
Assignment 3

EE 80724, Wide Bandgap Device Physics, Fall 2009

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1 Optical Transitions: The Quantum-Confined Stark Effect

When an electric field is applied across a quantum well, the fundamental optical transitions shift in energy. This ‘Stark’ shift of the confined levels in a quantum well can be calculated by using second-order perturbation theory. Consider the interaction between the electrons (effective mass m^*) in a quantum well of width d and a DC electric field of strength F_z applied along the z (growth) axis.

- a) Explain why the perturbation to the energy of an electron is given by $W = eF_z z$. Draw a band diagram to depict the situation.
- b) Explain why the first-order shift of the energy levels, given by

$$\Delta E_n^{(1)} = \int_{-\infty}^{+\infty} dz \phi_n^*(z) W \phi_n(z) \quad (1)$$

is ZERO. Use the Effective Mass Approximation to write down the wavefunctions in an infinitely deep quantum well for this problem.

- c) The second-order energy shift of the $n = 1$ level¹ is given by the Rayleigh-Schrödinger approximation

$$\Delta E_{n=1}^{(2)} = \sum_{n>1} \frac{|\langle 1|W|n \rangle|^2}{E_1 - E_n}, \quad (2)$$

where

$$\langle 1|W|n \rangle = \int_{-\infty}^{+\infty} dz \phi_1^*(z) W \phi_n(z). \quad (3)$$

Show that for an electron in a quantum well with infinitely high barriers, the Stark shift is given approximately by

$$\Delta E = -24 \left(\frac{2}{3\pi} \right)^6 \frac{e^2 m^* d^4}{\hbar^2} F_z^2. \quad (4)$$

- d) Note that the QCSE-shift goes as $\Delta E \sim m^* d^4 F_z^2$. Calculate and plot the shift (in meV) for a $d = 5nm$ thick AlGaIn/GaN/AlGaIn quantum well as a function of electric fields over a range typical in semiconductor devices. Comment on how this shifts the interband transition wavelength (red or blue?) by using same arguments for holes.
- e) The electric field F_z may be externally applied, or can arise due *internal* fields present in III-V Nitrides. Assuming a polarization field of $F_z \sim 2$ MV/cm, what are the shifts in energy eigenvalues of the ground state electrons and holes?

Contd...

¹Note the similarity to what we did in $\mathbf{k} \cdot \mathbf{p}$ theory due to interaction between the $n = 1$ state with all other states through the perturbation potential. This interaction led to the conclusion that the effective mass of CB electrons is proportional to the bandgap.

2 Transport of Bloch Electrons - ‘Ballistic’ Transport

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

$$E(k_x, k_y) = -E_0 \cdot [\cos k_x a + \cos k_y a] \quad (5)$$

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

$$T = \frac{\pi \hbar}{a F_x} \quad (6)$$

- d) Calculate and plot the x- and y-components of the velocity and the position of the electron, all functions of time, for $0 \leq t \leq 4T$.
- e) Make a graph of the trajectory of the electron in the x-y plane of real space. What is the net displacement of the electron in every cycle? Why is this type of motion called Bloch *oscillation*?
- f) We saw in class that electrons in typical semiconductors do not exhibit Bloch oscillations since the Brillouin Zone edge is too far in k -space; electrons are scattered before they make it to the BZ edge. However, it is possible to artificially engineer the bandstructure so that this problem can be solved. How can you change the bandstructure to achieve this? Search, and mention one reference paper that (experimentally) uses your approach.

3 Ballistic Transport: Quantized Conductance

- a) Show that the ballistic conductance due to electrons in a 1D band at the $T \rightarrow 0$ K limit is $G_0 = g_s g_v e^2 / h$, where g_s, g_v are the spin and valley degeneracies, e is the electron charge, and h ($= 2\pi \hbar$) is Planck’s constant.
- b) Argue why this result is correct whatever be the bandstructure.
- c) Examine how one can obtain Ohm’s law of conductance (or resistance, $R = \rho L / A$) in 2- and 3-dimensions, starting from the idea of quantized conductance of a single mode.

4 Time-Dependent Perturbation Theory: Fermi’s Golden Rule

- a) We derived the results of Fermi’s Golden Rule in class. Re-Derive Fermi’s Golden rule for the transitions from an initial state to a final state $|i\rangle \rightarrow |f\rangle$ (result: $\frac{1}{\tau_{i \rightarrow f}} \approx \frac{2\pi}{\hbar} |W_{if}|^2 \delta[E_f - E_i \pm \hbar\omega_0]$), as well as the result that gives the rate for transitions into a *continuum* of final states

(result: $\frac{1}{\tau} \approx \frac{2\pi}{\hbar} |W_{if}|^2 g(E_f - E_i \pm \hbar\omega_0)$, where $g(\dots)$ is the density of states). Show that one result can be derived from the other. Make special note that this is a ‘steady-state’ result, meaning as $t \rightarrow \infty$, and relate it with the actual time-evolution of Sinc-like functions.

- b) Discuss the restrictions under which one can apply the rule.
- c) Describe why the transitions ‘resonances’ are *not* indicative of energy not being conserved, but rather an interplay of the *total* energy of the *perturbed* and *perturbing* systems.

5 Application of Fermi’s Golden Rule: Scattering rates due to Point Defects

Assume that in a 3D semiconductor crystal of GaN (electron effective mass = $m^* \sim 0.2m_0$), 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.,

$$W(\mathbf{r}) = V_0\theta(R_0 - |\mathbf{r}|), \quad (7)$$

where $\theta(\dots)$ is the unit-step function. This is an example of what is called ‘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 *total* scattering rate ($\frac{1}{\tau}$) 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.
- c) Assuming that the mobility is given² by $\mu \sim e\tau/m^*$, plot the mobility for ‘thermal’ electrons with $\epsilon = E - E_c \sim k_B T$ at 300 K, as a function of the impurity density in the range $n_{imp} = 10^{15} \rightarrow 10^{20}/\text{cm}^3$ for various values of $V_0 = 0.1, 0.3, 0.5, 2.1$ eV. Assume an $R_0 \sim c/4$, where $c \sim 5.1\text{\AA}$ 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 AlGa_xN and InGa_xN 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 Al_xGa_{1-x}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.

6 Application of Fermi’s Golden Rule: Ionized Impurity Scattering

Now that you have done Problem (5), estimate the electron mobility in bulk GaN as a result of scattering from ionized donors of volume density N_D . Set up the *screened* potential³, find the matrix element, the single particle scattering rate, and estimate the mobility. Make representative plots (for example, mobility vs Temperature).

²We’ll see later that the momentum scattering rate needs a weighting factor and that the distribution function has to be considered in the general case, but the approximation here is reasonable.

³The screened Coulomb potential in 3D is $V_{scr}(r) = V_{unsc}(r) \times e^{-r/L_D}$, where L_D is the Debye screening length and $V_{unsc}(r)$ is the unscreened potential.