First-time User Guide
for Piecewise Constant Potential Barrier Tool

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The tool can simulate quantum mechanical tunneling through one or more barriers, which is otherwise forbidden by classical mechanics.

This tool calculates transmission probability (also called transmission co-efficient) through a set of one or more barriers. The resonance sits between barriers, giving rise to peaks in transmission.
This tool can also locate resonances, which are peaks in the transmission going to a value of one, and can see the formation of bands.
What if You Just Hit “Simulate”? 

You will get the listed plots.
Dips in reflection indicate resonances. Resonances are formed inside regions called “wells” that are surrounded by “barriers”.
Reflection approaches 0 at resonances.

Resonance index
Reducing the barrier height reduces confinement, which makes it easier for electrons to become unbounded. Any higher peak in transmission will result in an unbounded state. When running the simulation, you can use the “potential energy” tab to decrease the barrier height.
Increasing the length of the barrier increases the confinement in the well. Electrons need a higher energy to become unbounded. When running the simulation, you can use the “geometry” tab to make the well wider.
Thicker Barriers

Transmission for thicker barriers

Thicker barrier
Greater confinement in the well
Higher lifetime and sharper resonances

The dotted red line corresponds to default parameters. The blue line corresponds to thicker barriers. When running the simulation, use the “geometry” tab to make the barriers thicker.
Adding an identical well and barrier region splits these resonances. This splitting can be understood in terms of the coupled quantum well picture, where the resonances begin to "talk" to each other.
Band Formation: 1/3

2 barriers, 1 state
Band Formation: 3/3

25 barriers, 24 states
Bulk Band-Structure Plot and Particle in a Box

- 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.

Particle in a box energies

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

\[ n = 1, 2, 3, \ldots \]
Open Systems Versus 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; the particle in a box is a CLOSED system.
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

- The 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.

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

\[ n = 1, 2, 3, \ldots \]
Transfer Matrices : Analytical Solution

\[ Ce^{-\gamma_2 x} + De^{\gamma_2 x} \]

\[ Ge^{-\gamma_4 x} + He^{\gamma_4 x} \]

Barriers have decaying waves

\[ Ae^{ik_1x} + Be^{-ik_1x} \]

Wells have oscillating waves

\[ Ee^{ik_3x} + Fe^{-ik_3x} \]

\[ Ie^{ik_5x} + Ke^{-ik_5x} \]

\[ x = 0 \quad x = a \quad x = a + w \quad x = a + b + w \]

Following this procedure at each boundary we can write…

\[
\begin{bmatrix}
A \\
B
\end{bmatrix} = \begin{bmatrix}
M_1 & M_2 & M_3 \\
& \ddots & \\
& & M_n
\end{bmatrix}\begin{bmatrix}
I \\
K
\end{bmatrix}
\]

Thus transmission and reflectance can be calculated.

Source: Dragica Vasileska  
http://nanohub.org/resources/4829.

Note: Analytical solutions are derived using matrices. If effective, the mass varies and then the boundary conditions change.
The transfer matrix technique assumes a parabolic dispersion.

The tight-binding samples the space at discrete points, which could correspond to atomic locations.

The band structure given by tight-binding deviates from the parabolic assumption.

If the electronic properties vary in one given region, then the tight-binding will give superior results as compared to transfer matrices.
Comparison of Tight-binding and Transfer Matrices

In the transfer matrix method, the total system is broken down into adjacent sub-systems.

In tight-binding, the entire system is treated as a whole.

The peaks for tight-binding will be lower at higher energies because of non-parabolic bands.

More information about tight-binding can be found in the “Additional Resources” section.

• Vasileska, Dragica (2008), "Double Barrier Case," [link](https://nanohub.org/resources/4829).

• Tight Binding:
  • Agarwal, Samarth; Luisier, Mathieu; Jiang, Zhengping; McLennan, Michael; Klimeck, Gerhard (2008), "Resonant Tunneling Diode Simulation with NEGF," DOI: 10254/nanohub-r5237.11. [link](https://nanohub.org/resources/rtdnegf)