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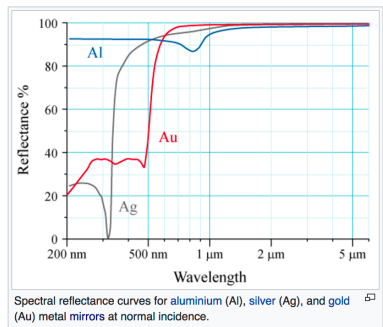
Spectral reflectance curves for aluminium (Al), silver (Ag), and gold (Au) metal mirrors at normal incidence.

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 $\boxed{\Gamma_r = \dfrac{E_r}{E_i} = \dfrac{\sqrt{\epsilon_0} - \sqrt{\epsilon(\omega)}}{\sqrt{\epsilon_0} + \sqrt{\epsilon(\omega)}}}$, 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 $\boxed{\epsilon(\omega) = \epsilon_0[1 + i\dfrac{\sigma(\omega)}{\omega\epsilon_0}]}$.

(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:

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

(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

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.

Fig. 4070.2: Electron on a ring

(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 $\int_0^L \cos^2\left(\frac{2\pi}{L}x\right)dx = \frac{L}{2}$. Does this superposition state have a definite momentum?
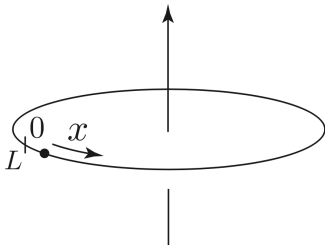
(d) We derived that the quantum expression for current flux is $\mathbf{j} = \frac{1}{2m}(\psi^\star \hat{\mathbf{p}}\psi - \psi \hat{\mathbf{p}}\psi^\star)$, where $\hat{\mathbf{p}} = -i\hbar\nabla$ is the momentum operator, which takes the form $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$ for the 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:

(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?

[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.

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. 4070.3: Andre Geim

(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.

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.

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

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

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

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

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

(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

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

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

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

(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

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!

[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 4070.6.

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)

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

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 4070.7, then find the trajectory of the electron in the **k**-space after the magnetic field has been switched on. Plot the trajectory in the **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 4070.8, 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.

Fig. 4070.7: 2D Electron k-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).

(d) Staring from the equation 4070.6, 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

Fig. 4070.8: 2D Electron real space

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

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

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

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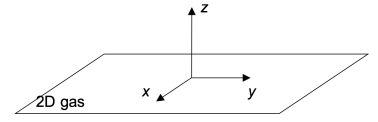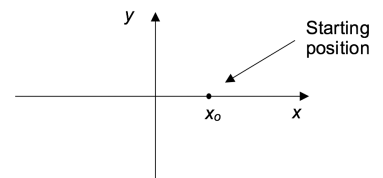
c) An electron is initially located at $\mathbf{k} = 0$ in $\mathbf{k}$-space, and $\mathbf{r} = 0$ is real space. At $t = 0$, a force $\mathbf{F}$ (from an electric field) is turned on which points in an oblique direction, such that $F_x = 2F_y$. Show the trajectory of the electron through the reduced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

$$T = \frac{\pi \hbar}{a F_x} \tag{4070.9}$$

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

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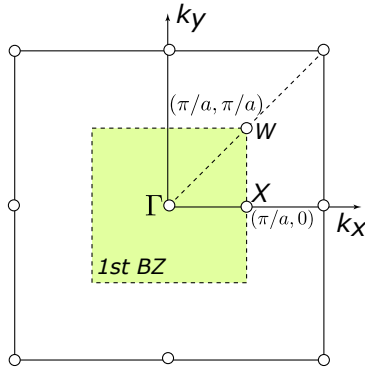
(a) Draw the nearly free-electron bandstructure from the BZ center in the $\Gamma - W$ direction slightly beyond the BZ edge. Identify the magnitude of k at the BZ edge, and express the energy in terms of $F = \hbar^2 \pi^2 / ma^2$. Include reciprocal lattice vectors smaller than $2 \times 2\pi/a$.

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

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.

Fig. 4070.9: 2D reciprocal lattice.

4070.3   HW 3

Posted: 03/02/2017, Due: 03/14/2017

Problem 11: Wigner-Seitz Cells and the Reciprocal Lattice

Figure 4070.10 shows the arrangement of atoms of a fictitious 2-dimensional crystal. All circles (filled and empty) represent the same atom.
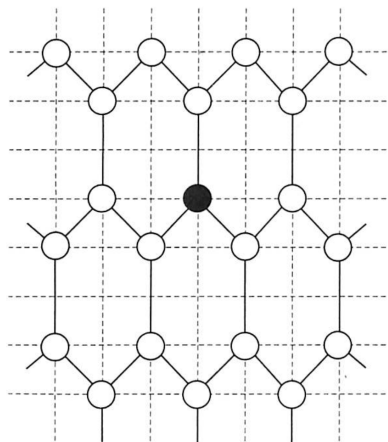
a) Using the filled 'atom' shown in black as the origin of the lattice, indicate the primitive translation vectors of this lattice. (There are several possible choices; use the simplest one, and explain.) How many atoms are there per lattice point?

b) Determine the reciprocal lattice vectors corresponding to this lattice, and sketch the reciprocal lattice as accurately as you can. Use the grid lines shown as an unit of measure.

Fig. 4070.10: Atomic arrangement of a fictitious 2-dimensional crystal.

c) Construct and show the 'Wigner-Seitz cell', or equivalently, the Brillouin zone clearly in the reciprocal lattice plot.

Problem 12: Energy Gap from a Square Wave Potential

#15·2-1: Energy Gap of a Square-Wave Periodic Potential

Using second-order Brillouin-Wigner perturbation theory, calculate the energy gap of a square-wave potential with the amplitude $\Delta V = F$, where F is again given by (14·3–17).
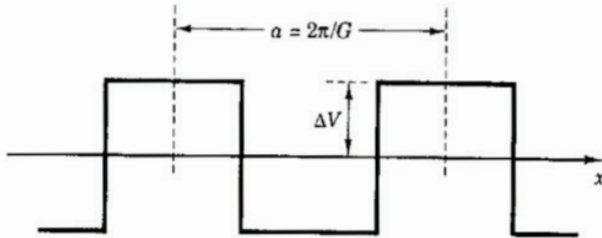
Fig. 4070.11: Square-wave perturbation to the particle in a box problem.

See Fig 4070.11. This problem is from Kroemer's QM Textbook. Note that the equation referred to is $F = \hbar^2 G^2 / 8 m_e$, the free-electron unperturbed energy at the Brillouin-zone edge. The given perturbation potential is applied on the *free electron*. Also test with the Rayleigh-Schrodinger (RS) approximation for the 2nd order energy corrections. Is the RS approximation a good one for this problem?

Problem 13: This crystal has no atoms! The Empty Lattice Bandstructure

a) Impossibility of indirect bandgaps in ideal 1D crystals: Argue why in an ideal 1D crystal, energy degeneracies (or band crossings) can *only* occur at $k = 0$ or at the Brillouin Zone edges, but never at any other k points. Since degeneracy points lead to bandgaps, what does this say about ideal 1D semiconductors: will they be direct or indirect bandgap? What about 2D and 3D crystals?

b) Now consider the ideal 2D crystal of graphene shown in Figure 4070.12. Identify the primitive real-space lattice vectors $(\mathbf{a_1}, \mathbf{a_2})$. Find the primitive reciprocal lattice vectors $(\mathbf{b_1}, \mathbf{b_2})$. The general reciprocal lattice vector may be written as $\mathbf{G} = n\mathbf{b_1} + m\mathbf{b_2}$, written more compactly as (n, m).

c) Starting from the expression for the energy bandstructure of the empty lattice model $\mathcal{E}(\mathbf{k}) = \frac{\hbar^2 (\mathbf{k}+\mathbf{G})^2}{2m_0}$, draw up a table with expressions of energy bands along the k_x and k_y directions. Associate each band with the respective (n, m) reciprocal lattice vector.

d) Plot the empty-lattice bandstructure along $(k_x, 0)$ for (n, m): (0,0) through (2, 2) with all possible ($\pm$) combinations. Also make a 2D plot of the energy bandstructure. Superimpose and compare with the known bandstructure of graphene and comment.
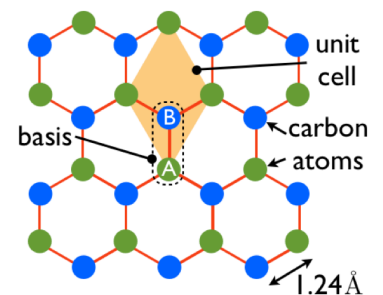
Fig. 4070.12: Atoms in the Graphene Crystal.

e) Do the same as in the previous problem, but for 3D Silicon (see Figure 4070.13). Use the diamond cubic crystal structure (you have 3 reciprocal lattice vectors). Plot the energy bands along the typical high-symmetry directions in the k-space. Superimpose and compare with the known bandstructure of Silicon and comment.
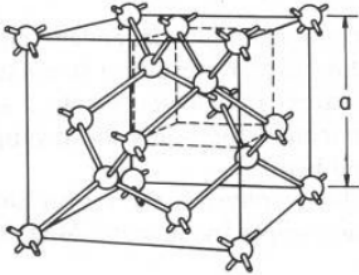
Diamond lattice (Si, Ge, Diamond)

Fig. 4070.13: Atoms in the Silicon Crystal.

Problem 14: Energy Bandstructure of 2D Graphene and BN

In this problem, we will quantitatively calculate the electronic bandstructure for 2D graphene and 2D Boron Nitride as our first 'elemental' and 'compound' semiconductors respectively.

a) Show that if the energies allowed for the electron in individual atoms A and B are E_A and E_B, and the lowering of energy because of hopping of the electron between the atoms between the atoms is U, the energies allowed for the electron after the formation of a chemical bond are $E_\pm = \frac{E_A + E_B}{2} \pm \sqrt{\overline{(\frac{E_A - E_B}{2})^2 + U^2}}$. Because each allowed electron state can hold *two* electrons of opposite spins, what is the *lowering* of energy due to the formation of the bond?

b) Now consider 2D Boron Nitride (or graphene), whose atomic basis has *two* atoms: B & N for BN (and C & C for graphene). We saw in class that the whole 2D crystal may be generated by repeating this two-atom basis, by translating by the two primitive lattice vectors $\mathbf{a_1} = a(\frac{3}{2}, \frac{\sqrt{3}}{2})$ and $\mathbf{a_2} = a(\frac{3}{2}, -\frac{\sqrt{3}}{2})$, where a is the distance between the A and B atoms. Sketch the basis, the lattice, and these vectors, and show that the three vectors from any atom to the three nearest neighbors are $\mathbf{n_1} = \frac{a}{2}(1, \sqrt{3})$, $\mathbf{n_2} = \frac{a}{2}(1, -\sqrt{3})$, and $\mathbf{n_3} = -a(1, 0)$. We will look at only the p_z orbital bands. For on-site orbital energies E_A and E_B and a hopping energy t, show that the off-diagonal (hopping) term is $h(\mathbf{k}) = -t(e^{i\mathbf{k} \cdot \mathbf{n_1}} + e^{i\mathbf{k} \cdot \mathbf{n_2}} + e^{i\mathbf{k} \cdot \mathbf{n_3}})$, and the resulting bandstructure is

$$E_\pm = A \pm \sqrt{B^2 + t^2[1 + 4\cos(\frac{3}{2}k_x a)\cos(\frac{\sqrt{3}}{2}k_y a) + 4\cos^2(\frac{\sqrt{3}}{2}k_y a)]} \,, \text{ where } A = \frac{E_A + E_B}{2}$$

and $B = \frac{E_A - E_B}{2}$.

c) Using the following parameters, underline{make 2D plots of the bandstructures of BN and graphene similar to shown in class. For BN: $E_A = +2.9$ eV, $E_B = -2.9$ eV, $t = -2.9$ eV, and $a = 0.15$ nm. For graphene, $E_A = E_B = 0$ eV, $t = 3.0$ eV, $a = 0.15$ nm. Describe the differences and similarities between them. Specifically, find the band-edge *effective masses* and *bandgap* for BN, and the *Fermi velocity* characterizing the slope of the $E - k$ Dirac cone of Graphene. Relate these analytically to the known parameters.

Problem 15: Energy Bandstructure of Silicon and GaAs

In this problem we extend the ideas of the last problem to calculate the tight-binding bandstructure of Silicon and GaAs, which are 3D semiconductors. The procedure is the same, just the matrices are larger. Do not be turned off by the forbidding looking matrix below-it is simpler than you think, and understanding it will put you in a select league! Silicon powers the electronics industry today, and GaAs the photonic industry - they together are the basis of the new information age. And within a month in this course, you are solving the quantum mechanical problem of both crystals! You will be able to get plots like the ones shown in Figures 4070.14 and 4070.15. Because the bandstructure is the allowed electron eigenvalues in the crystal, getting it means you have (almost) completely solved the full quantum mechanical problem of the two semiconductors. Since the bandstructure determines all the electronic and photonic properties of the semiconductor, it should be a memorable event when you get it to work!

Because for graphene and BN we looked at a single $|p_z\rangle$ orbital and a 2-atom basis, the matrix was 2×2. For Silicon and GaAs, the basis has two atoms too, but attached to each atom will be 4 orbitals: $|s\rangle, |p_x\rangle, |p_y\rangle, |p_z\rangle$, and the chemical bonding is sp^3. Thus, to get the energy bandstructure we have to solve a 8x8 matrix numerically.

a) Sketch the crystal structure, the atomic basis, and the nearest neighbor vectors $\mathbf{n}_1 = \frac{a}{4}(1,1,1)$, $\mathbf{n}_2 = \frac{a}{4}(-1,-1,1)$, $\mathbf{n}_3 = \frac{a}{4}(-1,1,-1)$, $\mathbf{n}_4 = \frac{a}{4}(1,-1,-1)$, where a is the lattice constant ($\neq$ nearest neighbor distance!). Sketch the orbitals centered at each site and identify the overlaps, and the angles between them.

b) Because of various orbital overlaps ss, $sp\sigma$, $pp\sigma$ and $pp\pi$, there are multiple hopping terms. Examine the matrix carefully and explain its structure. Specifically, explain all the diagonal terms, and the zeroes. Then explain the non-zero off-diagonal terms by invoking symmetries, geometries, and orbital overlaps.

Fig. 4070.14: Bandstructure of Silicon.

$$
\begin{array}{c c}
& \begin{array}{cccccccc} |s^A\rangle & |p_x^A\rangle & |p_y^A\rangle & |p_z^A\rangle & |s^B\rangle & |p_x^B\rangle & |p_y^B\rangle & |p_z^B\rangle \end{array} \\[4pt]
\begin{array}{c} \langle s^A| \\ \langle p_x^A| \\ \langle p_y^A| \\ \langle p_z^A| \\ \langle s^B| \\ \langle p_x^B| \\ \langle p_y^B| \\ \langle p_z^B| \end{array} &
\left(\begin{array}{cccccccc}
E_s^A & 0 & 0 & 0 & -V_0 g_0(\mathbf{k}) & V_1 g_1(\mathbf{k}) & V_1 g_2(\mathbf{k}) & V_1 g_3(\mathbf{k}) \\
0 & E_p^A & 0 & 0 & -V_1 g_1(\mathbf{k}) & V_2 g_0(\mathbf{k}) & V_3 g_3(\mathbf{k}) & V_3 g_2(\mathbf{k}) \\
0 & 0 & E_p^A & 0 & -V_1 g_2(\mathbf{k}) & V_3 g_3(\mathbf{k}) & V_2 g_0(\mathbf{k}) & V_3 g_1(\mathbf{k}) \\
0 & 0 & 0 & E_p^A & -V_1 g_3(\mathbf{k}) & V_3 g_2(\mathbf{k}) & V_3 g_1(\mathbf{k}) & V_2 g_0(\mathbf{k}) \\
\text{c.c.} & \text{c.c.} & \text{c.c.} & \text{c.c.} & E_s^B & 0 & 0 & 0 \\
\text{c.c.} & \text{c.c.} & \text{c.c.} & \text{c.c.} & 0 & E_p^B & 0 & 0 \\
\text{c.c.} & \text{c.c.} & \text{c.c.} & \text{c.c.} & 0 & 0 & E_p^B & 0 \\
\text{c.c.} & \text{c.c.} & \text{c.c.} & \text{c.c.} & 0 & 0 & 0 & E_p^B
\end{array}\right), \quad (4070.11)
\end{array}
$$

where c.c. stands for the complex conjugate (e.g. $H_{51} = H_{15}^\star$). The constants in this matrix are

$V_0 = V_{ss\sigma}$,
$V_1 = \frac{1}{\sqrt{3}} V_{sp\sigma}$,
$V_2 = \frac{1}{3} V_{pp\sigma} - \frac{2}{3} V_{pp\pi}$, and
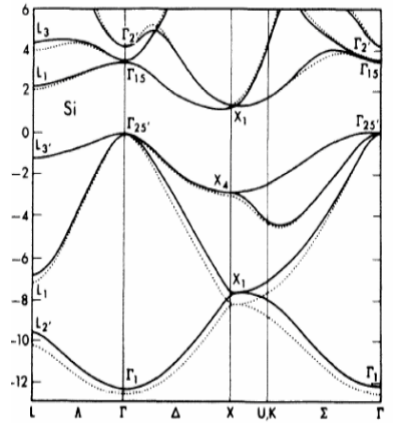$V_3 = \frac{1}{3} V_{pp\sigma} + \frac{1}{3} V_{pp\pi}$,

and the nearest neighbor 'hopping' phases are

$g_0(\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{n_1}} + e^{i\mathbf{k}\cdot\mathbf{n_2}} + e^{i\mathbf{k}\cdot\mathbf{n_3}} + e^{i\mathbf{k}\cdot\mathbf{n_4}}$,
$g_1(\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{n_1}} - e^{i\mathbf{k}\cdot\mathbf{n_2}} - e^{i\mathbf{k}\cdot\mathbf{n_3}} + e^{i\mathbf{k}\cdot\mathbf{n_4}}$,
$g_2(\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{n_1}} - e^{i\mathbf{k}\cdot\mathbf{n_2}} + e^{i\mathbf{k}\cdot\mathbf{n_3}} - e^{i\mathbf{k}\cdot\mathbf{n_4}}$, and
$g_3(\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{n_1}} + e^{i\mathbf{k}\cdot\mathbf{n_2}} - e^{i\mathbf{k}\cdot\mathbf{n_3}} - e^{i\mathbf{k}\cdot\mathbf{n_4}}$

for the 4 nearest neighbors. The eigenvalue spectrum of the 8×8 matrix above yields the bandstructure $E(\mathbf{k})$ of Silicon, GaAs, and all 3D semiconductors of the diamond-cubic or zinc-blende families. The electron wavevector $\mathbf{k} = (k_x, k_y, k_z)$ is three dimensional: the electron energy depends on the direction it moves.
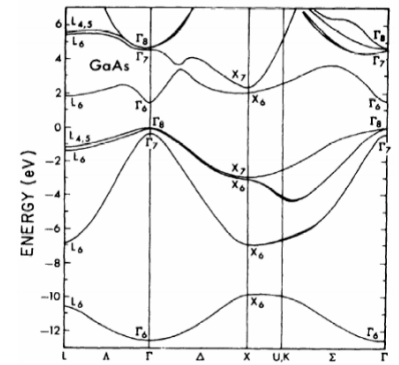
Fig. 4070.15: Bandstructure of GaAs.

c) Set up the matrix above in Mathematica, Matlab, Python (or any tool you love!) to plot the energy bandstructure $E(k)$ for k from $\mathbf{L} \leftrightarrow \boldsymbol{\Gamma} \leftrightarrow \mathbf{X} \leftrightarrow \mathbf{K} \leftrightarrow \boldsymbol{\Gamma}$. For Silicon, $E_s^A = E_s^B = -13.55$ eV, $E_p^A = E_p^B = -6.52$ eV, $V_{ss\sigma} = +2.03$ eV, $V_{sp\sigma} = +2.55$ eV, $V_{pp\sigma} = +4.55$ eV, $V_{pp\pi} = +1.09$ eV, and $a = 0.543$ nm.

d) Repeat the bandstructure plot for our first 3D compound semiconductor: GaAs! Use $E_s^{Ga} = -11.37$ eV, $E_s^{As} = -17.33$ eV, $E_p^{Ga} = -4.9$ eV, $E_p^{As} = -7.91$ eV, $V_{ss\sigma} = +1.70$

eV, $V_{sp\sigma} = +2.15$ eV, $V_{pp\sigma} = +3.44$ eV, $V_{pp\pi} = +0.89$ eV, and $a = 0.565$ nm. If you have worked your way to this stage, congratulations, your early hard work will pay off handsomely in the course.

e) From the 8×8 LCAO bandstructure matrix of GaAs, show that for the Γ point with $\mathbf{k} = 0$, the eight eigenvalues can be calculated analytically. Then prove that for GaAs, the conduction band edge state is at $E_c(\Gamma) = \frac{E_s^{Ga}+E_s^{As}}{2} + \sqrt{(\frac{E_s^{Ga}-E_s^{As}}{2})^2 + (4V_{ss\sigma})^2}$ composed of $|s\rangle$ orbital overlap between the Ga and As atoms, and no $|p\rangle$ orbitals are involved.

f) Similarly, show that for the states at the top of the valence band at the Γ point, only $|p\rangle$ orbitals are involved with no $|s\rangle$ orbital involvement. Use this property to argue why holes are anisotropic in most compound semiconductors, but electrons are isotropic.

4070.4   HW 4

Posted: 03/19/2017, Due: 03/29/2017

Problem 16: The deep-acceptor problem and the 2014 Physics Nobel Prize

a) Show that for a homogeneous semiconductor with electron mobility μ_n and hole mobility μ_p, the *lowest* conductivity that can be achieved at thermal equilibrium is $\sigma_{min} = 2qn_i\sqrt{\mu_n\mu_p}$, irrespective of the donor or acceptor doping.

Magnesium is a relatively deep acceptor in the wide bandgap semiconductor GaN. The acceptor ionization energy is $E_A \sim 160$ meV. Consider a GaN sample ($E_g = 3.4$ eV, $m_c^\star \sim 0.2m_0$, $m_v^\star \sim 1.4m_0$) doped with $N_A = 10^{18}/\text{cm}^3$ Magnesium acceptors. In the process of doping this sample with Magnesium, unintentional donors of density $N_D = 10^{14}/\text{cm}^3$ of donor ionization energy $E_D = 10$ meV also incorporate into the semiconductor.

b) For T=300K, Plot the log of n, p, N_A^-, N_D^+, $n+N_A^-$, and $p+N_D^+$ as a function of the Fermi level E_F. Remember the Fermi level can be within the gap, or in the conduction or valence bands. So in your plot vary the values of E_F from below E_c to above E_c. Indicate the donor and acceptor ionization energies and show in the plot where the real Fermi level at 300K is. Explain.

c) What are the densities and types of mobile carriers in the sample at 300K? Is the sample n- or p-type? Find the conductivity of the sample at 300K if the electron mobility is $\mu_n \sim 1000$ cm^2/V·s and the hole mobility is $\mu_p \sim 10$ cm^2/V·s.

d) Do an online research of the connection between the p-type doping problem of wide-bandgap semiconductors and the 2014 Physics Nobel prize and write a short summary of what you find.

Problem 17: Electric Current Flow in Semiconductor Crystals

In class, we have seen that the quantum mechanical current carried by Bloch states is found easily by using the concept of the **group velocity** which is obtained directly from the bandstructure $E(k)$. The second important concept of current flow is how the $k-$states are filled/emptied by metal contacts which are reservoirs of electrons, and determine the quasi-Fermi levels of the $|k\rangle$ states in the semiconductor. In this problem, you will gain practice in applying these concepts to find the quantum mechanical electric current in
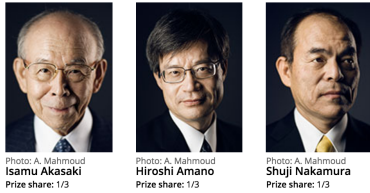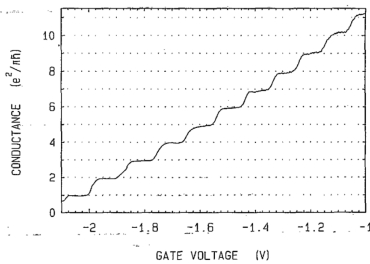

Fig. 4070.16: The 2014 Physics Nobel Prize went to the researchers who solved the p-type doping problem in GaN. This work made quantum well blue LEDs and Lasers and LED lighting possible.

Fig. 4070.17: Experimental evidence of conductance quantization measured in an Al-GaAs/GaAs quantum well structure with N parallel quantized conductors from 1998. The number of 1D conductors or subbands could be tuned by a gate voltage.

various situations.

a) Show that the ballistic conductance $G = I/V$ in any 1D metal or semiconductor at a low voltage V and at a low temperature $qV << k_bT$ is given by the *quantum of conductance*

$$\boxed{G_0 = g_s g_v \frac{q^2}{h}}$$, where g_s is the spin degeneracy and g_v the valley degeneracy of the 1D band,

q is the electron charge, and h is Planck's constant. In your derivation, show that rather remarkably this result is *independent* of the exact nature of the bandstructure! If there are N parallel 1D conductors or N uncoupled 1D bands, then the total conductance is NG_0.

b) Electrons sit in the n_z state of a heterostructure 2D quantum well of length L_z and infinite depth in the $z-$direction and are free to move in an area $L_x L_y$ in the $x - y$ directions. The energy bandstructure is $E(k_x, k_y) = \frac{\hbar^2(k_x^2 + k_y^2)}{2m^\star}$. Show that the probability current density for state $|\mathbf{k}\rangle = (k_x, k_y, k_{n_z})$ is the following:

$$\mathbf{j}(k_x, k_y, k_{n_z}) = \frac{1}{L_x L_y} \cdot \left[\frac{\hbar}{m^\star}(k_x \hat{x} + k_y \hat{y})\right] \cdot \frac{2}{L_z} \sin^2(k_{n_z} z). \qquad (4070.12)$$

c) Provide an expression for k_{n_z} and explain the result. Integrate the $z-$component to show that the 2D probability current is in the form $\mathbf{j}_{2d}(\mathbf{k}) = \frac{1}{L^d}\mathbf{v}_g(\mathbf{k})$, where $\mathbf{v}_g(\mathbf{k}) = \frac{1}{\hbar}\nabla_k E(\mathbf{k})$ is the group velocity. This is a more general result that applies also for particles that may appear 'massless'.

d) Now fill the quantum well (k_x, k_y) states so that the 2D carrier sheet density is n_s. This defines a Fermi level E_F: find how n_s is related to E_F at any temperature. Also, what happens to E_F if $\hbar \to 0$? Why?

e) Find the current per unit width flowing in the $+x$ direction as a function of temperature and n_s. Assume a spin degeneracy g_s and valley degeneracy g_v for each $\mathbf{k}$-state. This is of course equal to the current flowing in the $-x$ direction. Find the magnitude of the current density for $m^\star \sim 0.2 m_0$ and $n_s \sim 10^{13}/\text{cm}^2$, $g_s = 2$, and $g_v = 1$ (these values are typical for GaN transistors; g_v is larger for Silicon MOSFETs).

f) In some 2D semiconductors such as graphene, the energy bandstructure is not parabolic, but conical: $E(k_x, k_y) = \hbar v_F \sqrt{k_x^2 + k_y^2}$, where v_F is a characteristic 'Fermi' velocity. Find the $+x$ directed current per unit width for graphene as a function of temperature. Find the magnitude of the current per unit width for $v_F \sim 10^8$ cm/s, $n_s \sim 10^{13}/\text{cm}^2$, and $g_s = 2$, and $g_v = 2$, the values for 2D graphene.

Problem 18: To gap or not to gap, that is the question

A fictitious 2D semiconductor[5] has an energy dispersion $E(\mathbf{k}) = \pm \hbar v_F \sqrt{|\mathbf{k}|^2 + k_0^2}$, where $\mathbf{k} = (k_x, k_y)$, $\hbar$ is the reduced Planck's constant, v_F a characteristic velocity, and k_0 is a constant. Assume a spin degeneracy g_s and valley degeneracy g_v.

a) Find the energy bandgap E_g, and show that the effective mass m_{xx} at the band edge is related to the bandgap by $2m_{xx}v_F^2 = E_g$. Argue that if k_0 is externally tunable with a gate, the bandstructure of this material can be made to look like graphene and its gap can be made zero.

b) Find and sketch the density of states.

Hopping energy: $\gamma_0 \approx 3$ eV

sp^2 bonds

p_z orbitals

real space

$E(k_x, k_y)$

Dirac cone
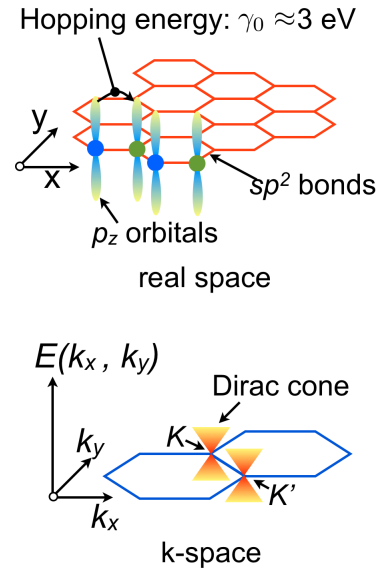
k_y

K

K'

k_x

k-space

Fig. 4070.18: Dirac cone bandstructure of graphene.

[5]Actually this is not fictitious any more - recently 2D crystal semiconductors with a broken symmetry in the direction perpendicular to the 2D plane have been discovered such as Silicene and Germanene - atomicaly thin versions of Silicon and Germanium that have this sort of a bandstructure. They have rather interesting *toplogical* properties that we are skipping in this course.

c) Find the group velocity $\mathbf{v}_g(\mathbf{k})$ of the state $\mathbf{k}$. Sketch the magnitude and direction of the group velocities in the $\mathbf{k}-$space.

d) Now the conduction band of this 2D semiconductor sheet is connected by ohmic contacts to a source and a drain. A voltage V is applied across these two terminals. Set up the expressions that will give the ballistic current in response to the applied voltage.

e) The temperature is held very low, $T \to 0$ K. Estimate the ballistic current as a function of voltage if $qV >> \hbar v_F k_0$.

Problem 19: Velocity saturation in Nanotubes and Semiconductors

a) If high energy electrons collide with the lattice and emit optical phonons at a very fast rate, they come to equilibrium with the lattice rather than the source and drain electrodes. Assume we have a metallic carbon nanotube that has a 1D energy dispersion $E(k) = \hbar v_F |k|$ with a spin degeneracy of $g_s = 2$ and a valley degeneracy $g_v = 2$. Show that if the optical phonon energy is $\hbar \omega_{op}$ and the above ultrafast optical phonon emission occurs, then the saturation current in the nanotube is given by $I_{sat} = \frac{q g_s g_v \omega_{op}}{2\pi}$. Find the magnitude of this current for $\hbar \omega_{op} \sim 160$ meV, and compare with experimental data (give references).

b) At low electric fields, the velocity v of electrons in a semiconductor increases linearly with the field F according to $v = \mu F$, where $\mu = q \tau_m / m^\star$ is the mobility, τ_m is the momentum scattering time and $m^\star$ the electron effective mass. But when the electric field is cranked up, the electron velocity saturates, because the electrons emit optical phonons each of energy $\hbar \omega_{op}$ every τ_E seconds, dumping the energy qFv they gain from the electric field every second. Setting up the equations for the conservation of momentum and energy, and solving for the steady state yields an estimate of this saturation velocity. Show that the saturation velocity obtained by this scheme is $v_{sat} = \sqrt{\frac{\hbar \omega_{op}}{m^\star}} \cdot \sqrt{\frac{\tau_m}{\tau_E}}$. Show that for a typical semiconductor for which $\hbar \omega_{op} \approx 60$ meV, $m^\star \sim 0.2 m_0$, and $\tau_m \sim \tau_E$, the electron saturation velocity is of the order of $\sim 10^7$ cm/s. This is a good rough number for the saturation velocity of most semiconductors.

Problem 20: Quantum Current across a Schottky Junction

The energy band diagram in Figure 4070.19 is of a metal/semiconductor junction of surface barrier height $a\phi_b$. In this problem you will calculate the ballistic (quantum) current flow across this junction as a function of the applied voltage. You will discover that the current is highly rectifying, and is given by $J = J_0(e^{\frac{qV}{k_b T}} - 1)$ - the famous rectifier equation in semiconductor devices. You will solve this problem in its full quantum mechanical glory.[6]

a) If the work function of the metal is $q\phi_M$, what is the work-function of the semiconductor? Why is there a depletion region in the semiconductor?

b) Sketch the distribution of electrons in the conduction band at the depletion edge plane indicated as a function of energy.

c) The semiconductor conduction bandstructure is given by $E(k_x, k_x, k_z) = E_c + \frac{\hbar^2}{2m_c^\star}(k_x^2 + k_y^2 + k_z^2)$ where E_c is the band-edge energy, and $m_c^\star$ is the conduction band effective mass. Find an expression for the (k_x, k_y, k_z) states *at the depletion edge plane* that can make it across the barrier. This defines a restricted volume Ω_k in the 3D $k-$space of electrons. Only electrons in this volume can make it ballistically to the metal.
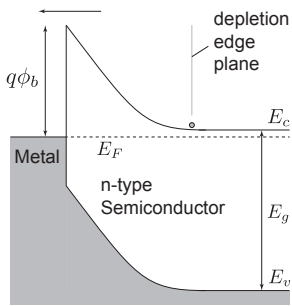
Fig. 4070.19: Schottky Diode

[6]This problem has been solved over the last century by Walter Schottky, Owen Richardson, Arnold Sommerfeld, Ralph Fowler, Lothar Nordheim, Hans Bethe, Nevill Mott, among others. The Schottky diode rectifier is an extremely important semiconductor device, and the rectifying property was one of the earliest to be used in crystal radios, and the earliest pointers to the existence of semiconductors - you can imagine why people have been interested in it for so long!

Fig. 4070.20: Walter Schottky was an early investigator of the metal-semiconductor junction. A semiconductor research institute in Munich is named after him.

d) Now use the expression for the quantum current $\mathbf{J} = \frac{1}{L^3}\sum_{\Omega_k}\mathbf{v_g}(\mathbf{k})f(k)$ to show that the *net* current as a function of the applied voltage is $\boxed{J = A^\star T^2 e^{-\frac{q\phi_b}{k_bT}}(e^{\frac{qV}{k_bT}} - 1)}$, where the prefactor $A^\star = \frac{4\pi q k_b^2 m_c^\star}{h^3}(1+\eta)$ is the famous Richardson constant when $\eta \to 0$; here $\eta = \frac{q\phi_b - qV - (E_c - E_F)}{k_bT}$.

e) The expression for the Schottky diode current is in the form $J = J_0(e^{\frac{qV}{k_bT}} - 1)$ if $\eta \to 0$. If the carriers suffer scattering and energy loss in the depletion region, only the carriers closest to the metal-semiconductor junction within a mean-free-path will make it to the metal. Argue why in this 'diffusive' limit, $\eta \to 0$. It is in this limiting form you will find the expression of the Schottky diode current in most books.

f) Assuming $\eta \to 0$, make a linear and a log-scale plot of J/T^2 vs voltage for a GaAs-metal Schottky diode of barrier height $q\phi_b = 1$ eV and $m_c^\star \sim 0.067m_0$ at $T = 300$K. In the log-plot, indicate the y-axis intercept. Argue why you can use such a plot to experimentally measure the conduction band effective mass $m_c^\star$. How would you measure ϕ_b?

Fig. 4070.21: Owen Richardson was awarded the 1928 Physics Nobel prize for thermionic emission; the Richardson constant is named after him.

4070.5   HW 5

Posted: 04/11/2017, Due: 04/28/2017

Problem 21: Effective Mass Methods: Doping and Quantum Dots

We derived the effective mass approximation in class, in which the complicated problem of a *free electron* in a periodic potential was mapped to a much simpler problem of an electron with an *effective mass* in a free potential. The key step was to create a wavepacket by constructing a linear combination of Bloch eigenstates $\psi_k(r) = u_k(r)e^{ikr}$ in the form $\phi_k(r) = \int \frac{dk}{2\pi}C(k)u_k(r)e^{ikr}$, and using Fourier transform properties with the Hamiltonian operator. The effective mass equation in the presence of *perturbations* to the periodic crystal potential then is written as

$$[E_n(-i\nabla) + W]C(r) = EC(r), \qquad (4070.13)$$

where $C(r)$ is the *envelope* function, and $E_n(-i\nabla)$ is an *operator* obtained from the bandstructure $E_n(k)$ of band n by replacing $k \to -i\nabla$. W is a time-dependent, or time-independent *perturbation* to the periodic potential of the crystal. Instead of the Bloch functions $\psi_k(r)$, we can now work with the envelope functions $C(r)$, remembering that the wavefunction of the wavepacket is the product of the envelope function and the periodic part of the Bloch-function, i.e., $\phi(r) = C(r)u_k(r)$. For this problem, consider the conduction band with a parabolic bandstructure characterized by an effective mass $m_c^\star$ and band-edge E_c, such that $E_c(k) = E_c + \frac{\hbar^2 k^2}{2m_c^\star}$.

a) Show that the effective mass equation is then

$$[-\frac{\hbar^2}{2m_c^\star}\nabla^2 + W]C(r) = (E - E_c)C(r). \qquad (4070.14)$$

Note that this is in the form of a modified Schrodinger equation, and is referred to as the effective mass Hamiltonian. Show that the solutions in the absence of the perturbation are simple plane waves, $C_k(r) = \frac{1}{\sqrt{V}}e^{ikr}$. Find k.

b) Doping: When we introduce a dopant atom in the semiconductor, the perturbation due to a single donor atom in a 3-Dimensional crystal semiconductor is a Coulomb potential $W(r) = -\frac{e^2}{4\pi\epsilon_s r}$ with ϵ_s the dielectric constant of the semiconductor. Argue that this

Fig. 4070.22: Walter Kohn with Joaquin Luttinger developed the effective mass theory for semiconductors. The effective mass theory arms us with a powerful method to design semiconductor nanostructures and enormously simplifies the design of quantum wells, wires, and dots. Kohn was awarded the Nobel Prize in 1998 for the development of Density Functional Theory (DFT). He passed away this week last year.
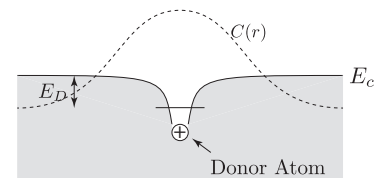
Fig. 4070.23: Schematic representation of a charged donor, its activation energy E_D and the envelope function of the donor electron $C(r)$.
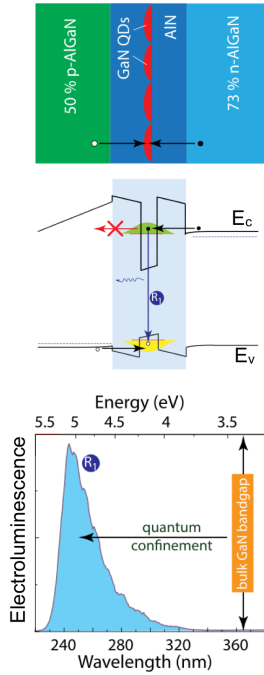
effective mass problem maps exactly to the Hydrogen atom problem, and show that the energy of the shallow donors are $E_n = E_c - Ry^\star/n^2$, where $Ry^\star = \frac{(m_c^\star/m_e)}{(\epsilon_s/\epsilon_0)^2} Ry^0$, where $Ry^0 = -13.6$ eV is the ground state energy of an electron in the Hydrogen atom. Also show that the radius of the donor electron is modified from the hydrogen electron radius to $a_B^\star = \frac{\epsilon_s/\epsilon_0}{m_c^\star/m_e} a_B^0$, where $a_B^0 = 0.53$ Angstrom is the Bohr radius of the electron in the Hydrogen atom. Estimate the ionization energy of the donor, and the radius in a semiconductor with $\epsilon_s = 10\epsilon_0$ and $m_c^\star = 0.1m_e$. From these considerations, argue why bands with heavy effective masses may be difficult to dope.

c) Quantum Dots: Suppose we have a narrow bandgap semiconductor quantum dot of size $L_x = L_y = L_z = L$ embedded in a wide-bandgap semiconductor matrix. Assume the conduction band offset ΔE_c and the valence band offset ΔE_v are very large, such that an electron in the conduction band and holes in the valence band of the quantum dot effectively see infinitely tall barriers. Find the allowed energies of the electrons and hole states in the quantum dot as a function of the dot size L, and the conduction and valence band effective masses $m_c^\star$ and $m_v^\star$. If the bulk bandgap of the narrow bandgap semiconductor is E_g, what is the energy of a photon that will be emitted if an electron transitions from the CB ground state to the VB ground state? Make a plot of the emitted photon energy as a function of the quantum dot size from 1 nm $\leq L \leq 10$ nm, for the following parameters of the narrow bandgap semiconductor: $m_c^\star = m_v^\star = 0.1m_e$, $E_g = 0.8$ eV.

Problem 22: Quantum Well Heterostructures

The finite quantum well problem is the basis of all quantized structures based on compound semiconductor heterostuctures. In this problem you evaluate some examples to gain insight, and collect some *very* useful formulae for the quantum design of heterostructure devices.

a) With relevant formulae and sketches, outline the graphical method for identifying the bound state eigenvalues and eigenfunctions in a finite quantum well of height U_0 and width L_w for a quantum well semiconductor material with effective mass $m^\star$. Show that the solution for allowed k values take the form $\sqrt{\frac{\theta_0^2}{\theta^2} - 1} = \tan\theta$ and $\sqrt{\frac{\theta_0^2}{\theta^2} - 1} = -\cot\theta$, where $\theta = \frac{kL_w}{2}$, and the characteristic constant $\theta_0^2 = \frac{m^\star L_w^2 U_0}{2\hbar^2}$.

b) Show that in the case of a vanishingly small barrier height $U_0 \to 0$, there is still at least one bound state for the 1D quantum well with a *binding energy* equal to $\boxed{U_0 - E_1 \approx \theta_0^2 U_0}$.

c) Show that the number of bound states is $\boxed{N = 1 + \text{Int}[\frac{2\theta_0}{\pi}]}$, where $\text{Int}[x]$ is the largest integer smaller than x. Show that the numerical value is $N = 1 + \text{Int}[1.63(\frac{L_w}{1\ \text{nm}})\sqrt{(\frac{m^\star}{m_0}) \cdot (\frac{U_0}{1\ \text{eV}})}]$.

d) Now consider the electron states in the conduction band of a heterostructure quantum well shown in Figure 4070.25, with $U_0 = \Delta E_c = 0.3$ eV, and $m_c^\star = 0.067m_e$. How many bound states does a well of thickness $L_w = 5$ nm hold? Write the effective mass wavefunctions $C(r)$ for electrons in the ground state of the quantum well, and find its characteristic penetration depth into the barrier layer.

e) Find the Fermi level in the quantum well if we fill the quantum well with electrons of 2D density $n_s = 10^{12}/\text{cm}^2$.

Fig. 4070.24: A quantum dot UV light-emitting diode realized by blue-shifting the emission from GaN by quantum confinement.
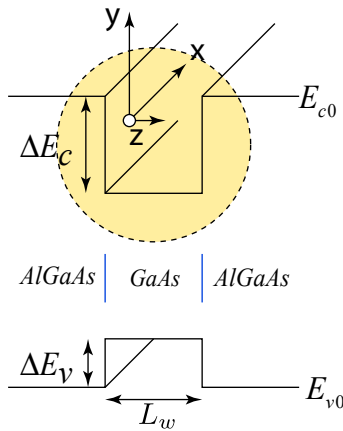

Fig. 4070.25: A quantum well Heterostructure realized in an Al-GaAs/GaAs/AlGaAs semiconductor system. Electrons are free to move in 2 dimensions in the (x, y) plane, but are confined in the z direction.

Problem 23: The Ballistic Field-Effect Transistor

In class, we derived the characteristics of a ballistic field-effect transistor. You are going to fill in a few steps, and solve a closely related problem.

a) Make log-scale and linear-scale plots of the gate-induced 2D electron gas (2DEG) carrier density at 300K and 77K vs the gate voltage V_{gs} of FETs for an insulating barrier of $t_b = 2$ nm, and $\epsilon_b = 10\epsilon_0$ for three semiconductor channels: one that has $m_c^\star = 0.2m_0$, $g_s = 2$ and $g_v = 2$, the second has $m_c^\star = 0.2m_0$, $g_s = 2$ and $g_v = 1$, and the third has $m_c^\star = 0.05m_0$, $g_s = 2$ and $g_v = 1$. What is the difference? Compare with the figure in the posted class notes.

b) Show why the ballistic current density is given by $J_{2d} = J_0[\mathcal{F}_{1/2}(\eta_s) - \mathcal{F}_{1/2}(\eta_s - v_d)]$, where $J_0 = q \cdot \frac{\hbar N_c}{m_c^\star}$, and all symbols have their usual meanings as they appear in the notes/handouts, and N_c is the effective conduction band edge DOS.

c) Make a plot of the ballistic FET currents of the three semiconductors of part (a). Make the drain current I_d vs gate voltage V_{gs} in the linear and log scales, and the drain current I_d vs drain voltage V_{ds} plots, similar to those shown in the class notes.

d) Describe qualitatively what sorts of changes in the device characteristics would you expect if instead of the 2DEG channel, you had a 1D channel in the ballistic FET. Remember you have shown before that the ballistic conductance per 1D channel is limited to the quantum of conductance $G_0 = g_s g_v \frac{q^2}{h}$, where h is the Planck's constant.

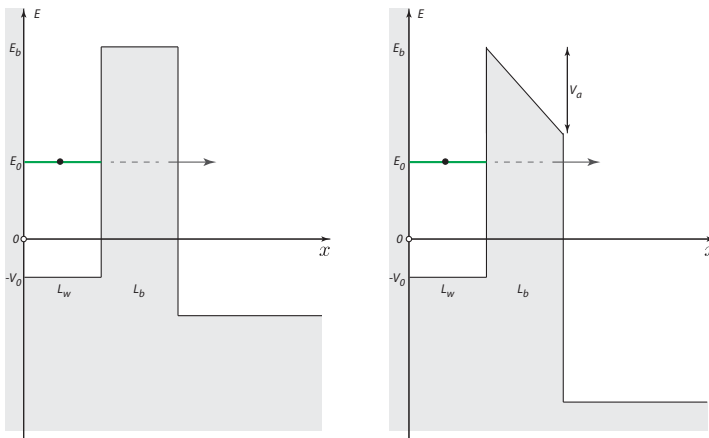## Problem 24: Vanishing Act: Tunneling Escape in a Flash Memory

Fig. 4070.26: Escape and field-emission by tunneling.

Figure 4070.26 shows a 1-dimensional potential for an electron, which is in the state with energy E_0 at $t = 0$. Since there is a lower potential for $x > L_w + L_b$, the state $|E_0\rangle$ is a *quasi-bound* state. The electron is destined to leak out.

a) Using WKB tunneling probability, and combining semi-classical arguments, find an analytical formula that estimates the time it takes for the electron to leak out. Find a value of this lifetime for $L_b \sim 3$ nm, $L_w \sim 2$ nm, $V_0 \sim 1$ eV, $E_0 \sim 2$ eV, and $E_b \sim 5$ eV. How many years does it take?

b) This feature is at the heart of *flash memory*, which you use in computers and cell phones. Find an analytical expression that describes how the lifetime changes if a voltage V_a is applied across the insulator. Estimate the new lifetime for $V_a \sim 2.8$ V. This is the *readout* of the memory.

Problem 25: Boltzmann Transport: Scattering and Mobility

a) We derived the solution to the Boltzmann transport equation in the relaxation-time approximation for elastic scattering events to be $f(\mathbf{k}) \approx f_0(\mathbf{k}) + \tau(\mathbf{k})(-\frac{\partial f_0(\mathbf{k})}{\partial \mathcal{E}(\mathbf{k})})\mathbf{v_k} \cdot \mathbf{F}$, where all symbols have their usual meanings. Use this to show that for transport in d dimensions in response to a constant electric field E, in a semiconductor with an isotropic effective mass $m^\star$, the current density is $J = \frac{nq^2 \langle \tau \rangle}{m^\star} E$, where $\langle \tau \rangle = \frac{2}{d} \cdot \frac{\int d\mathcal{E} \cdot \tau(\mathcal{E}) \mathcal{E}^{\frac{d}{2}} (-\frac{\partial f_0(\mathcal{E})}{\partial \mathcal{E}})}{\int d\mathcal{E} \cdot \mathcal{E}^{\frac{d}{2}-1} f_0(\mathcal{E})}$, where the integration variable $\mathcal{E} = \mathcal{E}(\mathbf{k})$ is the kinetic energy of carriers. You have now at your disposal the *most general form* of conductivity and mobility from the Boltzmann equation for semiconductors that have a parabolic bandstructure! *Hint:* You may need the result that the volume of a d-dimensional sphere in the k-space is $V_d = \frac{\pi^{\frac{d}{2}} k^d}{\Gamma(\frac{d}{2}+1)}$, and some more dimensional and Γ−function information from Problem 6 of the assignments.
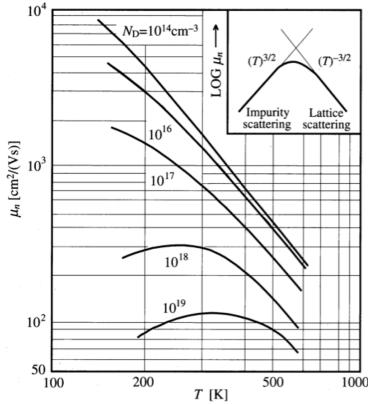

Fig. 4070.27: Electron mobility in a doped semiconductor at high temperatures is limited by phonon scattering, and by impurity and defect scattering at low temperatures. In this problem, you show that the ionized-impurity scattering limited mobility goes as $T^{\frac{3}{2}}/N_D$.

b) Scattering from uncorrelated events: Show using Fermi's golden rule that if the scattering rate of electrons in a band of a semiconductor due to the presence of ONE scatterer of potential $W(r)$ centered at the origin is $S(\mathbf{k} \to \mathbf{k}') = \frac{2\pi}{\hbar}|\langle \mathbf{k}'|W(r)|\mathbf{k}\rangle|^2 \delta(E_\mathbf{k} - E_{\mathbf{k}'})$, then the scattering rate due to N_s scatterers distributed *randomly and uncorrelated* in 3D space is $N_s \cdot S(\mathbf{k} \to \mathbf{k}')$. In other words, the scattering rate increases *linearly* with the number of uncorrelated scatterers, which implies that the mobility limited by such scattering will decrease as $1/N_s$. This argument is subtle, and effects of electron wave interference should enter your analysis. *Hint*: Add the potentials of each randomly distributed impurity for the total potential $W_{tot}(r) = \sum_i W(\mathbf{r} - \mathbf{R_i})$. Use the effective mass equation for the electron states to show that the matrix element is a Fourier transform. Then invoke the shifting property of Fourier transforms.

c) Impurity scattering: Using Fermi's golden rule, calculate the scattering rate for electrons due to a screened Coulombic charged impurity potential $V(r) = -\frac{Ze^2}{4\pi\epsilon_s r}e^{-\frac{r}{L_D}}$, where Ze is the charge of the impurity, ϵ_s is the dielectric constant of the semiconductor, and $L_D = \sqrt{\frac{\epsilon_s k_b T}{ne^2}}$ is the Debye screening length and n is the free carrier density. This is the scattering rate for just one impurity. Show using the result in parts (a) and (b), with a $1 - \cos\theta$ angular factor for mobility that if the charged-impurity density is N_D, the mobility for 3D carriers is $\mu_I = \frac{2^{\frac{7}{2}}(4\pi\epsilon_s)^2 (k_b T)^{\frac{3}{2}}}{\pi^{\frac{3}{2}} Z^2 e^3 \sqrt{m^\star} N_D F(\beta)} \sim \frac{T^{\frac{3}{2}}}{N_D}$. Here $\beta = 2\sqrt{\frac{2m^\star(3k_b T)}{\hbar^2}}L_D$ is a dimensionless parameter, and $F(\beta) = \ln[1 + \beta^2] - \frac{\beta^2}{1+\beta^2}$ is a weakly varying function. This famous result is named after Brooks and Herring who derived it first. Estimate the ionized impurity scattering limited mobility at $T = 300$ K for $m^\star = 0.2m_0$, $\epsilon_s = 10\epsilon_0$, $Z = 1$ and $N_D \sim 10^{17}, 10^{18}, 10^{19}/\text{cm}^3$. Are your values close to what is experimentally observed for these conditions as shown in Figure 4070.27?

Problem 26: Experiment I

Please form groups of 5-6 students and sign up for the available lab slots. The first experiment in the course is to measure the transport properties of semiconductors and metals. Please read the lab handout for an explanation of the experiment, and for directions on how to write a joint short report of your measurements.

4070.6   HW 6

Posted: 05/02/2017, Due: 05/15/2017

Problem 27: Fermi's Golden Rule: Mobility in Semiconductors

We now explain the complete temperature dependence of the electron mobility in some (not all!) doped 3D semiconductors. Figure 4070.27 shows the experimental result: at low temperatures, the electron mobility *increases* with temperature as $\mu(T) \sim T^{\frac{3}{2}}/N_D$, and at high temperature it *decreases* with temperature as $\mu(T) \sim 1/T^{3/2}$. We first connect the mobility to the scattering times via the Drude-like result $\mu = \frac{q\langle tau \rangle}{m_c^\star}$ where you found how to calculate the ensemble averaged scattering time $\langle \tau \rangle$ in Problem 25(a).

a) Phonon scattering: We showed in class that the scattering rate of electrons due to acoustic phonons in semiconductors is given by Fermis golden rule result for time-dependent oscillating perturbations $\frac{1}{\tau(\mathbf{k} \to \mathbf{k'})} = \frac{2\pi}{\hbar}|\langle \mathbf{k'}|W(\mathbf{r})|\mathbf{k}\rangle|^2 \delta(E_{\mathbf{k}} - E_{\mathbf{k'}} \pm \hbar\omega_q)$, where the acoustic phonon dispersion for low energy (or long wavelength) is $\omega_q \sim v_s q$ with v_s the sound velocity, and the scattering potential is $W(\mathbf{r}) = D_c \nabla_{\mathbf{r}} \cdot \mathbf{u}(\mathbf{r})$. Here D_c is the deformation potential (units: eV), and $\mathbf{u}(\mathbf{r}) = \hat{\mathbf{n}} u_0 e^{i\mathbf{q}\cdot\mathbf{r}}$ is the spatial part of the phonon displacement wave, $\hat{\mathbf{n}}$ is the unit vector in the direction of atomic vibration, and the phonon wavevector $\mathbf{q}$ points in the direction of the phonon wave propagation. We also justified why the amplitude of vibration u_0 may be found from $2M\omega_q^2 u_0^2 \approx N_{ph} \times \hbar\omega_q$, where $N_{ph} = 1/[e^{\frac{\hbar\omega_q}{k_b T}} - 1]$ is the Bose-number of phonons, and the mass of a unit cell of volume Ω is $M = \rho\Omega$, where ρ is the mass density (units: kg.m^{-3}). Show that a transverse acoustic (TA) phonon does *not* scatter electrons, but longitudinal acoustic (LA) phonons do.

b) By evaluating the scattering rate using Fermi's golden rule, and using the the ensemble averaging of Problem 25 (a), show that the electron mobility in three dimensions due to LA phonon scattering is $\mu_{LA} = \frac{2\sqrt{2\pi}}{3} \frac{q\hbar^4 \rho v_s^2}{(m_c^\star)^{\frac{5}{2}} D_c^2 (k_b T)^{\frac{3}{2}}} \sim T^{-\frac{3}{2}}$. This is a *very* useful result.

c) Now combine your work from parts (c) of problem 25 and (b) of this problem to explain the experimental dependence of mobility vs temperature and as a function of impurity density as seen in Figure 4070.27.

Problem 28: Semiconductor Heterojunctions and Band Offsets: Know what you are talking about

Here is Kroemers [see Fig 4070.28] Lemma of Proven Ignorance: *If, in discussing a semiconductor problem, you cannot draw an* **Energy-Band-Diagram**, *this shows that you don't know what you are talking about*, with the corollary *If you can draw one, but don't, then your audience won't know what you are talking about.*

In this problem we make sure we don't fall into this trap!

In Figure 4070.29 (a-f), energy band diagrams of several different semiconductor heterojunctions are shown (one on the left side and the other on the right side) *before* the two materials are put together, with their individual Fermi levels indicated. In each case sketch the equilibrium energy band diagram when a heterojunction is formed between the two semiconductors. In each case indicate the depletion and/or accumulation and/or inversion regions that may exist in equilibrium on either side of the heterointerface. The alignment shown corresponds to the electron affinity rule as shown explicitly in part (a).
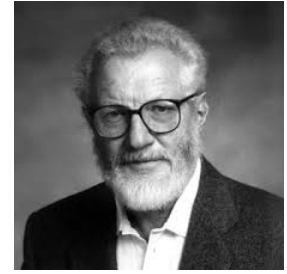

Fig. 4070.28: Herbert Kroemer, a pioneer in semiconductor hetero-junction based design of transistors and lasers was awarded the 2000 Nobel Prize in physics.
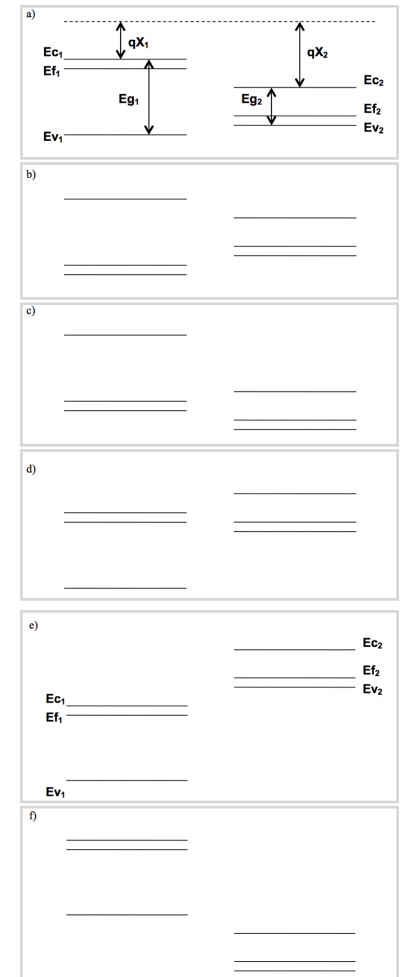

Fig. 4070.29: Various heterojunctions before reaching equilibrium.

All the labels are also shown in more detail in part (a), and which you can use for the other parts.

Problem 29: Population Inversion, Optical Gain, and Lasing

In class, we derived that the equilibrium optical absorption coefficient of a semiconductor is $\alpha_0(\hbar\omega) = C_0|\hat{e} \cdot \mathbf{p_{cv}}|^2 \rho_r(\hbar\omega - E_g)$, where $\rho_r(\hbar\omega - E_g)$ is the joint electron-photon DOS, $C_0 = \frac{\pi e^2}{n_r c \epsilon_0 m_0^2 \omega}$, and all symbols have their usual meanings. We also discussed that under *non-equilibrium* conditions, the optical absorption coefficient becomes $\alpha(\hbar\omega) = \alpha_0(\hbar\omega)[f_v(k) - f_c(k)]$, where the electron occupation functions of the bands are given by the Fermi-Dirac distributions $f_v(k) = \frac{1}{1+e^{\frac{E_v(k)-F_v}{k_b T}}}$ and $f_c(k) = \frac{1}{1+e^{\frac{E_c(k)-F_c}{k_b T}}}$, but with quasi-Fermi levels F_v for the valence band and F_c for the conduction band as the mathematical means to capture *non-equilibrium* conditions. Consider a semiconductor with parabolic bandstructures for the conduction band $E_c(k) = E_g + \frac{\hbar^2 k^2}{2m_c^\star}$ and valence band $E_v(k) = -\frac{\hbar^2 k^2}{2m_v^\star}$ for this problem.

a) Make a sketch of the equilibrium absorption coefficients $\alpha_0(\hbar\omega)$ for a bulk 3D semiconductor, and a 2D quantum well vs the photon energy $\hbar\omega$.

b) Plot the Fermi difference function $f_v(k) - f_c(k)$ as a function of the photon energy $\hbar\omega$ for a few choices of the quasi-Fermi levels F_v, F_c of the valence and conduction bands. Specifically, track the photon energy at which the difference function *changes sign* from ve to +ve.

c) Now combine (a) and (b) to plot the non-equilibrium absorption coefficient $\alpha(\hbar\omega)$ for the choices of F_v, F_c from part (b). Discuss the significance of a *negative* absorption coefficient.

d) Show that the requirement for population inversion is $F_c - F_v > E_c - E_v = \hbar\omega$. This is the famous Bernard-Duraffourg condition for *population inversion* in semiconductor lasers.

e) Based on your results above, explain why semiconductor heterostructure quantum wells have lower injection thresholds for lasing than 3D bulk semiconductors. This idea and demonstration won Herb Kroemer (Fig 4070.28) and Zhores Alferov (Fig 4070.31) the 2000 Nobel prize in physics.
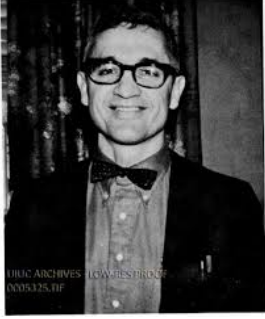

Fig. 4070.30: Nick Holonyak is a semiconductor pioneer, who first demonstrated the semiconductor light-emitting diode, and one of the first quantum well lasers.

Fig. 4070.31: Zores Alferov was awarded the 2000 Nobel Prize in physics for the demonstration of the double heterojunction semiconductor laser.

Problem 30: Gain in Quantum Wells

Instead of bulk semiconductors, if we have a quantum well of thickness L_z, the absorption coefficient still follows the joint density of states feature. To derive this, do the following: assume an infinite barrier height (this approximation can be relaxed in a numerical approach, we keep things analytical here). Then,

a) Write down the wavefunctions of electron states in the n_c^{th} subband if the conduction band $|n_c, \mathbf{k_c}\rangle$ as a product of the quantized envelope wavefunction $C(n_c, z)$ along the confinement $(z-)$direction, a free electron envelope wavefunction $t_c(x, y, \mathbf{k_c})$ in the transverse $(x - y-)$direction, and a CB Bloch periodic function $u_c(\mathbf{r})$. Do the same for the valence band states $|n_v, \mathbf{k_v}\rangle$, choosing the corresponding envelope functions $V(n_v, z)$, $t_v(x, y, \mathbf{k_v})$, and Bloch periodic function $u_v(\mathbf{r})$.

b) Argue why the transverse parts of the enveloped wavefunctions $t_c(x, y, \mathbf{k_c})$ and $t_v(x, y, \mathbf{k_v})$ must be the *same* for optical transitions.

c) The optical matrix element is given by $W_{op} = \langle n_c, \mathbf{k_c}| - \frac{e}{m_0}\mathbf{A} \cdot \mathbf{p}|n_v, \mathbf{k_v}\rangle$. Show that this can be written as the product $W_{op} = \frac{eA_0}{m_0} \times \hat{e} \cdot \underbrace{\langle u_c|\mathbf{p}|u_v\rangle}_{\mathbf{p_{cv}}} \times \delta_{\mathbf{k_c},\mathbf{k_v}} \times I^{c,n_c}_{v,n_v}$, where the

optical transition rules are dictated by the integral $I^{c,n_c}_{v,n_v} = \int_{-\infty}^{+\infty} C^\star(n_c, z)V(n_v, z)dz$.

d) Show that for infinite barrier quantum wells, the selection rule is $I^{c,n_c}_{v,n_v} = \delta_{n_v,n_c}$, i.e., the only transitions from valence band quantized states to conduction band quantized states that are allowed follow the selection rule $\Delta n = n_v - n_c = 0$ (for example, $1 \to 1$, $2 \to 2$ ...).

e) Based on part (d), show that the *equilibrium* absorption coefficient is then given by

$$\alpha_0(\hbar\omega) = \underbrace{\frac{\pi e^2}{n_r c\epsilon_0 m_0^2\omega}|\hat{e} \cdot \mathbf{p_{cv}}|^2}_{same-coeff-as-3D} \times \underbrace{\frac{m_r^\star}{\pi\hbar^2 L_z}}_{\rho_r^{2D}} \times \underbrace{\sum_n \theta[\hbar\omega - (E_g + E_n^c + E_n^v)]}_{staircase-function}, \qquad (4070.15)$$

where E_n^c, E_n^v are the conduction and valence band quantization energies and $n = n_c = n_v$.

f) Figure 4070.32 shows an experimentally measured optical gain spectrum of a lattice-matched InP/InGaAs/InP quantum well. Use the results of the this problem, and also figure 4070.33 to explain the gain spectrum.
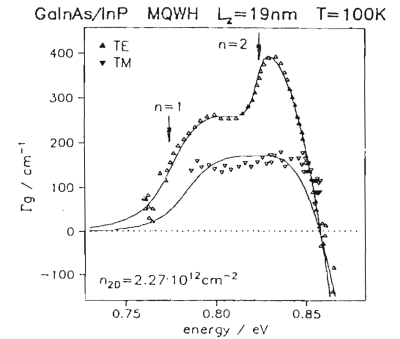
Fig. 4070.32: Experimentally measured optical gain in an InP/InGaAs/InP quantum well heterostructure.
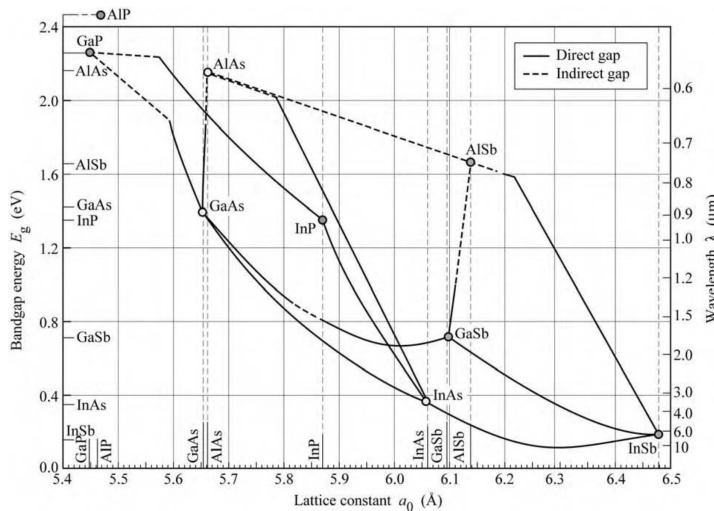
Problem 31: The Quantum Mechanic

Fig. 4070.33: Bandgaps and Lattice Constants of Compound Semiconductors (From Schubert's book on LEDs).

As the CTO of the stealth startup 'The Quantum Mechanics' you win a project from NASA to design an infrared photodetector for the detection of a very weak $\lambda_0 = 12.4$ μm radiation from a distant star. Because you have in your team the world's best group of III-V compound semiconductor MBE growers who can grow for you layered heterostructures of any combination of materials you can dream up from Figure 4070.33, you decide the design will be done using *intersubband transitions* in III-V quantum wells. Describe your design in quantitative detail - including plots, choices of materials, thicknesses, etc. Pay attention

to the *selection rules* for optical transitions, assume the 75%:25% $\Delta E_c : \Delta E_v$ band offset distribution, and use the rule of thumb that you cannot grow a strained layer thicker than $t_{cr} \sim \frac{a_0}{2\epsilon}$ where ϵ is the strain. Feel free to use the results of **Problem 22**. Explain if your IR photodetector will work at room temperature, or needs to be cooled. Cooling is *not* a problem, especially if it goes to space!

Problem 32: Experiment II

In the second experiment of this course, you will measure in the lab

a) the characteristics of a quantum well based semiconductor high electron mobility transistor (HEMT). You will measure the I_d vs V_{ds} and I_d vs V_{gs}, exhibiting on/off switching, and linear and current saturation regimes of the transistor,

and

b) the $I - V$ characteristics, and the electroluminescence spectrum $R_{sp}(\hbar\omega)$ of a quantum well semiconductor light-emitting diode.

Please read the lab handout for an explanation of the experiment, and for directions on how to write a joint short report of your measurements.

That is all for this semester!!

Fig. 4070.34: The 'Traitorous Eight', who left Bill Shockley's semiconductor company and formed Fairchild Semiconductors to make silicon transistors in the San Francisco bay area, giving birth to the Silicon Valley. See if you can spot Robert Noyce, the inventor of the Integrated Circuit, and Gordon Moore, known for Moore's law. A sub group later started Intel.