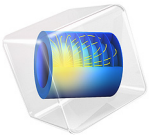


Model created in COMSOL Multiphysics 6.4

# Double Barrier 1D

This tutorial uses a simple 1D model of a double barrier structure to illustrate the essential steps to perform quantum mechanical simulations. Topics discussed include the eigenenergies and time evolution of quasi-bound states, resonant tunneling phenomenon, and transmission versus energy curves. The numerical results agree very well with analytical solutions.

## *Introduction*

The double barrier structure is of interest both because of its pedagogical function as an example to demonstrate the concepts of tunneling and quasi-bound stats to students of quantum mechanics, as well as its practical application in semiconductor devices such as resonant-tunneling diodes (Ref. 1).

To keep the relevance to semiconductor physics without losing generality, the model is assumed to be constructed from layers of GaAs and AlGaAs. The envelope function approximation (Chap. 1, Sec. 1.7 in Ref. 2) can be employed to justify the use of the single-particle Schrödinger equation. Note that not only the electron potential energy, but also the effective mass, is a function of material composition. To properly take care of the discontinuity in the effective mass, the **Schrödinger Equation** physics interface applies the BenDaniel–Duke boundary condition (Chap. 2, Sec. 2.6 in Ref. 2) by default.

## *Model Definition*

The fraction of Al in the AlGaAs material is assumed to be 0.32. The width of the well is assumed to be 10 nm and the width of the barriers 5 nm. The modeled domain has a width of 40 nm.

Four studies are set up to discuss different aspects related to the double barrier structure. First, the eigenenergies are solved for the quasi-bound states using an eigenvalue study, with open boundary conditions for outgoing waves at both ends of the modeling domain. Then, the time evolution of one of the quasi-bound states is solved in a time-dependent study. Next, the resonant tunneling condition is solved in an eigenvalue study, with a special type of open boundary condition for incoming waves on one end of the modeling domain. Finally, the transmission and reflection coefficients are computed using a stationary study, with regular open boundary conditions and a prescribed incoming wave from one end of the modeling domain.

## *Results and Discussion*

Figure 1 summarizes the result for the quasi-bound states: the electron potential energy (black solid line), the real part of the eigenenergies (black dotted line), and the real and imaginary parts of the wave functions shifted vertically to center around their eigenenergies (color solid and dashed curves).

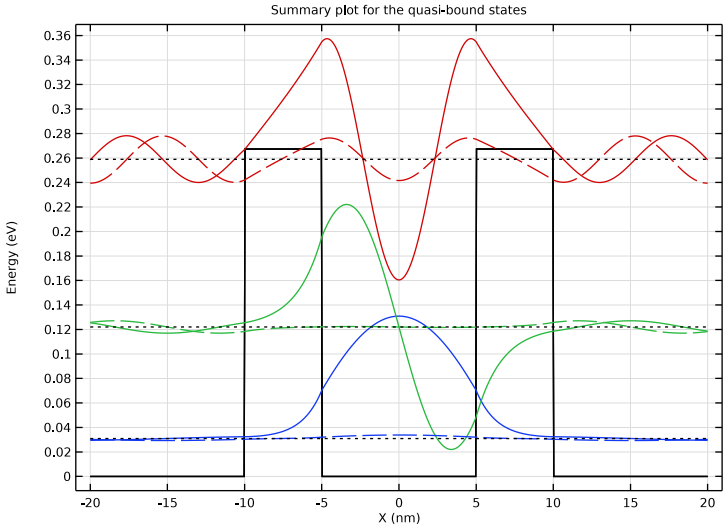



*Figure 1: Summary plot for the quasi-bound states, including the electron potential energy (black solid line), the real part of the eigenenergies (black dotted line), and the real and imaginary parts of the wave functions shifted vertically to center around their eigenenergies (color solid and dashed curves).*

The eigenenergies can be computed analytically using the transfer matrix method (Chap. 2, Sec. 2.10 in Ref. 2). We found that the numerical solution obtained using the eigenvalue study agree with the analytical solution to at least 6 significant digits for both the real and the imaginary part of the eigenenergies.

The time evolution of the quasi-bound states can be explicitly solved using a time-dependent study with one of the quasi-bound states' wave function as the initial condition. The result shows the wave function leaking out of the modeling domain as one would expect. It is best visualized with an animated movie as discussed in the Modeling Instructions below.

The decay of the total probability over time can be plotted as in Figure 2. The computed decay curve matches well with the analytical curve calculated from the imaginary part of the analytical eigenenergy.

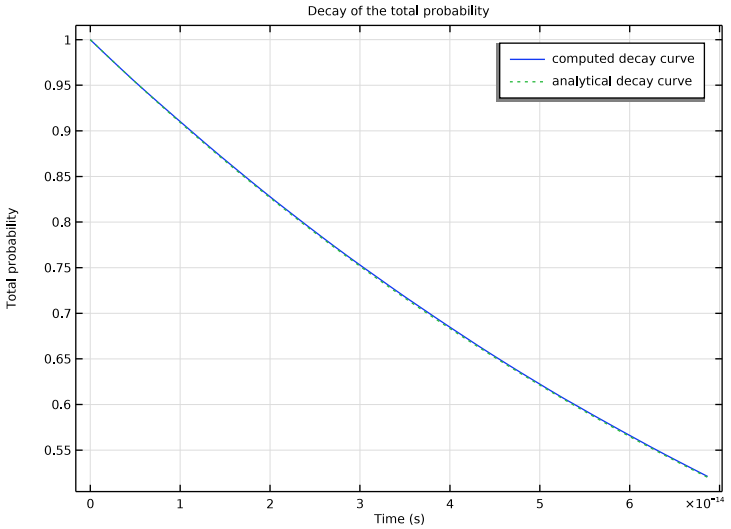



*Figure 2: The computed decay of the total probability over time matches well with the analytical solution.*

Figure 3 shows the summary of the resonant tunneling condition. The wave functions and the eigenenergies closely resemble those of the quasi-bound states, as one would expect. In this symmetric double barrier structure, the transmission is 100% under the resonant

tunneling condition, and the eigenenergies are real valued. The numerical solution agrees with the analytically solution to at least 7 digits for the eigenenergies.

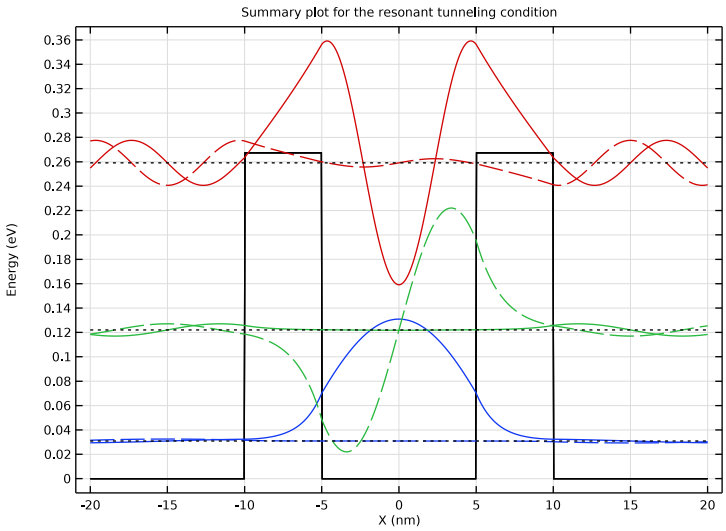



*Figure 3: Summary plot of the resonant tunneling condition.*

The final stationary study solves for the transmission versus energy curve by sweeping the total energy in the stationary Schrödinger equation. Figure 4 summarizes the wave functions for five different energies. The first, third, and fifth one are at resonant tunneling condition, and the wave functions resemble the ones from the previous study as expected.

The second and fourth one are at in-between energies, where the transmission probability is very small and most of the wave function is reflected back to the left-hand side. This is

clearly seen in the large amplitude of the wave function on the left and very small amplitude on the right.

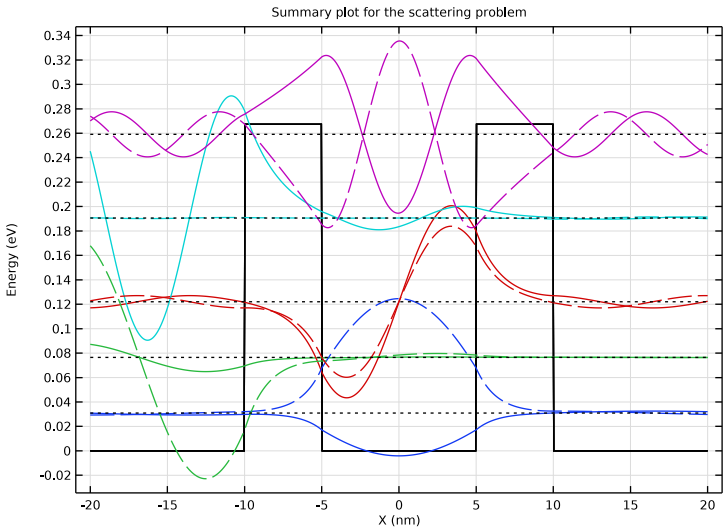



*Figure 4: Stationary study solutions of five selected energies.*

Figure 5 shows the computed transmission and reflection coefficients versus energy in colored curves and the analytical transmission coefficients in red circles. The agreement is very good.

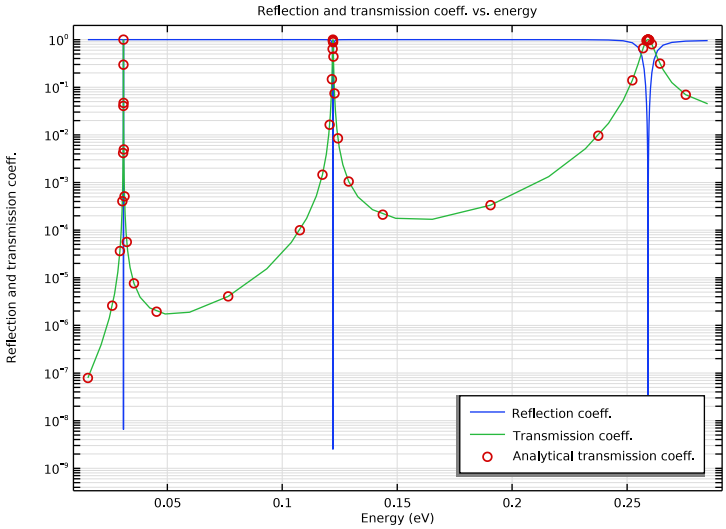



*Figure 5: Transmission curve matches very well with analytical result.*

## *References*

1. S. M. Sze and K. K. Ng, *Physics of Semiconductor Devices*, 3rd ed., John Wiley & Sons, Inc., 2007, Chap. 8, Sec. 8.4.

2. P. Harrison, *Quantum Wells, Wires and Dots*, 3rd ed., John Wiley & Sons, Inc., 2009.

**Application Library path:** `Semiconductor_Module/Verification_Examples/double_barrier_1d`

## *Modeling Instructions*

From the **File** menu, choose **New**.

**NEW**

In the **New** window, click **Model Wizard**.

### MODEL WIZARD

1 In the **Model Wizard** window, click — **1D**.

2 In the **Select Physics** tree, select **Semiconductor** > **Schrödinger Equation (schr)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces** > **Eigenvalue**.

6 Click **Done**.

### GEOMETRY 1

The Model Wizard starts the COMSOL Desktop with the **Geometry** node selected. We can take the chance to set the length unit to a more convenient one.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **nm**.

Now set up some global parameters.

### GLOBAL DEFINITIONS

*Parameters 1*

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `double_barrier_1d_parameters.txt`.

Next draw the geometry for the double barrier structure.

### GEOMETRY 1

*Interval 1 (i1)*

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Geometry 1** and choose **Interval**.

2 In the **Settings** window for **Interval**, locate the **Interval** section.

3 From the **Specify** list, choose **Interval lengths**.

4 In the **Left endpoint** text field, type `-L/2`.

5 In the table, enter the following settings:

| Lengths (nm) |
| --- |
| lw |
| lb |
| L-2*lw-2*lb |
| lb |
| lw |

6 Click **Build All Objects**.

Now we set up the physics. First enter the eigenvalue scale, which has the unit of energy. The eigenvalue returned by the eigenvalue study step is unitless. The eigenenergy is then given by the product of the eigenvalue and the eigenvalue scale.

### SCHRÖDINGER EQUATION (SCHR)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Schrödinger Equation (schr)**.

2 In the **Settings** window for **Schrödinger Equation**, locate the **Model Properties** section.

3 Find the **Eigenvalue study** subsection. In the $\lambda_{scale}$ text field, type `lmbd0`.

Then enter the effective mass and potential energy in the well regions. The selections are default to all domains but we will modify the barrier regions in later steps.

#### *Effective Mass 1*

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Schrödinger Equation (schr)** click **Effective Mass 1**.

2 In the **Settings** window for **Effective Mass**, locate the **Effective Mass** section.

3 In the $\mathbf{m}_{\mathrm{eff,e,11}}$ text field, type `mw`.

#### *Electron Potential Energy 1*

1 In the **Model Builder** window, click **Electron Potential Energy 1**.

2 In the **Settings** window for **Electron Potential Energy**, locate the **Electron Potential Energy** section.

3 From the $V_e$ list, choose **User defined**. In the associated text field, type `0`.

Now we enter the effective mass and potential energy in the barrier regions.

#### *Effective Mass 2*

1 In the **Physics** toolbar, click **Domains** and choose **Effective Mass**.

2 Select Domains 2 and 4 only.

3 In the **Settings** window for **Effective Mass**, locate the **Effective Mass** section.

4 In the $\mathbf{m}_{\text{eff},e,11}$ text field, type `mb`.

Note the red triangle appearing on the **Effective Mass 1** node where we set the effective mass in the well regions to all domains in an earlier step. This red triangle indicates that some selections in that node (**Effective Mass 1**) are overridden by the current node (**Effective Mass 2**).

We can see this by clicking on the **Effective Mass 1** node and observe that domains 2 and 4 in the selection box are now appended with "(overridden)".

*Effective Mass 1*

Also note the red triangle appearing on the **Effective Mass 2** node, indicating the source of the overriding feature.

*Electron Potential Energy 2*

1 In the **Physics** toolbar, click **Domains** and choose **Electron Potential Energy**.

2 Select Domains 2 and 4 only.

3 In the **Settings** window for **Electron Potential Energy**, locate the **Electron Potential Energy** section.

4 From the $V_e$ list, choose **User defined**. In the associated text field, type `Vb`.

Note the orange circle now appearing on the **Electron Potential Energy 1** node, indicating that the potential energy entered at the current node will be added to that node. This is called a "contributing" feature in COMSOL. In brief, an "overriding" feature (such as the **Effective Mass** node) replaces the value of the physical quantity being entered, and a "contributing" feature (such as the **Electron Potential Energy** node) adds to the value of the physical quantity being entered. Thanks to the "contributing" nature of the **Electron Potential Energy** node, a complicated potential profile can be conveniently built by using multiple nodes with overlapping selections.

For quasi-bound states, we look for solutions with wave functions leaking out of the modeling domain without reflection back from the end points of the modeling domain. This is done by using the **Open Boundary** condition.

*Open Boundary 1*

1 In the **Physics** toolbar, click **Boundaries** and choose **Open Boundary**.

2 In the **Settings** window for **Open Boundary**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **All boundaries**.

This boundary condition only applies to exterior boundaries, so we just selected "All boundaries" for convenience.

For verification purposes, we set up a fine mesh for better accuracy in the solution.

### MESH 1

*Edge 1*

In the **Mesh** toolbar, click  **Edge**.

*Distribution 1*

1 Right-click **Edge 1** and choose **Distribution**.

2 In the **Settings** window for **Distribution**, locate the **Distribution** section.

3 In the **Number of elements** text field, type `50`.

Now we set up the eigenvalue study. The **Open Boundary** condition introduces nonlinearity in the eigenvalue problem. This usually requires an iterative process, where the solution from a previous eigenvalue study step is entered as the linearization point for the next iteration, until the eigenvalue is converged. Here we take a shortcut by feeding the analytical solution as the linearization point.

### STUDY 1

*Step 1: Eigenvalue*

1 In the **Model Builder** window, under **Study 1** click **Step 1: Eigenvalue**.

2 In the **Settings** window for **Eigenvalue**, locate the **Study Settings** section.

3 In the **Desired number of eigenvalues** text field, type `1`.

4 In the **Search for eigenvalues around shift** text field, type `reE_anal/lmbd0`.

As mentioned earlier, the eigenenergy is given by the product of the eigenvalue and the eigenvalue scale. So here the analytical eigenenergy is divided by the eigenvalue scale to obtain the guess for the eigenvalue.

Show default solver to access the setting for the linearization point.

5 In the **Model Builder** window, click **Study 1**.

6 In the **Settings** window for **Study**, type `Study 1 Quasi-bound states` in the **Label** text field.

*Solution 1 (sol1)*

1 In the **Study** toolbar, click  **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Eigenvalue Solver 1**.

3 In the **Settings** window for **Eigenvalue Solver**, locate the **General** section.

4 Find the **Eigenvalue linearization point** subsection. In the **Value of eigenvalue linearization point** text field, type `reE_anal/1mbd0`.

Use a parametric sweep to solve for all three quasi-bound states in a sequence.

*Parametric Sweep*

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add** twice.

4 In the table, enter the following settings:

| Parameter name | Parameter value list | Parameter unit |
|---|---|---|
| reE_anal (Sweeping parameter for quasi-bound states) | `reE1anal reE2anal reE3anal` | J |
| imE_anal (Sweeping parameter for quasi-bound states) | `imE1anal imE2anal imE3anal` | J |

The parameter imE_anal is not used in the solution process. The purpose of including it in the parametric sweep is to easily compare with the analytical solution once the numerical solution is obtained.

5 In the **Study** toolbar, click **Compute**.

## RESULTS

*Normalized Wave Function (schr)*

The modeling result for the quasi-bound states is summarized in the 1D plot group **Potential Energy, Eigenenergy, and Wave Function**.

*Quasi-bound state summary plot*

1 In the **Model Builder** window, under **Results** click **Potential Energy, Eigenenergy, and Wave Function (schr)**.

2 In the **Settings** window for **1D Plot Group**, type `Quasi-bound state summary plot` in the **Label** text field.

3 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Summary plot for the quasi-bound states`.

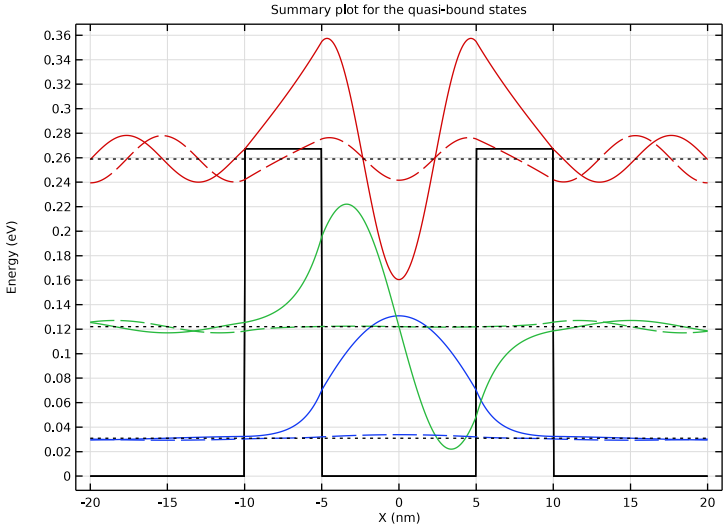
5 Locate the **Plot Settings** section.

6 Select the **x-axis label** checkbox. In the associated text field, type `X (nm)`.

7 Select the **y-axis label** checkbox. In the associated text field, type `Energy (eV)`.

8 Locate the **Legend** section. Clear the **Show legends** checkbox.

9 In the **Quasi-bound state summary plot** toolbar, click **Plot**.




We can also perform some global evaluations to compare the result with analytical solutions.

*Eigenvalue*

1 In the **Model Builder** window, expand the **Results** > **Derived Values** node, then click **Eigenvalue**.

2 In the **Settings** window for **Global Evaluation**, locate the **Expressions** section.

3 In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| `real(schr.Ei)/reE_anal-1` | 1 | `error of real part` |
| `imag(schr.Ei)/imE_anal-1` | 1 | `error of imaginary part` |

4 Click **Evaluate**.

### TABLE 1

1 Go to the **Table 1** window.

We see that both the real and the imaginary part of the eigenenergy agree with the analytical solution to 6 or more significant digits.

The wave functions of the quasi-bound states leak out of the double-barrier quantum well over time, and the probability density diminishes correspondingly. We can see this behavior explicitly by running a transient study. Add a time-dependent study with the initial condition set to the normalized wave function of the third quasi-bound state.

### ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies** > **Time Dependent**.

4 Click the **Add Study** button in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

### STUDY 2

*Step 1: Time Dependent*

1 In the **Settings** window for **Time Dependent**, click to expand the **Values of Dependent Variables** section.

2 Find the **Initial values of variables solved for** subsection. From the **Settings** list, choose **User controlled**.

3 From the **Study** list, choose **Study 1 Quasi-bound states, Eigenvalue**.

4 In the **Model Builder** window, click **Study 2**.

5 In the **Settings** window for **Study**, type `Study 2 Time evolution of the 3rd quasi-bound state` in the **Label** text field.

### SCHRÖDINGER EQUATION (SCHR)

*Initial Values 2 for time dependent study*

1 In the **Physics** toolbar, click **Domains** and choose **Initial Values**.

2 In the **Settings** window for **Initial Values**, type `Initial Values 2 for time dependent study` in the **Label** text field.

3 Locate the **Domain Selection** section. From the **Selection** list, choose **All domains**.

4 Locate the **Initial Values** section. In the *psi* text field, type `schr.Psi`.

The periodic cycle time `T3` and the decay time constant `tau3` for the 3rd quasi-bound state have been computed in the global parameters table. Set up the time steps accordingly, so that the time increment is small enough to show the oscillatory behavior of the wave function and the total simulation time is long enough to show the decay of the quasi-bound state.

## STUDY 2 TIME EVOLUTION OF THE 3RD QUASI-BOUND STATE

### *Step 1: Time Dependent*

1 In the **Model Builder** window, under **Study 2 Time evolution of the 3rd quasi-bound state** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

3 In the **Output times** text field, type `range(0,T3/10,tau3/3)`.

4 In the **Study** toolbar, click **Compute**.

## RESULTS

### *Wave Function (schr)*

The time evolution of the wave function and the probability density can be easily shown with COMSOL's animation functionality.

### *Animation 1*

1 In the **Wave Function (schr)** toolbar, click **Animation** and choose **Player**.

2 In the **Settings** window for **Animation**, locate the **Frames** section.

3 From the **Frame selection** list, choose **All**.

4 Click the **Play** button in the **Graphics** toolbar.

The outward propagating (leaking) of the wave function is clearly seen in the animation.

### *Animation 2*

1 Right-click **Animation 1** and choose **Duplicate**.

2 In the **Settings** window for **Animation**, locate the **Scene** section.

3 From the **Subject** list, choose **Probability Density (schr) 1**.

4 Click the **Play** button in the **Graphics** toolbar.

The decay of the probability density is also clearly seen in the animation.

We can also compare the decay of the total probability using a global plot. First remove some default plots to shorten the list of plot nodes in the Model Builder tree.

*Potential Energy (schr) 1*

In the **Model Builder** window, under **Results** right-click **Potential Energy (schr) 1** and choose **Delete**.

*Effective Mass (schr) 1*

Right-click **Effective Mass (schr) 1** and choose **Delete**.

*Compare decay of total probability*

1. In the **Results** toolbar, click **1D Plot Group**.
2. In the **Settings** window for **1D Plot Group**, type `Compare decay of total probability` in the **Label** text field.
3. Locate the **Data** section. From the **Dataset** list, choose **Study 2 Time evolution of the 3rd quasi-bound state/Solution 6 (sol6)**.
4. Locate the **Title** section. From the **Title type** list, choose **Manual**.
5. In the **Title** text area, type `Decay of the total probability`.
6. Locate the **Plot Settings** section.
7. Select the **y-axis label** checkbox. In the associated text field, type `Total probability`.

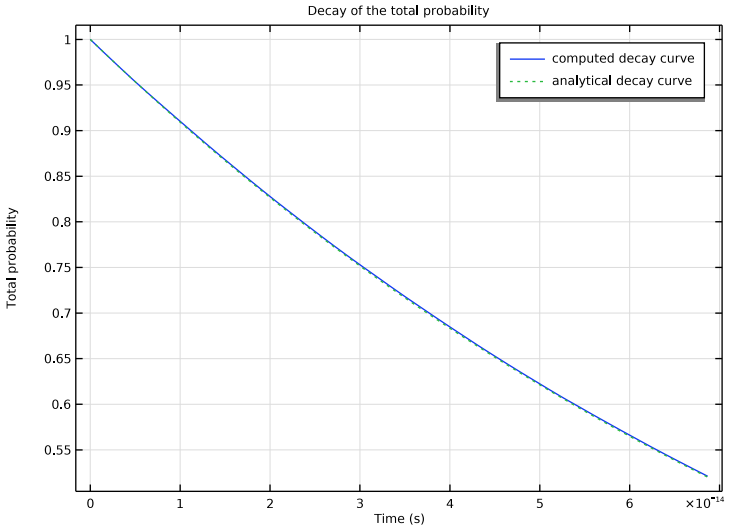
*Global 1*

1. Right-click **Compare decay of total probability** and choose **Global**.
2. In the **Settings** window for **Global**, locate the **y-Axis Data** section.
3. In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| `schr.int(schr.Pr)` | `1` | `computed decay curve` |
| `exp(-t/tau3)^2` | | `analytical decay curve` |

4. Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Cycle**.

5 In the **Compare decay of total probability** toolbar, click **Plot**.




In the next study, we look for the resonant tunneling solution. Unlike the quasi-bound states, where the wave function propagates outward on both open boundaries, for the resonant tunneling condition, the wave function propagates inward from one boundary and goes out of the other boundary. We will modify the boundary condition accordingly by overriding the left open boundary condition.

## SCHRÖDINGER EQUATION (SCHR)

*Open Boundary 2 for resonant tunneling study*

1 In the **Physics** toolbar, click **Boundaries** and choose **Open Boundary**.

2 In the **Settings** window for **Open Boundary**, type `Open Boundary 2 for resonant tunneling study` in the **Label** text field.

3 Select Boundary 1 only.

To reverse the wave function propagation direction across the open boundary, first turn on Advanced Physics Options, since this option is rarely used and normally hidden.

4 Click the **Show More Options** button in the **Model Builder** toolbar.

5 In the **Show More Options** dialog, in the tree, select the checkbox for the node **Physics** > **Advanced Physics Options**.

6 Click **OK**.

Now we can change the propagation direction.

7 In the **Settings** window for **Open Boundary**, click to expand the **Open Boundary Type** section.

8 From the list, choose **Incoming**.

Set up an eigenvalue study to solve for the resonant tunneling energies, following a procedure similar to the one for Study 1.

### ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **Preset Studies for Selected Physics Interfaces** > **Eigenvalue**.

4 Click the **Add Study** button in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

### STUDY 3

*Step 1: Eigenvalue*

1 In the **Settings** window for **Eigenvalue**, locate the **Study Settings** section.

2 In the **Desired number of eigenvalues** text field, type `1`.

3 In the **Search for eigenvalues around shift** text field, type `E_anal/1mbd0`.

4 Locate the **Physics and Variables Selection** section. Select the **Modify model configuration for study step** checkbox.

5 In the tree, select **Component 1 (comp1)** > **Schrödinger Equation (schr)** > **Initial Values 2 for time dependent study**.

6 Click **Disable**.

7 In the **Model Builder** window, click **Study 3**.

8 In the **Settings** window for **Study**, type `Study 3 Resonant tunneling` in the **Label** text field.

*Solution 7 (sol7)*

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 7 (sol7)** node, then click **Eigenvalue Solver 1**.

3 In the **Settings** window for **Eigenvalue Solver**, locate the **General** section.

4 Find the **Eigenvalue linearization point** subsection. In the **Value of eigenvalue linearization point** text field, type `E_anal/1mbd0`.

*Parametric Sweep*

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

| Parameter name | Parameter value list | Parameter unit |
|---|---|---|
| E_anal (Sweeping parameter for transmission=1 solutions) | `E1anal E2anal E3anal` | J |

5 In the **Study** toolbar, click **Compute**.

## RESULTS

*Normalized Wave Function (schr) 1*

Remove some default plots and examine the main summary plot.

1 Right-click **Results** > **Normalized Wave Function (schr) 1** and choose **Delete**.

*Effective Mass (schr) 1, Potential Energy (schr) 1, Probability Density (schr) 2*

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Probability Density (schr) 2**, **Potential Energy (schr) 1**, and **Effective Mass (schr) 1**.

2 Right-click and choose **Delete**.

*Resonant tunneling summary plot*

1 In the **Model Builder** window, under **Results** click **Potential Energy, Eigenenergy, and Wave Function (schr)**.

2 In the **Settings** window for **1D Plot Group**, type `Resonant tunneling summary plot` in the **Label** text field.

3 Locate the **Title** section. From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Summary plot for the resonant tunneling condition`.

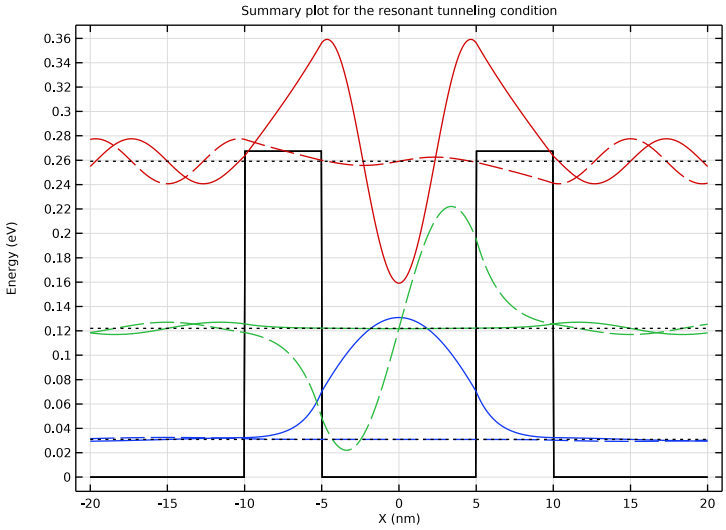
5 Locate the **Plot Settings** section.

6 Select the **x-axis label** checkbox. In the associated text field, type `X (nm)`.

7 Select the **y-axis label** checkbox. In the associated text field, type `Energy (eV)`.

8 Locate the **Legend** section. Clear the **Show legends** checkbox.

9 In the **Resonant tunneling summary plot** toolbar, click **Plot**.




As in the case of quasi-bound states, here we can also perform some global evaluations to compare the result with analytical solutions.

*Eigenvalue 1*

1 In the **Model Builder** window, under **Results** > **Derived Values** click **Eigenvalue 1**.

2 In the **Settings** window for **Global Evaluation**, locate the **Expressions** section.

3 In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| `real(schr.Ei)/E_anal-1` | 1 | `error of real part` |
| `imag(schr.Ei)/E_anal` | 1 | `error of imaginary part (exact imaginary part is zero)` |

4 Click **Evaluate**.

**TABLE 2**

1 Go to the **Table 2** window.

We see that the real part of the eigenenergy agrees with the analytical solution to 7 or more significant digits. The imaginary part is essentially zero within numerical precision, as one would expect from the fact that the exact solution is real valued.

The resonant tunneling condition discussed above are at specific energies with 100% transmission of the incoming wave function through the double barrier. To obtain the general curve of the transmission versus the energy, we solve the Schrödinger equation using a stationary study. First parameterize the energy of the incoming wave function.

### SCHRÖDINGER EQUATION (SCHR)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Schrödinger Equation (schr)**.

2 In the **Settings** window for **Schrödinger Equation**, locate the **Model Properties** section.

3 Find the **Stationary study** subsection. In the $E$ text field, type `E0`.

Then set up an ordinary open boundary condition (outgoing type by default). Add an incoming wave with a given amplitude `psi0`.

*Open Boundary 3 for transmission vs. energy study*

1 In the **Physics** toolbar, click **Boundaries** and choose **Open Boundary**.

2 In the **Settings** window for **Open Boundary**, type `Open Boundary 3 for transmission vs. energy study` in the **Label** text field.

3 Select Boundary 1 only.

4 Locate the **Open Boundary** section. Select the **Incoming wave** checkbox.

5 In the $\psi_0$ text field, type `psi0`.

Now set up a stationary study with an auxiliary sweep over the energy parameter E0. The list of values for E0 is chosen to capture the very sharp peaks in transmission around the resonant tunneling energies.

### ADD STUDY

1 In the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies** > **Stationary**.

4 Click the **Add Study** button in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

### STUDY 4

*Step 1: Stationary*

1 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

2 Select the **Modify model configuration for study step** checkbox.

3 In the tree, select **Component 1 (comp1)** > **Schrödinger Equation (schr)** > **Initial Values 2 for time dependent study**.

4 Click **Disable**.

5 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.

6 Click **Add**.

7 In the table, enter the following settings:

| Parameter name | Parameter value list | Parameter unit |
|---|---|---|
| E0 (Energy for stationary study) | `E1anal*(1-0.5*10^range(0,-0.2,-3)) E1anal E1anal+0.5*(E2anal-E1anal)*10^range(-3,0.2,-0.1) E2anal-0.5*(E2anal-E1anal)*10^range(0,-0.2,-3) E2anal E2anal+0.5*(E3anal-E2anal)*10^range(-3,0.2,-0.1) E3anal-0.5*(E3anal-E2anal)*10^range(0,-0.2,-3) E3anal E3anal*(1+0.1*10^range(-3,0.2,0))` | J |

8 In the **Model Builder** window, click **Study 4**.

9 In the **Settings** window for **Study**, type `Study 4 Transmission vs. energy` in the **Label** text field.

10 In the **Study** toolbar, click **Compute**.

## RESULTS

### *Wave Function (schr) 1*

Delete some default plots and examine the main summary plot at a few different energies.

1 Right-click **Results** > **Wave Function (schr) 1** and choose **Delete**.

### *Effective Mass (schr) 1, Potential Energy (schr) 1, Probability Density (schr) 2*

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **Probability Density (schr) 2**, **Potential Energy (schr) 1**, and **Effective Mass (schr) 1**.

2 Right-click and choose **Delete**.

*Transmission summary plot*

1 In the **Model Builder** window, under **Results** click **Potential Energy, Energy, and Wave Function (schr)**.

2 In the **Settings** window for **1D Plot Group**, type `Transmission summary plot` in the **Label** text field.

3 Locate the **Data** section. From the **Parameter selection (E0)** list, choose **Manual**.

4 In the **Parameter indices (1-97)** text field, type `17 33 49 65 81`.

5 Locate the **Title** section. From the **Title type** list, choose **Manual**.

6 In the **Title** text area, type `Summary plot for the scattering problem`.

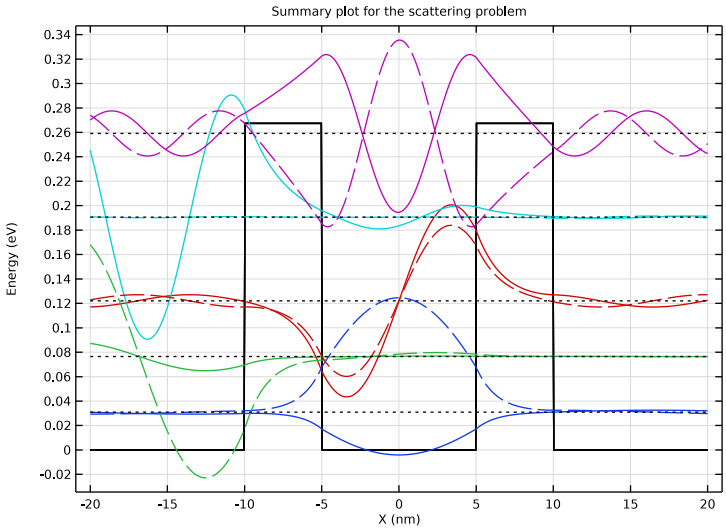
7 Locate the **Plot Settings** section.

8 Select the **x-axis label** checkbox. In the associated text field, type `X (nm)`.

9 Select the **y-axis label** checkbox. In the associated text field, type `Energy (eV)`.

10 Locate the **Legend** section. Clear the **Show legends** checkbox.

11 In the **Transmission summary plot** toolbar, click **Plot**.




The first, third, and last plotted energies are chosen to be the three resonant tunneling energies. It can be seen that the wave functions at these energies resemble the eigenfunctions from the previous study, which they should. The second and fourth plotted energies are between the resonant tunneling energies. From the profiles of the wave functions it can be seen that the transmission coefficient is very small at these energies.

We can also plot the transmission and reflection coefficients as functions of the energy, and compare with analytical results.

*Reflection & Transmission vs. Energy*

1 In the **Results** toolbar, click **1D Plot Group**.

2 In the **Settings** window for **1D Plot Group**, type `Reflection & Transmission vs. Energy` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 4 Transmission vs. energy/ Solution 12 (sol12)**.

*Global 1*

1 Right-click **Reflection & Transmission vs. Energy** and choose **Global**.

2 In the **Settings** window for **Global**, locate the **y-Axis Data** section.

3 In the table, enter the following settings:

| Expression | Unit | Description |
|---|---|---|
| `abs(schr.open3.int(psi/schr.psiI)-1)^2` | 1 | `Reflection coeff.` |
| `abs(schr.open1.int(psi)/psi0)^2` | 1 | `Transmission coeff.` |

4 Locate the **x-Axis Data** section. From the **Unit** list, choose **eV**.

5 In the **Reflection & Transmission vs. Energy** toolbar, click **Plot**.

6 Click the **y-Axis Log Scale** button in the **Graphics** toolbar.

*Reflection & Transmission vs. Energy*

1 In the **Model Builder** window, click **Reflection & Transmission vs. Energy**.

2 In the **Settings** window for **1D Plot Group**, locate the **Title** section.

3 From the **Title type** list, choose **Manual**.

4 In the **Title** text area, type `Reflection and transmission coeff. vs. energy`.

5 Locate the **Plot Settings** section.

6 Select the **x-axis label** checkbox. In the associated text field, type `Energy (eV)`.

7 Select the **y-axis label** checkbox. In the associated text field, type `Reflection and transmission coeff.`.

8 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

The very sharp peaks in transmission corresponding to the resonant tunneling condition are clearly seen in the plot.

Now import the analytical transmission coefficients and plot them on the same graph to compare with the numerical results.

*Analytical transmission coefficients*

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `Analytical transmission coefficients` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

4 Browse to the model's Application Libraries folder and double-click the file `double_barrier_1d_anal.csv`.

5 Locate the **Column Headers** section. In the table, enter the following settings:

| Column | Header |
|---|---|
| 1 | `E0 (eV)` |
| 2 | `Analytical transmission coeff.` |

### ANALYTICAL TRANSMISSION COEFFICIENTS

1 Go to the **Analytical transmission coefficients** window.

2 Click the **Table Graph** button in the window toolbar.

### RESULTS

*Table Graph 1*

Right-click **Results** > **1D Plot Group 14** > **Table Graph 1** and choose **Copy**.

*Table Graph 1*

In the **Model Builder** window, right-click **Reflection & Transmission vs. Energy** and choose **Paste Table Graph**.

*1D Plot Group 14*

In the **Model Builder** window, under **Results** right-click **1D Plot Group 14** and choose **Delete**.

*Table Graph 1*

1 In the **Model Builder** window, under **Results** > **Reflection & Transmission vs. Energy** click **Table Graph 1**.

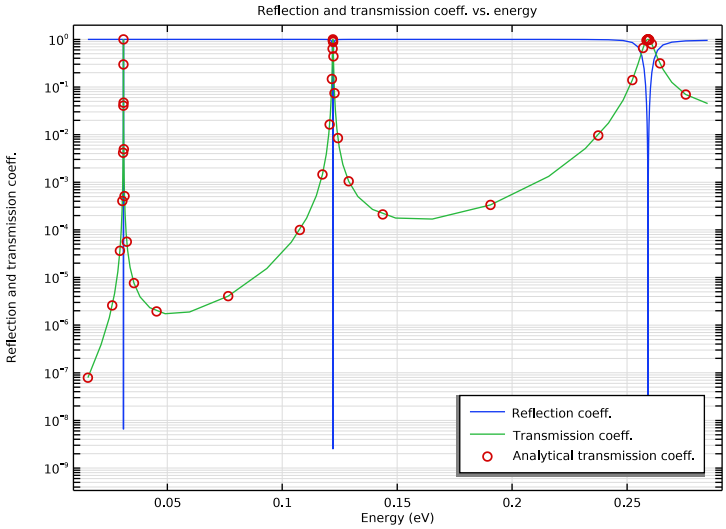
2 In the **Settings** window for **Table Graph**, locate the **Coloring and Style** section.

3 Find the **Line style** subsection. From the **Line** list, choose **None**.

4 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

5 Click to expand the **Legends** section. Select the **Show legends** checkbox.

6 In the **Reflection & Transmission vs. Energy** toolbar, click **Plot**.




It can be seen that the numerical and analytical transmission coefficients match very well.

This tutorial has been built incrementally, with new boundary and/or domain conditions added for subsequent studies. Therefore at this point if we try to solve one of the previous studies, it may not solve or may not give the correct answer, due to the change in boundary and/or domain conditions. This can be fixed by disabling the unwanted new boundary and/or domain conditions in each previous study step.

## STUDY 1 QUASI-BOUND STATES

### *Step 1: Eigenvalue*

1 In the **Model Builder** window, under **Study 1 Quasi-bound states** click **Step 1: Eigenvalue**.

2 In the **Settings** window for **Eigenvalue**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** checkbox.

4 In the tree, select **Component 1 (comp1)** > **Schrödinger Equation (schr)** > **Initial Values 2 for time dependent study**.

5 Click **Disable**.

6 In the tree, select **Component 1 (comp1)** > **Schrödinger Equation (schr)** > **Open Boundary 2 for resonant tunneling study**.

7 Click **Disable**.

8 In the tree, select **Component 1 (comp1)** > **Schrödinger Equation (schr)** > **Open Boundary 3 for transmission vs. energy study**.

9 Click **Disable**.

### STUDY 2 TIME EVOLUTION OF THE 3RD QUASI-BOUND STATE

*Step 1: Time Dependent*

1 In the **Model Builder** window, under **Study 2 Time evolution of the 3rd quasi-bound state** click **Step 1: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** checkbox.

4 In the tree, select **Component 1 (comp1)** > **Schrödinger Equation (schr)** > **Open Boundary 2 for resonant tunneling study**.

5 Click **Disable**.

6 In the tree, select **Component 1 (comp1)** > **Schrödinger Equation (schr)** > **Open Boundary 3 for transmission vs. energy study**.

7 Click **Disable**.

### STUDY 3 RESONANT TUNNELING

*Step 1: Eigenvalue*

1 In the **Model Builder** window, under **Study 3 Resonant tunneling** click **Step 1: Eigenvalue**.

2 In the **Settings** window for **Eigenvalue**, locate the **Physics and Variables Selection** section.

3 In the tree, select **Component 1 (comp1)** > **Schrödinger Equation (schr)** > **Open Boundary 3 for transmission vs. energy study**.

4 Click **Disable**.