ECE 4070, Spring 2017
Physics of Semiconductors and Nanostructures
Handout 4070

Problems

Present your solutions *neatly*. Do not turn in rough unreadable worksheets - learn to **take pride in your presentation**. Show the relevant steps, so that partial points can be awarded. $\boxed{\text{BOX}}$ your final answers where applicable. Draw figures wherever necessary. Always provide the analytical answer before finding numerical values. **Please print out the question sheet(s) and staple to the top of your homework.** Write your name, email address, and date/time the assignment is turned in on the cover. Assignments must be turned in before class on the due date. The time the assignment is turned in should be written. There will be a 10% penalty each day of delay, and assignments will not be accepted beyond 3 days after the due date. There will be no exceptions to this rule. You are allowed to work with other students in the class on your homeworks. The name(s) of the student(s) you worked with must be included in your homework. But what you turn in must be in your *own* writing, and have your *own* plots and figures. Turning in plots/figures/text that are exact replicas of others *is considered cheating*.

4070.1 HW 1

Posted: 02/04/2017, Due: 02/13/2017

Problem 1: Semiconductor History

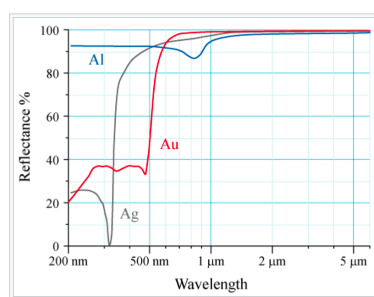
Write a short <1-page critique of the paper "The History of Semiconductors" handed out in class.

Problem 2: Mirror Mirror on the Wall

Believe it or not, coating glass with metal to make make a mirror was a *big* technological breakthrough back in the time [1]. In this problem, we answer why metals are shiny - why they reflect most of the visible light incident on them. Not surprisingly, this has to do with the conduction electrons in the metal. Here is our mode of attack: when the light wave experiences a mismatch in the refractive index, part of it is transmitted, and part reflected. So we will ask Maxwell's equations to give us the reflection coefficient when a light beam is incident from air on a metal. If we find that this reflection coefficient is very high for visible wavelengths, we have succeeded in explaining why metals are shiny.

The reflection coefficient Γ_r will depend on the refractive index $\sqrt{\epsilon(\omega)}$ of the metal, which in turn will depend on how the conduction electrons respond to the oscillating electric field of the light beam. This is where Drude's free electron model of the metal - the same model that explained electrical and thermal conductivity - will help us through.

Figure 4070.1 shows the measured reflectance of three common metals as a function of the wavelength of light incident on it. Your job in this problem is to calculate and make your own plot by standing on Maxwell, Drude, and Newton's shoulders. If things go right,



Spectral reflectance curves for aluminium (Al), silver (Ag), and gold (Au) metal mirrors at normal incidence.

Fig. 4070.1: Reflectance spectra of three metals from Wikipedia

[1] Quite possibly marking the birth of fashion?

you may even explain the dips and wiggles in figure 4070.1. I will roughly outline the method and trust you can finish the story:

The electric field of the light beam according to Maxwell oscillates in time as $E(t) = E_0 e^{i\omega t}$, where E_0 is the amplitude, and $\omega = 2\pi f$ is the radial frequency, $f = c\lambda$ with c the speed of light, and the wavelength λ of light is the $x-$axis in the plot. The reflection coefficient for light is $\boxed{\Gamma_r = \frac{E_r}{E_i} = \frac{\sqrt{\epsilon_0} - \sqrt{\epsilon(\omega)}}{\sqrt{\epsilon_0} + \sqrt{\epsilon(\omega)}}}$, where $\sqrt{\epsilon}$ is the refractive index of the media. The reflectance is $R = |\Gamma_r|^2$, which can be found for various wavelengths; this is the $y-$axis of the plot. Note that all symbols have their usual meanings.

(a) From Maxwell's equation $\nabla \times \mathbf{H} = \mathbf{J} + i\omega\epsilon_0 \mathbf{E}$ in material media, show that the dielectric constant of the metal is $\boxed{\epsilon(\omega) = \epsilon_0[1 + i\frac{\sigma(\omega)}{\omega\epsilon_0}]}$.

(b) Now if you have the frequency-dependent conductivity $\sigma(\omega)$, you can make your plot by looking up the properties of the metal! But we have only covered the DC Drude model for conductivity in class, where we obtained $\sigma(0) = \frac{nq^2\tau}{m_e}$. Here you need to use Newton's laws again and solve to show the following:

$$qE_0 e^{i\omega t} = m_e \frac{dv}{dt} - \frac{m_e v}{\tau} \implies \boxed{\sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau} = \underbrace{\frac{\sigma_0}{1 + (\omega\tau)^2}}_{\mathrm{Re}(\sigma(\omega))} + i \underbrace{\frac{\omega\tau\sigma_0}{1 + (\omega\tau)^2}}_{\mathrm{Im}(\sigma(\omega))}}. \tag{4070.1}$$

(c) Now you are close to the finish line. Use the above modified Drude ac conductivity, look up the required properties of the three metals, and plot the reflectances of all the three metals. Compare with figure 4070.1.

Problem 3: Lord of the Ring

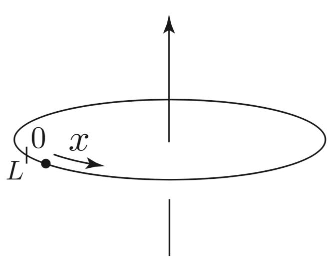


Fig. 4070.2: Electron on a ring

We derived in class that the allowed wavefunctions representing an electron on a circular ring of circumference L is $\psi_n(x) = \frac{1}{\sqrt{L}} e^{ik_n x}$, where $k_n = \frac{2\pi}{L} n$ are *quantized* because $n = 0, \pm 1, \pm 2, ...$ The *angular momentum* of a particle is defined as $\mathcal{L} = \mathbf{r} \times \mathbf{p}$, where $\mathbf{r}$ is the 'radius' of the circle, and $\mathbf{p}$ is the linear momentum.

(a) Show that the angular momentum of an electron in state $\psi_n(x)$ is $\mathcal{L}_n = n\hbar$, where $\hbar = \frac{h}{2\pi}$ is the 'reduced' Planck's constant. This implies that the angular momentum is *quantized* to values $0, \pm\hbar, \pm 2\hbar, ...$ Compare the quantized angular momentum $\mathcal{L}_1$ for $n = +1$ with the classical angular momentum $\mathcal{L}_{cl}$ of a mass $m = 1$ kg being spun by a string of length $R = 1$ m with tangential velocity $v = 1$ m/s to appreciate how 'nano' is the quantum of angular momentum.

(b) By balancing the classical centrifugal force and the electromagnetic Lorentz force, show that for an electron to be in the quantum state $\psi_n(x)$ on the ring, we need a *magnetic* field B_n such that the magnetic flux is $\Phi_n = B_n \cdot A = n \times \frac{h}{2e}$. Here A is the area of the ring, e is the electron charge and $h = 2\pi\hbar$. $\Phi_0 = \frac{h}{2e}$ is known as the *quantum of magnetic flux*, and has been measured experimentally in nanostructured rings.

(c) Consider the quantum state obtained by the superposition $\psi(x) = a[\psi_{n=1}(x) + \psi_{n=-1}(x)]$ from the eigenstates of the electron on the ring. Normalize the state to find the constant a. You may need the result $\int_0^L \cos^2(\frac{2\pi}{L}x)dx = \frac{L}{2}$. Does this superposition state have a definite momentum?

(d) We derived that the quantum expression for current flux is $\mathbf{j} = \frac{1}{2m}(\psi^\star \hat{\mathbf{p}}\psi - \psi\hat{\mathbf{p}}\psi^\star)$, where $\hat{\mathbf{p}} = -i\hbar\nabla$ is the momentum operator, which takes the form $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$ for the particle on the ring. Show that even though the states $\psi_{n=1}(x)$ and $\psi_{n=-1}(x)$ carry *net* currents, their superposition state of part (c) does not. Explain.

Problem 4: Born to be free

We discussed in class that because of the Pauli exclusion principle, Fermions must follow the Fermi-Dirac distribution, and they have half-integer spins. Now imagine we have a metal with $n = 10^{23}/\text{cm}^3$ electrons in a cubic box of side L, and we know that electrons are Fermions. Assume the electrons are completely free to move around in the box, meaning there are no atoms in their way. If that that much freedom is not enough for you, how about this: completely neglect the Coulomb interactions due the charge of the electrons![2] Find the following at $T = 0$K:

[2] This may all be very unsettling, but we will explain later why it is actually OK to do so - because with great freedom comes great responsibility! In fact this problem could be formulated for *any* Fermion - for example the uncharged neutron - and the analytical answers will be the same.

(a) The Fermi wavevector k_F.

(b) The Fermi momentum p_F.

(c) The Fermi energy E_F.

(d) The *average* energy of electrons $u = \frac{U}{N}$. What is the origin of this energy?

(e) What is the average energy of the electrons if they did not follow quantum mechanics, but were subject to classical mechanics?

Fig. 4070.3: Andre Geim

Problem 5: Graphene Density of States, Fermi-Dirac distribution

The electrons in the conduction band of graphene are free to move in 2-dimensions, forming a 2-dimensional electron gas (2DEG). The energy-momentum dispersion relationship for the 2DEG electrons in graphene is $E(k_x, k_y) = \hbar v_F\sqrt{k_x^2 + k_y^2}$, where v_F is a parameter with dimensions of velocity. For graphene, it is $v_F = 10^8$cm/s.

Fig. 4070.4: Kotsya Novoselov. Geim and Novoselov were awarded the Nobel prize in physics in 2010 for the discovery of graphene, the thinnest 2D crystal with remarkable electron transport properties.

(a) Make a sketch of the energy as a function of the (k_x, k_y) points in the 2D k-space plane, and show that the dispersion results in a conical shape.

(b) Show that the density of states for these electrons is $g(E) = \frac{g_s g_v}{2\pi(\hbar v_F)^2}|E|$, where $g_s = 2$ is the spin degeneracy of each (k_x, k_y) state, and g_v is the number of cones in the energy dispersion. For graphene, $g_v = 2$.

(c) Show that at thermal equilibrium, when the Fermi level is at $E_f = 0$, the number of conduction electrons per unit area in 2D graphene is $n_i = \frac{\pi}{6}(\frac{kT}{\hbar v_F})^2$. Make a plot of this density as a function of temperature for $0K \leq T \leq 500K$. Explain why your plot sets the bar on the lowest possible density of carriers achievable in graphene at those temperatures.

4070.2 HW 2

Posted: 02/18/2017, Due: 02/27/2017

Problem 6: Density of States of Electrons, Photons, and Phonons

(a) Show that for a parabolic bandstructure for electrons $E(k) = E_c + \frac{\hbar^2 k^2}{2m^\star}$ with band edge E_c and effective mass $m^\star$, the DOS for electron motion in d dimensions is

$$\boxed{g_d(E) = \frac{g_s g_v}{2^d \pi^{\frac{d}{2}} \Gamma(\frac{d}{2})} (\frac{2m^\star}{\hbar^2})^{\frac{d}{2}} (E - E_c)^{\frac{d}{2}-1}}, \tag{4070.2}$$

where g_s is the spin degeneracy, and g_v is the valley degeneracy. Here $\Gamma(...)$ is the Gamma function with property $\Gamma(x+1) = x\Gamma(x)$ and $\Gamma(\frac{1}{2}) = \sqrt{\pi}$. You may need the expression for the surface area of a $d-$dimensional sphere in $k-$space: $S_d = \frac{2\pi^{\frac{d}{2}} k^{d-1}}{\Gamma(\frac{d}{2})}$. Check that this reduces to the surface area of a sphere for $d = 3$ and the circumference of a circle for $d = 2$.

(b) Sketch the DOS for 3D, 2D, and 1D electron systems using the expression. Explain the roles of the valley degeneracy and the effective mass for Silicon and compound semiconductors.

(c) Show that the DOS for energy dispersion $E(k) = \hbar v k$ for 3 dimensions is

$$\boxed{g_\omega(\omega) = \frac{g_p \omega^2}{2\pi^2 \hbar v^3}}, \tag{4070.3}$$

where $\omega = vk$, and g_p is the polarization degeneracy. This is the dispersion for *waves*, such as photons and phonons moving with velocity v. The parabolic DOS of phonons and photons will play an important role in the thermal and photonic properties of semiconductors.

Problem 7: Sommerfeld's Coup

Fig. 4070.5: Arnold Sommerfeld introduced the quantum electron theory of the metal, and resolved the discrepancies of the Drude model. Was the advisor of a large cohort of Nobel prize winners, but was never awarded in spite of being nominated ∼80 times!

(a) Using the DOS you calculated in Problem 4070.6, find the *total energy* of N electrons in volume V at $T = 0$ K for 3D, 2D, and 1D electron gases with parabolic energy dispersion. Note that you already solved the 3D electron gas problem in Problem 4070.4.

(b) Now for the heat capacity $c_v = \frac{1}{V}\frac{dU}{dT}$, we need to find the total energy U at a non-zero temperature T. To do that, you can still use the fact that heating a bunch of electrons will not increase or decrease their number. Show[3] that for 3D electrons, the Fermi energy changes with temperature as

$$E_F(T) = E_F(0)[1 - \frac{1}{3}(\frac{\pi k_B T}{2E_F(0)})^2], \tag{4070.4}$$

(c) Show that the heat capacity of 3D 'quantum' electrons is then

$$c_v = \frac{\pi^2}{2} n k_B \frac{k_B T}{E_F(0)} \tag{4070.5}$$

(d) By comparing this form of the electron heat capacity with Drude's result $c_v = \frac{3}{2} n k_B$, can you explain why the heat capacity of the 'quantum' electrons is so much smaller than

[3] This is somewhat hard, but Sommerfeld did it ∼100 years ago!

the 'classical' electrons?

Problem 8: Quantum 2D Free Electrons in a Magnetic Field

Consider a 2D free electron gas confined to the x-y plane. In the Sommerfeld model, the energy of an electron with wavevector $\mathbf{k}$ is $E(\mathbf{k}) = \frac{\hbar^2 k^2}{2m_e}$, and the velocity is $\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}} E(\mathbf{k}) = \frac{\hbar \mathbf{k}}{m_e}$. Now suppose a DC magnetic field $\mathbf{B} = B_0 \mathbf{z}$ is switched on in the z-direction, as shown in Figure 4070.45.

In the presence of the magnetic field, because of the Lorentz force, the momentum of the electron satisfies the equation (assuming no electric field and no scattering)

$$q\mathbf{v}(\mathbf{k}) \times \mathbf{B} = \hbar \frac{d\mathbf{k}}{dt}, \tag{4070.6}$$

which is the quantum version of Newton's law, with the Lorentz force.

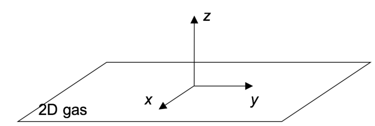


Fig. 4070.6: 2D Electron in a Perpendicular Magnetic Field

(a) In the k-space, if the starting position of the electron (before the magnetic field was switched on) is at $(k_{x0}, 0))$ as shown in Figure 4070.46, then find the trajectory of the electron in the $\mathbf{k}$-space after the magnetic field has been switched on. Plot the trajectory in the $\mathbf{k}$-space.

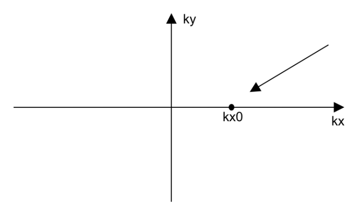


Fig. 4070.7: 2D Electron k-space

(b) Continuation of part (a): If in addition, the starting position of the electron (before the magnetic field was switched on) in real space is at $(x_0, 0)$ as shown in Figure 4070.47, then find the trajectory of the electron in real-space after the magnetic field has been switched on and plot it in the real space.

(c) If you did parts (a) and (b) correctly, you would have found that the motion of electron in both k-space and real space is *periodic*. Find the time period for the motion (i.e. the time taken by the electron to complete one period).

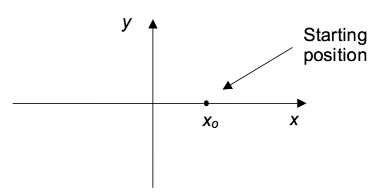


Fig. 4070.8: 2D Electron real space

(d) Staring from the equation 4070.149, prove that the energy of the electron is conserved (i.e. does not change) during its motion. Hint: The proof is just 1-2 lines of math.

(e) If instead of one electron, there were many, Before the magnetic field was switched the total current carrier by the electron gas (summing up contributions from all electrons) was given by

$$\mathbf{J} = 2q \int \frac{d^2 k}{(2\pi)^2} f(\mathbf{k}) \mathbf{v}(\mathbf{k}) = 0, \tag{4070.7}$$

where $f(\mathbf{k})$ was the equilibrium Fermi-Dirac distribution for electrons. Find the total current carried by the electron gas *after* the magnetic field has been switched on and explain your answer.

Problem 9: The Elusive Bloch Oscillator

In a fictitious 2-Dimensional crystal, the bandstructure of the lowest band with a square lattice (lattice constant a) is given by

$$E(k_x, k_y) = -E_0 \cdot [\cos k_x a + \cos k_y a]. \tag{4070.8}$$

a) Make a semi-quantitative contour plot of constant energies in the reduced Brillouin Zone, and highlight energies $E = 0, \pm E_0$.

b) Make a semi-quantitative plot of the effective mass in the (1,0) or $x-$direction, and the (2,1) direction in the reduced Brillouin Zone.

c) An electron is initially located at $\mathbf{k} = 0$ in $\mathbf{k}$-space, and $\mathbf{r} = 0$ is real space. At $t = 0$, a force $\mathbf{F}$ (from an electric field) is turned on which points in an oblique direction, such that $F_x = 2F_y$. Show the trajectory of the electron through the reduced zone in the $\mathbf{k}$-space, including umklapp processes, for the time interval $0 \leq t \leq 4T$, where

$$T = \frac{\pi\hbar}{aF_x} \tag{4070.9}$$

d) Calculate and plot the x- and y-components of the velocity and the position of the electron, all functions of time, for $0 \leq t \leq 4T$.

e) Make a graph of the trajectory of the electron in the x-y plane of real space.

f) Explain the phenomena in words. [4]

[4]If you have done the problem correctly, you will realize that *very mysteriously*, the electron is oscillating in real space in the presence of an *Electric* field! A DC electric field will lead to ac oscillation power - this idea is called a Bloch oscillator. The actual implementation has remained elusive in semiconductor quantum structures. They promise very high frequency (THz) output power, only if someone can make them!

Problem 10: Electrons get their Bands and Gaps

As shown in Figure 4070.9, in the $\mathbf{k}$-space of a 2D square lattice (lattice constant: a), denote the points $\Gamma : (k_x, k_y)$=(0,0), $X : (\pi/a, 0)$, and $W : (\pi/a, \pi/a)$. The nearly free electron bandstructure assumes no crystal potential, but a lattice.

(a) Draw the nearly free-electron bandstructure from the BZ center in the $\Gamma - W$ direction slightly beyond the BZ edge. Identify the magnitude of k at the BZ edge, and express the energy in terms of $F = \hbar^2\pi^2/ma^2$. Include reciprocal lattice vectors smaller than $2 \times 2\pi/a$.

(b) Label each band with the reciprocal lattice vector it is associated with. Clearly point out the *degeneracies* of each band.

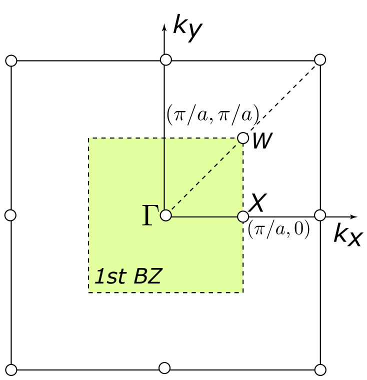


Fig. 4070.9: 2D reciprocal lattice.

Consider now that the basis atoms produce a 2-D potential

$$V(x, y) = -4V_0 \cos(\frac{2\pi x}{a}) \cos(\frac{2\pi y}{a}). \tag{4070.10}$$

(c) Find the bandgap at the W point due to this potential. Be judicious in choosing the basis set.

(d) The lowest energy at the $\Gamma : (k_x, k_y) = (0, 0)$ point *before* the potential was turned on was $E_\Gamma(0, 0) = 0$ eV. Give an estimate of the change in this energy eigenvalue due to the periodic potential.