Exercise Sheet 5

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1. (a) Use the lattice constants below to find the compositions of $In_xGa_{1-x}As$ and $In_xAl_{1-x}As$ that can be grown without strain on an InP substrate. Lattice constants in nm: InP: 0.5869; InAs: 0.6058; GaAs: 0.5653; AlAs: 0.5660. Why is the absence of strain an important consideration in realizing semiconductor heterostructures?
(b) Use Anderson's rule to estimate the energy offsets in the conduction and valence bands for two lattice-matched heterostructures: GaAs-AlAs and InAs-Alsb. Electron affinities in eV: GaAs:4.07; AlAs: 3.51; InAs: 4.92; AlSb:3.65. Sketch the band profile - conduction and valence band energy versus z - in the two cases.

2. Consider holes in a 5 nm quantum well of GaAs surrounded by AlGaAs. Estimate the lowest energy levels for light and heavy holes and their splitting using a simple model. How many holes can be put in the lowest "heavy" band before the "light" band becomes occupied? For GaAs, masses of heavy holes and light holes are $m_{hh} = 0.5m_0$ and $m_{lh} = 0.082m_0$ respectively where mass of electron m_0 is $9.109 * 10^{-31}$ Kg.

3. Consider free electrons in a finite 2D box of lengths L_x and L_y. The wavefunctions are travelling waves in each direction with periodic boundary conditions giving $\phi(x, y) = \frac{1}{\sqrt{L_x L_y}} \exp i(k_x x + k_y y)$. The allowed values of k_x and k_y are $(k_x, k_y) = (\frac{2\pi l}{L_x}, \frac{2\pi m}{L_y})$, $l, m = 0, \pm 1$,...Calculate the total density of states $(N(E))$ using the general definition $N(E) = 2\Sigma_{\mathbf{k}=-\infty}^{\mathbf{k}=\infty}\delta(E - \epsilon(\mathbf{k}))$. From $N(E)$, calculate the Fermi energy of a 2D electron gas with electron density N_{2D} at $T = 0$.

4. A quantum well is formed by embedding a 20 nm thick layer of InAs between AlSb layers. Assuming that the quantum well can be approximated as an infinite square well, calculate the electron confinement energies in eV for the first two confined electron states E_1 and E_2. The effective mass for InAs is $0.022m_0$. If the actual well depth is 1.27 eV, comment whether the infinite well approximation is appropriate in this case.
In addition to quantization in the growth direction, an electron in a quantum well has plane-wave behaviour in the perpendicular plane. Based on this, calculate and sketch the density of electron states as a function of energy where the energy range starts at the bottom of the quantum well and extends to a few tens of meV above the second electron state.
If the quantum well has an electron density of 10^{15} m^{-2}, determine the position of the Fermi energy above E_1 at a temperature of 0 K.

5. We can consider quantitatively the effect of the Coulomb attraction on the motion of electrons and holes in a semiconductor. We assume that the Coulomb attraction between electron and hole is weak due to screening by the valence electrons, so that the effective mass approximation is valid. The electron and hole in an exciton are localized relative to their centre of mass. Their relative motion can be shown to be described by $(-\frac{\hbar^2}{2\mu}\nabla_r^2 - \frac{e^2}{4\pi\epsilon_0\epsilon_r r})\phi(r) = E_r\phi(r)$, where μ, the reduced mass of the exciton, is defined by $\frac{1}{\mu} = \frac{1}{m_e} + \frac{1}{m_h}$ and $\phi(r)$ is the exciton envelope wavefunction. Equation is similar to the equation describing the motion of the electron in a hydrogen atom. For isotropic effective masses, E_r depends on the principal quantum number n only and is given by $E_r(n) = E_r(\infty) - \frac{R^*}{n^2}$, where $E_r(\infty)$ is the minimum energy of the continuum states, i.e, the energy gap, and R^* is the Rydberg constant for the exciton defined as $R^* = \frac{\mu e^4}{2\hbar^2(4\pi\epsilon_0\epsilon_r)^2} = \frac{\mu}{m\epsilon_r^2} * 13.6eV$. Two-dimensional excitons can also be considered. Their bound state energies (indexed by the quantum number n) E_{2D} are given by the series $E_{2D}(n) = E_{2D}(\infty) - \frac{R^*}{(n-\frac{1}{2})^2}$ for $n = 1, 2, ...$, where the effective Rydberg R^* is the same one as defined for three dimensional excitons. Sketch the binding energy of an exciton in an infinitely deep well as a function of the width L of the well considering particularly the limiting cases of $L = 0, \infty$. However, numerical results for finite wells in GaAs-AlGaAs systems (confinement depth $V_0 = 0.3eV$) show that the binding energy has a peak when $L = 5nm$, proving that the infinitely deep well is an unreliable model for narrow wells. Argue on dimensional grounds that the best confinement occurs when $L = 5nm$ ($m_e = 0.067m_0$ and $\epsilon_r = 13.2$ for GaAs). Explain qualitatively why the binding energy of an exciton in a real structure approaches the value corresponding to very wide wells as the width L goes to zero.

6. **Optional:** Estimate as follows the accuracy of the $'\Delta n = 0'$ rule for interband transitions in a GaAs quantum well of width 10 nm. For electrons, the depth is about 0.30 eV and the lowest state has energy 34 meV. The same energy would be found in an infinitely deep well if its width were 12.8 nm. Similarly, the holes sit in a well of depth 0.18 eV, which gives an energy of 5.9 meV, equivalent to an infinitely deep well of width 11.3 nm. Calculate the matrix element between the envelope functions (just their product!) using the wavefunctions in the equivalent infinite deep well.

For comparison, repeat this for the transition between the lowest electron and third hole states, using the same effective widths.

Calculate the wave functions in a finite well numerically, use these to evaluate the matrix element. How good is the rough approximation of adjusting the width of the well?