ECE606: Solid State Devices
Lecture 3

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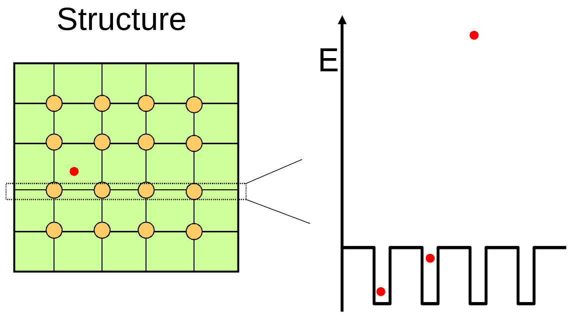
Motivation

Periodic Structure



Time-independent Schrodinger Equation

$$-\frac{\hbar^2}{2m_0}\frac{d^2\Psi}{dx^2}+U(x)\Psi=i\hbar\frac{d\Psi}{dt}$$

Assume

$$\Psi(x,t)=\psi(x)\,e^{-iEt/\hbar}$$

$$-e^{-\frac{iEt}{\hbar}}\frac{\hbar^2}{2m_0}\frac{d^2\psi(x)}{dx^2}+e^{-\frac{iEt}{\hbar}}U(x)\psi(x)=i\hbar\frac{-iE}{\hbar}\psi(x)e^{-\frac{iEt}{\hbar}}$$

$$-\frac{\hbar^2}{2m_0}\frac{d^2\psi}{dx^2}+U(x)\psi=E\psi$$

$$\frac{d^2\psi}{dx^2}+\frac{2m_0}{\hbar^2}(E-U)\psi=0$$

Time-independent Schrodinger Equation

$$\frac{d^2\psi}{dx^2}+\frac{2m_0}{\hbar^2}(E-U)\psi=0$$

If E >U, then ….

$$k\equiv\frac{\sqrt{2m_0[E-U]}}{\hbar}\qquad \frac{d^2\psi}{dx^2}+k^2\psi=0\qquad \psi(x)=A\sin(kx)+B\cos(kx)\equiv A_+e^{ikx}+A_-e^{-ikx}$$

If U>E, then ….

$$\alpha\equiv\frac{\sqrt{2m_0[U-E]}}{\hbar}\qquad \frac{d^2\psi}{dx^2}-\alpha^2\psi=0\qquad \psi(x)=De^{-\alpha x}+Ee^{+\alpha x}$$

A Simple Differential Equation

$$-\frac{\hbar^2}{2m_0}\frac{d^2\psi}{dx^2}+U(x)\psi=E\psi$$

- Obtain U(x) and the boundary conditions for a given problem.
- Solve the 2nd order equation – pretty basic
- Interpret $|\psi|^2=\psi^*\psi$ as the probability of finding an electron at x
- Compute anything else you need, e.g.,

$$p=\int_0^\infty \Psi^*\left[\frac{\hbar}{i}\frac{d}{dx}\right]\Psi\,dx \qquad E=\int_0^\infty \Psi^*\left[-\frac{\hbar}{i}\frac{d}{dt}\right]\Psi\,dx$$

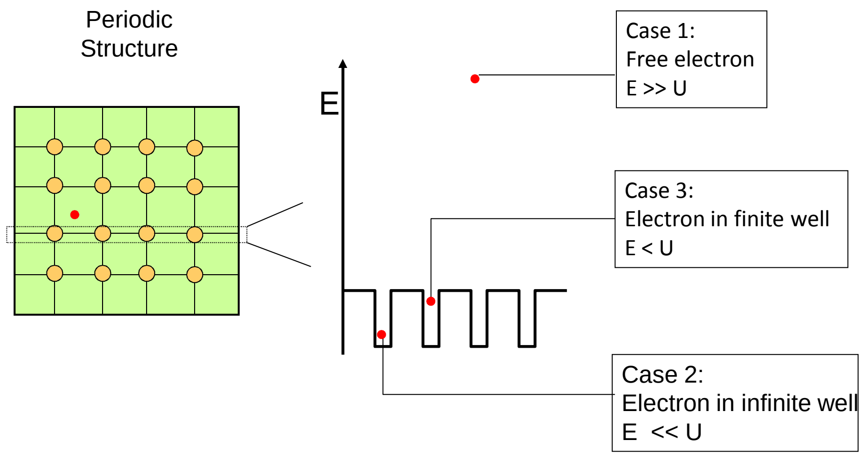
Presentation Outline

- Time Independent Schroedinger Equation
- Analytical solutions of Toy Problems
  - » (Almost) Free Electrons
  - » Tightly bound electrons – infinite potential well
  - » Electrons in a finite potential well
  - » Tunneling through a single barrier
- Numerical Solutions to Toy Problems
  - » Tunneling through a double barrier structure
  - » Tunneling through N barriers
- Additional notes
  - » Discretizing Schroedinger's equation for numerical implementations

Reference: Vol. 6, Ch. 2 (pages 29-45)

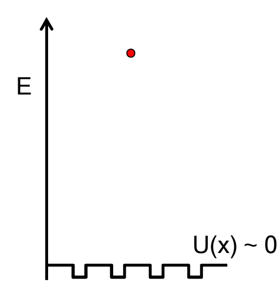
- piece-wise-constant-potential-barrier tool http://nanohub.org/tools/pcpbt

Full Problem Difficult: Toy Problems First



Case 1: Solution for Particles with E>>U

$$\frac{d^2\psi}{dx^2}+k^2\psi=0 \qquad k\equiv\frac{\sqrt{2m_0\left[E-U\right]}}{\hbar}$$



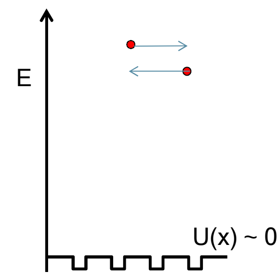
1) Solution $\psi(x)=A\sin(kx)+B\cos(kx)$
$$\equiv A_+e^{ikx}+A_-e^{-ikx}$$

2) Boundary condition $\psi(x)=A_+e^{ikx}$ positive going wave
$=A_-e^{-ikx}$ negative going wave

Free Particle ...

$$\psi(x) = A\sin(kx) + B\cos(kx)$$
$$\equiv A_+ e^{ikx} + A_- e^{-ikx}$$

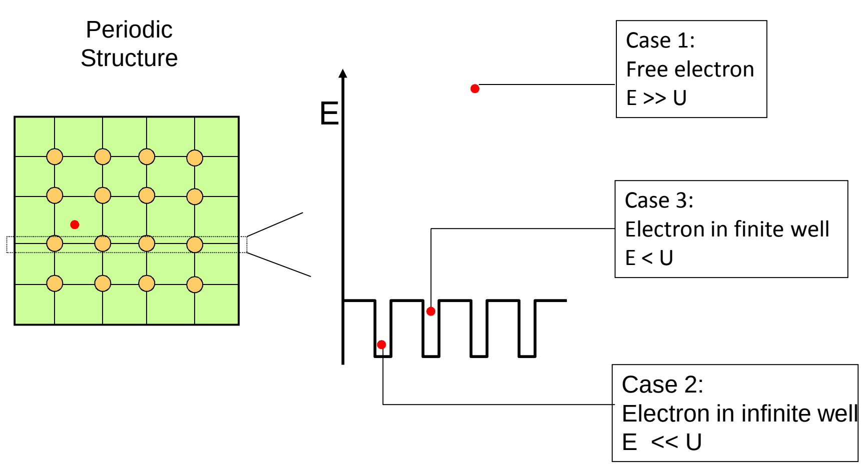
$$\psi(x) = A_+ e^{ikx} \quad \text{positive going wave}$$
$$= A_- e^{-ikx} \quad \text{negative going wave}$$



Probability: $|\psi|^2 = \psi\psi^* = |A_+|^2 \text{ or } |A_-|^2$

Momentum: $p = \int_0^{\infty} \Psi^* \left[\frac{\hbar}{i}\frac{d}{dx}\right] \Psi \, dx = \hbar k \text{ or } -\hbar k$

Full Problem Difficult: Toy Problems First

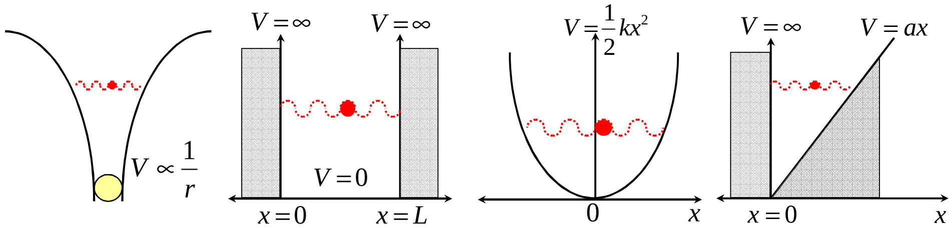


Case 2: Bound State Problems

- Mathematical interpretation of Quantum Mechanics(QM)

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = i\hbar\frac{\partial}{\partial t}\Psi$$

  - » Only a few number of problems have exact mathematical solutions
  - » They involve specialized functions



Coulomb Potential by nucleus in an atom	Particle in a box	Harmonic Oscillator	Triangular Potential Well
$\Psi_n(r) = AR_n(r)Y_n(\theta,\varphi)$	$\Psi_n(x) = A\sin(k_n x)$	$\Psi_n(x) = A\frac{1}{\sqrt{2^n n!}}H_n(Bx)e^{-\frac{Cx^2}{2}}$	$\Psi_n(x) = N\mathrm{Ai}(\xi_n)$

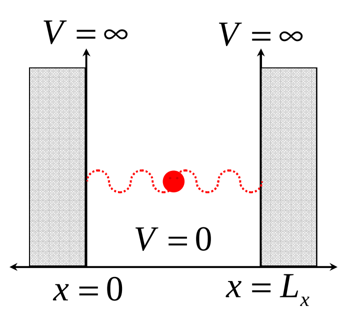
1-D Particle in a Box - A Solution Guess

- (Step 1) Formulate time independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x) \quad \text{where, } V(x) = \begin{cases} 0 & 0 < x < L_x \\ \infty & \text{elsewhere} \end{cases}$$

- (Step 2) Use your intuition that the particle will never exist outside the energy barriers to guess,

$$\psi(x) = \begin{cases} 0 & 0 \le x \le L_x \\ \ne 0 & \text{in the well} \end{cases}$$



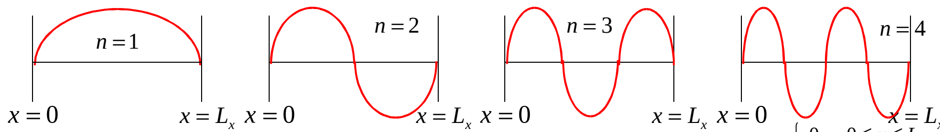
- (Step 3) Think of a solution in the well as:

$$\psi_n(x) = A\sin\left(\frac{n\pi}{L_x}x\right), \quad n = 1,2,3,\ldots$$

1-D Particle in a Box - Visualization

- (Step 4) Plot first few solutions

$$\psi_n(x) = A\sin\left(\frac{n\pi}{L_x}x\right), \quad n = 1,2,3,\ldots$$



Matches the condition we guessed at step 2!

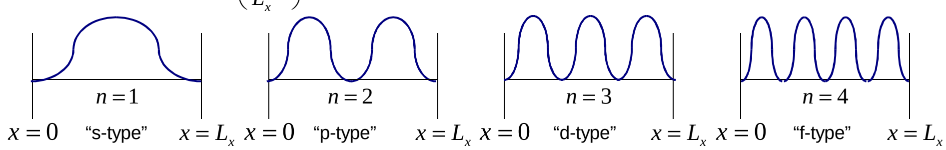
But what do the NEGATIVE numbers mean?

$$\psi(x) = \begin{cases} 0 & 0 \le x \le L_x \\ \neq 0 & \text{in the well} \end{cases}$$

- (Step 5) Plot corresponding electron densities

$$|\psi_n(x)|^2 = A^2 \sin^2\left(\frac{n\pi}{L_x}x\right), \quad n = 1,2,3,\ldots$$

➡ The distribution of SINGLE particle



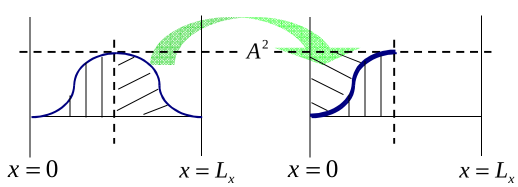
ONE particle => density is normalized to ONE

1-D Particle in a Box - Normalization to ONE particle

(Step 6) Normalization (determine the constant A)

Method 1) Use symmetry property of sinusoidal function

$$|\psi_n(x)|^2 = A^2 \sin^2\left(\frac{n\pi}{L_x}x\right)$$



$$(\text{Area}) = 1 = \frac{L_x}{2} \times A^2$$

$$\therefore A = \sqrt{\frac{2}{L_x}}$$

Method 2) Integrate $|\psi_n(x)|^2$ over $0 \sim L_x$

$$1 = \int_0^{L_x} |\psi_n(x)|^2 dx = \int_0^{L_x} A^2 \sin^2\left(\frac{n\pi}{L_x}x\right) dx = A^2 \int_0^{L_x} \frac{1-\cos\left(\frac{2n\pi x}{L_x}\right)}{2} dx = A^2 \frac{L_x}{2}$$

$$\therefore \psi_n(x) = \sqrt{\frac{2}{L_x}} \sin\left(\frac{n\pi}{L_x}x\right), \quad \begin{matrix} n = 1,2,3,\ldots \\ 0 < x < L_x \end{matrix}$$

1-D Particle in a Box - The Solution

(Step 7) Plug the wave function back into the Schrödinger equation

$$\psi_n(x) = \sqrt{\frac{2}{L_x}} \sin\left(\frac{n\pi}{L_x} x\right) \quad \Rightarrow \quad -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

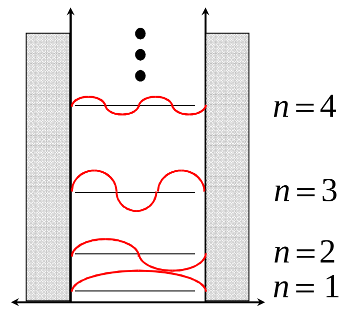
$$\frac{\hbar^2}{2m}\frac{n^2\pi^2}{L_x^2} \qquad\qquad = E_n$$

$$\psi_n(x) = \sqrt{\frac{2}{L_x}} \sin\left(\frac{n\pi}{L_x} x\right)$$

$$E_n = \frac{\hbar^2\pi^2}{2mL_x^2} n^2$$

$$n = 1, 2, 3, \ldots, \quad 0 < x < L_x$$

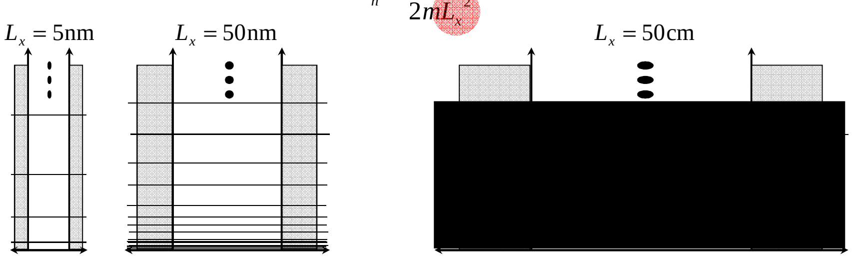
Discrete Energy Levels!



1-D Particle in a Box - Quantum vs. Macroscopic

- Quantum world → Macroscopic world
  - » What will happen with the discretized energy levels if we increase the length of the box?

$$E_n = \frac{\hbar^2\pi^2}{2mL_x^2} n^2$$



- Energy level spacing goes smaller and smaller as physical dimension increases.
- In macroscopic world, where the energy spacing is too small to resolve, we see continuum of energy values.
- Therefore, the quantum phenomena is only observed in nanoscale environment.

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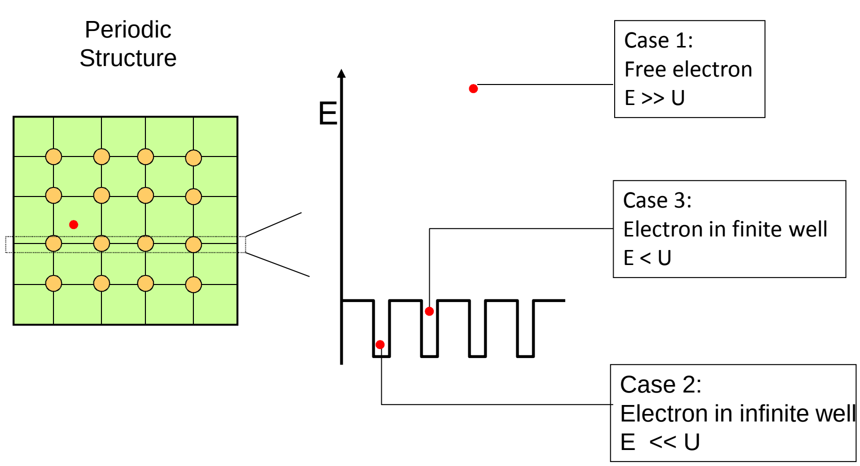


Five Steps for Closed System Analytical Solution

1) $\frac{d^2\psi}{dx^2}+k^2\psi=0$ → Solution Ansatz, 2N unknowns for N regions: $\psi(x)=A_+e^{ikx}+A_-e^{-ikx}$, $\psi(x)=De^{-\alpha x}+Ee^{+\alpha x}$

2) $\psi(x=-\infty)=0$, $\psi(x=+\infty)=0$ → Boundary Conditions at the edge. Reduces 2 unknowns

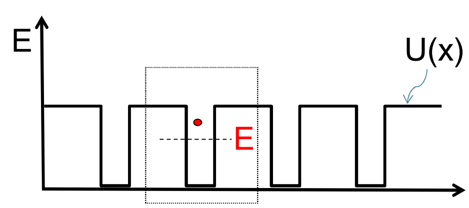
3) $\psi|_{x=x_B^-}=\psi|_{x=x_B^+}$, $\left.\frac{d\psi}{dx}\right|_{x=x_B^-}=\left.\frac{d\psi}{dx}\right|_{x=x_B^+}$ → Boundary Condition at each interface: Set 2N-2 equations for 2N-2 unknowns (for continuous U)

4) Det (coefficient matrix)=0 And find E by graphical or numerical solution

5) $\int_{-\infty}^{\infty}|\psi(x,E)|^2\,dx=1$

Normalization of unity probability for wave function

Case 2: Bound-levels in Finite Well (steps 1,2)

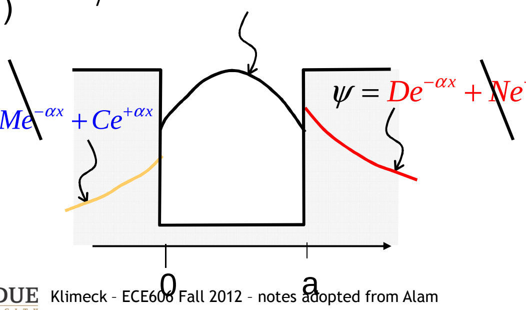


1)

$\psi = A\sin kx + B\cos kx$

$\psi = Me^{-\alpha x} + Ce^{+\alpha x}$

$\psi = De^{-\alpha x} + Ne^{+\alpha x}$



2) Boundary conditions at the edge

$\psi(x=-\infty)=0$

$\psi(x=+\infty)=0$

Case 2: Bound-levels in Finite Well (steps3)

3) Boundary at each interface

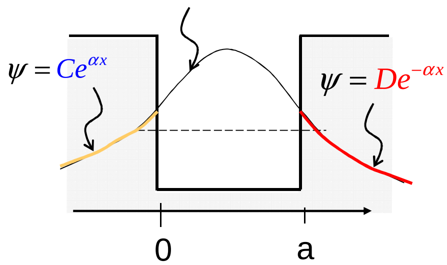
$$\psi\big|_{x=x_B^-} = \psi\big|_{x=x_B^+}$$

$$\frac{d\psi}{dx}\bigg|_{x=x_B^-} = \frac{d\psi}{dx}\bigg|_{x=x_B^+}$$

$$C = B$$
$$\alpha C = -kA$$

$$A\sin(ka) + B\cos(ka) = De^{-\alpha a}$$
$$kA\cos(ka) - kB\sin(ka) = -\alpha De^{-\alpha a}$$

$$\psi = A\sin kx + B\cos kx$$



$$\begin{pmatrix} 0 & 1 & -1 & 0 \\ k & 0 & \alpha & 0 \\ \sin(ka) & \cos(ka) & 0 & -e^{-\alpha a} \\ \cos(ka) & -\sin(ka) & 0 & \alpha e^{-\alpha a}/k \end{pmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Case 2: Bound-levels in Finite Well (step 4)

Only unknown is E

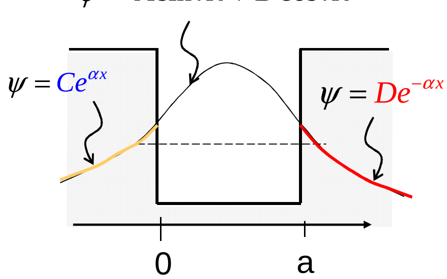
(i) Use Matlab function
(ii) Use graphical method

$$\tan(\alpha a\sqrt{\xi}) = \frac{2\sqrt{\xi(1-\xi)}}{2\xi - 1}$$

$$\xi \equiv \frac{E}{U_0} \qquad \alpha \equiv \sqrt{\frac{2mU_0}{\hbar^2}}$$

det (Matrix)=0

$$\psi = A\sin kx + B\cos kx$$

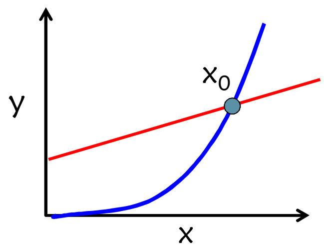


$$\begin{pmatrix} 0 & 1 & -1 & 0 \\ k & 0 & \alpha & 0 \\ \sin(ka) & \cos(ka) & 0 & -e^{-\alpha a} \\ \cos(ka) & -\sin(ka) & 0 & \alpha e^{-\alpha a}/k \end{pmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

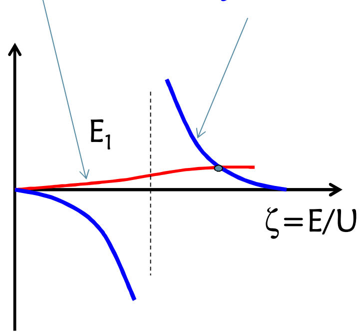
Case 2: Bound-levels in Finite Well (steps 4 graphical)

$$x^2 = x + 5$$

$$y_1 = x^2 \qquad y_2 = x + 5$$

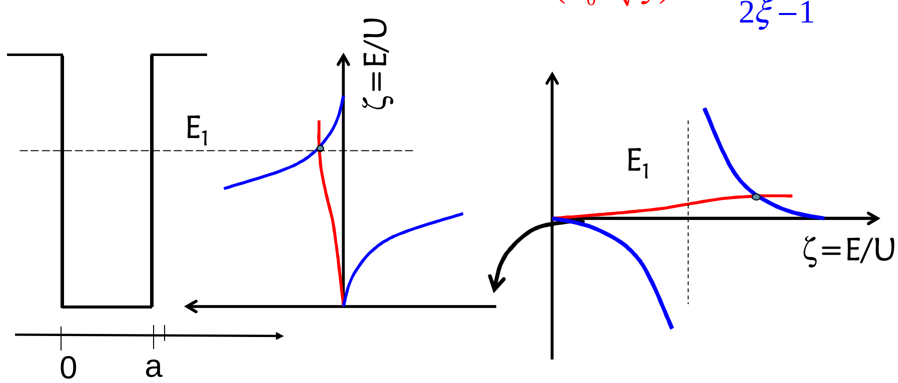


$$\tan(\alpha_0 a \sqrt{\xi}) = \frac{2\sqrt{\xi(1-\xi)}}{2\xi - 1}$$



Case 2: Bound-levels in Finite Well (steps 4 graphical)

$$\tan(\alpha_0 a \sqrt{\xi}) = \frac{2\sqrt{\xi(1-\xi)}}{2\xi - 1}$$



Obtained the eigenvalues
=> could stop here in many cases

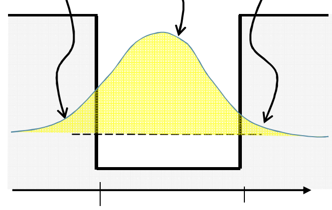
Case 2: Bound-levels in Finite Well (steps 5 wavefunction)

Need another boundary condition!

$$\begin{pmatrix} 0 & 1 & -1 & 0 \\ k & 0 & \alpha & 0 \\ \sin(ka) & \cos(ka) & 0 & e^{-\alpha a} \\ \cos(ka) & -\sin(ka) & 0 & -\alpha D e^{-\alpha a}/k \end{pmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$\psi = A\sin kx + B\cos kx$

$\psi = Ce^{\alpha x}$ $\psi = De^{-\alpha x}$



det (Matrix)=0

=> Linear dependent system
=> Only 3 variables are unique
=> One variable is undetermined
Let's assume A can be freely Chosen => can get B,C,D

Step 5: Wave-functions

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1 \quad \Rightarrow$$

Another boundary condition!
Non-linear => no simple linear algebra expression

$$\int_{-\infty}^{0} C^2 e^{2\alpha x} dx + \int_0^a \left[A\sin(kx) + B\sin(kx)\right]^2 dx + \int_a^{\infty} D^2 e^{-2\alpha x} dx = 1$$

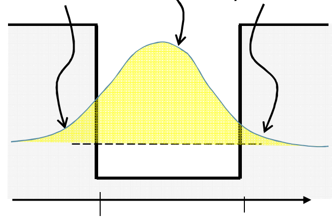
Get "A"

$$\begin{pmatrix} 0 & 1 & -1 & 0 \\ k & 0 & \alpha & 0 \\ \sin(ka) & \cos(ka) & 0 & e^{-\alpha a} \\ \cos(ka) & -\sin(ka) & 0 & -\alpha D e^{-\alpha a}/k \end{pmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{pmatrix} 1 & -1 & 0 \\ 0 & \alpha & 0 \\ \cos(ka) & 0 & e^{-\alpha a} \end{pmatrix} \begin{bmatrix} B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ -kA \\ -A\sin(ka) \end{bmatrix}$$

$\psi = A\sin kx + B\cos kx$

$\psi = Ce^{\alpha x}$ $\psi = De^{-\alpha x}$



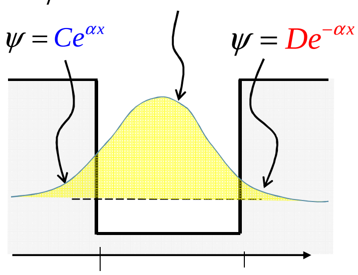
Get "B,C,D"

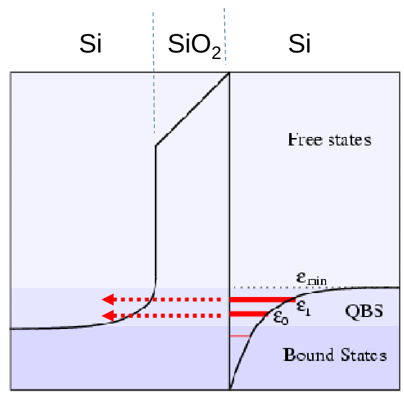
$$\begin{bmatrix} B \\ C \\ D \end{bmatrix} = \begin{pmatrix} 1 & -1 & 0 \\ 0 & \alpha & 0 \\ \cos(ka) & 0 & e^{-\alpha a} \end{pmatrix}^{-1} \begin{bmatrix} 0 \\ -kA \\ -A\sin(ka) \end{bmatrix}$$

Key Summary of a Finite Quantum Well

- **Problem is analytically solvable**
- **Electron energy is quantized and wavefunction is localized**
- **In the classical world:**
  - » **Particles are not allowed inside the barriers / walls => C=D=0**
- **In the quantum world:**
  - » **C and D have a non-zero value!**
  - » **Electrons can tunnel inside a barrier**

$$\psi = A \sin kx + B \cos kx$$





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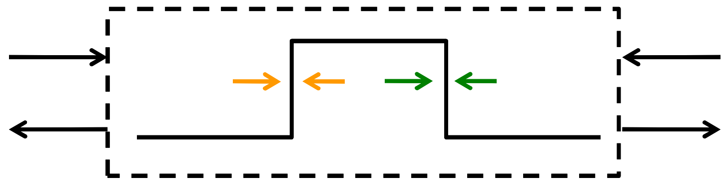
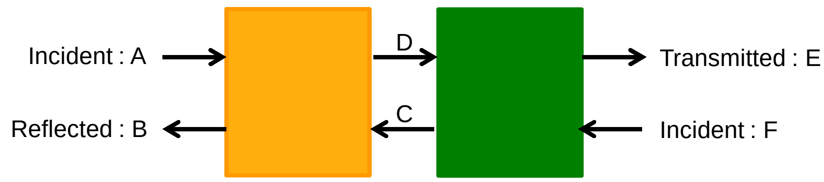
Transmission through a single barrier
Scattering Matrix approach

Define our system : Single barrier

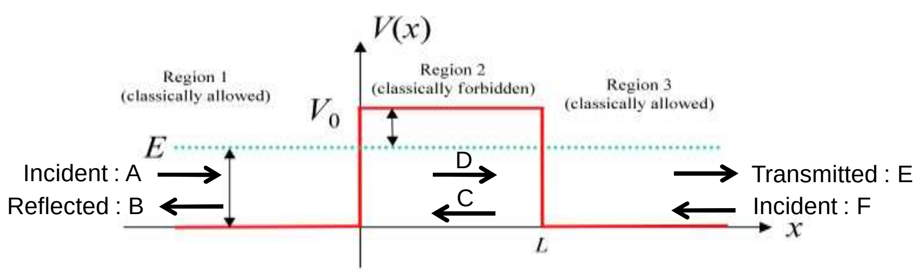


One matrix each for each interface: 2 S-matrices



No particles lost! Typically A=1 and F=0.

Tunneling through a single barrier



Wave-function each region,

$$\Psi_1(x) = Ae^{ikx} + Be^{-ikx}$$
$$\Psi_2(x) = Ce^{-\gamma x} + De^{\gamma x} \qquad k = \sqrt{\frac{2mE}{\hbar^2}} \qquad \gamma = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$
$$\Psi_3(x) = Ee^{ikx} + Fe^{-ikx}$$

Single barrier case

Applying boundary conditions at each interface (x=0 and x=L) gives,

$$\psi_1(0)=\psi_2(0) \quad\rightarrow\quad A+B=C+D$$
$$\psi_1'(0)=\psi_2'(0) \quad\rightarrow\quad ik(A-B)=-\gamma(C-D)$$
$$\psi_2(L)=\psi_3(L) \quad\rightarrow\quad Ce^{-\gamma L}+De^{\gamma L}=Ee^{ikL}+Fe^{-ikL}$$
$$\psi_2'(L)=\psi_3'(L) \quad\rightarrow\quad -\gamma\left(Ce^{-\gamma L}-De^{\gamma L}\right)=ik\left(Ee^{ikL}-Fe^{-ikL}\right)$$

Which in matrix can be written as,

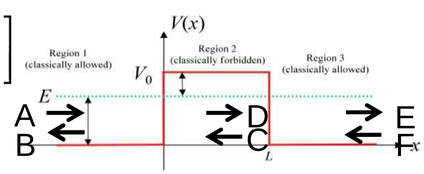
$$\begin{bmatrix}A\\B\end{bmatrix}=\begin{bmatrix}\frac{1}{2}\left(1+i\frac{\gamma}{k}\right) & \frac{1}{2}\left(1-i\frac{\gamma}{k}\right)\\ \frac{1}{2}\left(1-i\frac{\gamma}{k}\right) & \frac{1}{2}\left(1+i\frac{\gamma}{k}\right)\end{bmatrix}\begin{bmatrix}C\\D\end{bmatrix}=M_1\begin{bmatrix}C\\D\end{bmatrix}$$

$$\begin{bmatrix}C\\D\end{bmatrix}=\begin{bmatrix}\frac{1}{2}\left(1-i\frac{k}{\gamma}\right)e^{(ik+\gamma)L} & \frac{1}{2}\left(1+i\frac{k}{\gamma}\right)e^{-(ik-\gamma)L}\\ \frac{1}{2}\left(1+i\frac{k}{\gamma}\right)e^{(ik-\gamma)L} & \frac{1}{2}\left(1-i\frac{k}{\gamma}\right)e^{-(ik+\gamma)L}\end{bmatrix}\begin{bmatrix}E\\F\end{bmatrix}=M_2\begin{bmatrix}E\\F\end{bmatrix}$$

Generalization to Transfer Matrix Method

- The complete transfer matrix

$$\begin{bmatrix}A\\B\end{bmatrix}=M_1\begin{bmatrix}C\\D\end{bmatrix}=M_1M_2\begin{bmatrix}E\\F\end{bmatrix}=M\begin{bmatrix}E\\F\end{bmatrix}$$



- 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!

Single barrier case

Transmission can be found using the relations between unknown constants,

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

Case: $E<V_o$

$$T(E) = \left[1 + \left(\frac{\gamma^2 + k^2}{2k\gamma}\right)^2 sh^2(\gamma L)\right]^{-1}$$

Case(γL large): Strong barrier

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

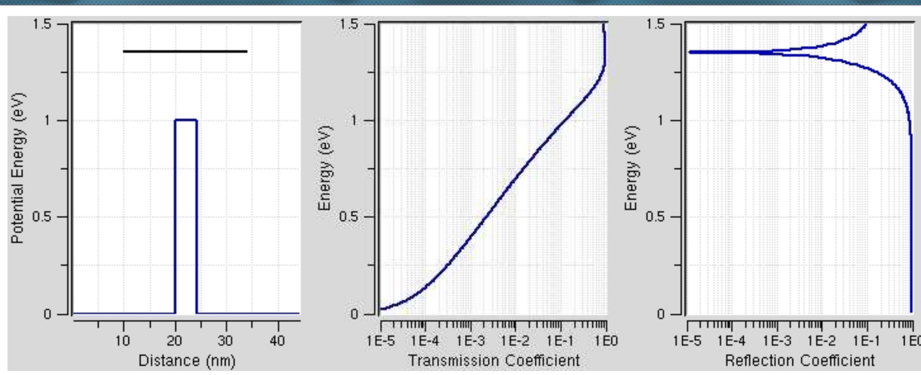
Case(γL<<1): Weak barrier

$$T(E) \approx \frac{1}{1 + (kL/2)^2}$$

Case: $E>V_o$

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

Single barrier : Concepts



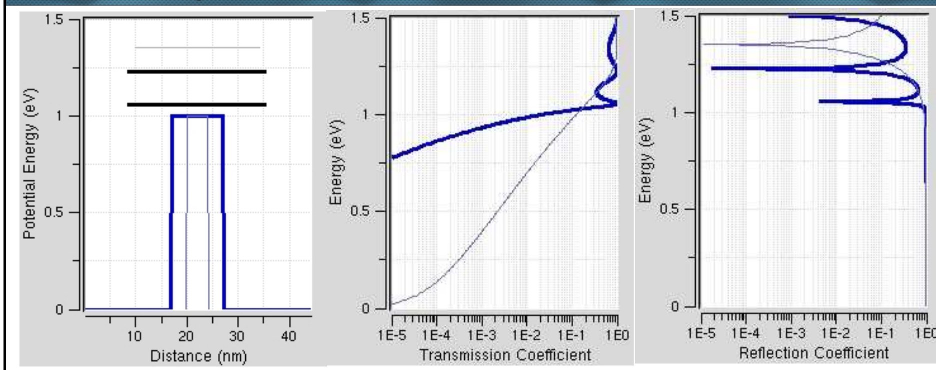
- Transmission is finite under the barrier – tunneling!
- Transmission above the barrier is not perfect unity!
- Quasi-bound state above the barrier. Transmission goes to one.

Case: $E>V_o$

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

- Computed with – http://nanohub.org/tools/pcpbt

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

Presentation Outline

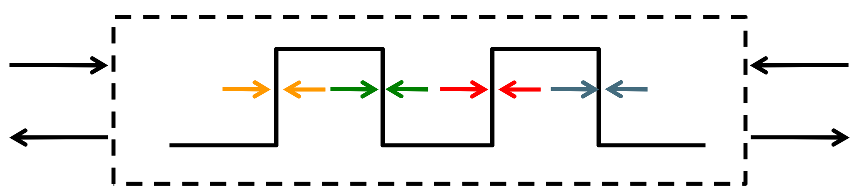
- Time Independent Schroedinger Equation
- Analytical solutions of Toy Problems
  - » (Almost) Free Electrons
  - » Tightly bound electrons – infinite potential well
  - » Electrons in a finite potential well
  - » Tunneling through a single barrier
- Numerical Solutions to Toy Problems
  - » Tunneling through a double barrier structure
  - » Tunneling through N barriers
- Additional notes
  - » Discretizing Schroedinger's equation for numerical implementations

Reference: Vol. 6, Ch. 2 (pages 29-45)

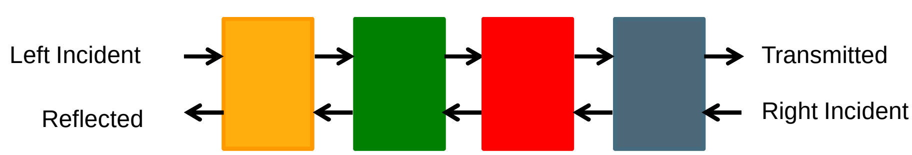
- piece-wise-constant-potential-barrier tool
  http://nanohub.org/tools/pcpbt

Double Barrier Transmission: Scattering Matrix approach

Define our system : Double barrier



One matrix each for each interface: 4 S-matrices

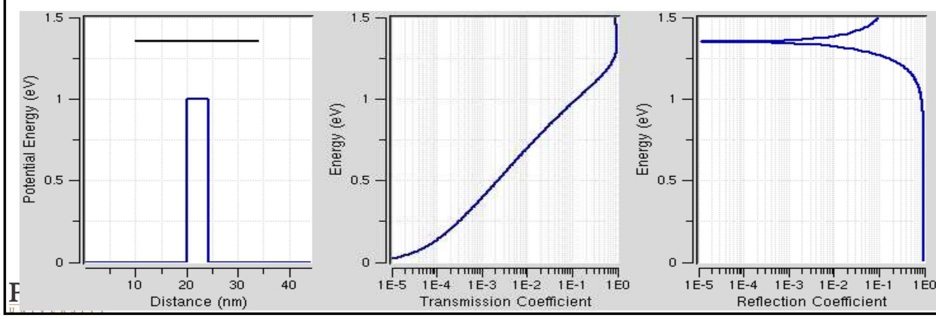


No particles lost!
Typically Left Incident wave is normalized to one.
Right incident is assumed to be zero.

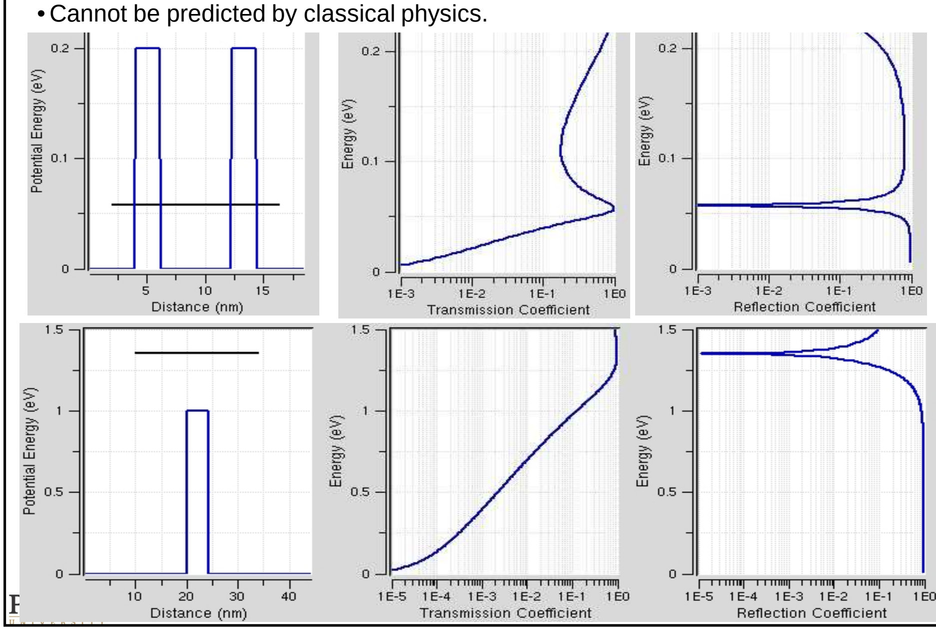
Also this problem is analytically solvable! => Homework assignment

Reminder: Single barrier

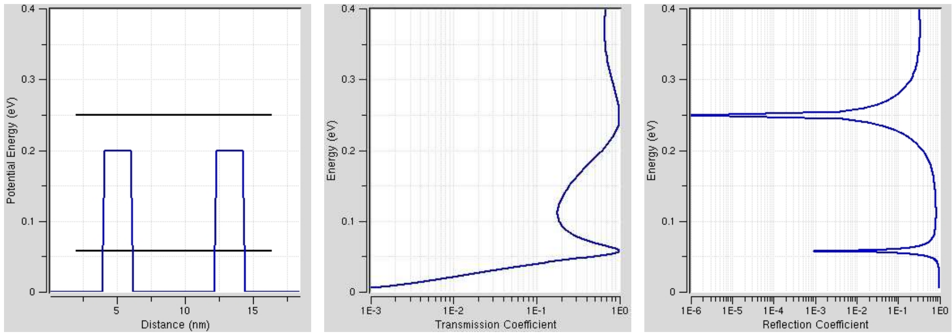
- •Transmission is finite under the barrier – tunneling!
- •Transmission above the barrier is not perfect unity!
- •Quasi-bound state above the barrier.
  Transmission goes to one.



- 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.

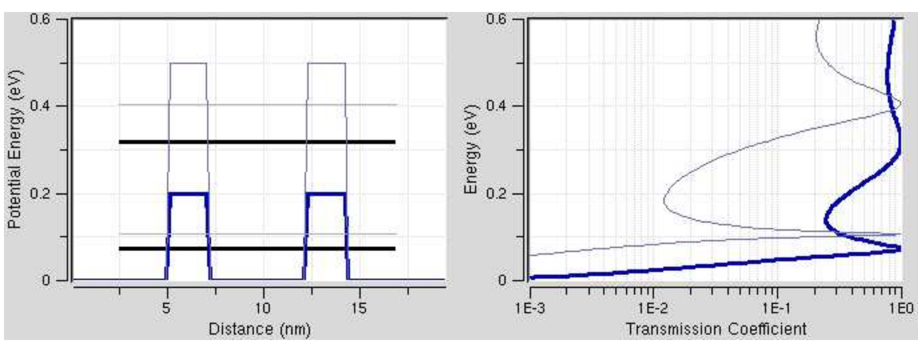


Double barrier: Quasi-bound states



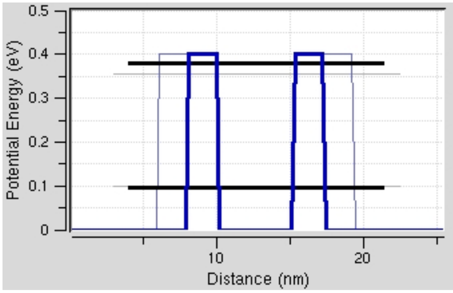
- In addition to states inside the well, there could be states above the barrier height.
- States above the barrier height are quasi-bound or weakly bound.
- How strongly bound a state is can be seen by the width of the transmission peak.
- The transmission peak of the quasi-bound state is much broader than the peak for the state inside the well.

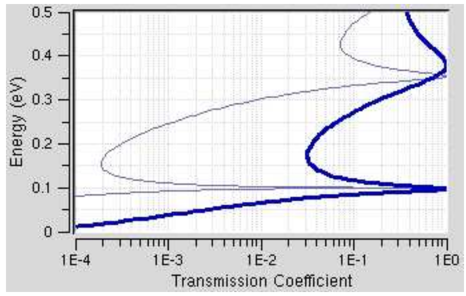
Effect of barrier height



- 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.

Effect of barrier thickness





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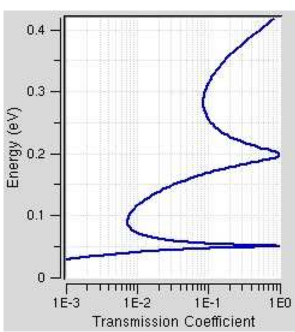
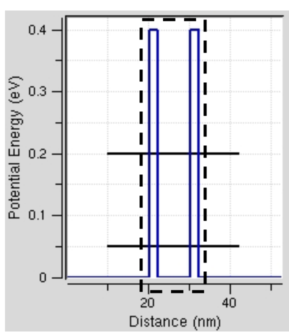
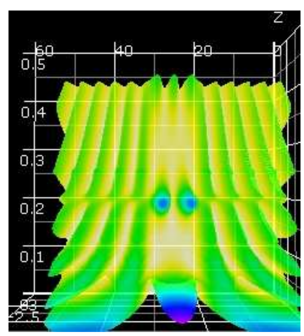
Double barrier energy levels Vs Closed system







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

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)+V(x)\psi(x)=E\psi(x) \quad \text{where, } V(x)=\begin{cases}0 & 0<x<L_x \\ \infty & \text{elsewhere}\end{cases}$$

- The solution in the well is:

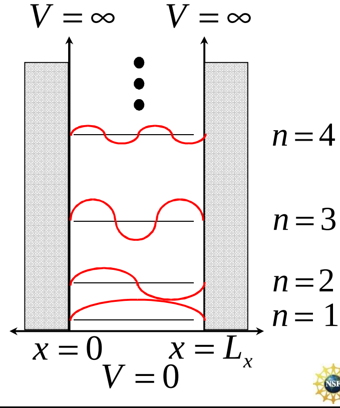
$$\psi_n(x)=A\sin\left(\frac{n\pi}{L_x}x\right),\quad n=1,2,3,\ldots$$

- Plugging the normalized wave-functions back into the Schrödinger equation we find that energy levels are quantized.

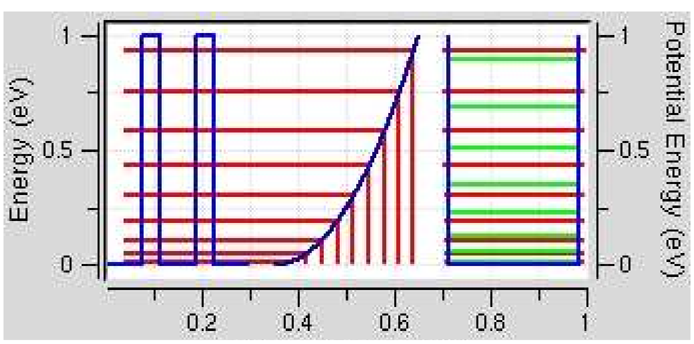
$$\psi_n(x)=\sqrt{\frac{2}{L_x}}\sin\left(\frac{n\pi}{L_x}x\right)$$

$$E_n=\frac{\hbar^2\pi^2}{2mL_x^2}n^2$$

$$n=1,2,3\ldots,\quad 0<x<L_x$$



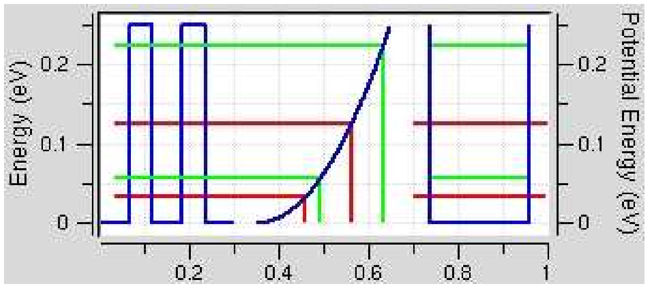
Double barrier & particle in a box



- 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.

Open systems Vs closed systems



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

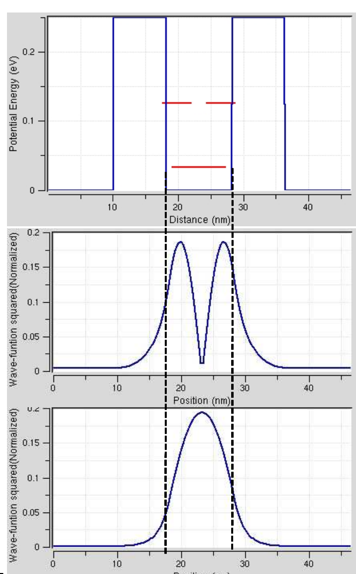
- Double barrier: Thinner Barriers(8nm), Shorter Barriers(0.25eV), Well(10nm).
- Even the first resonance energy does not match with the particle in a box energy.
- The well region does not resemble a particle in a box.
- A double barrier structure is an OPEN system, particle in a box is a CLOSED system.

Reason for deviation?

Potential profile and resonance energies using tight-binding.

First excited state wave-function amplitude using tight binding.

Ground state wave-function amplitude using tight binding.



- 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.

$$E_n = \frac{\hbar^2 \pi^2}{2mL_{well}^2} n^2$$

$$n = 1,2,3,\ldots, \quad 0 < x < L_{well}$$

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

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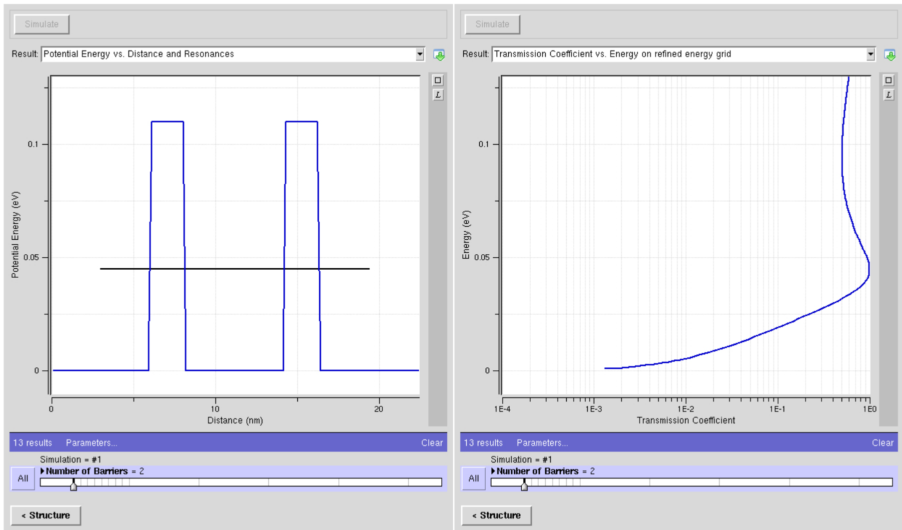
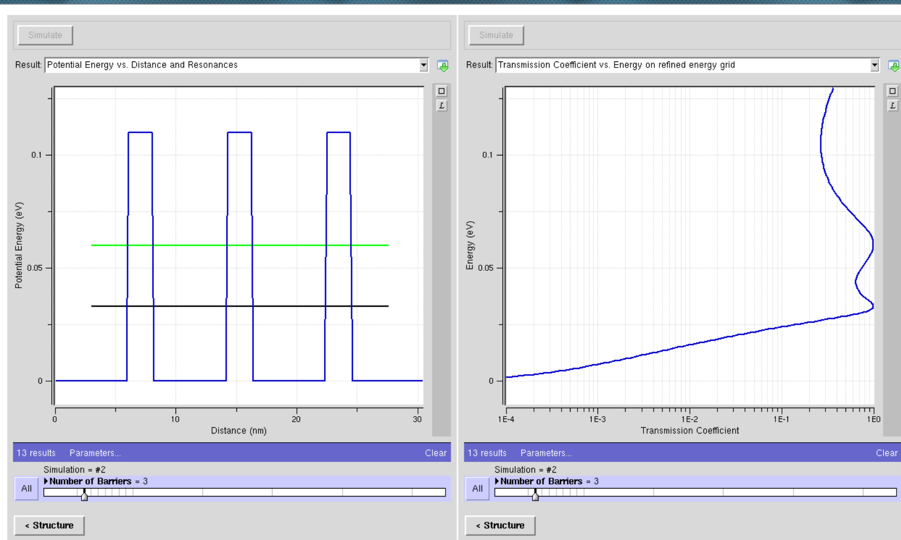
1 Well => 1 Transmission Peak



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

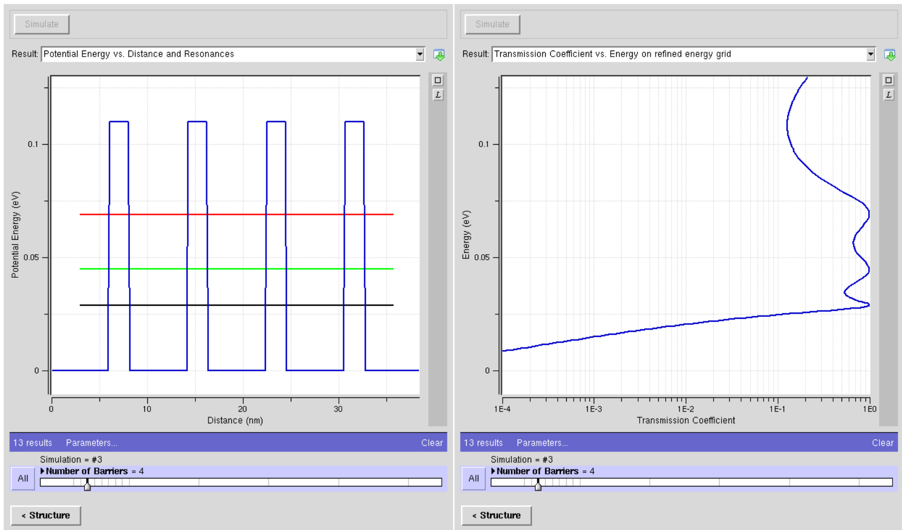
2 Wells => 2 Transmission Peaks



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

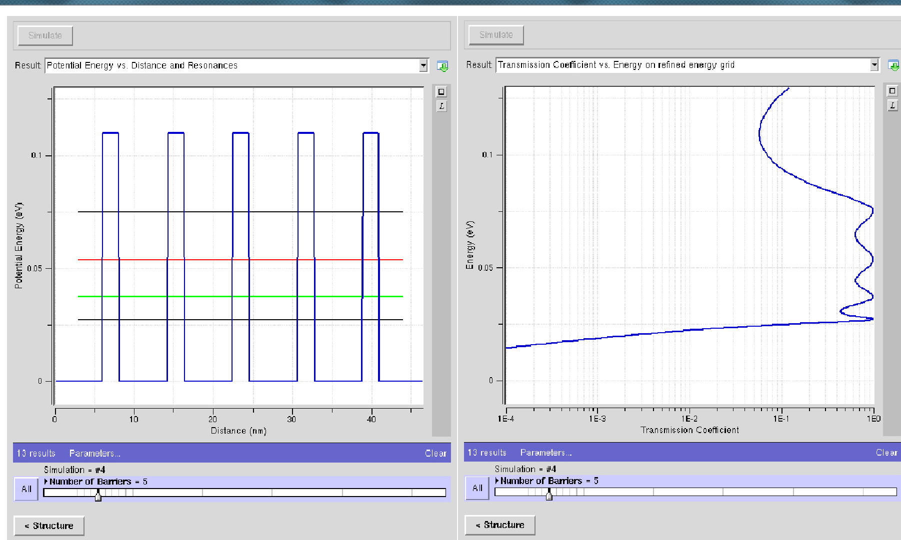
Bonding/Anti-bonding State

3 Wells => 3 Transmission Peaks



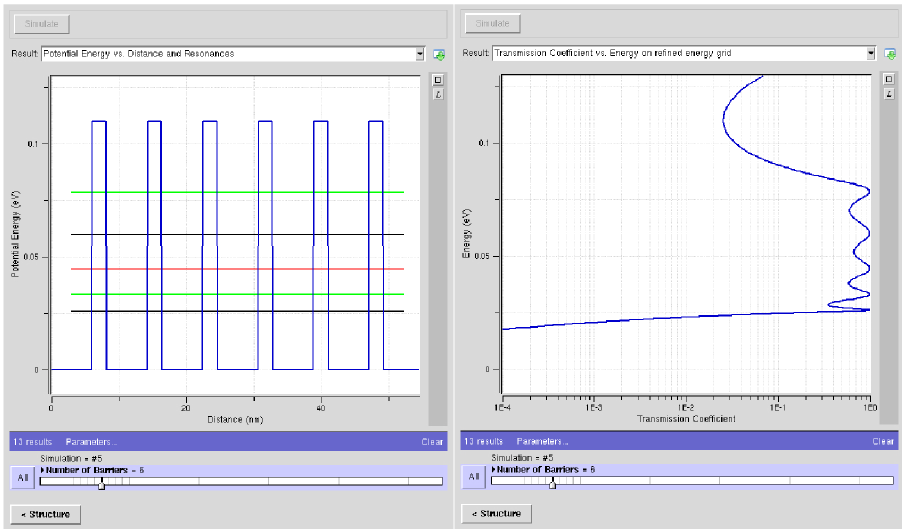
- Vb=110meV, W=6nm, B=2nm

4 Wells => 4 Transmission Peaks



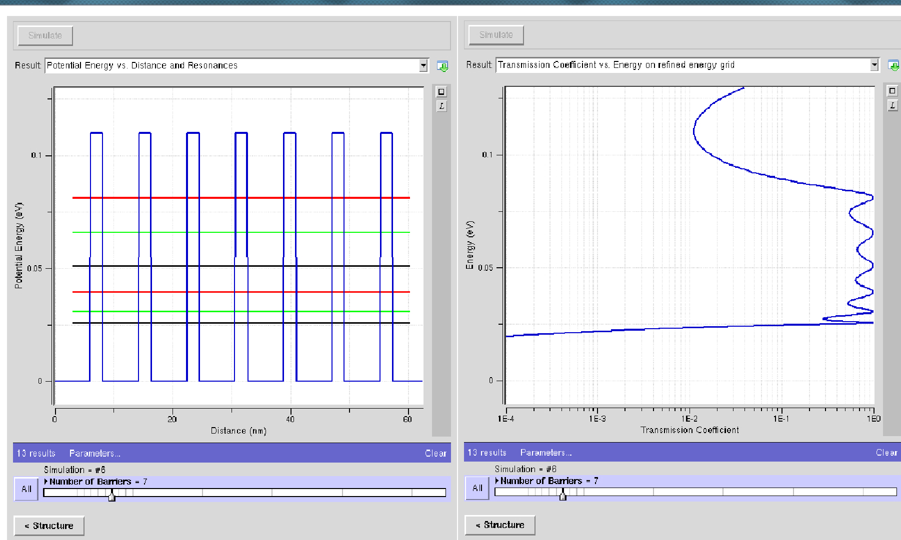
- Vb=110meV, W=6nm, B=2nm

5 Wells => 5 Transmission Peaks



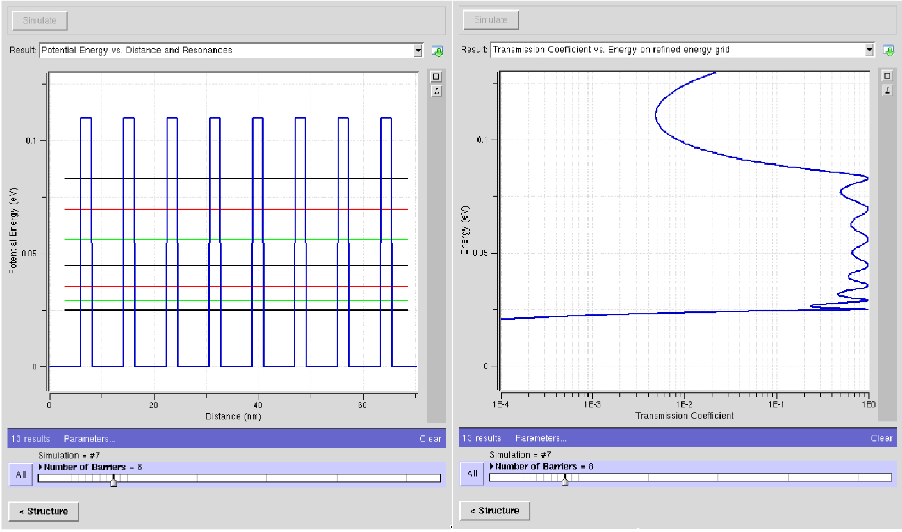
- Vb=110meV, W=6nm, B=2nm

6 Wells => 6 Transmission Peaks



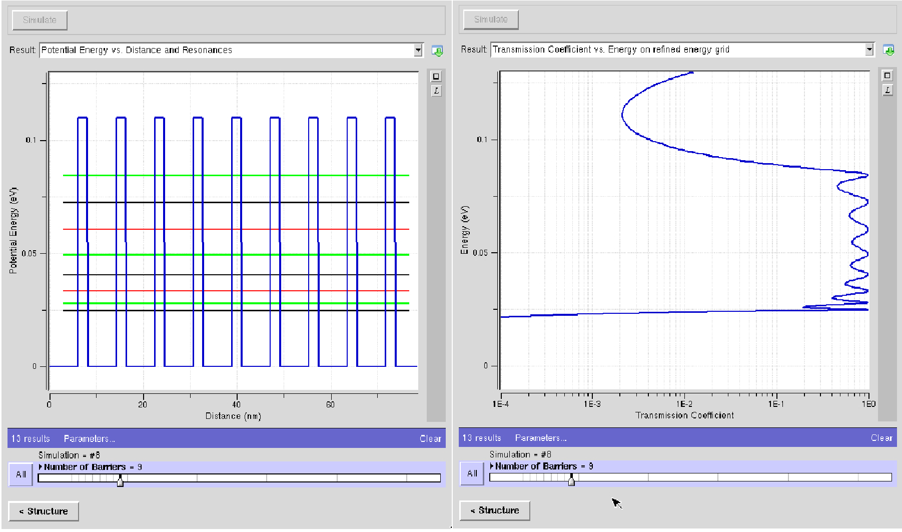
- Vb=110meV, W=6nm, B=2nm

7 Wells => 7 Transmission Peaks



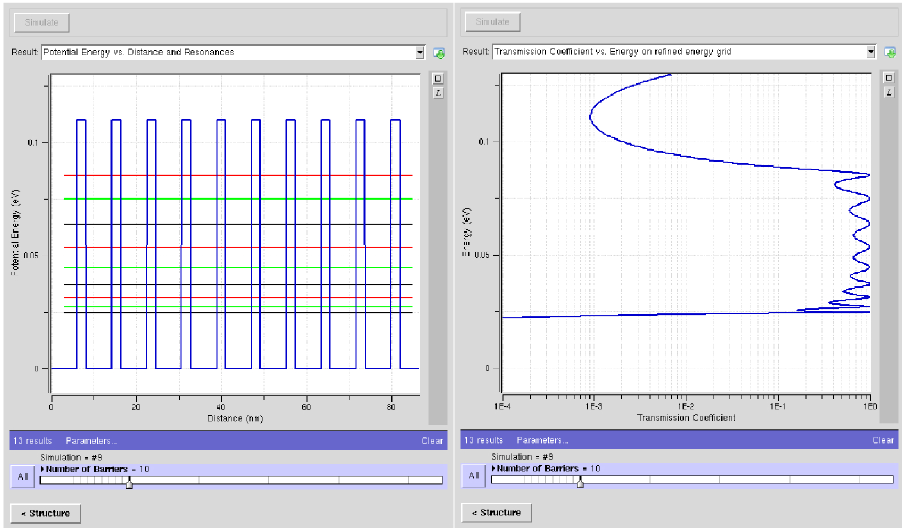
- Vb=110meV, W=6nm, B=2nm

8 Wells => 8 Transmission Peaks



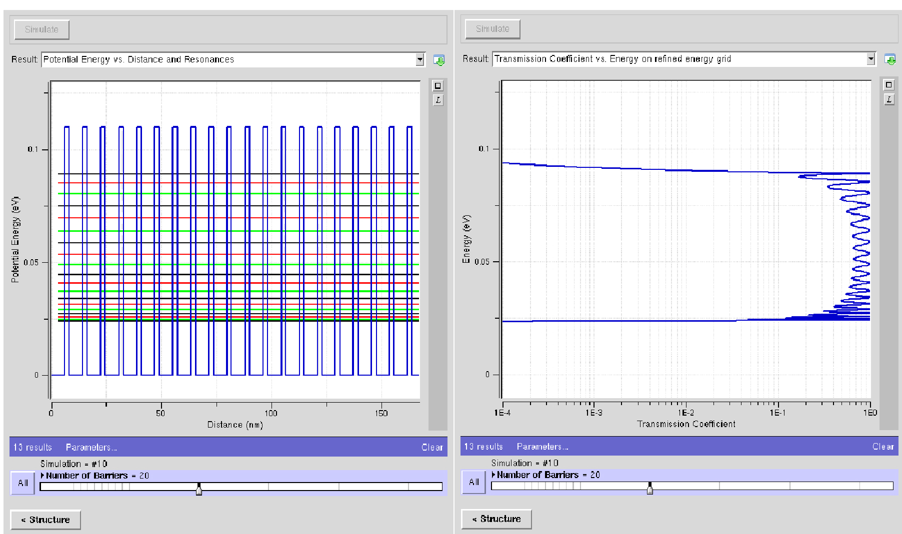
- Vb=110meV, W=6nm, B=2nm

9 Wells => 9 Transmission Peaks



- Bandpass filter formed
- Band transmission not symmetric

19 Wells => 19 Transmission Peaks



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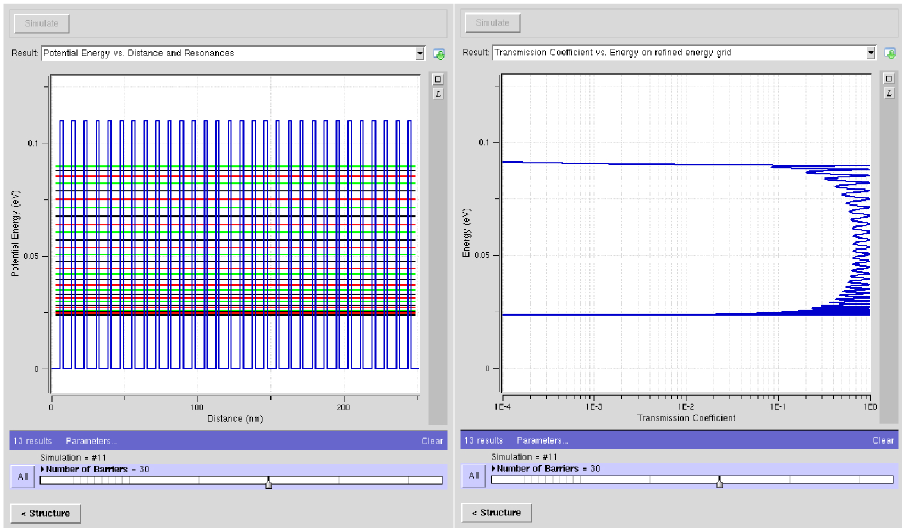
29 Wells => 29 Transmission Peaks



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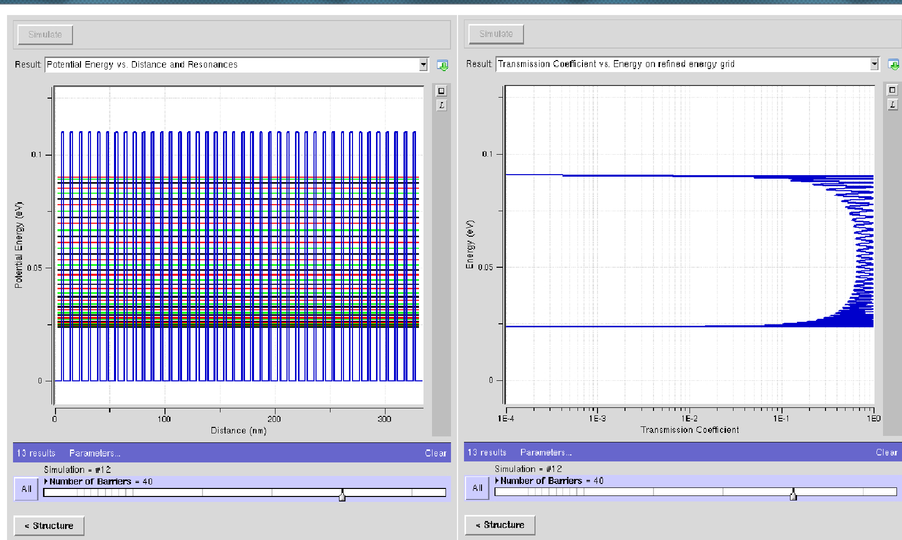
39 Wells => 39 Transmission Peaks



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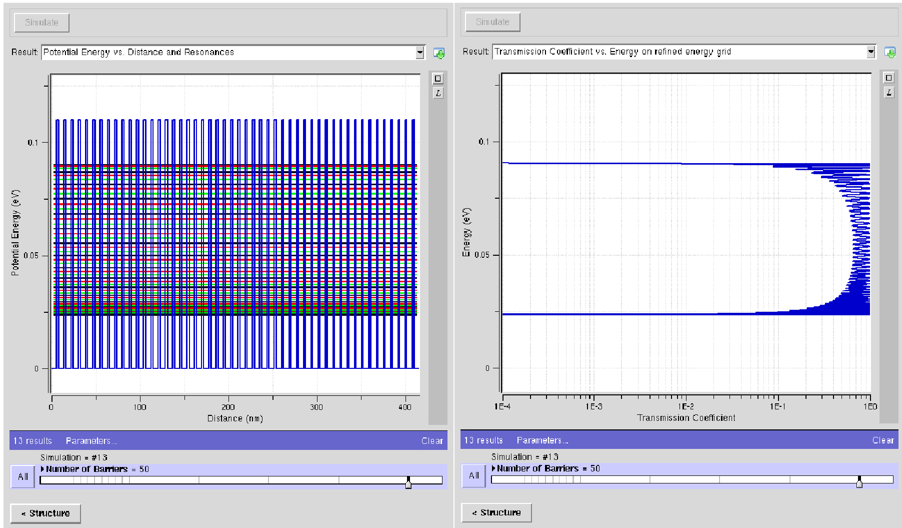
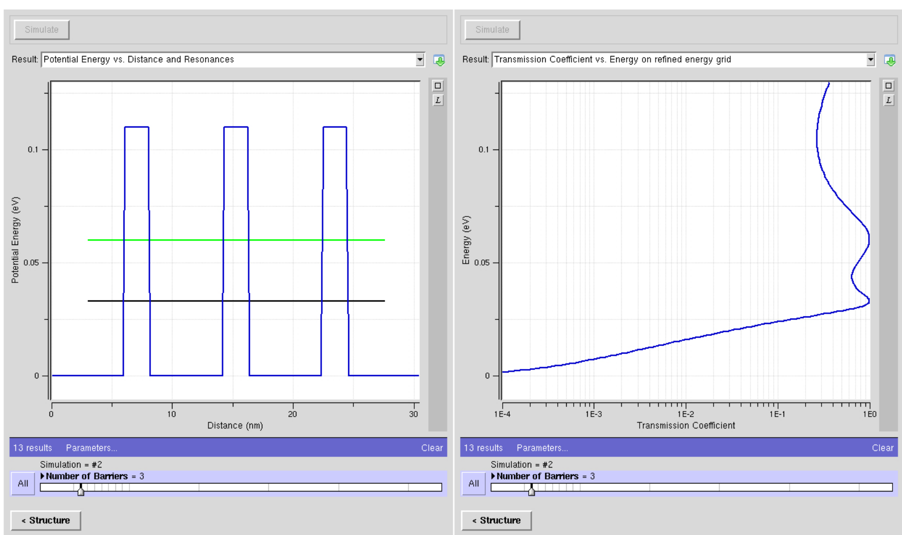
- Band transmission not symmetric

49 Wells => 49 Transmission Peaks



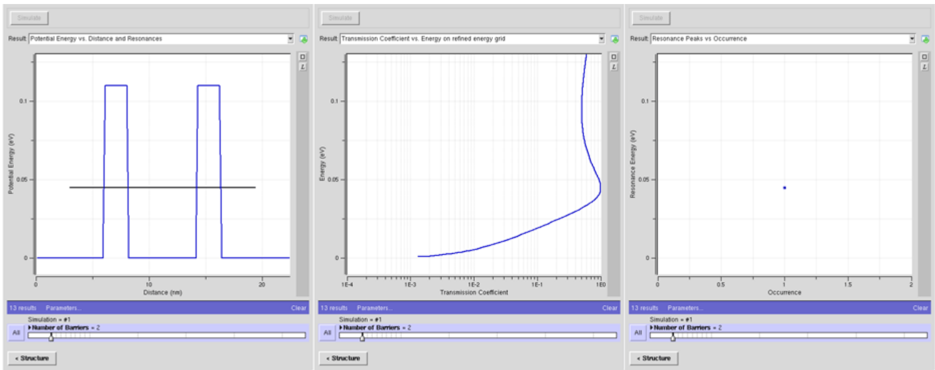
- Bandpass filter formed
- Band transmission not symmetric

N Wells => N Transmission Peaks



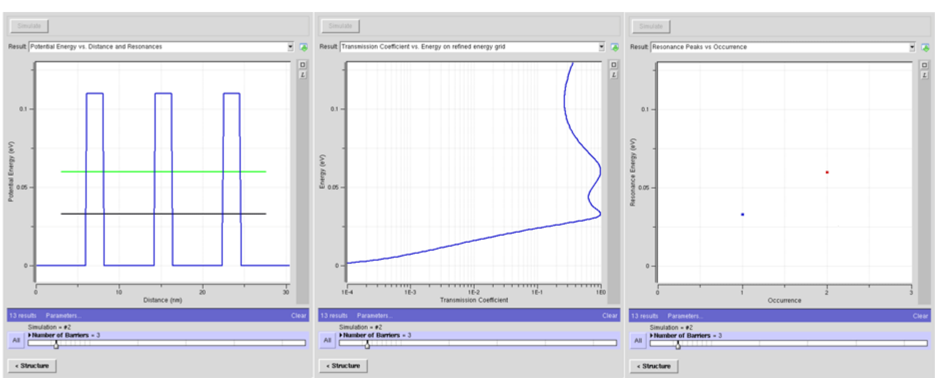
- Bandpass filter formed
- Band transmission not symmetric
- Bandpass sharpens with increasing number of wells

1 Well => 1 Transmission Peak => 1 State



- Bandpass filter formed
- Band transmission not symmetric
- Bandpass sharpens with increasing number of wells

2 Wells => 2 Transmission Peaks => 2 States



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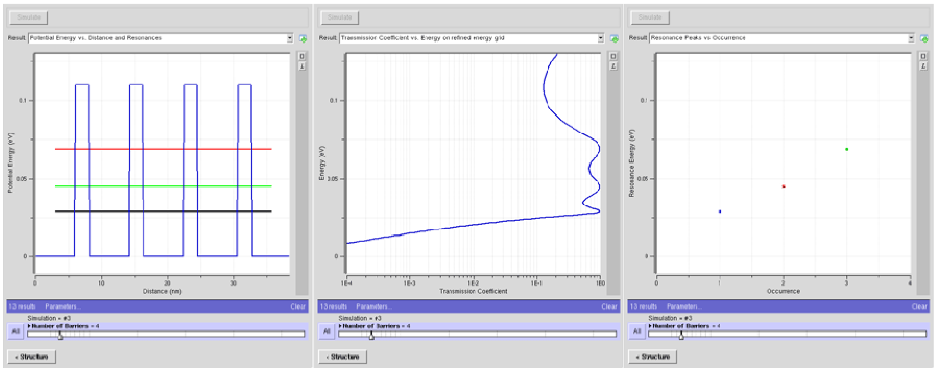
3 Wells => 3 Transmission Peaks => 3 States



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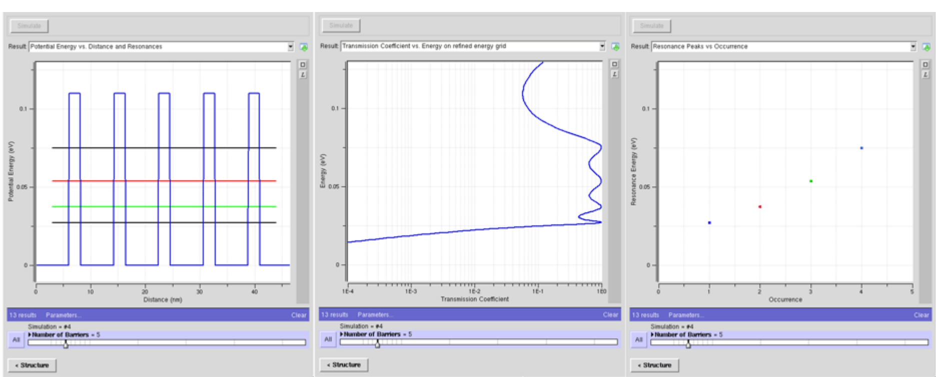

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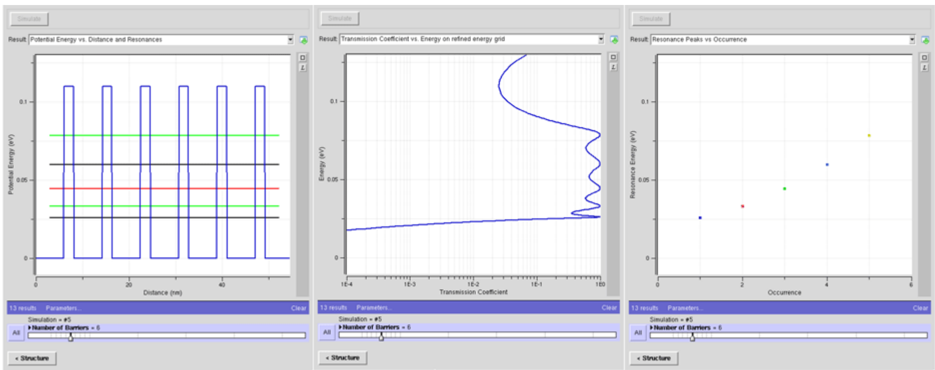

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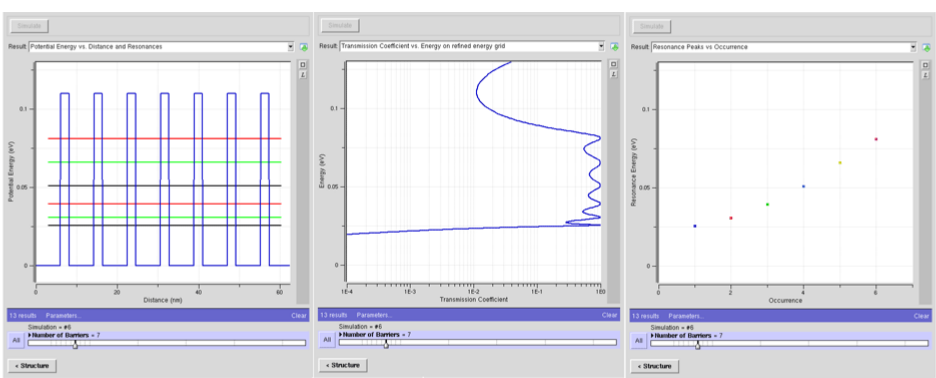

- Bandpass filter formed
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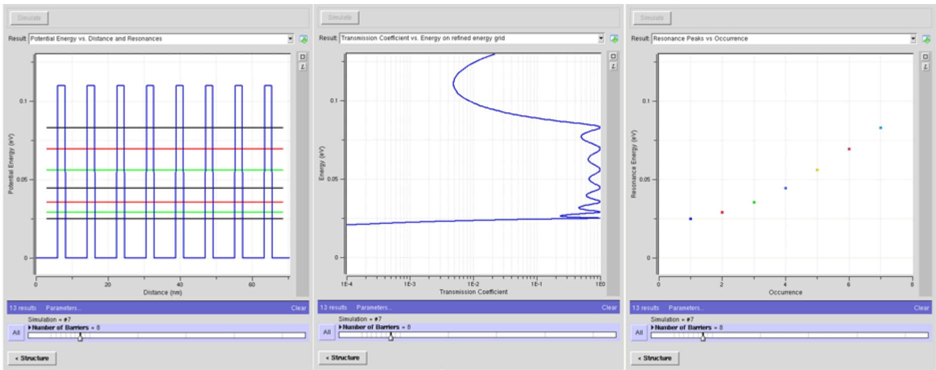

- Bandpass filter formed
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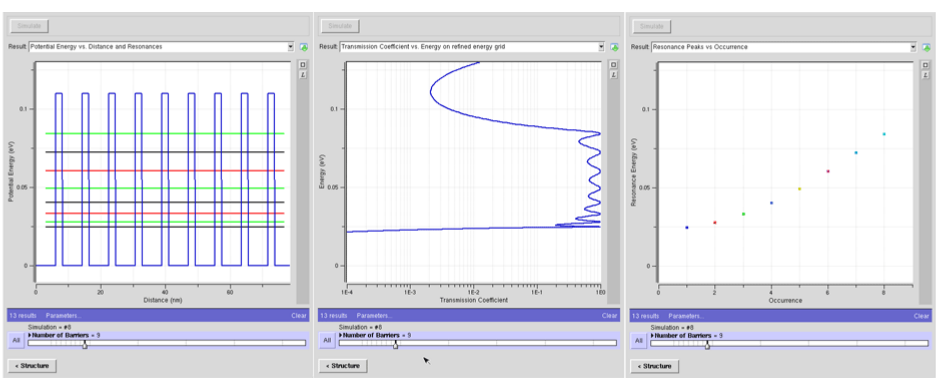
8 Wells => 8 Transmission Peaks => 8 States



- Bandpass filter formed
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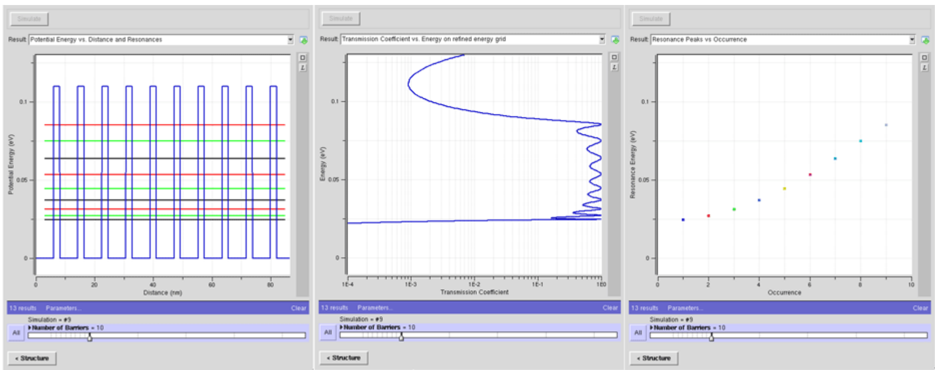
9 Wells => 9 Transmission Peaks => 9 States



- Bandpass filter formed
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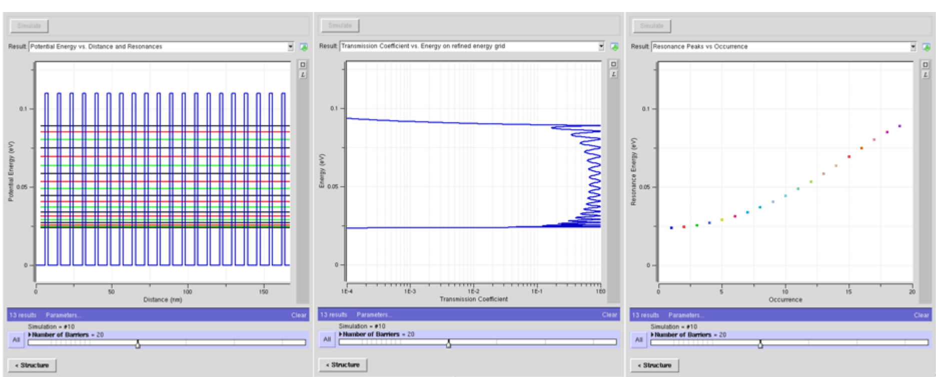
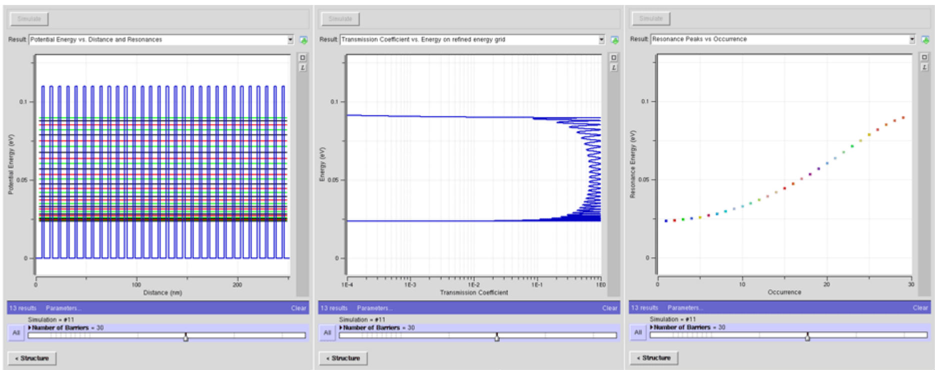


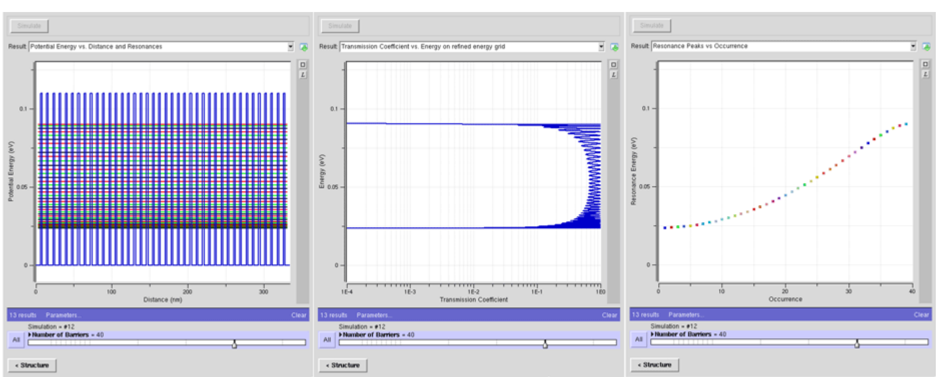
- Bandpass filter formed
- Band transmission not symmetric

29 Wells => 29 Transmission Peaks => 29 States



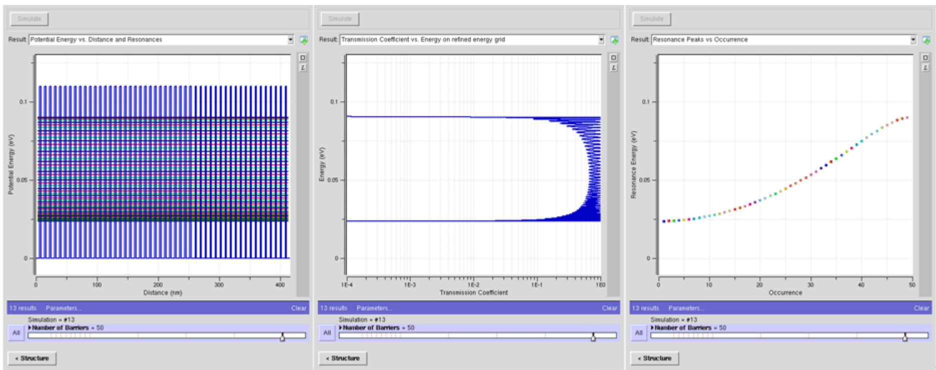
- Bandpass filter formed
- Band transmission not symmetric

39 Wells => 39 Transmission Peaks => 39 States



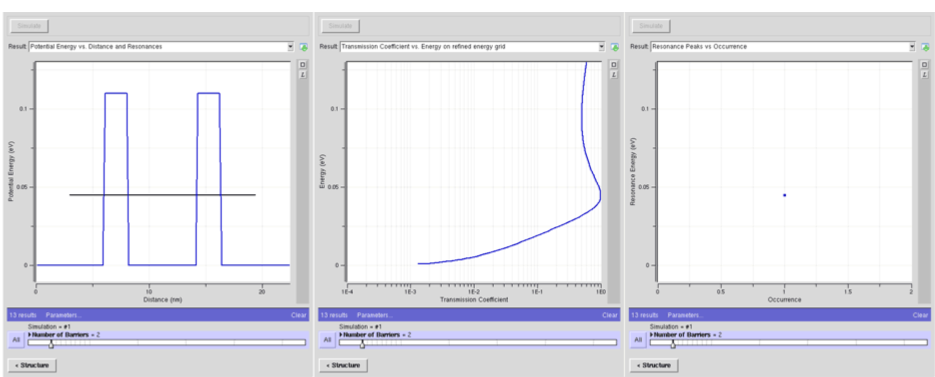
- Bandpass filter formed
- Band transmission not symmetric

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

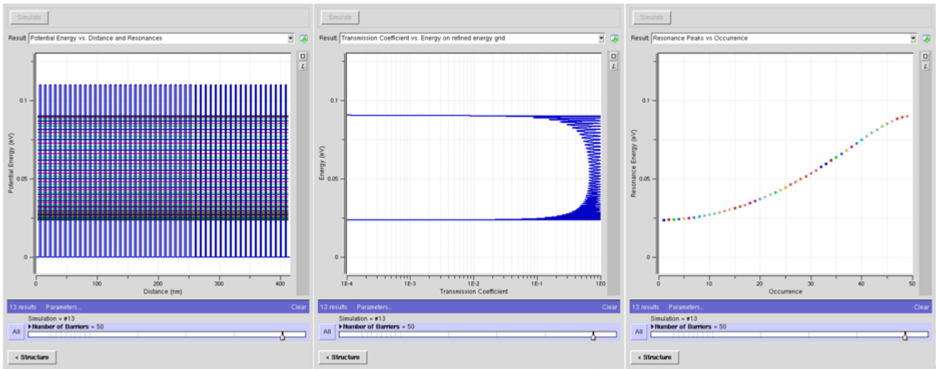


- Bandpass filter formed
- Band transmission not symmetric
- Cosine-like band formed
- Band is not symmetric

N Wells => N States => 1 Band

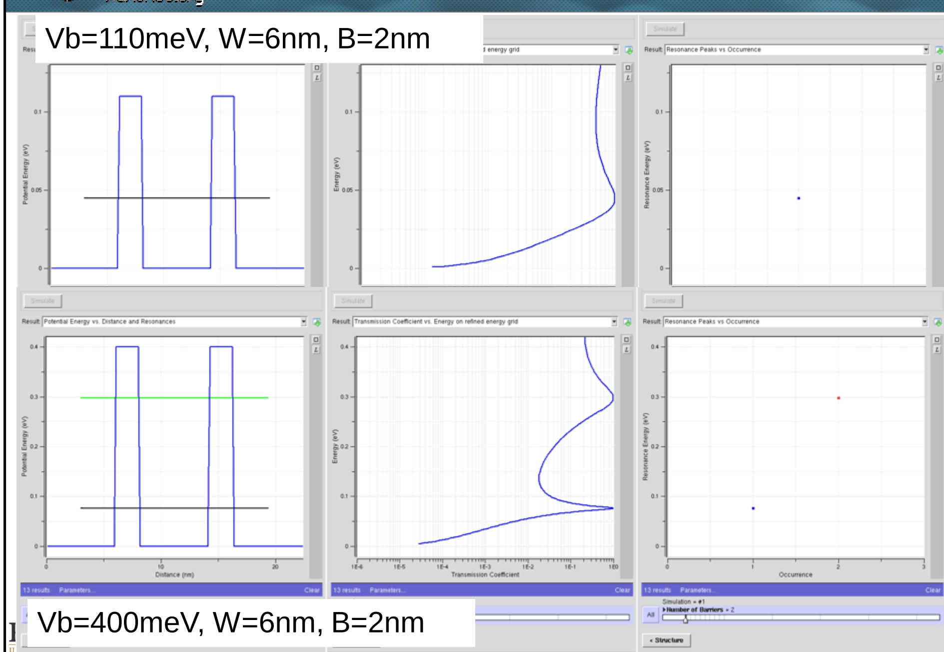
- Vb=110meV, W=6nm, B=2nm => ground state in each well

=> what if there were excited states in each well => Vb=400meV

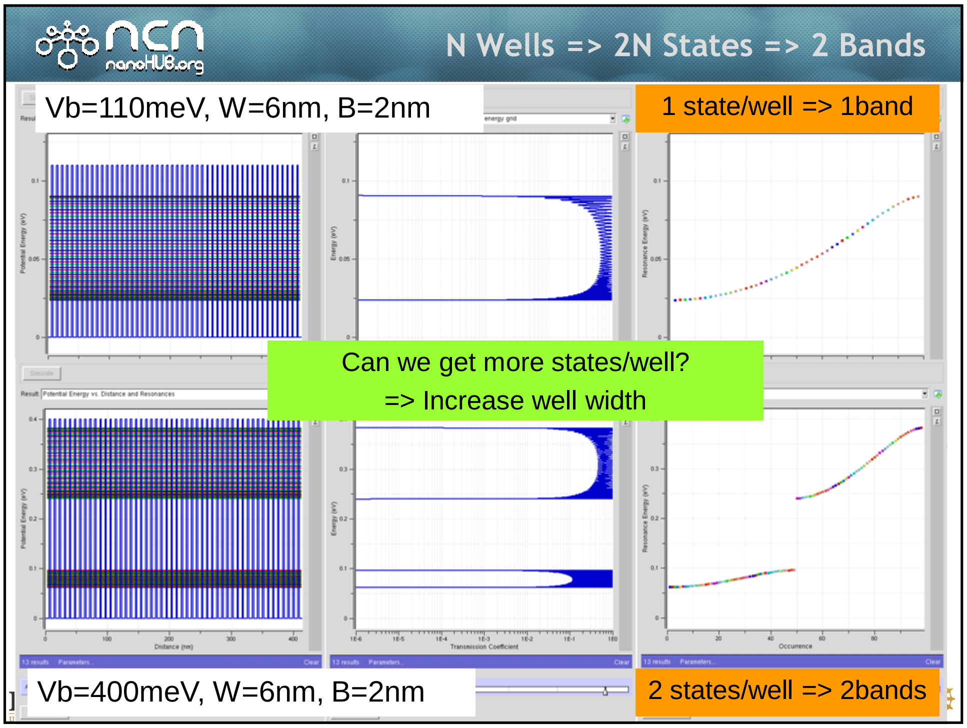


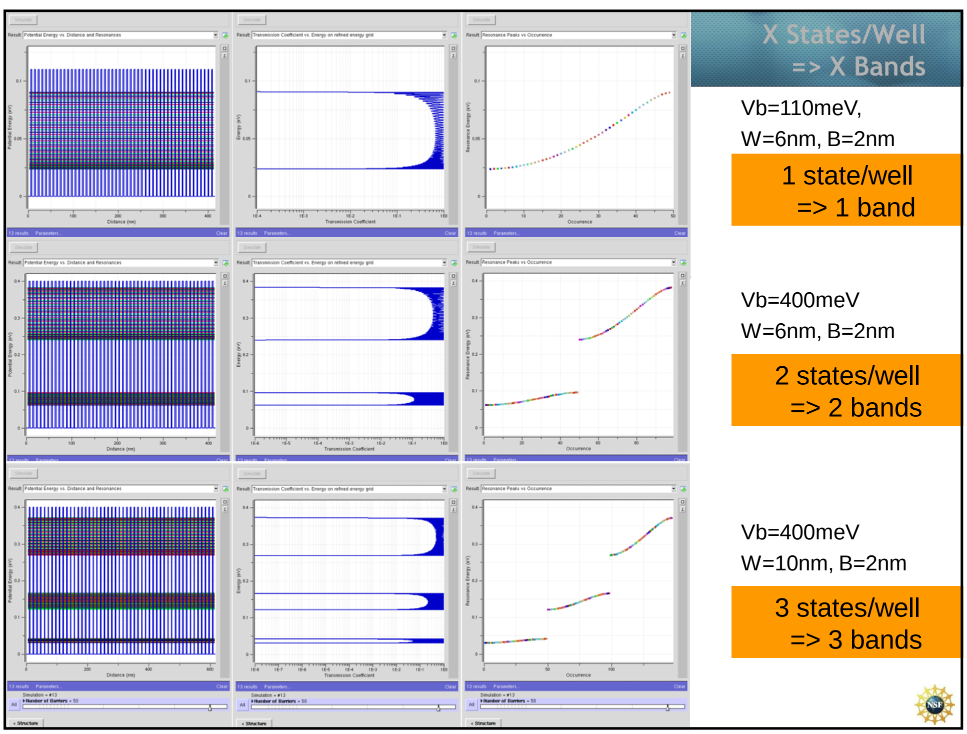
N Wells => 2N States => 2 Bands

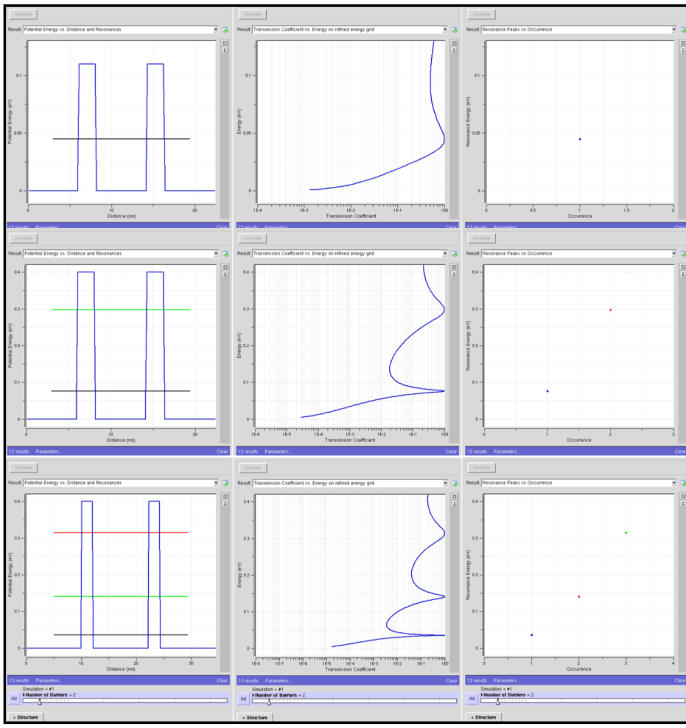
Vb=110meV, W=6nm, B=2nm



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


nanoHUB.org
N Wells => 2N States => 2 Bands
Vb=110meV, W=6nm, B=2nm
1 state/well => 1band
Can we get more states/well?
=> Increase well width
Vb=400meV, W=6nm, B=2nm
2 states/well => 2bands


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



X States/Well => X Bands

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

1 state/well => 1 band

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

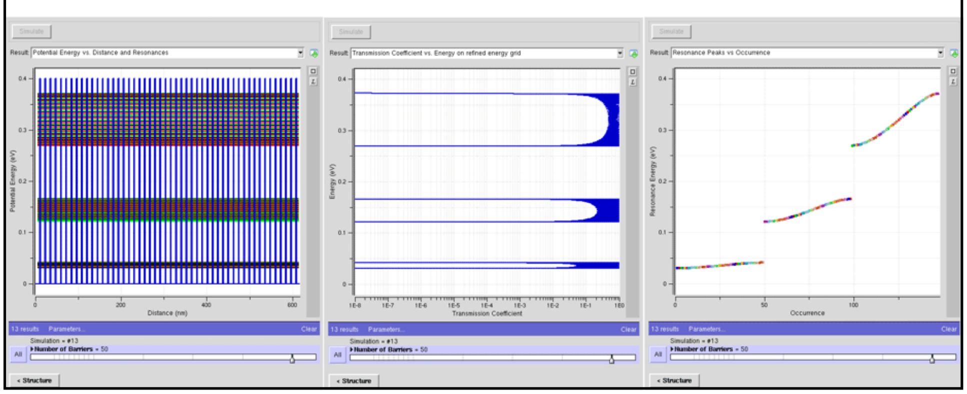
2 states/well => 2 bands

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

- Time Independent Schroedinger Equation
- Analytical solutions of Toy Problems
  - » (Almost) Free Electrons
  - » Tightly bound electrons – infinite potential well
  - » Electrons in a finite potential well
  - » Tunneling through a single barrier
- Numerical Solutions to Toy Problems
  - » Tunneling through a double barrier structure
  - » Tunneling through N barriers
- Procedure Summary
- Additional notes
  - » Discretizing Schroedinger's equation for numerical implementations

Reference: Vol. 6, Ch. 2 (pages 29-45)

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

Five Steps for Closed System Analytical Solution

1) $$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$ ⟶ Solution Ansatz, 2N unknowns for N regions

$$\psi(x) = A_+ e^{ikx} + A_- e^{-ikx}$$
$$\psi(x) = De^{-\alpha x} + Ee^{+\alpha x}$$

2) $$\psi(x = -\infty) = 0$$ $$\psi(x = +\infty) = 0$$ ⟶ Boundary Conditions at the edge. Reduces 2 unknowns

3) $$\psi\Big|_{x=x_B^-} = \psi\Big|_{x=x_B^+}$$ $$\frac{d\psi}{dx}\Big|_{x=x_B^-} = \frac{d\psi}{dx}\Big|_{x=x_B^+}$$ ⟶ Boundary Condition at each interface: Set 2N-2 equations for 2N-2 unknowns (for continuous U)

4) Det (coefficient matrix)=0 And find E by graphical or numerical solution

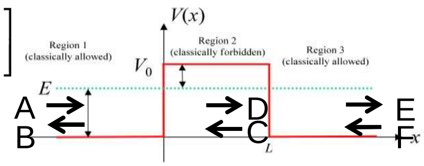
5) $$\int_{-\infty}^{\infty} |\psi(x,E)|^2 dx = 1$$

Normalization of unity probability for wave function

Open System: Generalization to Transfer Matrix Method

- 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

$$\begin{pmatrix} A_N \\ B_N \end{pmatrix} = \prod_{j=2..N} \underline{T}_j \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} .$$

- Looks conceptually very simple and analytically pleasing
- Use it for your homework assignment for a double barrier structure!

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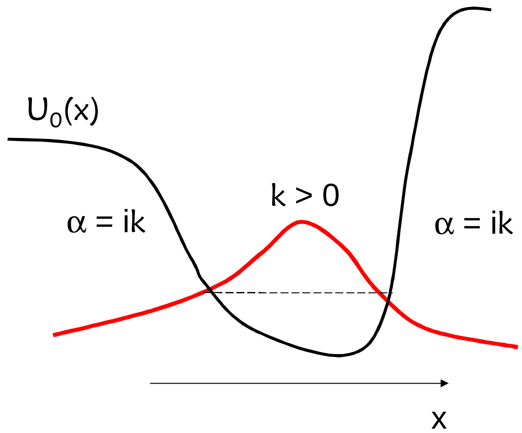
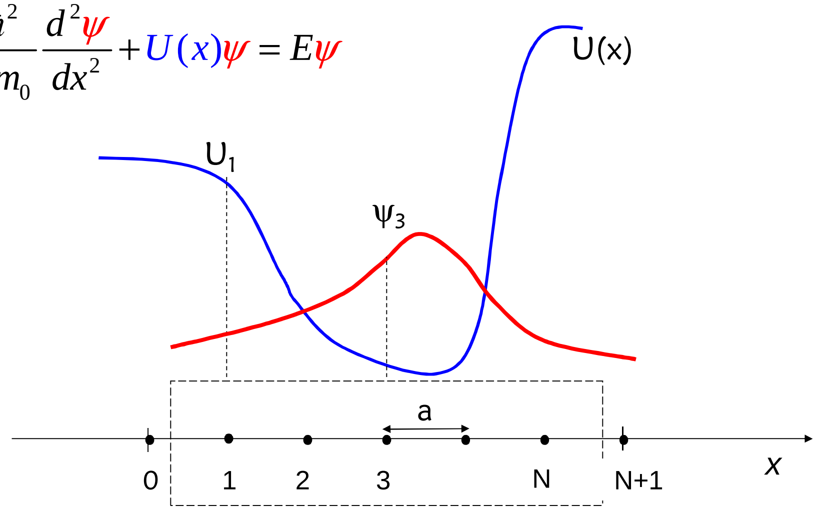
Numerical solution of Schrodinger Equation

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad k \equiv \sqrt{2m_0\left[E - U(x)\right]}/\hbar$$



(1) Define a grid ...

$$-\frac{\hbar^2}{2m_0}\frac{d^2\psi}{dx^2} + U(x)\psi = E\psi$$



Second Derivative on a Finite Mesh

$$\psi(x_0+a)=\psi(x_0)+a\left.\frac{d\psi}{dx}\right|_{x_0=a}+\frac{a^2}{2}\left.\frac{d^2\psi}{dx^2}\right|_{x_0=a}+\ldots$$

$$\psi(x_0-a)=\psi(x_0)-a\left.\frac{d\psi}{dx}\right|_{x_0=a}+\frac{a^2}{2}\left.\frac{d^2\psi}{dx^2}\right|_{x_0=a}-\ldots$$

$$\psi(x_0+a)+\psi(x_0-a)-2\psi(x_0)=a^2\left.\frac{d^2\psi}{dx^2}\right|_{x_0=a}$$

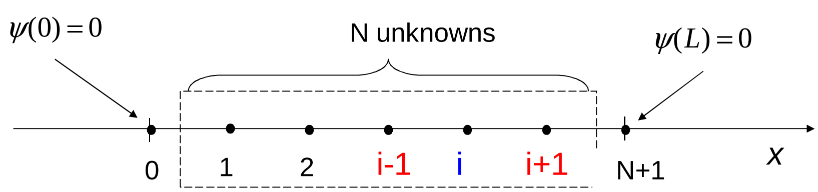
$$\left.\frac{d^2\psi}{dx^2}\right|_i=\frac{\psi_{i-1}-2\psi_i+\psi_{i+1}}{a^2}$$

(2) Express equation in Finite Difference Form

$$-\left(t_0a^2\right)\frac{d^2\psi}{dx^2}+U(x)\psi=E\psi \qquad t_0\equiv\frac{\hbar^2}{2m_0a^2}$$

$$\left.\frac{d^2\psi}{dx^2}\right|_i=\frac{\psi_{i-1}-2\psi_i+\psi_{i+1}}{a^2}$$

$$\left[-t_0\psi_{i-1}+\left(2t_0+U_i\right)\psi_i-t_0\psi_{i+1}\right]=E\psi_i$$



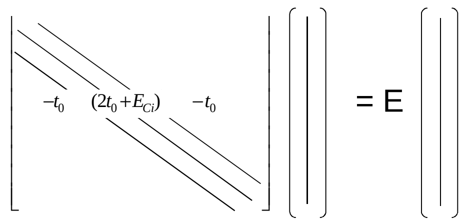
$$\left[-t_0\psi_{i-1} + (2t_0 + E_{Ci})\psi_i - t_0\psi_{i+1}\right] = E\,\psi_i \qquad \text{(i = 2, 3…N-1)}$$

$$\left[-t_0\psi_0 + (2t_0 + E_{Ci})\psi_1 - t_0\psi_2\right] = E\psi_i \qquad \text{(i = 1)}$$

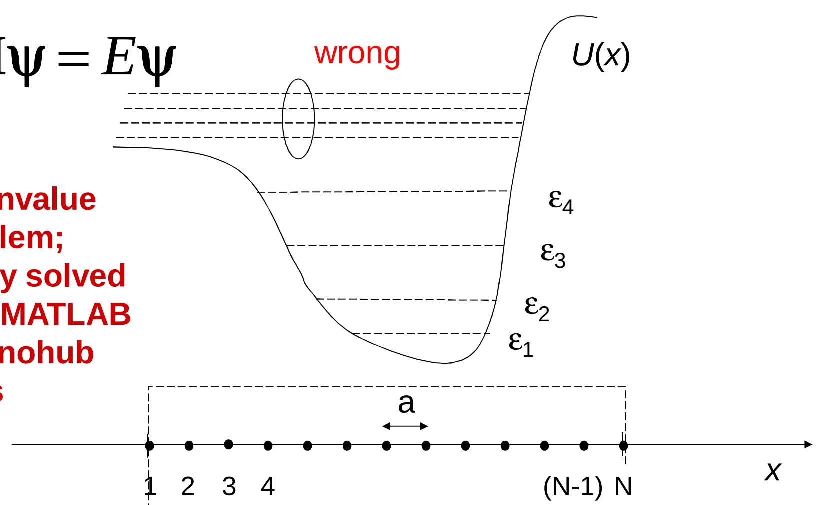
$$\left[-t_0\psi_{N-1} + (2t_0 + E_{Ci})\psi_N - t_0\psi_{N+1}\right] = E\psi_i \qquad \text{(i = N)}$$

$$\mathbf{H}\psi = E\psi$$

N x N N x 1



$$\mathbf{H}\psi = E\psi$$



Eigenvalue problem; easily solved with MATLAB & nanohub tools