DELTA-FUNCTION WELL - SCATTERING

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Sec 2.5.2.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.4, Exercise 5.4.2 (b).

The delta-function well always has exactly one bound state, where the energy of the particle is less than zero. If we consider states where the energy is greater than zero, we can investigate the phenomenon of scattering.

The potential function we are using is

$$V(x) = -\alpha\delta(x) \tag{1}$$

where α is a positive constant that gives the strength of the well. In this case, the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi \tag{2}$$

At all points except $x = 0$ this equation becomes

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \tag{3}$$

With $E > 0$, we can write this as

$$\frac{d^2\psi}{dx^2} = -k^2\psi \tag{4}$$

where

$$k \equiv \frac{\sqrt{2mE}}{\hbar} \tag{5}$$

Since $E > 0$, k is real and can be taken to be positive. As in the case of the bound state, because of the singularity at $x = 0$ we need to consider solutions on either side of this point separately.

The general solution of 4 is

$$\psi(x)=Ae^{ikx}+Be^{-ikx} \tag{6}$$

so we can take this as the solution for $x<0$ and call it $\psi_{-}(x)$:

$$\psi_{-}(x)=Ae^{ikx}+Be^{-ikx} \tag{7}$$

For $x>0$, we can write

$$\psi_{+}(x)=Ce^{ikx}+De^{-ikx} \tag{8}$$

Because the potential is zero in these two regions, the solutions are those of the free particle and, as we saw when we considered that case, these solutions are not normalizable so cannot, on their own, represent a physically realizable state. However, because any linear combination of solutions is also a solution, we found in the case of the free particle that we could create a wave packet and that such a packet, although not itself a stationary state, *was* normalizable and represented a particle travelling through space.

Unfortunately, we also saw that the mathematics rapidly becomes pretty horrible when we attempt to work with wave packets, so much of what is known about them is derived through computer simulations. When dealing with scattering problems, the same problems arise, and realistic problems (that is, ones involving wave packets rather than single, non-normalizable functions) can be solved only by simulation.

We will work through the problem using stationary states to see how scattering problems are handled, but it should always be kept in mind that this is not a physically realizable situation. The problem is that we will be doing the analysis for only a single value of k (and hence, of E), whereas a wave packet consists of contributions from many different values of k, and thus from many different energies. As we will see, the probabilities of reflection from the potential and of transmission through it both depend on k, so each value of k behaves differently. A proper wave packet therefore scatters in quite a complex manner, and it's a non-trivial problem to work this out in detail.

With that warning, let's see how we solve a scattering problem for a single value of k. The idea behind a scattering experiment is that we imagine a particle coming in from one direction (say, coming in from the left, so moving towards the positive x direction). When this particle hits the potential well, it may bounce back towards $-x$, or it may go through the $x=0$ point and emerge on the other side, still travelling in the direction of $+x$.

Remember that the full solution of the Schrödinger equation in this case is

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar} \tag{9}$$

For $x < 0$, this becomes

$$\Psi_-(x,t) = Ae^{i(kx-Et/\hbar)} + Be^{i(-kx-Et/\hbar)} \tag{10}$$

and for $x > 0$:

$$\Psi_+(x,t) = Ce^{i(kx-Et/\hbar)} + De^{i(-kx-Et/\hbar)} \tag{11}$$

In each of these functions, the first term represents a wave travelling to the right, and the second term a wave travelling to the left. (A reminder of how to see this: consider the motion of a fixed point on the wave, where the exponent is a constant, and consider how x must change as t increases to see which way the wave is moving. If $kx - Et/\hbar =$constant, then x must increase as t increases; just the opposite is true if $-kx - Et/\hbar =$constant.)

Therefore, to represent the experiment we described above, with a particle coming in from the left and possibly reflecting back from or passing through the potential well, we need to include terms with waves travelling in both directions for $x < 0$ and only one direction (travelling to the right) for $x > 0$. Therefore, we can say that $D = 0$ since there are no waves travelling to the left when $x > 0$.

Requiring the wave function to be continuous at $x = 0$ gives us one more condition:

$$A + B = C \tag{12}$$

We can get another condition by using the same integration technique that we applied in the case of the bound state. Integrating the Schrödinger equation across the origin we get:

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{\varepsilon}\frac{d^2\psi}{dx^2}dx - \alpha\int_{-\varepsilon}^{\varepsilon}\delta(x)\psi dx = E\int_{-\varepsilon}^{\varepsilon}\psi dx \tag{13}$$

$$-\frac{\hbar^2}{2m}\frac{d\psi}{dx}\Big|_{-\varepsilon}^{\varepsilon} - \alpha\psi(0) = E\int_{-\varepsilon}^{\varepsilon}\psi dx \tag{14}$$

Taking the limit as $\varepsilon \to 0$ gives us

$$-\frac{\hbar^2 ik}{2m}(C-A+B)-\alpha C=0 \tag{15}$$

We can now use 12 and 15 to eliminate two of the three constants, and we can express C and B in terms of A:

$$B = \frac{i\beta}{1-i\beta}A \tag{16}$$

$$C = \frac{1}{1-i\beta}A \tag{17}$$

$$\beta \equiv \frac{m\alpha}{\hbar^2 k} \tag{18}$$

It might look as though we're stuck at this point, since we can't normalize the wave function, so we can't determine A. However, what we really want is the probability that the particle will be reflected or transmitted, and we can get that by comparing B and C with A. Remember that the term $Ae^{i(kx-Et/\hbar)}$ represents the incoming particle, $Be^{i(-kx-Et/\hbar)}$ the reflected particle and $Ce^{i(kx-Et/\hbar)}$ the transmitted particle. For the region $x<0$, the probability that the particle is travelling to the left *relative* to the probability that it is travelling to the right should give the probability that it has been reflected. Comparing the probability that the particle is found in the region $x>0$ to the probability that it is travelling to the right in the region $x<0$ should give the probability that it has been transmitted.

At this point, you might be thinking there is something wrong with the logic here. After all, the particle can't be *both* travelling to the right *and* to the left at the same time in the region $x<0$, nor can it be on both sides of the origin at the same time. Not only that, but we are analyzing an explicitly time-dependent problem using only stationary states, and these states are just waves of constant amplitude that extend out to infinity, rather than wave packets describing real particles. There is no honest way around this problem; essentially we are fudging the answer since we are analyzing a non-physical system anyway. One way of thinking about it that might make you feel a bit better is, instead of imagining a single particle travelling in and either bouncing off or passing through the well, imagine a steady stream of particles being beamed at the well from the left. In that case, we would reach a steady state in which a certain fraction of particles would get reflected and the remainder would get transmitted. This situation at least gets rid of any explicit time dependence, although the problem of non-normalizability of the wave function is still there.

In the final analysis, the only honest way of analyzing this problem is by constructing a wave packet out of multiple values of k, doing the normalization properly and then working out the probabilities. However, as you might imagine, that is far from easy.

In the meantime, we can get expressions for our steady state reflection and transmission probabilities R and T by finding the appropriate ratios:

$$R = \frac{|B|^2}{|A|^2} \tag{19}$$

$$= \frac{\beta^2}{1+\beta^2} \tag{20}$$

$$= \frac{1}{1+2\hbar^2 E/m\alpha^2} \tag{21}$$

$$T = \frac{|C|^2}{|A|^2} \tag{22}$$

$$= \frac{1}{1+\beta^2} \tag{23}$$

$$= \frac{1}{1+m\alpha^2/2\hbar^2 E} \tag{24}$$

after substituting for β and then for k in terms of E. Note that $R+T=1$ so the particle must be either reflected or transmitted.

The derivation of R and T is also valid for a delta function barrier if we set $\alpha<0$, since nothing in the derivation relied on α being positive, and the final values of R and T depend only on α^2.

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