

11. Scattering from a Barrier

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As a final topic in one-dimensional wave mechanics, let us now consider what happens when a wavepacket, freely traveling at first, hits a localized potential energy barrier of some sort. After the wavepacket hits the barrier, we would expect some of it to reflect and some to be transmitted, in analogy to light hitting a pane of glass. The “Barrier Scattering” web application (linked from our course web page) simulates and animates this process.

That simulation uses the simplest (but most computationally intensive) possible method: brute-force integration of the time-dependent Schrödinger equation. It discretizes the x axis into 720 points, storing the real and imaginary parts of ψ in separate arrays. It calculates $d^2\psi/dx^2$ at each point by comparing the value there to the two neighboring values, and then incorporates the value of $V(x)$ into a calculation of the amount by which $\psi(x)$ changes during each discrete time step. You can see the details if you look at the code using your browser’s View Source or Page Source command (usually hidden in a Developer section of the menus). Most of the physics is in the `doStep` function.

Note that because the simulation starts with a *wavepacket*, the energy of the incoming quantum particle is not precisely defined. Technically that’s always true in the real world, but real-world wavepackets are often much wider in space, and hence narrower in momentum space and energy resolution, than in the simulation.

The more common approach to analyzing barrier scattering is therefore to take the limit where the wavepackets become perfect sinusoidal waves, $e^{ipx/\hbar}$, where p is positive for a right-moving wave and negative for a left-moving wave. These waves fill all of space and their probability densities don’t change with time, so the “scattering” becomes a steady-state process that’s harder to visualize. But the approach is entirely analogous to the way we analyze reflection and transmission of monochromatic light in optics.

In the sinusoidal-wave limit, the wavefunctions are simple sinusoidal functions wherever $V(x) = 0$. But inside the barrier they can be quite different, depending on the barrier’s potential energy function $V(x)$. Because these wavefunctions now have well-defined energy, however, we can find them by solving the time-*independent* Schrödinger equation.

I’ll illustrate the approach for an incident wave of energy E that comes in from the left. Then, to the left of the barrier, the total wavefunction should be a superposition of the incident and reflected waves:

$$\psi_{\text{left}}(x) = Ae^{ikx} + Be^{-ikx}, \quad (1)$$

where $k = \sqrt{2mE}/\hbar$ and the amplitudes A and B are complex numbers (that is, they can incorporate phase shifts of the form $e^{i\phi}$). Meanwhile, to the right of the

barrier, we should have only a right-moving transmitted wave:

$$\psi_{\text{right}}(x) = F e^{ikx}, \quad (2)$$

for the same k and some complex amplitude F . (My notation follows that of Griffiths, 2nd edition, page 81.)

Inside the barrier, the wavefunction is still unknown. But because the entire wavefunction has well-defined energy, it must be a solution of the TISE. Our job, therefore, is to find a solution of the TISE that matches equations 1 and 2, and thus to determine the relationships between the amplitudes A , B , and F . The square moduli of these amplitudes are proportional to the corresponding probability densities, so the probabilities of reflection and transmission are given, respectively, by the ratios

$$R = \frac{|B|^2}{|A|^2} \quad \text{and} \quad T = \frac{|F|^2}{|A|^2}. \quad (3)$$

Conservation of probability requires $T + R = 1$.

And how do we actually find the desired solution of the TISE? As usual, we can either do it numerically (for essentially any barrier potential function $V(x)$), or analytically (for idealized special cases).

The numerical approach is to start with boundary conditions on the right of the barrier, using equation 2 with an arbitrary value of F (for example, $F = 1$). Then it is straightforward for a computer to integrate the TISE leftward, through the barrier and beyond. (Since E is specified from the start, and any positive E is allowed, there is no hunting for eigenvalues as there is when you're trying to find bound states.) To the left of the barrier, the solution should match equation 1 for some complex coefficients A and B . The logic for determining these coefficients from the numerical data requires a bit of thought, but otherwise the process is extremely straightforward. Once A and B are known, the reflection and transmission probabilities are given by equations 3.

The analytic approach is feasible only for reasonably simple barrier shapes, and is simplest when the barrier potential is constant: $V(x) = V_0$. Then, if $V_0 < E$, the wavefunction inside the barrier must also be sinusoidal; we could write it as a superposition of complex exponentials, or alternatively (following Griffiths), we can express it as a superposition of a sine and a cosine:

$$\psi_{\text{inside}}(x) = C \sin(lx) + D \cos(lx) \quad \text{for } V_0 < E, \quad (4)$$

where $l = \sqrt{2m(E - V_0)}/\hbar$ is the wavenumber inside the barrier and the amplitudes C and D can again be complex. We've now solved the TISE everywhere except at the two boundaries, where $V(x)$ is discontinuous. At those points, the TISE simply requires that both the wavefunction $\psi(x)$ and its derivative $d\psi/dx$ be continuous; otherwise the second derivative, $d^2\psi/dx^2$, would be infinite. So, for example, we can set equations 2 and 4 equal when we evaluate both of them at the right edge

of the barrier, and we can also set their derivatives equal at that point, and these two equations allow us to solve for C and D in terms of F . Then we similarly set equations 1 and 4 equal at the left edge of the barrier, to relate A and B to F and to each other. The results are quite interesting, with certain special “resonant” energies where the transmission probability is 100% (see Griffiths for details).

In the case of a constant barrier potential that is *greater* than E , the solution inside the barrier is instead exponential:

$$\psi_{\text{inside}}(x) = Ce^{lx} + De^{-lx} \quad \text{for } V_0 > E, \quad (5)$$

where now $l = \sqrt{2m(V_0 - E)}/\hbar$. The procedure and the logic, however, are otherwise the same. As you might guess, the exponential behavior can make the transmitted wave negligible, in comparison to the incident wave, when the barrier is sufficiently wide or “high.” But for “low” and narrow barriers, the probability of transmission (also called *tunneling* in this case) can be significant.