Lecture 18:
Scattering from a Step Potential

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In this section, we are going to consider the problem of scattering of a particle from a step potential of height $V_0$. The complication here is that, physically, we want to start with incoming particles with well-defined position and momentum, send them into the barrier to interact, and calculate the outgoing particle state. But such initial and final states are not eigenstates of the Hamiltonian. So we will first solve for the eigenstates and then construct a wave-packet initial state, similar to what we did for the free particle.

We do things in a somewhat different order than Shankar, but the basic ideas are the same. Shankar begins with wave packets, which can be confusing since he a) has to fudge some things (e.g., the packet width must be small compared to its initial distance from the step but large enough that the packet does not spread during the time it takes to reach the step) and b) considering the wave packet first violates our normal procedure of writing the Hamiltonian and finding the eigenstates first.
Scattering from a Step Potential: Basic Solution (cont.)

Setting up the Hamiltonian

We consider a potential

\[ V(x) = \begin{cases} 
0 & x < 0 \\
V_0 & x \geq 0 
\end{cases} \]  \hspace{1cm} (5.46)

We assume \( V_0 \geq 0 \) without lack of generality: if \( V_0 < 0 \), then one can reverse the \( x \)-axis to make the step orientation the same and adjust the solutions accordingly. The Hamiltonian is of course

\[ H = \frac{p^2}{2m} + V(X) \]

As we did for the particle in a box, we assume the existence of an eigenstate of \( H \) of energy \( E \), denoted by \( |\psi_E\rangle \). The eigenvalue equation for \( H \) is identical in form to the one we wrote for the particle in a box except for the specific form of \( V(x) \):

\[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_{E,x}(x) + V(x) \psi_{E,x}(x) = E \psi_{E,x}(x) \]
Solving for the Eigenstates, $E > V_0$

The stepwise nature of the potential suggests that we should solve the equation separately in the two regions: region I, $x < 0$; and region II, $x \geq 0$. In each region, the potential is constant, leading us to write the usual complex exponential form for the solution:

$$\psi^I_E, x(x) = A e^{i k_1 x} + B e^{-i k_1 x} \quad k_1 = \sqrt{\frac{2m}{\hbar^2} E}$$

$$\psi^{II}_E, x(x) = C e^{i k_2 x} + D e^{-i k_2 x} \quad k_2 = \sqrt{\frac{2m}{\hbar^2} (E - V_0)}$$

We restrict $k_1 \geq 0$ and $k_2 \geq 0$ because the sign-flip freedom in $k_1$ and $k_2$ is already allowed by having the two conjugate complex exponentials in each solution.

Since $H$ is Hermitian, we are assured $E$ is real and thus $k_1$ and $k_2$ are pure real or pure imaginary. Recall, though, that for $H$ to be Hermitian, we need $P$ to be Hermitian. When we consider functions on the entire real line, $P$ is only Hermitian if the solutions either vanish or are exponentials with purely imaginary arguments at $\pm \infty$. For $E > V_0$, these conditions are all met without restricting the freedom in any of the coefficients. We will see that there will be restrictions when $E \leq V_0$. 
As usual, to connect the solutions in the two regions, we need matching conditions. We showed even for the infinite well that the wavefunction must be continuous at the interface. The same result will hold here; the same proof goes through, and is in fact less subtle because everything stays finite. We can show that, in the case of a finite step, the first derivative of the wavefunction must also be continuous:

\[
\left. \frac{d}{dx} \psi_{E,x}(x) \right|_{-\epsilon}^{\epsilon} = \int_{-\epsilon}^{\epsilon} dx \frac{d^2}{dx^2} \psi_{E,x}(x) \\
= \frac{2m}{\hbar^2} \int_{-\epsilon}^{0} dx (-E) \psi_{E,x}^{I}(x) + \frac{2m}{\hbar^2} \int_{0}^{\epsilon} dx (V_0 - E) \psi_{E,x}^{II}(x) \\
\approx \frac{2m}{\hbar^2} \epsilon \left[ (-E)\psi_{E,x}^{I}(-\epsilon) + (V_0 - E)\psi_{E,x}^{II}(\epsilon) \right]
\]

where we have used the eigenvalue equation to replace \( \frac{d^2}{dx^2} \psi_{E,x}(x) \) and then rewritten the integrals assuming \( \epsilon \) is small enough that \( \psi \) does not change appreciably over it. Since we have already shown \( \psi_{E,x}(x) \) must be continuous across the boundary, we are guaranteed the difference in the parentheses will remain finite as \( \epsilon \to 0 \). Thus, as we let \( \epsilon \to 0 \), the entire expression is guaranteed to vanish, implying continuity of \( \frac{d}{dx} \psi_{E,x}(x) \).
Scattering from a Step Potential: Basic Solution (cont.)

So our conditions for matching the wavefunction and its derivative are:

\[ A + B = C + D \quad i k_1 (A - B) = i k_2 (C - D) \]  \hspace{2cm} (5.49)

We have four conditions (real and imaginary) and eight total degrees of freedom (real and imaginary of \(A, B, C,\) and \(D\)), so we have too much freedom. Recalling our discussion of the free particle and bound states, the excess freedom is in the fact that there are right-going and left-going states with the same energy; there is degeneracy for free states. Initially, one sees this from the fact that \(k_1\) and \(k_2\) could take on positive or negative values, though we restricted that freedom above, saying that it was already provided in the form of the solution. We apply this freedom here by making the ansatz that, for a given \(E\), there should be two solutions, one that has \(D = 0\) and one that has \(A = 0\), corresponding to a right-going solution and a left-going solution. The right-going solution allows for a left-going solution in region I to allow for reflection at the interface, but no left-going solution in region II; and vice versa for the left-going solution. For each solution, we are left with four conditions and six degrees of freedom. The extra two are, as always, normalization and phase. *There is no need for quantization of \(k_1\) or \(k_2\) because there are enough coefficient degrees of freedom.*
Let’s do the right-going solution explicitly; the left-going solution will be analogous. To eliminate the normalization and phase degrees of freedom explicitly, we take ratios, letting \( b_\to = B/A \) and \( c_\to = C/A \). We use \( \to \) subscripts to indicate “right-going”. So we have

\[
1 + b_\to = c_\to \\
k_1 (1 - b_\to) = k_2 c_\to \\
k_1 (1 - b_\to) = k_2 (1 + b_\to) \\
\]

\[
b_\to = \frac{k_1 - k_2}{k_1 + k_2} \\
c_\to = \frac{2 k_1}{k_1 + k_2} \tag{5.50}
\]

The analogy to a wave on a string reaching an interface where the speed of propagation changes (due to a change in the string density) is clear. The situation is also similar to electromagnetic wave propagation across a boundary between two media with different indices of refraction. For the right-going solution, the left-going wave vanishes if \( k_1 = k_2 \), which corresponds to no step.
Before worrying about the time evolution, which, as we know, puts a simple
time-dependent complex exponential in front, let’s discuss the interpretation of these
two states and their components. These solutions do not decay at infinity, so
discussing the total probability is nonsense. We can, however, consider the probability
currents that we defined in the previous section. Let us calculate them for the
right-going state (c.c. = complex conjugate):

\[
j_{\rightarrow}(x) = -\frac{i}{2} \frac{\hbar}{m} \left[ (A^* e^{-i k_1 x} + B^* e^{i k_1 x}) \frac{\partial}{\partial x} (A e^{i k_1 x} + B e^{-i k_1 x}) - c.c \right]
\]

\[
= -\frac{i}{2} \frac{\hbar}{m} \left[ (A^* e^{-i k_1 x} + B^* e^{i k_1 x}) i k_1 (A e^{i k_1 x} - B e^{-i k_1 x}) \right.
\]
\[
\left. - (A e^{i k_1 x} + B e^{-i k_1 x}) i k_1 (-A^* e^{-i k_1 x} + B^* e^{i k_1 x}) \right]
\]

\[
= \frac{1}{2} \frac{\hbar k_1}{m} \left[ |A|^2 - |B|^2 + A B^* e^{2i k_1 x} + A^* B e^{-2i k_1 x} \right.
\]
\[
\left. + |A|^2 - |B|^2 - A B^* e^{2i k_1 x} - A^* B e^{-2i k_1 x} \right]
\]
\[
= \frac{\hbar k_1}{m} \left[ |A|^2 - |B|^2 \right] = |A|^2 \frac{\hbar k_1}{m} \left[ 1 - |b_{\rightarrow}|^2 \right]
\]
The same calculation for region II is much easier because there is only one component to the wavefunction:

$$j_{\rightarrow}^{II}(x) = -\frac{i}{2} \frac{\hbar}{m} \left[ C^* e^{-i k_2 x} \frac{\partial}{\partial x} C e^{i k_2 x} - c.c. \right]$$

$$= \frac{\hbar k_2}{m} |C|^2 = |A|^2 \frac{\hbar k_2}{m} |c_{\rightarrow}|^2$$

When thinking in terms of probability currents, then, it becomes clear that the current breaks into three terms (where we now drop $x$ because the currents have shown themselves to be constant in each region):

$$j_{\rightarrow, I}^{in} = |A|^2 \frac{\hbar k_1}{m}$$  (5.51)

$$j_{\rightarrow, I}^{out} = -|A|^2 \frac{\hbar k_1}{m} |b_{\rightarrow}|^2 \equiv -R j_{\rightarrow, I}^{in} \quad R = |b_{\rightarrow}|^2$$  (5.52)

$$j_{\rightarrow, II}^{out} = |A|^2 \frac{\hbar k_2}{m} |c_{\rightarrow}|^2 \equiv T j_{\rightarrow, I}^{in} \quad T = |c_{\rightarrow}|^2 \frac{k_2}{k_1}$$  (5.53)
The definitions of $R$ and $T$ ensure

$$R + T = |b_{\rightarrow}|^2 + \frac{k_2}{k_1} |c_{\rightarrow}|^2 = \left( \frac{k_1 - k_2}{k_1 + k_2} \right)^2 + \frac{k_2}{k_1} \left( \frac{2k_1}{k_1 + k_2} \right)^2 = 1 \quad (5.54)$$

which then implies

$$j_{\text{in},I} + j_{\text{out},I} = j_{\text{out},II} \quad (5.55)$$

That is, we have conservation of the probability current at the step, as we expect.

The probability currents thus guide us in the interpretation of the states. The $A$ term yields a right-going current in region I. The $C$ term yields a right-going current in region II, which is clearly the part of the probability current that gets transmitted to region II. The $B$ term yields a left-going current in region I, which we interpret as a reflected current. The interpretation of the $B$ term as reflection is supported by the fact that $R = 1 - T$, which is consistent with conservation of probability current at the step.
Solving for the Eigenstates, $0 < E < V_0$

How do we solve the problem when $0 < E < V_0$? (We will consider $E < 0$ later.) Here, the allowed form for our solution is now

$$\psi_{E,x}^I(x) = A e^{i k_1 x} + B e^{-i k_1 x} \quad k_1 = \sqrt{\frac{2m}{\hbar^2}} E$$

$$\psi_{E,x}^{II}(x) = C e^{-\kappa_2 x} + D e^{\kappa_2 x} \quad \kappa_2 = \sqrt{\frac{2m}{\hbar^2}} (V_0 - E)$$

The solution for region I is the same as Equation 5.47, while the solution for region II has changed from a complex exponential in Equation 5.48 to a real exponential. The exponential constant $\kappa_2$ is related to the original version $k_2$ by $\kappa_2 = i k_2$. Again, we restrict $k_1 \geq 0$ and $\kappa_2 \geq 0$ because the sign flip freedom is already in the solution.

Since the solution is real exponential in region II, there is no longer a concept of right-going or left-going waves in that region. We shall see that we obtain a decaying *evanescent wave* in region II and that the probability current there vanishes.
Before continuing, we must set $D = 0$ to ensure the state is normalizable and hence belongs to the Hilbert space; left-going incoming states are thereby eliminated for this range of $E$ and polarity of potential. One can also view this condition as being enforced by Hermticity of $P$, which requires that the wavefunction vanish or behave like an imaginary exponential at $\pm \infty$.

Our matching conditions then become

$$A + B = C \quad i k_1 (A - B) = -\kappa_2 C$$

(5.58)

The degrees of freedom now correspond to the $E > V_0$ case after we have picked either a left-going or right-going solution: there are four constraints and six complex coefficient degrees of freedom. This loss of degeneracy is because there is no left-going solution for $E < V_0$ and is consistent with our generic discussion of states that are unbound on one side. As before, two degrees of freedom go to phase and normalization, so we have a fully constrained problem without any quantization requirement on $k_1$ or $\kappa_2$. 

Section 5.5 Simple One-Dimensional Problems: Scattering from a Step Potential
Again, we set $b \to = B/A$ and $c \to = C/A$ and rewrite the above equations:

\begin{align*}
1 + b \to &= c \to \\
&= i k_1 (1 - b \to) = -\kappa_2 c \to \\
i k_1 (1 - b \to) &= -\kappa_2 (1 + b \to)
\end{align*}

\begin{align*}
b \to &= \frac{i k_1 + \kappa_2}{i k_1 - \kappa_2} = -\frac{(i k_1 + \kappa_2)^2}{k_1^2 + \kappa_2^2} = \frac{k_1^2 - \kappa_2^2}{k_1^2 + \kappa_2^2} - \frac{2 i k_1 \kappa_2}{k_1^2 + \kappa_2^2} \\
c \to &= \frac{2 k_1^2}{k_1^2 + \kappa_2^2} - \frac{2 i k_1 \kappa_2}{k_1^2 + \kappa_2^2}
\end{align*} \quad (5.59)

(5.60)

The coefficients are more complicated than in the $E > V_0$ case, but the matching procedure was the same. Notice that here $b \to$ and $c \to$ can pick up a phase shift, whereas in the $E > V_0$ case, they were real.
Let’s calculate the probability currents again. The region I probability current keeps the same form because, though the formula for $b_→ = B/A$ has changed, the form of the solution is unchanged. On the right side, though, our functional form has changed and so we have to recalculate. The calculation is trivial though, now that the form on the right side is a real exponential. For this case, $ψ_{E,x}^{II}(x)$ and $ψ_{E,x}^{II*}(x)$ differ only in their coefficients, not in the arguments of the exponentials, so

$$ψ_{E,x}^{II*}(x) \frac{d}{dx} ψ_{E,x}^{II}(x) = ψ_{E,x}^{II}(x) \frac{d}{dx} ψ_{E,x}^{II*}(x)$$

(the conjugation of $C$ does not matter because one gets $|C|^2$ in each term). Hence, the current on the right side vanishes! Moreover, one can easily see that $|b_→| = 1$ because its numerator and denominator are complex conjugates of one another. To summarize, we have

$$j^{in}_{→,I} = |A|^2 \frac{ℏ k_1}{m} \quad j^{out}_{→,I} = -|A|^2 \frac{ℏ k_1}{m} = -j^{in}_{→,I} \quad j^{out}_{→,II} = 0$$

(5.61)

$$R = 1 \quad T = 0$$

(5.62)
As one would expect classically for $E < V_0$, the right-going probability current in region II vanishes — the particle cannot escape to infinity on the right side because it does not have enough energy — and the reflected probability current is equal to the incoming probability current. However, there is a finite relative probability of measuring the particle's position to be in the barrier (relative to being in any finite interval in region I)! This is a completely quantum phenomenon that results from the fact that the particle state is a vector in a Hilbert space, not a definite position and momentum. If there step barrier were finite in length and dropped back to zero energy, we would find the probability current would not be zero in that region, indicating some probability for the incoming particle to tunnel through the barrier to a free-particle state on the right side. This is a good toy model for $\alpha$ decay in a nucleus.
Special Cases: $E = V_0$, $E = 0$, and $E < 0$

$E < 0$: The solutions must now be real exponential in both regions, and both the $A$ and $D$ coefficient terms must be eliminated to make the solution normalizable. The matching conditions now become impossible to meet:

\[
B = C \quad \kappa_1 B = -\kappa_2 C \\
\implies \kappa_1 B = -\kappa_2 B
\]

(5.63)

(5.64)

Since both $\kappa_1$ and $\kappa_2$ are positive numbers, one is left with $B = C = 0$. The solution becomes nonexistent, since the Hamiltonian acting on a state whose $\{|x\rangle\}$-basis representation vanishes everywhere returns zero, not a negative $E$. 


$E = 0$: Here, one must reconsider the differential equation in region I; it is now
\[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_{E=0,x}(x) = 0\]

This is directly integrable; the general solution is
\[\psi_{E=0,x}(x) = A + B x \quad (5.65)\]

We must exclude the second term because it blows up at $-\infty$. So we just have a constant in region I. This is ok, as a constant wavefunction is delta-function normalizable (we included $p = 0$ in our discussion of the free particle). The region II solution is the same as the $0 < E < V_0$ case because that part of the problem does not care about the value of $E$ as long as $E < V_0$. The matching conditions become
\[A = C \quad 0 = -\kappa_2 C \quad (5.66)\]

Since $\kappa_2 \neq 0$, we thus have $A = C = 0$. This ends up being the same as the $E < 0$ case.
\( E = V_0 \): Here, the region II differential equation simplifies as the region I equation did for \( E = 0 \), so we have

\[
\psi_{E=V_0,x}(x) = C \quad (5.67)
\]

(Again, the linear term must be discarded because it blows up at \(+\infty\).) The solution in region I is the same as for \( 0 < E < V_0 \) or \( E > V_0 \). Our matching conditions become

\[
A + B = C \quad i k_1 (A - B) = 0 \quad (5.68)
\]

So we have \( A = B \) and \( C = 2A \). This is a rather bizarre state. The probability currents are simple and take on the same values that they do for the \( 0 < E < V_0 \) case:

\[
\begin{align*}
j_{\rightarrow,\text{I}} & = |A|^2 \frac{\hbar k_1}{m} \\
-j_{\rightarrow,\text{I}} & = -|A|^2 \frac{\hbar k_1}{m} = -j_{\rightarrow,\text{I}} \\
j_{\rightarrow,\text{II}} & = 0 \quad R = 1 \quad T = 0 \quad (5.69)
\end{align*}
\]
The current vanishes not because the probability density vanishes, but because the state has no momentum in region II. But there is non-zero probability for finding the particle there. Here, our attempt to understand time-dependent behavior — incoming particles, transmission, reflection — using time-independent energy eigenstates breaks down. The probability currents still tell us something reasonable, but the wavefunction is not easily interpretable for time-dependent behavior. The right way to handle this is to construct a wave packet, which we will do next.