ECE 5390/MSE 5472, Fall Semester 2017
Quantum Transport in Electron Devices & Novel Materials

Debdeep Jena (djena@cornell.edu), Depts. of ECE and MSE, Cornell University

Assignment 3 and Prelim

Policy on assignments: Please turn them in by 5pm of the due date. The due date for this assignment is **Monday, Oct 30th, 2017**. The due date for the Prelim question 3.6 is **Friday Nov 3rd**.

General notes: 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. Draw figures wherever necessary. Please print out this question sheet and staple to the top of your homework. Write your name and email address on the cover. Some problems may lead to publishable results - be on the lookout!

Problem 3.1) Designer digital and analog Ballistic FETs

In class we discussed that for a Ballistic FET with a 2D electron gas channel, a parabolic bandstructure $E(k_x, k_y) = \frac{\hbar^2}{2m^\star}(k_x^2 + k_y^2)$ leads to a current $\frac{I_d}{W} \propto (V_{gs} - V_T)^{\frac{3}{2}}$, leading to a gain or transconductance $g_m = \frac{\partial I_d}{\partial V_{gs}} \propto (V_{gs} - V_T)^{\frac{1}{2}}$.

(a) Using the on-state current as the primary metric, discuss the effects of the band-edge effective mass $m^\star$ and k-valley degeneracy g_v on the FET on-current. Using your program for Problem 2.6 in Assignment 2, show that the dependence can be *non-monotonic*, meaning a lighter effective mass does guarantee the highest on-current, and a higher valley degeneracy does not always mean a higher on-current. What is the reason?

(b) Show why if the gate of the FET is driven by a monochromatic input signal $V_{gs} = V_{gs}^{dc} + v_\omega e^{i\omega t}$, the output ac current has many frequencies, not just the frequency of the input signal.

(c) Assume $v_\omega << V_{gs}^{dc}$. Can you design a bandstructure that will remove these higher harmonics? This will make the transistor more linear. If you have a good strategy, you can make an impact on communication electronics, where transistors with high *linearity* are in demand.

Problem 3.2) The Boltzmann Transport Equation

In class, we discussed the Boltzmann transport equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f + \mathbf{F} \cdot \nabla_{\mathbf{p}} f = \hat{C} f \tag{1}$$

where the symbols have the usual meanings. The collision term on the right is

$$\hat{C} f = \sum_{k'} [S(k' \to k) f_{k'} (1 - f_k) - S(k \to k') f_k (1 - f_{k'})], \tag{2}$$

where $S(k \to k') = \frac{2\pi}{\hbar} |\langle k'|W(r)|k\rangle|^2 \delta(E_{k'} - E_k \pm \hbar\omega)$ are the scattering rates given by Fermi's golden rule. In this problem, we discuss a few details of this recipe of solving diffusive transport problems. For *any* scattering potential, we found that $\frac{S(k\to k')}{S(k'\to k)} = \exp(\frac{E_k - E_{k'}}{kT})$, which led us to distinguish between elastic and inelastic scattering events.

a) Under what conditions can we make the relaxation time approximation (RTA), where $\hat{C}f \approx -(f - f_0)/\tau$? Discuss for both elastic and inelastic scattering events.

b) Outline how from the RTA of the distribution function f, one may obtain charge transport properties such as the electrical conductivity, and thermoelectric properties.

c) For a force $\mathbf{F} = q\mathbf{F_e}$ due to an electric field *alone*, the RTA solution of the BTE took the form

$$f \approx f_0 + \tau(-\frac{\partial f_0}{\partial E})\mathbf{v}\cdot\mathbf{F}. \quad (3)$$

However, in the presence of a crossed electric and magnetic field, the net force is the Lorentz force, $\mathbf{F} = q(\mathbf{F_e} + \mathbf{v}\cdot\mathbf{B})$. Work out a solution for f in the RTA for this situation. You may refer to Wolfe/Holonyak/Stillman's book on the Physics of Semiconductors for this part. Realize that this is the situation encountered in a Hall-effect measurement.

d) Outline how magnetoresistance properties may be obtained from the BTE from your discussion above.

Problem 3.3) Application of Fermi's Golden Rule: Scattering rates due to Point Defects, and Alloy Disorder Scattering

Assume that in a 3D semiconductor crystal of GaN (electron effective mass = $m^\star \sim 0.2m_0$), point defects of volume density $n_{imp} = N_{imp}/V$ are present. Also, assume that the perturbation V_0 to the crystal potential due to each point defect is confined to a radius R_0 around its location, i.e.,

$$W(\mathbf{r}) = V_0\theta(R_0 - |\mathbf{r}|), \quad (4)$$

where $\theta(...)$ is the unit-step function. This is an example of a 'short-range' scatterer.

a) Find the matrix element for scattering of electrons by all the point defects.

b) Assume the single-electron picture, and a parabolic bandstructure. Find an expression for the *momentum* scattering rate $1/\tau_m(E)$ of an electron due to the point defects as a function of its energy above the conduction band edge ($\epsilon = E - E_c$). Make necessary assumptions in the process. Show that the momentum and quantum scattering rates are the same for this form of isotropic scattering potentials.

c) Plot the mobility for 'thermal' electrons with $\epsilon = E - E_c \sim k_BT$ at 300 K, as a function of the impurity density in the range $n_{imp} = 10^{15} \to 10^{20}/\text{cm}^3$ for various values of $V_0 = 0.1, 0.3, 0.5, 2.1$ eV. Assume an $R_0 \sim c/4$, where $c \sim 0.51$ nm is the c-axis lattice constant of GaN.

d) This is a reasonable model for things such as alloy scattering, for example, for charge transport of electrons in AlGaN and InGaN layers. Explain why an disordered alloy can be considered to be a perfect crystal with a high density of point defects. Then, estimate the mobility for electrons in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ layers as a function of the alloy composition x, by using your results in part (c). Find any references where this might have been done.

Problem 3.4) Flash Memory Design by Fermi's golden rule

Figure 1 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.

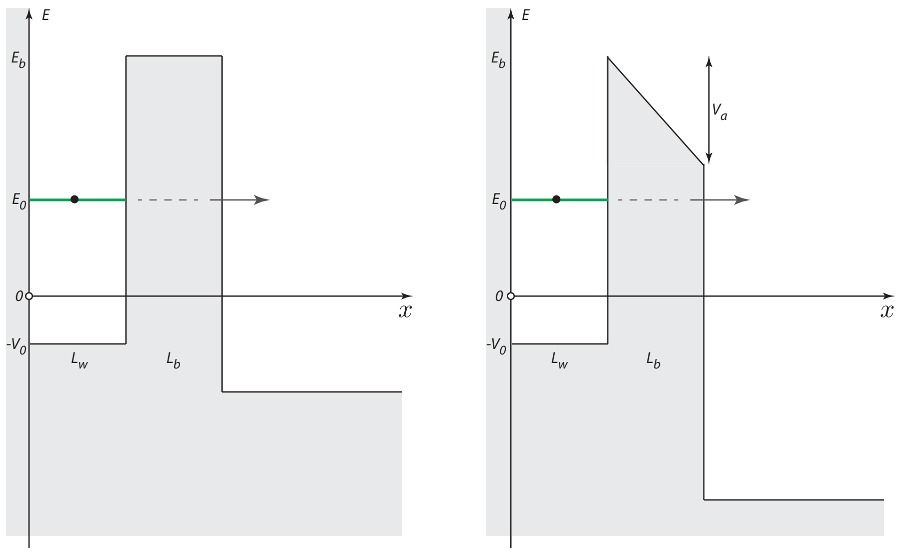

Figure 1: Escape and field-emission by tunneling.

(c) In the last two parts you invoked semi-classical arguments to estimate the tunneling escape time there. Now try solving the *same* problem using Fermi's golden rule. Model the problem carefully so that you can apply Fermi's golden rule. Discuss your approximations and their validity.

Problem 3.5) Higher-order time-dependent perturbation theory: Dyson series and diagrams

In class, we used the *interaction representation* to write the perturbed quantum state at time t as $|\psi_t\rangle = e^{-i\frac{H_0}{\hbar}t}|\psi(t)\rangle$, where H_0 is the unperturbed Hamiltonian *operator*. This step helped us recast the time-dependent Schrodinger equation $i\hbar\frac{\partial}{\partial t}|\psi_t\rangle = (H_0 + W_t)|\psi_t\rangle$ to the simpler form $i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = W(t)|\psi(t)\rangle$, where $W(t) = e^{+i\frac{H_0}{\hbar}t}W_t e^{-i\frac{H_0}{\hbar}t}$ is the time-evolution operator. This equation was integrated over time to yield the Dyson series

$$|\psi(t)\rangle = \underbrace{|0\rangle}_{|\psi(t)\rangle^{(0)}} + \underbrace{\frac{1}{i\hbar}\int_{t_0}^{t} dt' W(t')|0\rangle}_{|\psi(t)\rangle^{(1)}} + \underbrace{\frac{1}{(i\hbar)^2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' W(t')W(t'')|0\rangle}_{|\psi(t)\rangle^{(2)}}$$
$$+ \underbrace{\frac{1}{(i\hbar)^3}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \int_{t_0}^{t''} dt''' W(t')W(t'')W(t''')|0\rangle}_{|\psi(t)\rangle^{(3)}} + ..., \tag{5}$$

where $|\psi(t_0)\rangle = |0\rangle$ is the initial state. Restricting the Dyson series to the 1st order term in W for a perturbation of the the form $W_t = e^{\eta t} W(r)$, we derived Fermi's golden rule for the transition rate $\Gamma^{(1)}_{0\to n} = \frac{2\pi}{\hbar}|\langle n|W(r)|0\rangle|^2 \delta(\epsilon_0 - \epsilon_n)$. We used the relation $\lim_{\eta\to 0^+} \frac{2\eta}{x^2+\eta^2} = 2\pi\delta(x)$ in this process.

a) Show that the second and third order terms in W in the Dyson series lead to a modified golden rule result

$$\Gamma_{0\to n} = \frac{2\pi}{\hbar}|\langle n|W|0\rangle + \sum_m \frac{\langle n|W|m\rangle\langle m|W|0\rangle}{\epsilon_0 - \epsilon_m + i\eta\hbar} + \sum_{k,l} \frac{\langle n|W|k\rangle\langle k|W|l\rangle\langle l|V|0\rangle}{(\epsilon_0 - \epsilon_k + 2i\eta\hbar)(\epsilon_0 - \epsilon_l + i\eta\hbar)} + ...|^2 \delta(\epsilon_0 - \epsilon_n), \tag{6}$$

where in the end we take $\eta \to 0^+$. We identify the Green's function propagators of the form $G = \sum_m \frac{|m\rangle\langle m|}{\epsilon_0 - \epsilon_m + i\eta\hbar}$. Thus, the result to higher orders may be written in the compact form

$$\Gamma_{0\to n} = \frac{2\pi}{\hbar}|\langle n|W + WGW + WGWGW + ...|0\rangle|^2 \delta(\epsilon_0 - \epsilon_n). \tag{7}$$

5.23 A one-dimensional harmonic oscillator is in its ground state for $t < 0$. For $t \geq 0$ it is subjected to a time-dependent but spatially uniform *force* (not potential!) in the x-direction,

$$F(t) = F_0 e^{-t/\tau}.$$

(a) Using time-dependent perturbation theory to first order, obtain the probability of finding the oscillator in its first excited state for $t > 0$. Show that the $t \to \infty$ (τ finite) limit of your expression is independent of time. Is this reasonable or surprising?

(b) Can we find higher excited states? You may use

$$\langle n'|x|n\rangle = \sqrt{\hbar/2m\omega}(\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}).$$

Figure 2: Harmonic oscillator perturbed by a time-dependent field.

b) Sketch the 'Feynman' diagrams[1] corresponding to the terms in the series, showing the *virtual* states explicitly for the higher order terms.

c) Solve the above problem in Figure 2 from Sakurai (Modern Quantum Mechanics). Note that for part (b), you will need to invoke higher-order perturbation terms as discussed in this problem, the 1st order Fermi's golden rule result term will not be enough.

[1] More accurately, Goldstone diagrams.

Problem 3.6) Prelim: Electron Mobility in Semiconductors

The purpose of this question is to reproduce the theoretical calculation of electron mobility vs temperature as shown in Figure 3 and explain the physics of electron transport underlying what is measured in the experiment. This requires you to calculate the scattering rates due to phonons, ionized impurities, and neutral impurities, and applying the Boltzmann transport equation to evaluate the electron mobility vs temperature. On the class website I have provided you with a handout from Wolfe / Holonyak / Stillman to help you in this problem, and the paper from where this plot is taken, so you have everything you need to solve this problem.

(a) Boltzmann Transport Equation 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. $\mu = \frac{q\langle\tau\rangle}{m^\star}$ is the mobility. 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 $\Gamma-$function information.

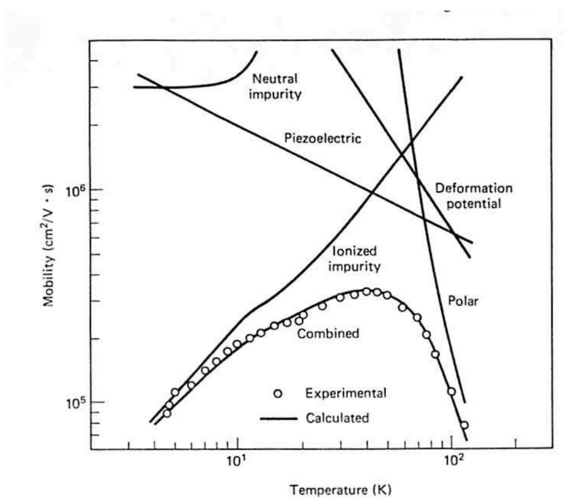

Figure 6.7 Temperature dependence of the mobility for *n*-type GaAs showing the separate and combined scattering processes. [From C. M. Wolfe, G. E. Stillman, and W. T. Lindley, *J. Appl. Phys. 41*, 3088 (1970).]

Figure 3: Electron mobility in doped GaAs semiconductor at high temperatures is limited by phonon scattering, and by impurity and defect scattering at low temperatures. In this problem, you will calculate the solid lines of this plot.

(b) Spatially uncorrelated scattering points: 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.] Now calculate the neutral impurity scattering limited mobility for GaAs and compare with Figure 3.

(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. Calculate the ionized impurity scattering limited mobility and compare: are your values close to what is experimentally observed for these conditions as shown in Figure 3?

(d) Acoustic Phonon scattering: The scattering rate of electrons due to acoustic phonons in semiconductors is given by Fermis golden rule result for time-dependent oscillating perturbations $\frac{1}{\tau(\mathbf{k}\rightarrow\mathbf{k}')} = \frac{2\pi}{\hbar}|\langle\mathbf{k}'|W(\mathbf{r})|\mathbf{k}\rangle|^2 \delta(E_{\mathbf{k}} - E_{\mathbf{k}'} \pm \hbar\omega_q)$, 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. 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. Calculate and explain the acoustic deformation potential and acoustic piezoelectric phonon scattering rates for GaAs and compare with Figure 3.

(e) Discuss how polar optical phonon scattering is different from acoustic phonon scattering, and calculate the phonon scattering limited mobility for GaAs and compare with Figure 3.

(f) Now combine all the above parts of to explain the experimental dependence of mobility vs temperature and as a function of impurity density as seen in Figure 3. If you have succeeded in getting it to work, you have built a very powerful transport tool - because now you can use it to explain electron transport properties in *any* semiconductor! This is because the material parameters may change, but the transport formalism remains the same.