HW2 Finite barrier quantum well energy levels

Q. 1. (a) Determine the electron and hole (both light and heavy) energy levels and wavefunctions in the well of an Al\textsubscript{x}Ga\textsubscript{1-x}As-GaAs multiple quantum well layer. Assume well thickness of 50 Ångstrom. Use 30% aluminum in AlGaAs. Assume energy band discontinuity $\Delta E_c/\Delta E_v$ ratio to be 60 to 40 in conduction and valence bands, respectively. (b) What is the effective well width $L_{eff}$ of an infinite well which would give the same location of the first level in the conduction band as in the finite well problem done above in part (a). Given:

Effective masses: GaAs well

- $m_e = 0.0665 m_o$
- $m_{hh} = 0.34 m_o$
- $m_{lh} = 0.094 m_o$

AlGaAs barrier [$m_{hh}$=heavy holes, $m_{lh}$=light holes]

- $m_e = 0.0916 m_o$
- $m_{hh} = 0.466 m_o$
- $m_{lh} = 0.107 m_o$

$E_g$ as a function of aluminum fraction $Al_{x}Ga_{1-x}As = 1.424 + 1.247 \times (x)$

Reference: Notes pp. 70-78.

Q1. Hint/Solution attached

Write your program and confirm the values shown in the solution/hint set.
Wave function and energy level in a finite well:
(a) Determine the electron and hole (both light and heavy) energy levels and wavefunctions in the well of an Al$_x$Ga$_{1-x}$As-GaAs multiple quantum well layer. Assume well thickness of 50 Angstrom. Use the effective masses as given on page 95 of the Ref. (S. Chuang, Physics of Optoelectronic Devices, Wiley, 1995). Use 30% aluminum in AlGaAs. For $E_g$ in AlGaAs, use the relation given in 980 nm design set or notes or Chuang**. Assume energy band discontinuity to be 60 to 40 in conduction and valence bands, respectively.

Reference: S. Chuang, Chapter 3, John Wiley.
(b) What is the effective well width $L_{eff}$ of an infinite well which would give the same location of the first level in the conduction band as in the finite well problem done above in part (a).

Given:
Effective masses: GaAs well AlGaAs barrier
$m_e = 0.0665m_0$ $m_e = 0.0916m_0$
$m_{hh} = 0.34 m_0$ $m_{hh} = 0.466 m_0$
$m_h = 0.094 m_0$ $m_h = 0.107 m_0$

$E_g$ as a function of aluminum fraction $Al_xGa_{1-x}As = 1.424 + 1.247(x)$

(Find equations, which provide effective masses as a function of composition)

$m_{hh} =$ heavy holes, $m_b =$ light holes.

Computation of conduction band $\Delta E_c$ and valence band $\Delta E_v$ discontinuities:
Find the band gap difference $\Delta E_g$.

Solutions (a)

\[ \Delta E_g = 0.6 \Delta E_g \]
\[ \Delta E_v = 0.4 \Delta E_g \]

$E_g = 1.424 + 1.247x$

\[ \Delta E_g = 1.247x \]
\[ = 1.247(0.3) \]
\[ = 0.3741 \text{ eV} \]

$\Delta E_c = 0.6 \Delta E_g$
\[ = 0.6(0.3741) = 0.2246 \text{ eV} \]
\[ \Delta E_v = 0.4 \Delta E_g = 0.4(0.3741) = 0.1496 \text{ eV} \]

Schrödinger equation:

\[
\left[-\frac{\hbar^2}{2m} \nabla^2 + V(z)\right] \psi(x, y, z) = E \phi(x, y, z) \quad (1)
\]

The Schrödinger equation in a system with multiple layers. (the m_e values are different in the well \(m_{ew}\) and barrier \(m_{eb}\)):

\[
\left[-\frac{\partial}{\partial z} \frac{1}{m} \frac{\partial}{\partial z} + V(z)\right] \phi(z) = E \phi(z) \quad (2)
\]

Schrodinger equation in a well:

\[
-\frac{\hbar^2}{2m_{ew}} \frac{\partial^2 \phi(z)}{\partial z^2} = E \phi(z)
\]

\[
\frac{\partial^2 \phi(z)}{\partial z^2} = -\frac{2m_{ew}}{\hbar^2} E \phi(z)
\]

\[
= -k^2 \phi(z) \quad (3)
\]

\[
k^2 = \frac{2m_{ew}E}{\hbar^2} \quad (4)
\]

**Boundary Conditions**

1. \( \phi \left( z = \frac{L}{2}^+ \right) = \phi \left( z = \frac{L}{2}^- \right) \) \quad (5)

2. \( \frac{1}{m_{eb}} \frac{d}{dz} \phi \left( z = \frac{L}{2}^+ \right) = \frac{1}{m_{ew}} \frac{d}{dz} \phi \left( z = \frac{L}{2}^- \right) \)

\[
-\frac{L}{2} < z < \frac{L}{2}
\]

In the well the solution of Equation (3) is: \( \phi(z) = C_1 \cos kz + C_2 \sin kz \) \quad (7)

**Even Wavefunction:** \( \phi(z) = C_2 \cos kz \) \quad (7a)

**Odd Wavefunction:** \( \phi(z) = C_2 \sin kz \) \quad (7b)
In the barrier \( |z| > \frac{L}{2} \), Equation (2) reduces to:

\[
\left[ -\frac{\hbar^2}{2m_e} \frac{\partial^2 \phi(z)}{\partial z^2} + V_0 \phi(z) \right] = E \phi(z)
\]

\[-\frac{\hbar^2}{2m_e} \frac{\partial^2 \phi(z)}{\partial z^2} + (V_0 - E) \phi(z) = 0, \text{ where } V_0 = \Delta E_c\]

\[
\frac{\partial^2 \phi}{\partial z^2} = + \frac{2m_e}{\hbar^2} (V_0 - E) \phi(z) \quad (8)
\]

\[
\alpha^2 = \frac{2m_e}{\hbar^2} (V_0 - E) \quad (9)
\]

For \( z > \frac{L}{2} \), the solution is: \( \phi(z) = C_1 e^{-\alpha (z - \frac{L}{2})} + C_1 e^{\alpha (z - \frac{L}{2})} \)

At \( z = \infty \), the second term becomes infinite. For a physical solution \( C_1 = 0 \), therefore:

\( \phi(z) = C_1 e^{-\alpha (z - \frac{L}{2})} \) for \( z > \frac{L}{2} \)

or \( \phi(z) = C_1 e^{\alpha (z + \frac{L}{2})} \) for \( z < \frac{-L}{2} \)

**Evaluation of \( C_2, C_1 \) for even wavefunction**

**First boundary condition, Equation (5):**

\[
\phi \left( z = \frac{L^*}{2} \right) = \phi \left( z = \frac{-L}{2} \right)
\]

\[
C_1 e^{-\alpha \left( \frac{L - L}{2} \right)} = C_2 \cos k \frac{L}{2}
\]

\[
C_1 = C_2 \cos k \frac{L}{2} \quad (10)
\]

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Using the second boundary condition,

\[
\frac{1}{m_{eb}} \frac{d}{dz} C_1 e^{-\alpha(z - \frac{L}{2})} \bigg|_{z = \frac{L}{2}} = \frac{1}{m_{ew}} \frac{d}{dz} C_2 \cos k z \bigg|_{z = \frac{L}{2}}
\]

\[
\frac{1}{m_{eb}} C_1 (-\alpha) = -\frac{1}{m_{ew}} C_2 k \sin k \frac{L}{2}
\]

\[
C_1 = C_2 \frac{m_{eb} k}{m_{ew} \alpha} \sin k \frac{L}{2} \quad (11)
\]

Dividing (11) by (10), we get the Eigenvalue equation:

\[
l = \frac{m_{eb} k}{m_{ew} \alpha} \tan \frac{kL}{2}
\]

Eigenvalue equation: \[
\tan \frac{kL}{2} = \frac{m_{ew}}{m_{eb}} \frac{\alpha L}{k L/2} \quad (12)
\]

Odd wave function Eigen equation is:

\[
\cot k \frac{L}{2} = -\frac{m_{ew}}{m_{eb}} \left( \frac{\alpha L/2}{k L/2} \right) \quad (13)
\]

Determination of \( k \) and \( \alpha \):

In addition to the Eigenvalue equation, we need one more equation. By definition \( k \) and \( \alpha \) are defined by Equation (9) and (4).

\[
\alpha^2 = \frac{2m_{eb} (V_0 - E)}{\hbar^2} \quad (9)
\]

\[
k^2 = \frac{2m_{ew} E}{\hbar^2} \quad (4)
\]

\[
E = \frac{\hbar^2 k^3}{2m_{ew}}, \text{ substitute in (4)}:
\]
\[ \alpha^2 = \frac{2m_{eb}}{h^2} V_0 - \frac{2m_{eb}}{h^2} \frac{\hbar^2 k^2}{2m_{ew}} \] (14)

\[ k^2 \frac{2m_{eb}}{2m_{ew}} \alpha^2 = 2 \frac{m_{ew}}{h^2} V_0 \]

\[ k^2 + \frac{m_{ew}}{m_{eb}} \alpha^2 = 2 \frac{m_{eb}}{h^2} V_0 \]

Multiply by \( \left( \frac{L}{2} \right)^2 \): \( \left( k \frac{L}{2} \right)^2 + \frac{m_{ew}}{m_{eb}} \left( \frac{\alpha L}{2} \right)^2 = 2 \frac{m_{eb}}{h^2} V_0 \left( \frac{L}{2} \right)^2 \)

\[ \alpha^* = \sqrt{\frac{m_{ew}}{m_{eb}}} \alpha \]

\[ \left( k \frac{L}{2} \right)^2 + \left( \frac{\alpha^* L}{2} \right)^2 = 2 \frac{m_{eb}}{h^2} V_0 \left( \frac{L}{2} \right)^2 \] (15)

\( V_0 = \Delta E_C \) in the conduction band.

\( k_0 \) and \( \alpha \) are found for even and odd wave functions using the Eigenvalue and equation 6.

The Matlab code on the following page plots \( \alpha \) vs. \( E \). The eigenenergy is the point of intersection of the two lines (see page 8 for plots).

Input: \( V_0 = \Delta E_C, L = 50 \text{ Å}, m_{eb}, m_{ew} \)

Output: Equation (15) and (12), give \( k, \alpha^* \) (or \( \alpha \)). Once \( k \) is known, using Equation (4) we get:

\[ E = \frac{\hbar^2 k^2}{2m_{ew}} \] (4)

\[ \phi(z) = C_2 \cos k z \] (7a)

The points of intersection are:

<table>
<thead>
<tr>
<th>Electrons</th>
<th>( E_{C1} = 72.5 \text{ meV} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heavy Holes</td>
<td>( E_{HH1} = 22.3 \text{ meV} )</td>
</tr>
<tr>
<td>Light Holes</td>
<td>( E_{LH1} = 52.9 \text{ meV} )</td>
</tr>
</tbody>
</table>
\[ m_0 = 9.109 \times 10^{-31}; \]
\[ h = 6.626 \times 10^{-34} / (2 \times 3.1415); \]
\[ q = 1.6 \times 10^{-19}; \]
\[ l = 50 \times 10^{-10}; \]

% for electrons
\[ v_0 = 0.22446 \times q; \]
\[ m_b = 0.0916 \times m_0; \]
\[ m_w = 0.0665 \times m_0; \]

% for Heavy holes
\[ v_0 = 0.14964 \times q; \]
\[ m_b = 0.466 \times m_0; \]
\[ m_w = 0.34 \times m_0; \]

% for Light holes
\[ v_0 = 0.1496 \times q; \]
\[ m_b = 0.107 \times m_0; \]
\[ m_w = 0.094 \times m_0; \]

\[ e_1 = 0.001; \]
\[ e_2 = 0.001; \]

\[ \alpha_1 = (m_b / m_w) \times \sqrt{\left(2 \times m_w \times e_1 \times q / h^2\right) \times \tan\left(\sqrt{\left(2 \times m_w \times e_1 \times q / h^2\right) \times (1/2)}\right)}; \]
\[ \alpha_2 = \sqrt{2 \times m_b \times (v_0 - e_2 \times q / h^2)}; \]
\[ \text{plot}(e_1, \alpha_1, e_2, \alpha_2); \]
\[ \text{xlabel}("\text{E}_1 \text{ (eV)}"); \]
\[ \text{ylabel}("\text{Alpha}"); \]
\[ \text{title}("\text{Alpha vs E}_1 \text{ (eV) For Heavy Holes}"); \]
(b) $L_{\text{eff}}$ is the length of an infinite well which has the same energy levels as a finite well.

The effective width, $L_{\text{eff}}$ can be found by:

$$L_{\text{eff}} = \sqrt{\frac{\pi^2 h^2}{2m^*E}}$$

$E_1$ is the first energy level.

$E_{\text{C1}}$: electrons  
$E_{\text{HH1}}$: heavy holes  
$E_{\text{LH1}}$: light holes

$$L_{\text{eff}} = \sqrt{\frac{\pi^2 (1.06 \times 10^{-34})^2}{2(0.065)(9.11 \times 10^{-31})(1.16 \times 10^{-20})}} = 88.3 \text{ Å}$$

$$L_{\text{eff}} = \sqrt{\frac{\pi^2 (1.06 \times 10^{-34})^2}{2(0.034)(9.11 \times 10^{-31})(3.57 \times 10^{-21})}} = 70.4 \text{ Å}$$

$$L_{\text{eff}} = \sqrt{\frac{\pi^2 (1.06 \times 10^{-34})^2}{2(0.094)(9.11 \times 10^{-31})(8.48 \times 10^{-21})}} = 86.9 \text{ Å}$$