Exercises:
1) Formation of Bandstructure in Finite Superlattices
2) RTDs
• Analytical solutions of Toy Problems
  » Tunneling through a single barrier

• Numerical Solutions to Toy Problems
  » Tunneling through a double barrier structure
  » Tunneling through N barriers

Reference:
• piece-wise-constant-potential-barrier tool
  http://nanohub.org/tools/pcpbt
Define our system: Single barrier

One matrix each for each interface: 2 S-matrices

Incident: A → Reflected: B 
Transmitted: E

No particles lost! Typically A=1 and F=0.
Wave-function each region,

\[ \psi_1(x) = Ae^{ikx} + Be^{-ikx} \]
\[ \psi_2(x) = Ce^{-\gamma x} + De^{\gamma x} \]
\[ \psi_3(x) = Ee^{ikx} + Fe^{-ikx} \]

\[ k = \sqrt{\frac{2mE}{\hbar^2}} \]
\[ \gamma = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \]
Applying boundary conditions at each interface (x=0 and x=L) gives,

\[ \psi_1(0) = \psi_2(0) \quad \Rightarrow \quad A + B = C + D \]
\[ \psi_1(0) = \psi_2(0) \quad \Rightarrow \quad ik(A - B) = -\gamma(C - D) \]
\[ \psi_2(L) = \psi_3(L) \quad \Rightarrow \quad Ce^{-\gamma L} + De^{\gamma L} = Ee^{ikL} + Fe^{-ikL} \]
\[ \psi_2(L) = \psi_3(L) \quad \Rightarrow \quad -\gamma(Ce^{-\gamma L} - De^{\gamma L}) = ik(Ee^{ikL} - Fe^{-ikL}) \]

Which in matrix can be written as,

\[
\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \left(1 + i \frac{\gamma}{k}\right) & \frac{1}{2} \left(1 - i \frac{\gamma}{k}\right) \\ \frac{1}{2} \left(1 - i \frac{\gamma}{k}\right) & \frac{1}{2} \left(1 + i \frac{\gamma}{k}\right) \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix} = M_1 \begin{bmatrix} C \\ D \end{bmatrix}
\]
\[
\begin{bmatrix} C \\ D \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \left(1 - i \frac{k}{\gamma}\right)e^{(ik + \gamma)L} & \frac{1}{2} \left(1 + i \frac{k}{\gamma}\right)e^{-(ik - \gamma)L} \\ \frac{1}{2} \left(1 + i \frac{k}{\gamma}\right)e^{(ik - \gamma)L} & \frac{1}{2} \left(1 - i \frac{k}{\gamma}\right)e^{-(ik + \gamma)L} \end{bmatrix} \begin{bmatrix} E \\ F \end{bmatrix} = M_2 \begin{bmatrix} E \\ F \end{bmatrix}
\]
The complete transfer matrix

\[
\begin{bmatrix}
A \\
B
\end{bmatrix} = M_1 \begin{bmatrix}
C \\
D
\end{bmatrix} = M_1 M_2 \begin{bmatrix}
E \\
F
\end{bmatrix} = M \begin{bmatrix}
E \\
F
\end{bmatrix}
\]

In general for any intermediate set of layers, the TMM is expressed as:

\[
\begin{pmatrix}
A_{n-1}^+ \\
A_{n-1}^-
\end{pmatrix} = \begin{pmatrix}
M_{11} & M_{12} \\
M_{21} & M_{22}
\end{pmatrix} \begin{pmatrix}
A_n^+ \\
A_n^-
\end{pmatrix}
\]

For multiple layers the overall transfer matrix will be

\[
\begin{pmatrix}
A_N \\
B_N
\end{pmatrix} = \prod_{j=2}^{N} T_j \begin{pmatrix}
A_1 \\
B_1
\end{pmatrix}.
\]

Looks conceptually very simple and analytically pleasing

Use it for your homework assignment for a double barrier structure!
Transmission can be found using the relations between unknown constants,

\[
\begin{bmatrix}
A \\
B
\end{bmatrix} = M_1 \begin{bmatrix}
C \\
D
\end{bmatrix} = M_1 M_2 \begin{bmatrix}
E \\
F
\end{bmatrix} = M \begin{bmatrix}
E \\
F
\end{bmatrix} \quad T(E) = \left| \frac{E}{A} \right|^2 = \frac{1}{|m_{11}|^2}
\]

Case: \( E < V_0 \)

\[ T(E) \approx \frac{1}{1 + \left( \frac{kL}{2} \right)^2} \]

Case (\( \gamma L \ll 1 \)): Weak barrier

\[ T(E) \approx \left( \frac{4k\gamma}{k^2 + \gamma^2} \right)^2 \exp(-2\gamma L) \]

Case (\( \gamma L \) large): Strong barrier

Case: \( E > V_0 \)

\[ T(E) = \left[ 1 + \left( \frac{k^2 - k_2^2}{2kk_2} \right)^2 \sin^2(k_2L) \right]^{-1} \]
Single barrier: Concepts

- Transmission is finite under the barrier – tunneling!
- Transmission above the barrier is not perfect unity!
- Quasi-bound state above the barrier. Transmission goes to one.

Case: $E > V_o$

$$T(E) = \left[ 1 + \left( \frac{k_2^2 - k_1^2}{2kk_2} \right)^2 \sin^2 (k_2 L) \right]^{-1}$$

Effect of barrier thickness below the barrier

- Increased barrier width reduces tunneling probability
- Thicker barrier increase the reflection probability below the barrier height.
- Quasi-bound states occur for the thicker barrier too.
- Computed with – http://nanohub.org/tools/pcpbt

Case: $E > V_o$

$$T(E) = \left[ 1 + \left( \frac{k^2 - k_2^2}{2kk_2} \right)^2 \sin^2(k_2L) \right]^{-1}$$
Single Barrier - Key Summary

• Quantum wavefunctions can tunnel through barriers
• Tunneling is reduced with increasing barrier height and width

• Transmission above the barrier is not unity
  » 2 interfaces cause constructive and destructive interference
  » Quasi bound states are formed that result in unity transmission
• Analytical solutions of Toy Problems
  » Tunneling through a single barrier

• Numerical Solutions to Toy Problems
  » Tunneling through a double barrier structure
  » Tunneling through N barriers

Reference:
• piece-wise-constant-potential-barrier tool
  http://nanohub.org/tools/pcpbt
Define our system: Double barrier

One matrix each for each interface: 4 S-matrices

No particles lost!
Typically Left Incident wave is normalized to one.
Right incident is assumed to be zero.

Also this problem is analytically solvable! => Homework assignment
Reminder: Single barrier

- Transmission is finite under the barrier – tunneling!
- Transmission above the barrier is not perfect unity!
- Quasi-bound state above the barrier. Transmission goes to one.
• Double barriers allow a transmission probability of one / unity for discrete energies (reflection probability of zero) for some energies below the barrier height.
• This is in sharp contrast to the single barrier case
• Cannot be predicted by classical physics.
In addition to states inside the well, there could be states above the barrier height. States above the barrier height are quasi-bound or weakly bound. How strongly bound a state is can be seen by the width of the transmission peak. The transmission peak of the quasi-bound state is much broader than the peak for the state inside the well.
Effect of barrier height

- Increasing the barrier height makes the resonance sharper.
- By increasing the barrier height, the confinement in the well is made stronger, increasing the lifetime of the resonance.
- A longer lifetime corresponds to a sharper resonance.
Increasing the barrier thickness makes the resonance sharper.
By increasing the barrier thickness, the confinement in the well is made stronger, increasing the lifetime of the resonance.
A longer lifetime corresponds to a sharper resonance.
The well region in the double barrier case can be thought of as a particle in a box.
Particle in a box

- The time independent Schrödinger equation is
  \[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x) = E\psi(x) \]
  where, \( V(x) = \begin{cases} 0 & 0 < x < L_x \\ \infty & \text{elsewhere} \end{cases} \)

- The solution in the well is:
  \[ \psi_n(x) = A \sin \left( \frac{n\pi}{L_x} x \right), \ n = 1, 2, 3, \ldots \]

- Plugging the normalized wave-functions back into the Schrödinger equation we find that energy levels are quantized.
  \[ \psi_n(x) = \sqrt{\frac{2}{L_x}} \sin \left( \frac{n\pi}{L_x} x \right) \]
  \[ E_n = \frac{\hbar^2 \pi^2}{2mL_x^2} n^2 \]
  \( n = 1, 2, 3, \ldots \)
• Double barrier: Thick Barriers (10nm), Tall Barriers (1eV), Well (20nm).
• First few resonance energies match well with the particle in a box energies.
• The well region resembles the particle in a box setup.

• Green: Particle in a box energies.
• Red: Double barrier energies
Open systems Vs closed systems

Double barrier & particle in a box

- Green: Particle in a box energies.
- Red: Double barrier energies.

- Double barrier: Thick Barriers (10nm), Tall Barriers (1eV), Well (20nm).
- First few resonance energies match well with the particle in a box energies.
- The well region resembles the particle in a box setup.
Wave-function penetrates into the barrier region.
• The effective length of the well region is modified.
• The effective length of the well is crucial in determining the energy levels in the closed system.

\[ E_n = \frac{\hbar^2 \pi^2}{2mL_{\text{well}}^2} n^2 \]

\[ n = 1, 2, 3, \ldots, \quad 0 < x < L_{\text{well}} \]
Double Barrier Structures - Key Summary

• Double barrier structures can show unity transmission for energies BELOW the barrier height
  » Resonant Tunneling

• Resonance can be associated with a quasi bound state
  » Can relate the bound state to a particle in a box
  » State has a finite lifetime / resonance width

• Increasing barrier heights and widths:
  » Increases resonance lifetime / electron residence time
  » Sharpens the resonance width
• Analytical solutions of Toy Problems
  » Tunneling through a single barrier

• Numerical Solutions to Toy Problems
  » Tunneling through a double barrier structure
  » Tunneling through N barriers

Reference:
• piece-wise-constant-potential-barrier tool
  http://nanohub.org/tools/pcpbt
• $V_b=110\text{meV}$, $W=6\text{nm}$, $B=2\text{nm}$
2 Wells => 2 Transmission Peaks

1 Well => 1 Transmission Peak

- $V_b = 110 \text{meV}$, $W = 6 \text{nm}$, $B = 2 \text{nm}$

- $V_b = 110 \text{meV}$, $W = 6 \text{nm}$, $B = 2 \text{nm}$
  
  Bonding/Anti-bonding State
• $V_b=110\text{meV}$, $W=6\text{nm}$, $B=2\text{nm}$
4 Wells $\Rightarrow$ 4 Transmission Peaks

- $V_b=110\text{meV}$, $W=6\text{nm}$, $B=2\text{nm}$
5 Wells => 5 Transmission Peaks

- $V_b = 110 \text{meV}$, $W = 6 \text{nm}$, $B = 2 \text{nm}$
6 Wells => 6 Transmission Peaks

- $V_b = 110 \text{meV}$, $W = 6 \text{nm}$, $B = 2 \text{nm}$
7 Wells => 7 Transmission Peaks

- $V_b = 110\text{meV}$, $W = 6\text{nm}$, $B = 2\text{nm}$
8 Wells => 8 Transmission Peaks

- $V_b = 110\text{meV}$, $W = 6\text{nm}$, $B = 2\text{nm}$
• Bandpass filter formed

• Band transmission not symmetric
• Bandpass filter formed
• Band transmission not symmetric
• Bandpass filter formed
• Band transmission not symmetric
• Bandpass filter formed
• Band transmission not symmetric
• Bandpass filter formed
• Band transmission not symmetric
N Wells => N Transmission Peaks

- Bandpass filter formed
- Band transmission not symmetric
- Bandpass sharpens with increasing number of wells
1 Well => 1 Transmission Peak => 1 State

- Bandpass filter formed
- Band transmission not symmetric

- Bandpass sharpens with increasing number of wells
• Bandpass filter formed
• Band transmission not symmetric
3 Wells => 3 Transmission Peaks => 3 States

• Bandpass filter formed
• Band transmission not symmetric
• Bandpass filter formed
• Band transmission not symmetric
• Bandpass filter formed
• Band transmission not symmetric
6 Wells => 6 Transmission Peaks => 6 States

- Bandpass filter formed
- Band transmission not symmetric

Klimeck - ECE606 Spring 2010 - notes adopted from Alam
• Bandpass filter formed
• Band transmission not symmetric
• Bandpass filter formed
• Band transmission not symmetric
- Bandpass filter formed
- Band transmission not symmetric
• Bandpass filter formed
• Band transmission not symmetric
• Bandpass filter formed
• Band transmission not symmetric
• Bandpass filter formed
• Band transmission not symmetric
49 Wells => 49 Transmission Peaks => 49 States

- Bandpass filter formed
- Band transmission not symmetric
- Cosine-like band formed
- Band is not symmetric
N Wells => N Transmission Peaks => N States

- Bandpass filter formed
- Band transmission not symmetric
- Cosine-like band formed
- Band is not symmetric
• $V_b=110\text{meV}, W=6\text{nm}, B=2\text{nm}$ => ground state in each well

=> what if there were excited states in each well => $V_b=400\text{meV}$
N Wells $\Rightarrow$ 2N States $\Rightarrow$ 2 Bands

$V_b=110\text{meV}, \ W=6\text{nm}, \ B=2\text{nm}$

$V_b=400\text{meV}, \ W=6\text{nm}, \ B=2\text{nm}$
N Wells => 2N States => 2 Bands

Vb=110meV, W=6nm, B=2nm

1 state/well => 1 band

Can we get more states/well?
=> Increase well width

Vb=400meV, W=6nm, B=2nm

2 states/well => 2 bands
$V_b = 110\text{meV, } W = 6\text{nm, } B = 2\text{nm}$

1 state/well => 1 band

$V_b = 400\text{meV, } W = 6\text{nm, } B = 2\text{nm}$

2 states/well => 2 bands

$V_b = 400\text{meV, } W = 10\text{nm, } B = 2\text{nm}$

3 states/well => 3 bands
X States/Well => X Bands

Vb=110meV, W=6nm, B=2nm
1 state/well => 1 band

Vb=400meV, W=6nm, B=2nm
2 states/well => 2 bands

Vb=400meV, W=10nm, B=2nm
3 states/well => 3 bands
Formation of energy bands

- Each quasi-bond state will give rise to a resonance in a well. (No. of barriers -1)
- Degeneracy is lifted because of interaction between these states.
- Cosine-like bands are formed as the number of wells/barriers is increased.
- Each state per well forms a band.
- Lower bands have smaller slope = > heavier mass.
Presentation Outline

• Analytical solutions of Toy Problems
  » Tunneling through a single barrier
• Numerical Solutions to Toy Problems
  » Tunneling through a double barrier structure
  » Tunneling through N barriers

Reference:
• piece-wise-constant-potential-barrier tool
  http://nanohub.org/tools/pcpbt