Midterm Exam, Fall 2009

ECSE-6220 – Physical Foundations of Solid-State Devices, Prof. E. F. Schubert

Note: (*i*) Put your name on paper, show your work, underline results, and always show units.
(*ii*) Textbook, manuscript, excerpts, and calculators are allowed.

1. The Bohr radius of an electron occupying the ground state of a hydrogen atom is r_{Bohr} = 0.53 Å = 0.053 nm.
   (a) Calculate the de Broglie wavelength of the electron.
   (b) Calculate the momentum p of the electron.
   (c) Calculate the classical velocity v of the electron.
   (d) Calculate the ratio of the electron velocity to the speed of light (2.99×10^8 m/s).
   (e) Calculate the ratio of the electron velocity to the speed of sound (340 m/s).

   (a) Electronic orbitals are allowed, only if the circumference is an integer multiple of the electron de Broglie wavelength

$$S = (n + 1)\,\lambda$$

   For ground state, n = 0. Therefore,

$$\lambda_{0,\text{hydrogen}} = S = 2\pi r_{\text{Bohr}} = 2\pi \times 0.53\text{ Å} = 3.33\text{ Å}$$

   (b) According to the de Broglie relation, the momentum is given as

$$p = \frac{h}{\lambda} = 1.99 \times 10^{-24}\text{ kg m/s}$$

   (c) The classical velocity of the electron can be calculated using the following relation,

$$p = mv$$

   where m is the mass of the electron. Therefore,

$$v = \frac{p}{m_e} = \frac{1.99 \times 10^{-24}}{9.1094 \times 10^{-31}} = 2.18 \times 10^6\text{ m/s}$$

   (d) The ratio of the electron velocity to the speed of light is

$$\frac{v_e}{v_{light}} = \frac{2.18 \times 10^6}{2.99 \times 10^8} = 7.3 \times 10^{-3}$$

   (e) The ratio of the electron velocity to the speed of sound is

$$\frac{v_e}{v_{sound}} = \frac{2.18 \times 10^6}{340} = 6.4 \times 10^3$$

2. An electron occupies the ground state of a quantum well in the GaN conduction band. Assume that the quantum well has a width of L_{QW} = 20 Å and that the quantum well walls are infinitely high.
   (a) Calculate the ground-state energy.
   (b) Calculate the de Broglie wavelength of the electron.
   (c) Calculate the velocity v of the electron.
   (d) Give two differences between the *classical velocity* of a classical particle and a *quantum-mechanical velocity* (the group velocity) of an electron.

(a) The ground-state (n = 0) energy of an infinite potential quantum well is given by,

$$E_n = \frac{\hbar^2}{2m_e^*}\left[\frac{\pi}{L_{QW}}\right]^2 = \frac{(1.0546\times 10^{-34})^2}{2\times 0.2\times 9.1094\times 10^{-31}}\left[\frac{\pi}{20\times 10^{-10}}\right]^2$$
$$= 7.53\times 10^{-20}\ \text{J} = 470\ \text{meV}$$

(b) The de Broglie wavelength of the electron in the ground state of an infinite potential quantum well can be calculated using the relation

$$\lambda = 2L_{QW} = 2\times 20 = 40\ \text{Å}$$

(c) Since the energy is purely kinetic, the velocity v of the electron can be calculated using

$$E_n = \frac{1}{2}m_e^* v^2$$

Therefore,

$$v = \sqrt{\frac{2E_n}{m_e^*}} = \sqrt{\frac{2\times 7.53\times 10^{-20}}{0.2\times 9.1094\times 10^{-31}}} = 9.09\times 10^5\,\text{m/s}$$

(d) *First difference*: The group velocity of a quantum-mechanical particle has an uncertainty associated with it. The velocity of a classical object has no uncertainty associated with it.
Second difference: The group velocity of a quantum-mechanical particle has a phase velocity associated with it. The velocity of a classical object does not have a phase velocity associated with it.
Third difference: The group velocity of a quantum-mechanical particle is non-deterministic. The velocity of a classical object is deterministic.

3. Assume a dispersion relation of an electron in a one-dimensional (1D) periodic potential is given by: $E = 2\,\Delta E_0\,[1 - \cos(ka)]$, where a = 5 Å = 0.5 nm is the lattice constant of a one-dimensional lattice and ΔE_0 = 10 meV.
   (a) Calculate the phase velocity at the points $k = 0$, $k = \pi/(2a)$, and $k = \pi/a$.
   (b) Calculate the group velocity at the points $k = 0$, $k = \pi/(2a)$, and $k = \pi/a$.
   (c) Assume that it takes the electron the time 10^{-10} s to go from $k = 0$ to $k = \pi/a$. What is the electric field that is applied to the 1D periodic potential?

(a) The phase velocity is given by

$$v_{ph} = \frac{\omega}{k} = \frac{E}{\hbar k} = \frac{2\times 10\times 10^{-3}\times 1.6022\times 10^{-19}}{1.0546\times 10^{-34}}\frac{[1-\cos(k\times 5\times 10^{-10})]}{k}$$

For the case of k = 0, we use the following relation

$$\lim_{x\to 0}\frac{1-\cos(x)}{x} = 0$$

Therefore,

$$v_{ph,k=0} = 0\ \text{m/s}$$
$$v_{ph,k=\pi/2a} = 9.67\times 10^3\ \text{m/s}$$
$$v_{ph,k=\pi/a} = 9.67\times 10^3\ \text{m/s}$$

(b) The group velocity is given by

$$v_{gr} = \frac{1}{\hbar}\frac{\mathrm{d}E}{\mathrm{d}k} = \frac{1}{\hbar}2a\Delta E_0 \sin(ka)$$

$$= \frac{2 \times 5 \times 10^{-10} \times 10 \times 10^{-3} \times 1.6022 \times 10^{-19}}{1.0546 \times 10^{-34}} \sin(ka)$$

Therefore,

$$v_{gr,k=0} = 0 \text{ m/s}$$

$$v_{gr,k=\pi/2a} = 1.52 \times 10^4 \text{ m/s}$$

$$v_{gr,k=\pi/a} = 0 \text{ m/s}$$

(c) The rate of change of k value of the electron is given as

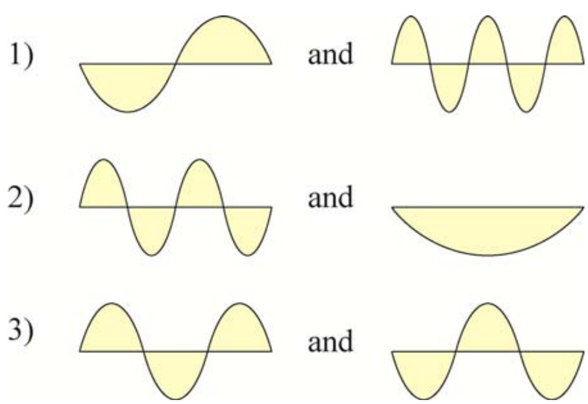
$$\frac{\mathrm{d}k}{\mathrm{d}t} = -\frac{1}{\hbar} eE$$

Therefore, the applied electric field, E, can be calculated as

$$E = -\frac{\hbar}{e}\frac{\mathrm{d}k}{\mathrm{d}t} = -\frac{1.0546 \times 10^{-34}}{1.6022 \times 10^{-19}} \frac{[\frac{\pi}{5 \times 10^{-10}} - 0]}{1 \times 10^{-10}} = -4.14 \times 10^4 \text{ V/m}$$

4. Selection rule for optical transitions

(a) State whether transition between the following pairs of wave functions due to an odd-symmetry perturbation function are allowed or disallowed.



(b) Is an intraband optical transition allowed in a bulk semiconductor? Explain.

(a) Transition is
1) Allowed
2) Allowed
3) Disallowed

(b) No. The perturbing potential energy caused by an oscillating electromagnetic field (such as light wave) is an odd-symmetry function of the special coordinate x given by

$$U(x) = -eE_0 x$$

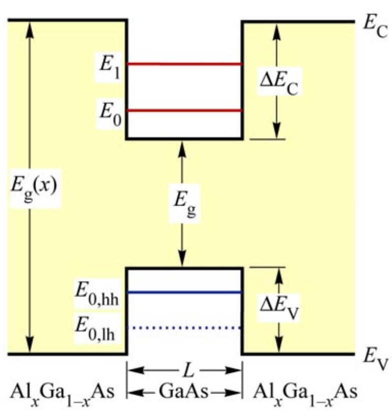
The transition matrix element is given as

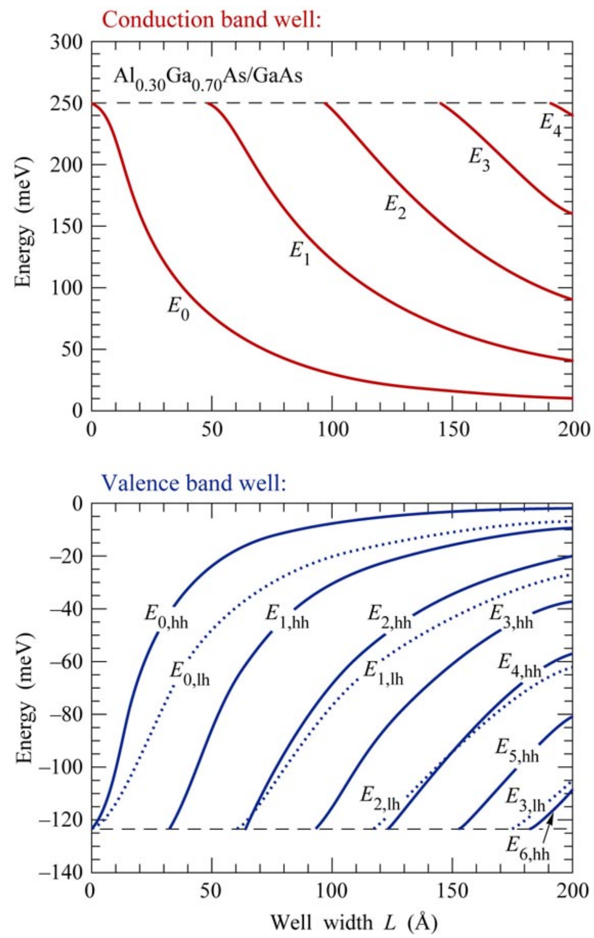
$$H'_{mj} = \int_{-\infty}^{\infty} \Psi_m^*(x) H'(x) \Psi_j(x) \mathrm{d}x$$

Therefore, for an intraband transition, when the initial and final state have the same symmetry (either odd or even) the resultant integrand is of odd-symmetry. The integration thus evaluates to zero, disallowing any such intraband transition.

5. Consider a symmetric finite $Al_{0.30}Ga_{0.70}As$ / GaAs conduction band potential well, as shown in the figure below.
   (a) How many quantized energy states does a 12 nm wide potential well have in the conduction band and the valence band?
   (b) If the width of the well is decreased, will the energy of the quantized states increase or decrease?
   (c) If the width of the well is decreased, will it contain fewer or more quantized energy states?
   (d) Can the well width be adjusted so that it contains zero quantized energy states?

   (a) The conduction band has 3, the light-hole valence band has 3, and the heavy-hole valence band has 4 quantized energy states.
   (b) Increase.
   (c) Fewer.
   (d) No. A symmetric potential well will always have at least one bound state.





$E_{g,\,Al_xGa_{1-x}As} = (1.424 + 1.247 \times x)$ eV

$\Delta E_c = (2/3)\,\Delta E_g$

$\Delta E_v = (1/3)\,\Delta E_g$

$m^*_{e,\,Al_xGa_{1-x}As} = (0.067 + 0.083 \times x)\,m_0$

$m^*_{hh,\,Al_xGa_{1-x}As} = (0.45 + 0.30 \times x)\,m_0$

$m^*_{lh,\,Al_xGa_{1-x}As} = (0.08 + 0.057 \times x)\,m_0$

Fig. 7.6. Quantized energies of subbands in the conduction band and valence band of an $Al_xGa_{1-x}As$/GaAs single quantum well structure at room temperature. There are different subbands for heavy holes (hh) and light holes (lh) in the valence band.

6. An electron with effective mass $m^* = 0.5\ m_0$ tunnels through a barrier that is 100 meV high and 10 nm wide.
   (a) Calculate the tunneling probability of the electron.
   (b) What is the tunneling probability if only the barrier height is doubled?
   (c) What is the tunneling probability if only the barrier width is doubled?
   (d) What is the tunneling probability if only the electron effective mass is doubled?
   (e) Which of the three parameters (barrier height, barrier width, electron effective mass) has the strongest effect on the tunneling probability?
   (f) Which of the three parameters has the weakest effect on the tunneling probability?

   (a) The tunneling probability is given by

$$T = e^{-\int_{x=0}^{L_B}\frac{2}{\hbar}\sqrt{2m^*[U(x)-E]}\mathrm{d}x}$$

$$= e^{-\frac{2}{1.0546\times10^{-34}}\sqrt{2\times0.5\times9.1094\times10^{-31}[100\times10^{-3}\times1.6022\times10^{-19}]}\times[10\times10^{-9}-0]}$$

$$= e^{-22.9} = 1.12\times10^{-10}$$

   (b) If only the barrier height is doubled, the tunneling probability is

$$T = e^{-22.9\times\sqrt{2}} = 8.61\times10^{-15}$$

   (c) If only the barrier width is doubled, the tunneling probability is

$$T = e^{-22.9\times2} = 1.28\times10^{-20}$$

   (d) If only the electron effective mass is doubled, the tunneling probability is

$$T = e^{-22.9\times\sqrt{2}} = 8.61\times10^{-15}$$

   (e) Doubling the barrier width has the strongest effect on the tunneling probability.
   (f) Of the three parameters doubling the barrier height and doubling the effective mass has the exact same effect on the tunneling probability. The effect of both these parameters is weaker compared to doubling the barrier height.