sigma\mathbf{E}$, so $\sigma = -ne\mathbf{v}/\mathbf{E}$

where $q = -e$ for an electron, E_o is the amplitude of the oscillating applied electric field, ω is the angular frequency of the oscillating applied electric field, and τ is the collision time, **to show that the conductivity (σ) at frequency ω is**:

$\sigma(\omega) = \sigma_o\,[\{1+i\omega\tau\}/\{1+(\omega\tau)^2\}]$ where $\sigma_o = ne^2\tau/m$.

HINT: Assume v has the same frequency dependence as E, so try $v = v_o e^{i\omega t}$ **.** This will relate v to E.
As you can see, this gives a complex answer when it should be a real answer.
The extra credit opportunity below problem 26 shows how to remove this "complexity".

26. Frequency Dependence of the Electrical Conductivity (alternate way)

(a) Do the above problem except this time assume $\mathbf{E}(t) = \mathbf{E_o}\sin(\omega t)$ instead of $\mathbf{E_o}e^{i\omega t}$ and show that the conductivity (σ) at frequency ω is:

$\sigma(\omega) = \sigma_o\,[\{1+(\omega\tau)^2\}^{1/2}/\{1+(\omega\tau)^2\}] = \sigma_o/\sqrt{[1+(\omega\tau)^2]}$

and

$v(t) = v_o\sin(\omega t+\theta)$ where $\theta = \tan^{-1}(-\omega\tau)$.

HINT: Assume that $v(t) = v_o\sin(\omega t+\theta)$ and see if it works. Recall these trig identities:
$\sin(a+b) = \sin(a)\cos(b) + \sin(b)\cos(a)$ and $\cos(a+b) = \cos(a)\cos(b) - \sin(a)\sin(b)$, and
recall that $A\sin(\omega t) + B\cos(\omega t) = 0$ only if A=0 and B=0.

Extra credit: Show that the answers to problems 25 and 26 are equivalent.
To do this, assume $v = v_o e^{i\omega t+i\theta}$, substitute into Newton's 2nd Law, and solve. You will have to have the real parts to solve and the imaginary parts to solve. This gives you two equations for two unknowns: v_o and θ.

27. (a) From the DC conductivity, $\sigma_o = ne^2\tau/m$, calculate τ at room temperature using values for σ_o at room temperature for Aluminum = 3.65×10^5 (ohm-cm)$^{-1}$ = 3.65×10^7 (ohm-m)$^{-1}$ and using $n=1.806\times10^{23}/cm^3 = 1.806\times10^{29}/m^3$ for Aluminum.

(b) Using your value of τ from part a above, and using the results of homework problem 26 for $\sigma(\omega)$: $\sigma(\omega) = \sigma_o / \sqrt{[1 + (\omega\tau)^2]}$, find:

b-1) $\sigma(f = 60\text{ Hz})$ and then compare to σ_o;

b-2) $\sigma(f = 10\text{ GHz})$ and then compare to σ_o.

b-3) at what frequency will $\sigma(\omega) = \frac{1}{2}\sigma_o$?

(c) Find the mean free path, ℓ using the relation $\ell = v_F * \tau$ and your value for τ from part a and your value for v_F for Aluminum in problem 21.

28. Derive the expression: $K_{thermal} = (1/3)C\,v\,\ell$ for the thermal conductivity of particles of velocity v, heat capacity C, and mean free path ℓ. (This was done for phonons in the Thermal Conductivity section of Part 2, but the same process should also apply to electrons.)

29. (a) Use values previously obtained for C, v and ℓ for electrons and calculate $K_{thermal}$ due to the electrons. [Assume heat capacity = $3Nk_B$ in high T limit, v = v_F, and $\ell = v^*\tau$ where τ was calculated in problem 27.]

(b) Use values previously obtained for C, v and ℓ for phonons to calculate $K_{thermal}$ due to the phonons. [You may assume the same heat capacity as in part a; for ℓ, you may assume a value of about 10 nm; you have previously determined v for the phonons for Aluminum in problem 18.]

(c) Compare the values for $K_{thermal}$ due to the electrons and the phonons, and then comment on the thermal properties of conductors versus insulators.

30. Demonstrate that the equations:

$$a_1x + b_1y + c_1z = 0$$

$$a_2x + b_2y + c_2z = 0$$

$$a_3x + b_3y + c_3z = 0$$

(a) have a solution if:

$$\begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} = 0$$

HINT: choose values for x, y, and z (such as x=3, y=2, and z=1) then choose values for the a_i, b_i, and c_i that make the above equations work.)

(b) do not have a solution if:

$$\begin{vmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{vmatrix} \neq 0$$

HINT: for this part, simply change one of the a_i so that the determine does not = 0 and show that the equations can not work except for the trivial solution x=0=y=z.

that is, pick numbers for the a,b,c's such that the determinate is zero and show that the equations can be solved for x,y,z; then pick other numbers for the a,b,c's such that the determinate is not zero and show that the equations can not be solved for x,y,z [other than x=0, y=0 and z=0].