Solid State Question of students
PHYS5340

1.
(a) Let's consider a metallic sample with free electrons. Using pictures, and key equations, explain the Hall Effect in your own words. Note: no calculations are needed, only a qualitative explanation.

(b) What, if anything, would be different if we were to instead assume that the metallic sample had free holes (positive charge carriers), not electrons

(c) Assuming that the electrons are the charge carrier in a metallic sample, if the Lorentz force is equal to $1.6 \; x \; 10^{-24} N$, the magnetic field on the sample is $1 \, T = 1 \; \frac{kg}{As^2}$, and the current density applied is $0.4 \; \frac{A}{m^2}$, find the Hall Coefficient R_H. Assume that the steady state has been established. Express your answer in $\frac{cm^3}{C}$. You can neglect the sign.

(d) Using your result from (c), find the carrier concentration n. Express your answer in cm^{-3}.

Key:
(a) Let's consider a rectangular shaped sample as shown below with an applied current density $\vec{J}_x$
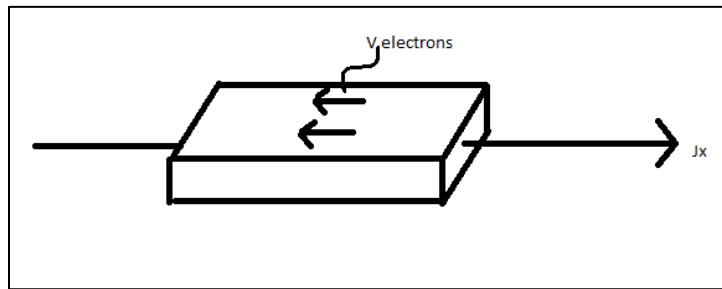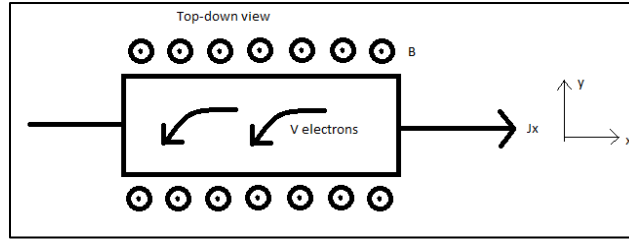

Now we place the sample under the influence of a magnetic field B in the $\hat{z}$ direction
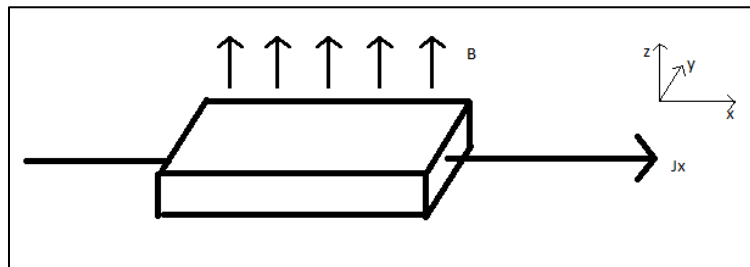

According to the Lorentz Force, given by
$$\vec{F} = -e(\vec{E} + \vec{v} \; x \; \vec{B})$$
The trajectory of the electrons will be deflected. According to this equation and the specific geometry of this set up, the electrons will be deflected in the $-\hat{y}$ direction.

Top-down view

B

V electrons

Jx

y

x

The deflection of the electron trajectory will cause a buildup of electronic charge on one side of the sample and a buildup of positive ion charge on the other

Top-down view

+ + + + +

− − − − −

Jx

y

x
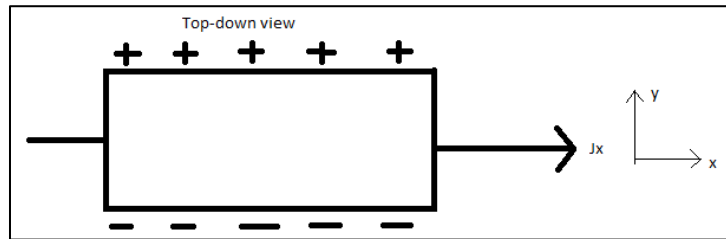
This creates its own Electric field E_y. This buildup of charge will continue to happen until the electric field E_y (the Hall Field) cancels out the Lorentz Force due to the magnetic field on the electrons. In the steady state, it will look like

Ex

B

+ + + + +

− − − − −

V electrons

Ey

Jx
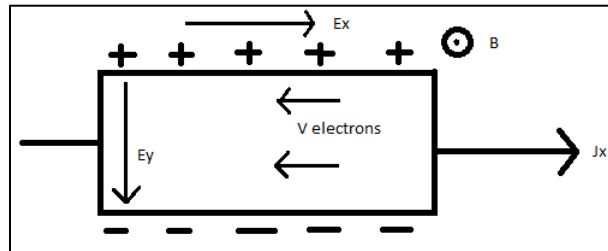
This buildup of charge due to an external magnetice field and an applied current density is the essence of the Hall Effect. The quantity given by

$$R_H = \frac{E_y}{J_x B}$$

Is the Hall Coefficient. For this set up, the Hall Coefficient should be negative because E_y is negative.

(b) There are a couple of differences when assuming positive charge carriers. The first is that the holes will travel in the same direction as J_x
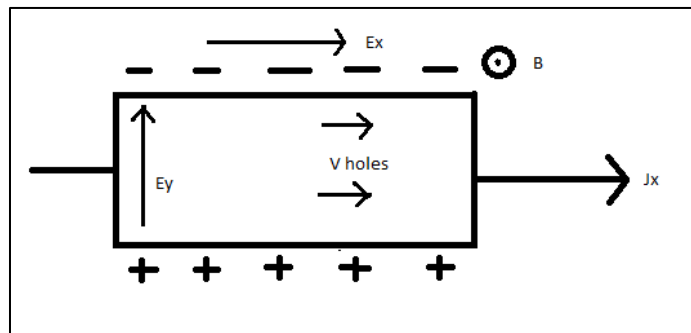
V holes

Jx
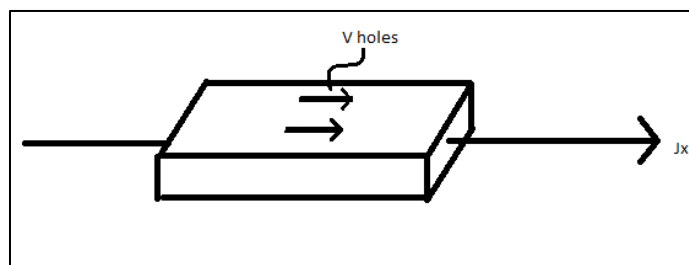
The second is that the Lorentz Force will be given by
$$\vec{F} = e(\vec{E} + \vec{v} \times \vec{B})$$
When the magnetic field is applied, the holes will be deflected as follows:
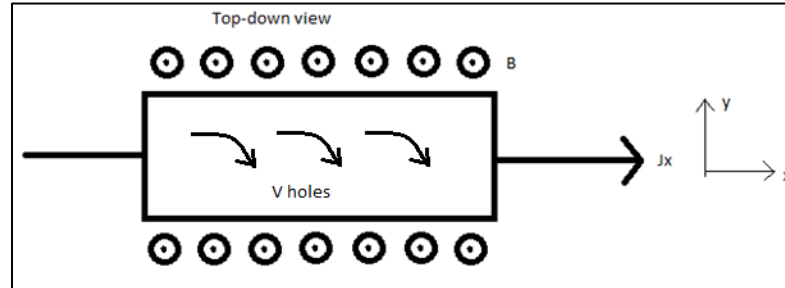
This results in the following steady state configuration:

This time the charge build up is flipped, meaning that the Hall Coefficient will now be positive

(c) When the steady state has been established
$$\vec{F}_{Lorentz} = \vec{F}_{Hall\ Field} = eE_y$$

$$E_y = \frac{F_{Lorentz}}{e} = \frac{(1.6\ x\ 10^{-24}\ N)}{(1.6\ x\ 10^{-19}\ C)}$$
$$E_y = 1\ x\ 10^{-5}\frac{N}{C}$$

Now we can use the relation
$$R_H = \frac{E_y}{J_x B}$$
To find the Hall Coefficient. Plugging in, we find

$$R_H = \frac{1\ x\ 10^{-5}\frac{N}{C}}{\left(0.4\ \frac{A}{m^2}\right)(1\ T)} = \frac{1\ x\ 10^{-5}\frac{kg\ *\ m}{C\ *\ s^2}}{\left(0.4\ \frac{A}{m^2}\right)\left(1\ \frac{kg}{A\ *\ s^2}\right)} = 2.5\ x\ 10^{-5}\frac{m^3}{C}$$
$$R_H = \left(2.5\ x\ 10^{-5}\frac{m^3}{C}\right)\left(\frac{100\ cm}{1\ m}\right)^3$$

$$R_H = 25 \, \frac{cm^3}{C}$$

(d) Recall that the Hall Coefficient is related to the carrier concentration through

$$R_H = \frac{1}{ne}$$

So then

$$n = \frac{1}{R_H e}$$

$$n = \frac{1}{\left(25 \, \frac{cm^3}{C}\right)(1.6 \, x \, 10^{-19} \, C)}$$

$$n = 2.5 \, x \, 10^{17} \, \frac{electrons}{cm^3}$$

2. Kittel states that almost any simple attempt to improve upon the free electron model is enormously profitable. With this in mind,
   (a) What must be taken into account to extend the free electron model to the nearly free electron model and understand the difference between conductors and insulators?
   (b) What effect may possibly emerge in the electronic structure of the solid as a consequence of this extension?
   (c) What is the cause of this emergent phenomenon?
   (d) In terms of parts (b-c), why does this phenomenon occur?
   (e) Given the potential energy function

$$U(x) = U cos\left(\frac{2\pi x}{a}\right),$$

And the probability densities at the first Brillouin zone boundary:

$$p(+) \approx cos^2\left(\frac{\pi x}{a}\right)$$

and,

$$p(-) \approx sin^2\left(\frac{\pi x}{a}\right)$$

Find the difference (band gap energy) between the two solutions at the 2nd Brillouin zone boundary i.e. $k=2\pi/a$ (Hint: $cos^2(x) - sin^2(x) = cos(2x)$.
   (f) Now assume that the potential has a 2nd order periodic component that has a period a/2 and redo problem.
   i.e. $k=\pi/a$ (Hint: $cos^2(x) - sin^2(x) = 2cos^2(x) - 1$

Key: (a) The periodic nature of a crystal structure so we need to introduce a periodic potential energy function with a periodicity equal to the lattice. Since it is a periodic function we can most probably write

it as a Fourier series in terms of reciprocal lattice vectors (similar to the way we described the electron density in chapter 2, equation 9 page 28)

(b) I expect that the electronic structure of the solid will show energy bands and band gaps in between them. The energy bands will be areas of large density of states. The bandgaps indicates energy intervals for which no stationary states do exist in the material.

(c) The bandgaps emerge because of the periodic nature of the potential energy function of the valence electrons.

(d) Wavelike stationary solutions of the Schrodinger equation do not exist for certain energy intervals referred to as the bandgaps. States still exists in those energy intervals but they are not stationary (not steady states) that means an electron in the bandgap will lose energy as a function of time. Quantum mechanically an electron with an energy in the bandgap will be Bragg relflected because of the periodic potential from the positive ion cores. Wave-function are no longer traveling waves but standing waves near the Brillouin zone boundary.

(e) Note that my probability densities are now

$$P(+) = A\cos^2\left(\frac{2\pi x}{a}\right)$$

$$P(-) = A\sin^2\left(\frac{2\pi x}{a}\right)$$

$$E_g = A^2\int_0^a dx\, U\cos\left(\frac{2\pi x}{a}\right)\left(\cos^2\left(\frac{2\pi x}{a}\right) - \sin^2\left(\frac{2\pi x}{a}\right)\right) = A^2\int_0^a dx\, U\cos\left(\frac{2\pi x}{a}\right)\left(2\cos^2\left(\frac{2\pi x}{a}\right) - 1\right) =$$

$$A^2\int_0^a dx\, U\cos\left(\frac{2\pi x}{a}\right)2\cos^2\left(\frac{2\pi x}{a}\right) - A^2\int_0^a dx\, U\cos\left(\frac{2\pi x}{a}\right) = 2UA^2\int_0^a dx\cos^3\left(\frac{2\pi x}{a}\right) = 0$$

Since the cosine cube function is periodic with period a and symmetrical around zero.

(f) Note that we are still looking at the 2nd zone boundary so probability density functions are still:

$$P(+) = A\cos^2\left(\frac{2\pi x}{a}\right)$$

$$P(-) = A\sin^2\left(\frac{2\pi x}{a}\right)$$

However the potential is now described by:

$$U(x) = U_o\cos\left(\frac{4\pi x}{a}\right)$$

$$E_g = A^2 U_o\int_0^a \cos\left(\frac{4\pi x}{a}\right)\left(\cos^2\left(\frac{2\pi x}{a}\right) - \sin^2\left(\frac{2\pi x}{a}\right)\right)dx = A^2 U_o\int_0^a \cos\left(\frac{4\pi x}{a}\right)\left(\cos\left(\frac{4\pi x}{a}\right)\right)dx = A^2\frac{a}{2}U_o$$

The normalization constant can be calculated from the normalization condition over one period, i.e.

$$\int_0^a \psi^*\psi dx = \int_0^a A^2\cos^2\left(\frac{2\pi x}{a}\right)dx = A^2\frac{a}{2} = 1 \Rightarrow A = \frac{\sqrt{2}}{a}$$

Or in other words the bandgap at the 2nd Brillouin zone boundary is equal to Uo, i.e. the amplitude of the a/2 sinusoidal component in the potential energy. Note that in general the potential energy is not sinusoidal but contains all kind of higher harmonics (see also fig. 3 page 166 in Kittel. The higher harmonics determine the bandgaps at higher zone boundaries in the extended zone scheme. Furthermore notice that one normally only refers to the gap between the highest occupied band and the lowest unoccupied band as the bandgap of the material.

3. Consider the Kronig-Penney model. For the delta-function potential and with P≪1, find at k=0 the energy of the lowest energy band.

Key: From eq. (21b) on chapter 7 on pag. 169 on kittel, we have:

$$\left(\frac{P}{Ka}\right)\sin(Ka) + \cos(Ka) = \cos(ka)$$

When k=0, then cos (ka) = 1,

When P=0, then K=0, so when P≪1 → Ka≪1

Then, for a small Ka:

$$\left(\frac{P}{Ka}\right)[Ka+(Ka)^3] + \left[1 - \frac{1}{2}(Ka)^2+(Ka)^4\right] = 1$$

If we ignore the quadratic term in Ka we get

$$P + P(Ka)^2 + 1 - \frac{1}{2}(Ka)^2 = 1 \rightarrow P = \left(\frac{1}{2} - P\right)(Ka)^2 \rightarrow K^2 = \frac{P}{\left(\frac{1}{2} - P\right)a^2}$$

So we have that the energy is:

$$\varepsilon = \frac{\hbar^2 K^2}{2m}$$

$$\varepsilon \approx \frac{\hbar^2 P}{(1 - 2P)ma^2}$$

Note that 1-2P is approximately equal to 1.

4. Consider free electron gas in two dimensions.

(a) Write down the free-particle Schrödinger equation in two dimensions by using wavefunction ψ(r).

(b) If the electrons are confined to a cube of edge L, the wave function is the form of a traveling wave. Write down the wave-function by using the exponential function and wave-vector k.

(c) Show that the component of the wave-vector k_x and k_y are 0, $\pm\frac{2\pi}{L}, \pm\frac{4\pi}{L}$ ... by using periodic boundary conditions.

(d) In the ground state of a system of N free electrons, the occupied orbitals may be represented as points inside a circle in k space. The energy at the edge of the circle is the Fermi energy. Find the density of states $D(\varepsilon)$ in two dimensions and show that $D(\varepsilon)$ is independent of energy ε.

Key: (a) $-\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2})\psi(r) = \varepsilon\psi(r)$

(b) $\psi(r) = e^{ik\cdot r}$

(c) Boundary condition: $\psi(x+L,y) = \psi(x,y)$ and $\psi(x,y+L) = \psi(x,y)$

$e^{ik_xL} = 1$ then k_x are 0, $\pm\frac{2\pi}{L}, \pm\frac{4\pi}{L}$ ... and similarly for k_y

(d) $D(\varepsilon) = \frac{dN}{d\varepsilon}$ where N is the total number of orbitals. $N = 2\frac{\pi K_F^2}{(\frac{2\pi}{L})^2} = 2\frac{\pi\frac{2m\varepsilon}{\hbar^2}}{\frac{4\pi^2}{A}} = \frac{Am\varepsilon}{\pi\hbar^2}$

$D(\varepsilon) = \frac{Am}{\pi\hbar^2}$ is independent of ε.

5. Consider a simple cubic metal with lattice constant a and one free electron per atom at 0K temperature.
   (a) find Fermi energy ε_f and k_f, $D(\varepsilon)$
   (b) find the total electronic thermal kinetic energy.
   (c) prove that $p = 2U/3a^3$

Key:

(a) $k_f = (3\pi^2 N/v)^{1/3} = (3\pi_2/a^3)^{1/3}$
   $\varepsilon_f = h^2 k_f^2/2m = h^2(3\pi^2/a^3)^{2/3}/2m$
   $D(\varepsilon) = dN/d\varepsilon = d((v/3\pi^2)(2m\varepsilon/h^2)^{3/2})/d\varepsilon = (v/2\pi^2)(2m\varepsilon/h^2)^{3/2}\varepsilon^{1/2} = (a^3/2\pi^2)(2m\varepsilon/h^2)^{3/2}\varepsilon^{1/2}$

(b) $U = \int_0^{\varepsilon f} \varepsilon D(\varepsilon)d\varepsilon = (V/2\pi^2)(2m/h^2)^{3/2}(2/5 \varepsilon_f)^{5/2} = (a^3/2\pi^2)(2m/h^2)^{3/2}(2/5 \varepsilon_f)^{5/2}$
(c) $W = dU = -pdV$
   $P = -dU/dV = -d((V/2\pi^2)(2m/h^2)^{3/2}(2/5 \varepsilon_f)^{5/2})/dV = 2U/3a^3$
   ($\varepsilon_f = h^2 k_f^2/2m = h^2(3\pi^2/a^3)^{2/3}/2m = constant*1/V^{2/3}$)

6. The atom He^3 has spin ½ and is a fermion. The density of liquid He3 is 0.081 g cm-3 near absolute zero. Calculate the Fermi energy eF and the Fermi temperature TF.

Key:

5. The number of moles per cm^3 is $81 \times 10^{-3}/3 = 27 \times 10^{-3}$, so that the concentration is 16×10^{21} atoms cm^{-3}. The mass of an atom of He^3 is (3.017) $(1.661) \times 10^{-24} = 5.01 \times 10^{-24}$ g. Thus $\varepsilon_F = [(1.1 \times 10^{-54})/10^{-23}][(30)(16) \times 10^{21}]^{2/3} \approx 7 \times 10^{-16}$ erg, or $T_F \approx 5K$.

7. (a) The Fermi energy of the highest occupied state is given by:

$$E_F = \frac{\hbar^2}{2m} k_F^2 = \frac{\hbar^2}{2m} \left(3\pi^2 \frac{N}{V}\right)^{2/3}$$

Assume that the density of copper is 8.96 gm/cm3, that the atomic weight of copper is 63.5 gm/mol, and that each copper atom contributes one conduction electron.

(b) What is the corresponding electron velocity? Is it safe to assume that the electrons in copper are non-relativistic?

(c) At what temperature would the characteristic thermal energy ($k_B T$) be equal to the Fermi energy for copper? Show that this temperature is substantially below the Fermi temperature.

Key: (a) EF=7 eV, N/V=8.5E28 electrons/cm3.

(b) Use $E_F = \frac{1}{2} m_e v^2 \Rightarrow v = \sqrt{\frac{2E_F}{m_e}}$, plugging in the numbers give 1.6E6 m/s, so v=5.3E-3c,

so no relativistic corrections are required.

(c) kB=1.38E-23 J/K, EF=kBTF, TF=8.1E4 K. Note that the copper melting temperature is 1356 K so the Fermi temperature is very high.

8. Describe the principle physical processes that account for the resistivity and explain the temperature dependence of the resistivity in the low and the high temperature region. Assume that the free carrier concentration stays constant (note that this is often not the case for semiconductor materials). Use in your discussion mean free path, mean time between collisions, and scattering cross section. The latter parameter was not discussed in Kittel but is of used to describe scattering phenomena between two particles. One of the particles is kept fixed (target) while the other is treated as an incident projectile. In our case the target particles are the defects and the incident particles are the electrons. The cross sectional area of the fixed particles (expressed in m²) tells you how easily it is to hit the particle. The cross sectional area can be calculated from the number of target particles N, the incident particle flux Φ, and 1/τ, the scattering frequency (scattering rate):

$$\frac{1}{\tau} = \sigma N \Phi \Rightarrow \sigma = \frac{1}{\Phi N \tau} \qquad\qquad [1]$$

Note that the unit of flux is m⁻²s⁻¹ and that τ has the units of seconds, so σ should have the units of m². The cross sectional area depends on the type of interaction between the target and incident particles: for example the scattering of an electron of an impurity is much larger for a charged impurity as for a neutral impurity. Even if the electron will pass the charged impurity at 5 lattice distances, it still feels the impurity's presence. Equation [1] is well known in particle physics. Assuming that the incident particle flux is one particle per

sec per A m^2 (where A is the cross sectional area), we can write for a single incident particle:

$$\sigma = \frac{A}{N\tau}$$ [2]

We can replace the mean time between scattering events by an expression in mean free path and average speed. For electrons it is best to use the Fermi velocity for the speed since only the electrons around the Fermi-level significantly contribute to the charge transport (see also discussion 147-152 in Kittel); so we will replace τ by l_o/v_F where l_o is the mean free path and v_F is the Fermi velocity, i.e. the velocity of the electrons near the Fermi level. For the velocity of the electrons I take the Fermi velocity, i.e. v_F, as it are only the electrons around the Fermi-level that contribute to the electric conduction as they are the only electrons that can find an unoccupied state at approximately the same energy. Electrons far below the Fermi-level will not contribute to charge transport as they will not be able to change state as they cannot find an empty state with a different momentum vector but with approximately the same energy that is unoccupied. We also multiply by A on both sides:

$$\sigma = \frac{Av_F}{Nl_o}$$ [3]

Note that the incident particle has a chance to hit any imperfection in the volume AvF. So N/(AvF) is the concentration of defects n. So I can rewrite [3] by:

$$n = \frac{1}{\sigma l_o} \Rightarrow \sigma = \frac{1}{nl_o}$$ [4]

This equation is often used in materials physics as it related defect concentration mean free path and cross sectional area. Notice that an electron moving towards the right will definitely scatter after it moved lo toward the right, so I need one defect in that volume defined by σ and l_o. which explains equation [4].

λo
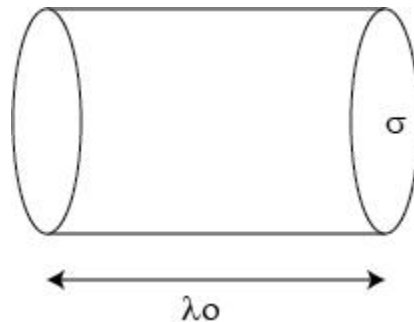
Key: If the lattice of a metal is perfect and there are no lattice vibrations, electron waves would pass through the lattice un-scattered without resistance. In the actual metal the free electrons suffer scattering by distortions of the periodic potential field due to thermal vibrations of the lattice atoms and by some structural irregularities such as impurities and

defects in the crystal, giving rise to an electrical resistivity. Thus the resistivity of a metal can be considered as the sum of the effect of phonons and the effect of imperfections in the crystal structure, i.e.

$$\rho = \rho_{phonon} + \rho_{impurity}$$

Notice that resistivity is caused by imperfections and scales proportional to the concentration of the imperfections. So the more imperfections the larger the resistivity.

At low temperature I expect the scattering by phonons to be negligible. So the mean time between phonon scattering becomes infinitiy and thus ρ will go to zero (see also equation [43] in the text):

$$\rho_i = \frac{m}{ne^2\tau} = \frac{m}{ne^2\tau_i} = \frac{mv_F}{ne^2l_i} = \frac{mv_F}{ne^2}n_i\sigma_i$$

Where n is the free electron concentration, n_i is the impurity concentration, v_F is the Fermi velocity and σ_i the impurity cross section. Note that ρ_i is constant independent of the temperature for this case.

For high temperature: as T increase scattering by phonons becomes more effective. When T become sufficiently large scattering by phonons dominate, i.e.

$$\rho = \rho_{phonons}$$

For phonons, calculating ρ_{phonon} involves electron-phonon interaction. However we can write:

$$l_{phonon} = \frac{1}{n_a\sigma_a}$$

Where l_{phonon} is the mean free path of an electron that is eventually scattered by a phonon, σ_a is the cross section per atom because of phonon scattering, and n_a is the concentration of host atoms in the lattice. Notice that this is a very simple model as it assumes that each individual atom is a harmonic oscillator and has a cross sectional area unequal to zero that can scatter a conduction electron. If we assume that the cross sectional area of the atom is proportional to the expectation value of x square, i.e. $<x^2>$, and we estimate $<x^2>$ to be proportional to k_BT (equipartition theorem) we get:

$$\sigma_a \propto \left\langle x^2 \right\rangle \propto \frac{k_BT}{C}$$

Where C is the elastic stiffness constant. So after substituting this in the expression for the resistivity we see that the resistivity is time dependent:

$$\rho_{phonon} = \frac{mv_F}{ne^2 l_{phonon}} = \frac{mv_F}{ne^2} n_a \sigma_a \propto \frac{mv_F}{ne^2} n_a \frac{2k_B T}{C}$$

Of course we can use a more advanced model and assume that phonons are traveling waves, i.e. the neighboring atoms interact following Debye's approach but now for electrical resistivity. Such approach will show that for Silicon and Germanium the electrons mainly interact with acoustical phonons resulting in a temperature dependence of the resistivity following $T^{3/2}$ behavior, while for the phonon scattering of optical phonons shows a $T^{0.5}$ temperature dependence.

9. Calculate the density of states for electrons in 1D. Use the following steps:

a. Find the Fermi level.

b. Find the number of orbitals in terms of energy ε.

c. Find the density of states in terms of energy ε.

Key: a. For periodic boundary conditions I find the following k-vectors for 1D:

$\quad\quad$ k=0, k=+/- 2π/L, +/- 4π/L, ... $\hfill$ [1]

So in k-space there are L/2π grid points per unit length. My k-space are below the Fermi level is $-k_F < k < k_F$, so 2 k_F which results in the following number of grid points:

$\quad\quad$ L/(2π) * 2 k_F = Lk_F/π $\hfill$ [2]

Number of quantum states. I have spin up and spin down so I have totally:

$\quad\quad$ 2L/(2π) * 2k_F = N $\hfill$ [3]

So in other words:

$$N = \frac{2Lk_F}{\pi} \rightarrow k_F = \frac{N\pi}{2L} \hfill [4]$$

In 1D the relation between k_F and ε_F is given by:

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m} \rightarrow \varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{N\pi}{2L}\right)^2 = \left(\frac{\hbar^2 \pi^2 N^2}{8mL^2}\right) \hfill [5]$$

b. We can convert equation [5] into an expression for the number of orbitals below an arbitrary ε, i.e.

$$N(\varepsilon) = \frac{2L}{\pi}\sqrt{\frac{2m\varepsilon}{\hbar^2}} \hfill [6]$$

c. Now take the derivative of N(e) we find:

$$D(\varepsilon) = \frac{dN}{d\varepsilon} = \frac{d}{d\varepsilon}\left[\frac{2L}{\pi}\sqrt{\frac{2m}{h^2}}\sqrt{\varepsilon}\right] = \frac{L}{\pi}\sqrt{\frac{2m}{h^2}}\frac{1}{\sqrt{\varepsilon}}$$ [7]

10. The free electron model for metal suggests that the conduction electrons can be approximated by a gas of free electrons where the only important parameters for the gas are n, the number of density of electrons and τ the time between collisions. Show that in the model the electric conductivity of a metal can be expressed as,

$\sigma = (ne^2\tau)/m$ [1]

Estimate the collision time for an electron in copper. The resistivity in copper metal is 1.7 x 10^{-6} ohm cm and the atomic density of copper is 8.5 X 10^{22} atoms /cm.

Key: For a free electron the momentum p and the wave vector k are related by, p =hk. The equation if its motion in an applied force field F is given by the Newton's second law.

F = dp/dt = (ℏ)dk/dt

While the vectors of all electrons increase parallel to the applied force , an equilibrium state will be reached with the electron reverting to their original states by collations with the lattice ions in a relaxation time for collision τ , given by ,

$\delta k = \tau F/ℏ$

δk is the change is in wave vector k from the equilibrium value. The corresponding change in velocity is ,

$\delta v = \delta p/m = k\delta k/m = \tau F/m$

If the applied electric field is E, the force acting on each electron is given by ,

F = -eE

Hence the induced current density is given by,

J = -neδv = ne$^2\tau$E/m = σE, this implies that, σ = ne$^2\tau$/m

The collision time τ is given by,

$\tau = m\sigma/ne^2 = m/ne^2\rho$

b. If each copper atom contributes one free electron, then n = 8.5 x 10^{28} m^{-3}

τ = (9.11 x 10^{-31})/(8.5 x 10^{28}x(1.6 x 10^{-19})^2 x1.7 x 10^{-8}) = 2.5 x 10^{-14} s

11. Find the magnitude of the energy gap for a square potential energy assuming the wave-function are standing waves near the first Brillouin zone boundary, i.e. the wave-functions

have a period equal to twice the lattice parameter, i.e. 2*(2a)=4a. Assume that the potential energy function is –Uo between –a/2 and a/2, is 0 between a/2 and 3a/2, is again –Uo between 3a/2 and 5a/2, etc. Proceed with the following steps:

a. Sketch the low energy wave-function Ψ+(x) and its probability |Ψ+(x)|² in the figure below (i.e. we are looking for the wave-function at the first Brillouin zone boundary).

b. Sketch the low energy wave-function Ψ-(x) and its probability |Ψ-(x)|² in the figure below (i.e. we are looking for the wave-function at the first Brillouin zone boundary).

 c. Are |Ψ+(x)|² and |Ψ-(x)|² consistent with the Bloch theorem?

d. Calculate the expectation value for the potential energy near the first Brillouin boundary.
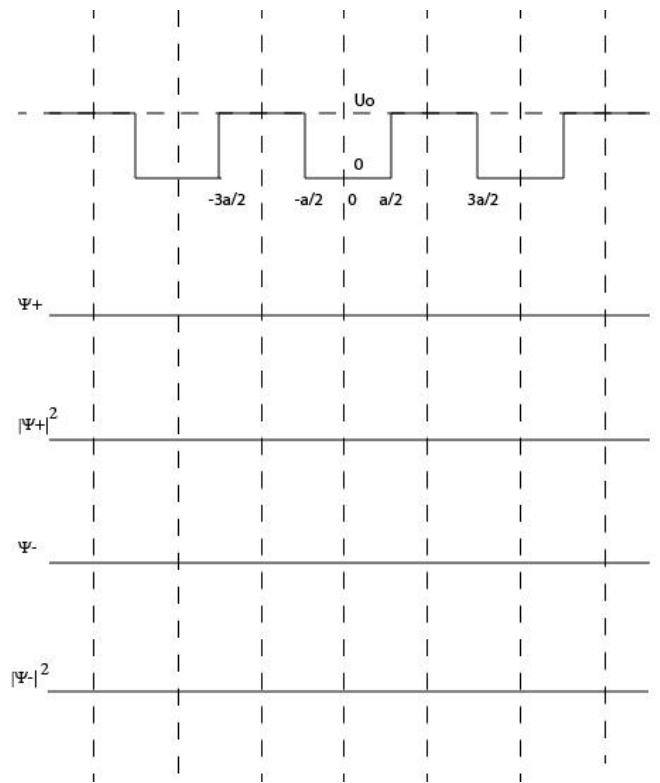
a. See figure below.
b. See Figure below.
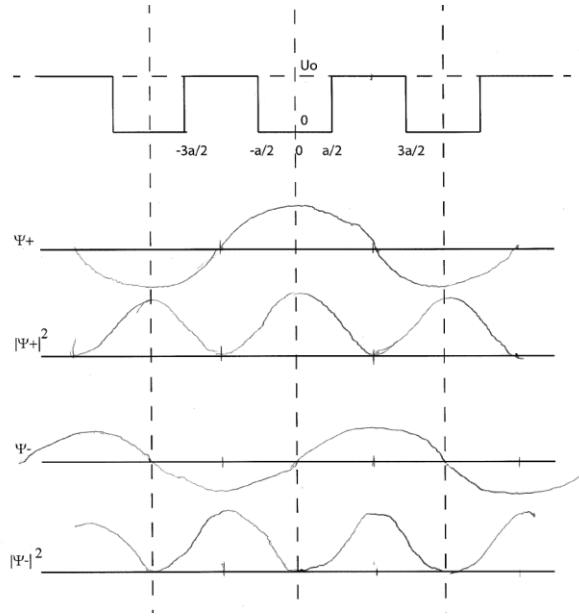
c. I expect the probability density function to be the same around each lattice point, i.e. at x=2a, x=4a etc. because of the Bloch theorem, i.e.

$$\psi^*\psi = \left(u_k(\vec{r})e^{i\vec{k}\bullet\vec{r}}\right)^*\left(u_k(\vec{r})e^{i\vec{k}\bullet\vec{r}}\right) = \left((u_k(\vec{r}))^* e^{-i\vec{k}\bullet\vec{r}}\right)\left(u_k(\vec{r})e^{i\vec{k}\bullet\vec{r}}\right) = \left|u_k(\vec{r})\right|^2\left(e^{-i\vec{k}\bullet\vec{r}}e^{i\vec{k}\bullet\vec{r}}\right) = \left|u_k(\vec{r})\right|^2$$

d. Now:

$$E_g = \int_{-a/2}^{a/2} U_o A^2\left(\cos^2\left(\frac{\pi x}{2a}\right) - \sin^2\left(\frac{\pi x}{2a}\right)\right)dx = \int_{-a/2}^{a/2} U_o A^2 \cos\left(\frac{\pi x}{a}\right)dx$$

.

$$= U_o A^2 \frac{a}{\pi}\sin\left(\frac{\pi x}{a}\right)\Bigg|_{-a/2}^{a/2} = 2U_o A^2 \frac{a}{\pi}$$

We can find the A from the normalization condition similarly as shown in problem 2 above, so A = $\sqrt{2}/a$, resulting in E$_g$=U$_o$/π. Note that for this problem it can be easily shown that there are also band gaps at the higher zone boundaries.

12. Consider one dimensional metal of length (L) with atoms regularly spaced in a distance σ apart in the tight binding approximation, with one electron per atom. The atomic wave functions are of the form $\psi(r - r_i)$, with r_i being the position of the nucleus of the ith atom. ($r_i = i\sigma$, the nucleus will be considered to be fixed in space). Assume that,

$\int \psi * (r - r_i) H\psi(r - r_i)dr = -E_0$

$\int \psi * (r - r_i) H\psi(r - r_{i+1})dr = -V$

$\int \psi * (r - r_i) H\psi(r - r_{i+j})dr = 0$, with $j \geq 2$, where H is the Hamiltonian

a) Calculate and plot the electronic band structure (E_k vs. k), (plot of band structure in the first Brillouin zone only).

b) Calculate and plot the electronic density of states (ρ vs. E)