Reflection of Quantum Waves off of a Step Potential

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1 Waves at Material Boundaries

Imagine a particle that is free to move in one direction in a region of constant potential U_I traveling to the right. At $x = 0$, suddenly the potential jumps up to a different value U_T, as shown figure 1. This situation could describe an electron that is traveling in free space, and then suddenly runs into a piece of metal, striking it at normal incidence, for example (the symmetry of striking it at normal incidence makes this effectively a one-dimensional problem).

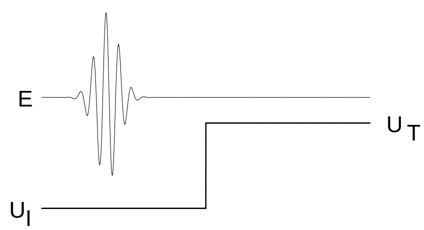

Figure 1: A wave packet approaching a sudden potential change.

What happens to a the particle when it "hits the wall"? First, let's consider what would happen according to *Newtonian mechanics*. In the picture I have drawn the particle's wave packet in a position which suggests that the total energy of the particle will be greater than the potential energy of the particle after it passes $x = 0$. Classically, if a particle has enough energy to "climb out of the potential well," it will. It will simply slow down (if the potential increases at $x = 0$) or speed up (if the potential decreases). And with 100% certainty the particle should pass the potential step without reflecting. If the particle's total energy was less than the new potential energy the particle would reflect off of the step with 100% certainty. In other words, if I try to roll a ball over a hill, it will either have enough energy to get over, or it won't. Period.

Things work out a little differently, however, when we take the particle's wave nature into account. Lets first consider the analogous problem of light striking a piece of glass at normal incidence. In this case, some of the wave is transmitted into the glass, and some of it is reflected off of the surface. If the incoming beam of light is a pure sine wave, then the transmitted and reflected beams will also be pure sine waves. If you have seen this problem before, you may remember that the transmitted and reflected beams will oscillate at the same frequency as the incident beam. But because the transmitted beam is travelling through a material with a different index of refraction, it will have a different wavelength than the incident beam.

To work the problem of a quantum wave running into a potential step, we are going to assume a wave function which is a pure momentum state. This will give us an answer which is approximately true for a particle whose wave function extends over a large space, such that it has little momentum uncertainty. Furthermore, since I can write any wave packet as a sum of pure momentum waves, if I can work this problem for a general sine wave, I can understand what will happen to an arbitrary wave packet.

Imagine that I have a wave propagating from $x = -\infty$ of the form

$$\Psi_I(x, t) = A_I e^{i(k_I x - \omega t)} \tag{1}$$

(the I in Ψ_I, A_I, and k_I stands for "incident"). Now, the question is, what will happen to this incident wave as it passes through the point where the potential changes? In analogy with the light wave hitting a piece of glass, we might expect that the total wave function will be a sum of the incident wave plus a reflected wave to the left of the potential step and a transmitted wave to the right of the step:

$$\Psi = \begin{cases} \Psi_I + \Psi_R & \text{for} \quad -\infty < x < 0 \\ \Psi_T & \text{for} \quad x > 0 \end{cases} \tag{2}$$

Whatever happens, four simple rules must be obeyed:

1. To be a well behaved wave function, it must be continuous (otherwise the second x derivative blows up, and that corresponds to infinite kinetic energy).
2. To be a well behaved wave function, it's first derivative in x must be continuous (for the same reason).
3. Energy must be conserved.
4. Probability must be conserved.

We can learn a lot from the third rule, energy conservation. For the classical problem this basically says that if you roll a ball up a hill, regardless of whether you detect the ball rolling along the top of the hill or rolling back down the hill, the total energy of the ball will be the energy it started with before it encountered the hill. In quantum mechanics, energy is related to the frequency ω. So the third rule tells us that, whatever happens, the frequency of the wave will not change — the rate at which the wave function "evolves" will be the same on both sides of the barrier. Furthermore, since the potential energy is known on both sides of the barrier and the total energy is conserved, we can find what the kinetic energy, and therefore the momentum of the wave, will be on both sides of the barrier.

For a particle in a pure momentum state with a given energy E, we know that $E = E_k + U = p^2/2m + U$. Furthermore, since $p = \hbar k$, we know that the wavenumber k for an incident particle with energy E will be given by

$$k_I = \frac{\sqrt{2m(E - U_I)}}{\hbar} \tag{3}$$

The reflected wave travels in the same potential as the incident wave. So the kinetic energy should be the same, and therefore the magnitude of the momentum and the wavenumber will be the same as well. But the reflected wave will travel in the opposite direction. The fact that the wavenumber for the reflected wave is well defined implies that the reflected wave will be a pure momentum plane wave, just like the incident wave but traveling in the opposite direction with possibly a different amplitude and phase:

$$\Psi_R = A_R e^{i(-k_I x - \omega t + \phi_R)}. \tag{4}$$

I can simplify this expression by noting that

$$A_R e^{i(-k_I x - \omega t + \phi_R)} = A_R e^{i\phi} e^{i(-k_I x - \omega t)} \tag{5}$$

and realizing that $e^{i\phi}$is just a constant. If I define a complex number $\tilde{A}_R \equiv A_R e^{i\phi}$ (where the tilde simple means "this number might be complex"), I can write the form of the reflected wave as

$$\Psi_R = \tilde{A}_R e^{i(-k_I x - \omega t)}. \tag{6}$$

This makes it so that I don't have to deal with the phase as a separate term in the math that lies ahead, without taking away any generality from our derivations.

If any wave is transmitted through the step, it should have the same total energy: $\hbar^2 k_T^2/2m + U_T = E = \hbar^2 k_I^2/2m + U_I$. So we can find what the wavenumber k_T will be on the transmitted side of the step:

$$k_T = \sqrt{k_I^2 + \frac{2m}{\hbar}(U_I - U_T)} = \frac{\sqrt{2m(E - U_T)}}{\hbar}. \tag{7}$$

The fact that the wavenumber is well defined implies that the transmitted wave will be a pure momentum plane wave just like the incident wave, but with a different wavelength and with possibly a different amplitude and phase:

$$\Psi_T = \tilde{A}_T e^{i(k_T x - \omega t)}. \tag{8}$$

2 When $E > U_T$

First lets consider the case when the particle has enough energy to get past the step.

2.1 A Bad Guess

In Newtonian physics, if the total energy of the particle is greater than the potential energy beyond the step, we would expect compete transmission of the particle. As such, we might imagine (incorrectly) that as our quantum wave passes through the junction, the wave simply changes its momentum and moves on. There may be a change in the amplitude and phase of the wave as it crosses the junction, but no reflection. Let's see if this model follows our three rules...

If our intuition is right, the wave function to the left of the step will just be the incident wave

$$\Psi_{left}(x,t) = A_I e^{i(k_I x - \omega t)}, \tag{9}$$

and the wave function on the "transmitted" side of the step will have the form

$$\Psi_{right}(x,t) = \tilde{A}_T e^{i(k_T x - \omega t + \phi_T)}. \tag{10}$$

What is wrong with this assumption? Lets consider the first rule. Can we choose $\tilde{A}_T$ in such a way that the wave function is continuous across $x = 0$ at all times: $\Psi_{left}(0,t) = \Psi_{right}(0,t)$? When we plug in the assumed forms of $\Psi_{left}(0,t)$ and $\Psi_{right}(0,t)$ we get:

$$A_I e^{-i\omega t} = \tilde{A}_T e^{i(-\omega t)} \tag{11}$$

For this equality to be true at any time t, $\tilde{A}_T$ must equal A_I. Note that this condition could not be met if we didn't have the same frequency ω in both terms.

Now let's consider the second rule for the junction: $d\Psi_{left}/dt$ is equal to $d\Psi_{right}/dt$. When we plug in our assumptions for Ψ_{left} and Ψ_{right} and take the derivative of each, we find that:

$$ik_1 A_I e^{i(k_I x - \omega t)}\Big|_{x=0} = ik_2 \tilde{A}_T e^{i(k_T x - \omega t)}\Big|_{x=0} \tag{12}$$

$$\Rightarrow \quad k_I A_I e^{-i\omega t} = k_T \tilde{A}_T e^{i(-\omega t)} \tag{13}$$

But if $\tilde{A}_T = A_I$, this equality can only be true if $k_I = k_T$, which is not the case! So we need something more...

2.2 Incident, Transmitted, and Reflected Waves (a Better Guess)

We saw that a solution which was just the incident wave on one side and a transmitted wave on the other didn't work. So lets include the possibility that part of the incident wave will be reflected back toward $-\infty$. We will write the wave on the left hand side (the sum of the incident and reflected waves) as

$$\Psi_{left}(x,t) = A_I e^{i(k_I x - \omega t)} + \tilde{A}_R e^{i(-k_I x - \omega t)}. \tag{14}$$

The wave on the right hand side (the transmitted wave) will be of the form

$$\Psi_{right}(x,t) = \tilde{A}_T e^{i(k_T x - \omega t)}. \tag{15}$$

Now to find the appropriate values for $\tilde{A}_R$ and $\tilde{A}_T$, we turn to our continuity rules. The first rule gives us:

$$\Psi_{left}(0,t) = \Psi_{right}(0,t) \Rightarrow A_I + \tilde{A}_R = \tilde{A}_T \tag{16}$$

The second rule gives us:

$$k_I A_I - k_I \tilde{A}_R = k_T \tilde{A}_T \tag{17}$$

So now we have 2 equations, 2 unknowns. We solve for the two unknowns, and we get:

$$\boxed{A_T = \frac{2k_I}{k_I + k_T} A_I} \tag{18}$$

$$\boxed{A_R = \frac{k_I - k_T}{k_I + k_T} A_I} \tag{19}$$

I have dropped the tildes because, as you can see, these amplitudes turned out to be real. (In other words, ϕ_R and ϕ_T turned out to be zero — or 180 degrees for the reflected wave in the case that $k_I < k_T$. This is exactly what happens with classical waves, like our example of light hitting a piece of glass. If the wave speed increases past the barrier, $k_T < k_I$ and the reflected light comes back in phase. If the wave speed decreases, the reflected wave is inverted.)

If we assume that we know A_I (the amplitude of the wave we are sending in), we can use the above relations to find the other two amplitudes.

2.3 Reflection Probability

The probability of finding a particle within a given region dx is $\Psi^*\Psi dx$. If our particle had a wave function which was not a pure sine wave, but which had a finite extent in space, then at some time t we can be reasonably sure that the particle hasn't "passed" the step. At this time, there is no reflected or transmitted part of the wave function, and Ψ is just the incident part. If I integrate $\Psi_I^*\Psi_I$ from $-\infty$ to 0, I would get 1. At some later time we can be sure that the particle has completely passed the step. At this time there is no more incident wave, just the reflected and transmitted wave. At this time if I integrate $\Psi_R^*\Psi_R$ from $-\infty$ to 0 I would get the probability of finding that the particle had reflected off of the step. Since both Ψ_I and Ψ_R have the same form, it can be seen that the probability of reflecting is just

$$\boxed{P_{reflect} = \frac{A_R^* A_R}{A_I^* A_I} = \left(\frac{k_I - k_T}{k_I + k_T}\right)^2}. \tag{20}$$

The probability of transmission is just $1 - P_{reflect}$. We could also find it from A_T, but it is not as simple as the reflection probability because the incident and transmitted waves travel at different velocities. The reflection and transmission probabilities are plotted as a function of particle energy in figure 2 below.

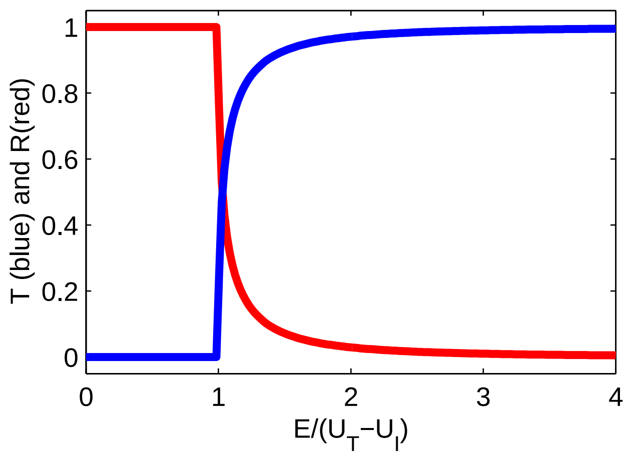

Figure 2: The transmission and reflection probabilities for a particle travelling from left to right which encounters a sudden increase in the potential. The probabilities are plotted as a function of $E/(U_T - U_I)$ where U_T is the potential to the right of the step and U_I is the potential to the left of the step.

The neat thing here is that, unlike classical physics, even if the particle has enough energy to "climb up" to the new potential energy, sometimes it doesn't. Sometimes it reflects back. Or, rather, the wave function contains both reflected and transmitted components, and when we measure the location of the particle it is possible that we will find it has transmitted, and it is possible that we will find that it reflected. But, in agreement with the correspondence principle, in the limit of large energy (compared to the potential step), the reflection probability goes to zero.

3 When $E < U_T$

Now lets consider the case when $E < U_T$. In Newtonian physics, this is the case where the ball doesn't have enough kinetic energy to roll up the hill. Once again we will assume a reflected and transmitted wave: $\Psi_R = \tilde{A}_R e^{i(-k_I x - \omega t)}$ and $\Psi_T = \tilde{A}_T e^{i(k_T x - \omega t)}$. But when $E < U_T$, the wavenumber of the transmitted wave is imaginary (see equation 7). To deal with this I define $\alpha \equiv k_T/i$, which will be real if k_T is imaginary. From equation 7 above, we find that

$$\alpha \equiv \frac{k_T}{i} = \frac{\sqrt{2m(E - U_T)}}{\hbar\sqrt{-1}} = \frac{\sqrt{2m(U_T - E)}}{\hbar}.$$

When we plug α in for the ik_T in the transmitted wave, we end up with $\Psi_T = \tilde{A}_T e^{-\alpha x} e^{-i\omega t}$. In this form it is obvious what will happen: the "transmitted" wave decays exponentially with x. As such, there is no probability of finding the particle at $x = \infty$, and we conclude that, just like the classical case, there is 100% reflection when a particle runs into a barrier for which $U_T > E$.

Before we draw conclusions, lets make sure that our rules for good wave functions are followed. First of all, the wave function can be continuous if

$$A_I e^{-i\omega t} + \tilde{A}_R e^{-i\omega t} = \tilde{A}_T e^{-i\omega t}.$$

So once again $A_I + \tilde{A}_R = \tilde{A}_T$. If the first derivative is to be continuous at $x = 0$, then

$$iA_I k_I - i\tilde{A}_R k_I = \tilde{A}_T \alpha.$$

These two equations can be solved for A_R and A_T. If you work through it, you will find that

$$\tilde{A}_R = \frac{ik_I - \alpha}{ik_I + \alpha} A_I$$

and that

$$\tilde{A}_R^* \tilde{A}_R = A_I^* A_I.$$

So the probability of reflection is, indeed, 100%. But there is a phase shift in the reflected beam, evident by the fact that $\tilde{A}_R$ is complex. Furthermore, although there is no probability of having a particle transmitted to infinity, there is an exponentially decaying probability of finding the particle in the "classically forbidden" region (where the kinetic energy is negative)! It turns out that uncertainty saves the day — the probability falls off just rapidly enough to keep you from being sure that you've detected a negative kinetic energy particle. To be sure that the particle is to the right of the step puts a limit on how big Δx can be, which in turn puts a limit on how small Δp can be.

4 Tunneling

Your textbook has a section on tunneling. But since the book doesn't derive any of the equations, I just wanted to point out that you can solve the tunneling problem just like we solved the "reflection from a step potential" problem. You assume an incident and reflected pure momentum state to the left, and a transmitted pure momentum state to the right, and a decaying exponential in the middle region. Then you have to find the right amplitudes in order to match up the waves properly at the boundaries. The tunneling problem is considerably harder than what we have done. It involves two boundaries. Also, $Ae^{-\alpha x}$ and $Ae^{\alpha x}$ are both legitimate solutions in the "classically forbidden" region (since $x = \infty$ is not in this region), and we have to consider them both.