ECE 4070/MSE 6050
Physics of Semiconductors and Nanostructures
Exam 2, April 11, 2017

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Instructions:

- There are **THREE** problems in this exam
- Every problem must be done in the booklet provided
- Always solve **analytically first** before finding numerical values
- Only work done on exam booklets will be graded. Do not attach your own sheets to the exam booklets under any circumstances
- To get partial credit you must show all the relevant work
- Correct answers with wrong reasoning will not get points
- All questions do not carry equal points
- All questions do not have the same level of difficulty, use your time judiciously
- Common Physical Constants: [Planck's constant: $h = 6.63 \times 10^{-34}$ J·s and $\hbar = h/(2\pi)$], [Electron charge: $q = 1.6 \times 10^{-19}$ Coulomb], [Free electron mass: $m_e = 9.1 \times 10^{-31}$ kg], [Speed of light in vacuum: $c = 3 \times 10^8$ m/s], [Permittivity of vacuum: $\epsilon_0 = 8.85 \times 10^{-12}$ F/m], [Boltzmann constant: $k_b = 1.38 \times 10^{-23}$ J/K], [Room temperature $k_bT \sim 1/40$ eV ~ 26 meV].

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1 Miscellaneous [25 points]

Give *very* short answers to the following questions. All symbols have their usual meanings.

a) Explain the origin of electron energy bands and gaps using a sketch of the $E(k)$ bandstructure of a free electron, and of an electron in a periodic crystal,.

b) What determines if a crystal is a metal or a semiconductor? Do metals have more *net* electrons than a semiconductor?

c) If I sum the expression for the quantum current $J = q\sum_k v_g(k)f(k)$ over all k states of the bandstructure in a *completely filled band*, what do I get?

d) Show by using the quantum expression of current $J = q\sum_k v_g(k)f(k)$ that the current due to an *empty* electron state at the top of a valence band flows in a direction *opposite* to *filled* electron states at the bottom of the conduction band. What does this imply about the *effective charge* of a hole?

e) Silicon has a bandgap $E_g = 1.1$ eV, and $T = 300$K intrinsic carrier concentration due to interband thermal generation $n_i \sim 10^{10}/\text{cm}^3$. Find the *hole density* p and the electron density n in Silicon if I dope it with shallow ($E_D << k_bT$) *donors* of density $N_D \sim 10^{14}/\text{cm}^3$. Use suitable approximations.

2 Quantum Transport of Bloch Electrons [30 points]

In class, we derived the rather remarkable results that if we know the bandstructure $E(k)$ of any crystal, the velocity of an electron in state k is its group velocity $v_g(k) = \frac{1}{\hbar}\frac{dE(k)}{dk}$ with suitable generalization to higher dimensions, and the motion of the states in $k-$space is given simply by $F = \hbar\frac{dk}{dt}$ where F is the force. In this problem, consider an electron on a ring of length L moving through an extremely weak periodic crystal potential of lattice constant a such that the periodicity of the crystal is imprinted on the electron wavefunctions.

(a) Show that in the limit of a vanishing crystal potential, the wavefunction of the electron must be of the form $\psi(x) = \frac{1}{\sqrt{L}} e^{i(k+G)x}$, where $G = \frac{2\pi}{a} n$ is a reciprocal lattice vector with $n = ... -1, 0, +1, ...$

(b) The Bloch wavefunction is of the form $\psi_k(x) = e^{ikx} u(x)$ such that $u(x+a) = u(x)$. Show that the electron wavefunction of part (a) is in the Bloch form. Identify $u(x)$ and prove that indeed $u(x+a) = u(x)$.

(c) Show that the allowed electron eigenvalues are $E(k) = \frac{\hbar^2 (k+G)^2}{2m_e}$. Write expressions for several values of G, and sketch the corresponding nearly free electron energy bands for $-3\frac{\pi}{a} \leq k \leq +3\frac{\pi}{a}$. Show on this bandstructure why at any k, there are several possible energy states with various group velocities.

(d) If an electron starts at $k = 0$ in the band indexed by $G = 0$ and experiences a force F, find the time it will take to reach an energy level degenerate with the band indexed by $G_2 = -\frac{4\pi}{a}$. Can the electron jump or transition to the other bands in the absence of a periodic potential?

(e) What does a periodic potential do to the bandstructure of part (c) and to the transport of part (d)?

3 Physics of a 1-D Semiconductor Crystal [45 points]

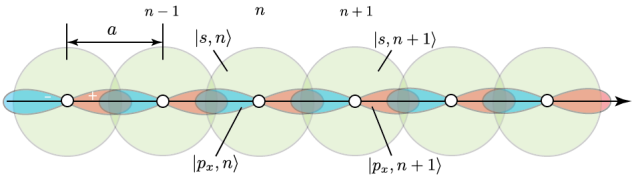

Figure 1: Orbitals and overlaps for a 1D tight-binding lattice.

In this problem, you will calculate the simplified bandstructure of a 1D semiconductor using the tight-binding model. Then you will find the density of states, band-edge effective mass, and solve a quantum transport problem for the semiconductor. Assume a circular ring of atoms with lattice constant a as shown in Figure 1 and N sites, such that $L = Na$. Electrons can occupy two atomic orbitals per lattice site: one $|s\rangle$ and the other $|p_x\rangle$. When the atoms are not in the crystal, the energies of electrons in these orbitals are $H_0|s\rangle = E_S|s\rangle$ and $H_0|p_x\rangle = E_P|p_x\rangle$, such that $E_S > E_P$. Upon forming chemical bonds, the nearest neighbor $|s\rangle$ orbitals hybridize with hopping energy $\langle s, n \pm 1|H_{crystal}|s, n\rangle = -V_{ss\sigma}$, and the nearest neighbor $|p_x\rangle$ orbitals hybridize with hopping energy $\langle p_x, n \pm 1|H_{crystal}|p_x, n\rangle = +V_{pp\sigma}$. Assume in this problem that there is no bonding of $|s, n\rangle$ with $|p_x, n \pm 1\rangle$, meaning $\langle s, n|H_{crystal}|p_x, n \pm 1\rangle = V_{sp\sigma} = 0$.

(a) Show that the two bands formed have bandstructures $E_c(k) = E_S - 2V_{ss\sigma}\cos(ka)$ and $E_v(k) = E_p + 2V_{pp\sigma}\cos(ka)$. We will call the s-band the conduction band, and the p-band the valence band.

(b) Sketch the bandstructure of the crystal in the first Brillouin zone $-\frac{\pi}{a} \leq k \leq +\frac{\pi}{a}$ (remember $E_S > E_P$). Label the extrema points of the bandstructure. Under what conditions will the crystal have no energy gap? Exactly how many electrons can the 1st BZ hold?

(c) Assume the hopping terms are such that there is a bandgap. What is the bandgap? With how many electrons will you fill the crystal to make it an intrinsic semiconductor?

(d) Using a Taylor expansion of $\cos x \approx 1 - \frac{x^2}{2}$ for $x << 1$, show that the effective mass of the conduction band edge at the $\Gamma-$point, i.e. at $k = 0$ is $m_c^\star = \frac{\hbar^2}{2V_{ss\sigma}a^2}$. Relate this effective mass to the total energy bandwidth of the conduction band. Does it make intuitive sense?

(e) By some means, you have managed to populate with $f(k) = 1$ the conduction band states between $-k_L \leq k \leq +k_R$ where $-k_L$ is the highest left-going state, and k_R is the highest right-going state. What is the net quantum current flowing in the crystal?

(f) Show that the exact conduction band DOS is given by $g_c(E) = \frac{g_s}{2\pi a\sqrt{(2V_{ss\sigma})^2 - (E-E_S)^2}}$. Make a sketch of this DOS on the side of your bandstructure sketch of part (b) of this problem.