

Piecewise Potentials I

Lecture 14

Physics 342
Quantum Mechanics I

Wednesday, February 24th, 2010

We saw that the Dirac delta potential admits a single bound state and a continuum of scattering states. Technically, we can make any potential out of a sequence of finite approximations to the delta function, so in a sense, we are done. But there are some interesting physical and mathematical points that can usefully be discussed in the context of simple step and finite barrier potentials.

14.1 Finite Step

The finite step problem is defined by a potential of the form:

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x \geq 0. \end{cases} \quad (14.1)$$

The Schrödinger equation can then be split in two, with one equation relevant for the region $x < 0$ (call this region I), and the other acting for $x \geq 0$, region II:

$$-\frac{\hbar^2}{2m} \psi_I''(x) = E \psi_I(x) \quad -\frac{\hbar^2}{2m} \psi_{II}''(x) + V_0 \psi_{II}(x) = E \psi_{II}(x). \quad (14.2)$$

Continuity of the wave-function and its derivative give the two boundary conditions:

$$\psi_I(0) = \psi_{II}(0) \quad \psi_I'(0) = \psi_{II}'(0). \quad (14.3)$$

The problem, then, is to solve the wavefunction in each region, then patch them together.

14.2 Negative Energy States

By assumption, in the above, we have $V_0 > 0$. Then there are three basic regimes for the energy of the wavefunction: $E < 0$, $0 < E < V_0$ and $E > V_0$. First take $E < 0$ – then the solution on the left will be:

$$\psi_I(x) = A e^{\kappa x} + B e^{-\kappa x} \quad (14.4)$$

with $\kappa^2 \equiv \frac{2m|E|}{\hbar^2}$. We reject the growing solution for $x < 0$ by setting $B = 0$.

On the right, we can write:

$$\psi_{II}''(x) = \frac{2m(|E| + V_0)}{\hbar^2} \psi_{II}(x), \quad (14.5)$$

and once again, the solution is growing and decaying exponentials, this time with $\bar{\kappa}^2 \equiv \frac{2m(|E| + V_0)}{\hbar^2}$:

$$\psi_{II}(x) = F e^{\bar{\kappa} x} + G e^{-\bar{\kappa} x}. \quad (14.6)$$

For $x > 0$, where this solution lives, we must set $F = 0$ to obtain a solution that does not grow at spatial infinity.

Now we have to impose the boundary conditions – continuity for the wavefunction tells us immediately that $A = G$, but then, for the derivative, we must have

$$A \kappa = -G \bar{\kappa} \longrightarrow \kappa = -\bar{\kappa} \quad (14.7)$$

and this cannot be satisfied unless both κ and $\bar{\kappa}$ are equal to zero, leading to a contradiction.

Conclusion: We cannot have finite solutions for the wavefunction if $E < 0$. Then we need only consider $E > 0$, and the two remaining energy regimes can be handled simultaneously.

14.3 Positive Energy Solutions

For $E > 0$, we have the usual plane wave solutions for region I – there are two independent solutions, neither of which decay to zero at infinity, but each *is* bounded (at infinity), which is good enough for forming a basis. Our solution is:

$$\psi_I(x) = A e^{i k x} + B e^{-i k x} \quad (14.8)$$

with $k \equiv \sqrt{\frac{2mE}{\hbar^2}}$. In region II, we get

$$\psi_{II}(x) = F e^{\bar{k}x} + G e^{-\bar{k}x} \quad \bar{k} \equiv \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}. \quad (14.9)$$

Now we can see how the relative size of V_0 and E will play a role – for $E < V_0$, we will have $\bar{k} \in \mathbb{R}$, and the solutions will again be growing and decaying exponentials. For $E > V_0$, \bar{k} will be purely imaginary, and the solutions represent oscillation.

14.3.1 Solution for $E < V_0$

In this case, we have a solution on the left that is oscillatory, and on the right, a (necessarily) decaying exponential. Our boundary conditions can be written as:

$$A + B = F + G \quad ikA - ikB = \bar{k}F - \bar{k}G \quad F = 0. \quad (14.10)$$

There are a number of ways to express these linear equations, depending on what input we are given. As we shall see when we tack on the time-dependence, the solutions in region *I* represent left and right-traveling waves. So one common approach is to “send in” a wave of amplitude A , then we get a “reflected” wave traveling to the left with amplitude B , and the “tunneling” solution on the right governed by G .

We can write our algebraic relations as

$$\begin{aligned} A + B &= G \\ A - B &= \frac{i\bar{k}}{k} G \end{aligned} \quad (14.11)$$

and the solution (obtained by adding and subtracting these two equations is:

$$G = \frac{2A}{1 + \frac{i\bar{k}}{k}} \quad B = \frac{1}{2} G \left(1 - \frac{i\bar{k}}{k} \right) = \frac{A \left(1 - \frac{i\bar{k}}{k} \right)}{\left(1 + \frac{i\bar{k}}{k} \right)}. \quad (14.12)$$

As a stationary solution, it is not clear how we should interpret the coefficients above.

Traveling Waves

The solution on the left, $\psi_I(x)$, when accompanied by its time-dependence looks like:

$$\Psi_I(x, t) = \psi_I(x) e^{-\frac{iEt}{\hbar}} = A e^{ik(x - \frac{\hbar k}{2m} t)} + B e^{ik(-x - \frac{\hbar k}{2m} t)}. \quad (14.13)$$

If we look at the units, it is pretty clear that $\frac{\hbar k}{m}$ has units of $\frac{J s^{1/m}}{kg} = m/s$, a velocity (as it must be). This is reminiscent of the solutions to the one-dimensional wave equation: $-\frac{1}{v^2} \frac{\partial^2 \phi}{\partial t^2} + \frac{\partial^2 \phi}{\partial x^2} = 0$, which are

$$\phi(x, t) = f(x - vt) + g(x + vt), \quad (14.14)$$

for functions $f(y)$ and $g(y)$. In this setting, the $x - vt$ contribution is a right-traveling waveform – think of the value of the function f at time $t = 0$, location $x = 0$, this is just $f(0)$. Now, at a time $t = \epsilon$ later, the value $f(0)$ is at $x = v\epsilon$ (clear from $f(x - v\epsilon) = f(0)$). The combination appearing in $g(x + vt)$ corresponds to a left-traveling solution. Referring to $\Psi_I(x, t)$, then, we can identify the A portion of the solution as a right traveling wave, the B portion as a left-traveling wave. Then the quaint story we tell ourselves is: A wave of magnitude A travels to the right, interacts with the step potential, and gives rise to a “reflected” wave of magnitude B . This is difficult to justify in the context of an infinite plane wave superposition, but is a useful decomposition in the case of, for example, wave packets that we make out of positive or negative k solutions.

Finally, we have to be a little careful with our wave interpretation – the big difference between the plane “waves” represented by $\Psi_I(x, t)$ and the plane waves of, for example, E&M is the velocity – in E&M, waves travel in vacuum according to the fundamental velocity of the vacuum: c . In our quantum mechanical example, the waves travel with a k -dependent velocity.

We have the complete solution $\Psi_I(x, t)$, and the time-dependent analogue on the right:

$$\Psi_{II}(x, t) = G e^{-\bar{k}x} e^{-i \frac{V_0 - \frac{\bar{k}^2 \hbar^2}{2m}}{\hbar} t}, \quad (14.15)$$

and we can relate \bar{k} to k using $E = \frac{\hbar^2 k^2}{2m} = V_0 - \frac{\hbar^2 \bar{k}^2}{2m}$. We know that, since these are stationary states, $\Psi^* \Psi$ is time-independent (as you can verify explicitly). Then our conservation of probability equation reads:

$$\frac{\partial(\Psi^* \Psi)}{\partial t} = 0 = \frac{d}{dx} \underbrace{\left[\left(-\frac{i\hbar}{2m} \right) \left(\frac{d\psi}{dx} \psi^* - \frac{d\psi^*}{dx} \psi \right) \right]}_{\equiv J}, \quad (14.16)$$

and the current $J(x)$ must be a constant. We calculate this on the left and right-hand sides of the potential discontinuity:

$$J_I = \frac{1}{m} (|A|^2 - |B|^2) \hbar k \quad J_{II} = 0. \quad (14.17)$$

The value of the current on the right: $J_{II} = 0$ gives $J_I = 0$ (J is constant), and tells us immediately that $|B|^2 = |A|^2$, which is already true of our solution.

14.3.2 Solution for $E > V_0$

In this case, the general solution (14.9) still holds, but now \bar{k} is imaginary. Let's write $\bar{k} = iK$ for K real, then:

$$\psi_{II}(x) = F e^{iKx} + G e^{-iKx} \quad K = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}. \quad (14.18)$$

Our story now goes: "A wave comes in from the left with amplitude A , hits a wave coming in from the right with amplitude G , and this gives a reflected wave for $x < 0$ of amplitude B , and a reflected wave in $x > 0$ of amplitude F ." From the continuity conditions, we have:

$$A + B = F + G \quad (A - B) ik = (F - G) iK. \quad (14.19)$$

There are, again, a number of ways to tabulate this result. If we imagine that we know the magnitude of the incoming waves on the left and right, then our interest is in the reflected waves, and we would obtain the solution by inverting the following:

$$\begin{pmatrix} 1 & -1 \\ ik & -iK \end{pmatrix} \begin{pmatrix} A \\ F \end{pmatrix} = \begin{pmatrix} -1 & 1 \\ ik & -iK \end{pmatrix} \begin{pmatrix} B \\ G \end{pmatrix}, \quad (14.20)$$

giving:

$$\begin{pmatrix} B \\ G \end{pmatrix} = \begin{pmatrix} \frac{k+K}{k-K} & \frac{-2K}{k-K} \\ \frac{2k}{k-K} & -\frac{k+K}{k-K} \end{pmatrix} \begin{pmatrix} A \\ F \end{pmatrix}. \quad (14.21)$$

The traditional optics configuration, where we send in a wave and calculate the reflected and transmitted amplitudes, corresponds here to setting $G = 0$, then:

$$F = \frac{2kA}{k+K} \quad B = \frac{k-K}{k+K} A. \quad (14.22)$$

What can we say about continuity? We once again know that the probability current must be a constant. On the left, we recover

$$J_I = \frac{1}{m} (|A|^2 - |B|^2) \hbar k \quad (14.23)$$

which is now not necessarily zero. On the right, we have, by analogy:

$$J_{II} = \frac{1}{m} (|F|^2 - |G|^2) \hbar K. \quad (14.24)$$

Setting $G = 0$, we have:

$$|A|^2 - |B|^2 = |F|^2 \frac{K}{k}. \quad (14.25)$$

In light of the continuity requirement, then, we call $\frac{|B|^2}{|A|^2}$ the “reflection coefficient”, and $\frac{|F|^2}{|A|^2} \frac{K}{k}$ the “transmission coefficient”.

Finally, fun facts aside, think of the picture – we have an oscillatory solution on the left, and an oscillatory solution on the right – they have different wavelengths (and frequencies, although we cannot see this in a stationary diagram) and match smoothly at $x = 0$.

Homework

Reading: Griffiths, pp. 78–84.

Problem 14.1

For the finite step potential:

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x \geq 0 \end{cases}, \quad (14.26)$$

find the solution to the time-independent Schrödinger equation for energy $E = V_0$.

Problem 14.2

We have seen how to make a “traveling” Gaussian wavepacket out of free particle stationary states, by starting from an initial wavefunction $\bar{\psi}(x)$ that had $\langle p \rangle = p_0$. But it was not clear, without actually calculating the expectation value of momentum for the complete solution $\Psi(x, t)$, that we would have constant $\langle p \rangle = p_0$ for all time. Using an appropriate version of Ehrenfest’s theorem, show that in fact, for free particles, it is the case that $\langle p \rangle = p_0 \forall t$, so the initial momentum expectation value holds for all time.

Problem 14.3

We have the delta well potential: $V(x) = -\alpha \delta(x)$. If we start with an initial wavefunction that is Gaussian:

$$\bar{\psi}(x) = A e^{-ax^2}, \quad (14.27)$$

compute the probability that we will make an energy measurement of

$$E = -\frac{m\alpha^2}{2\hbar^2}. \quad (14.28)$$

(write your answer in terms of $z \equiv \frac{m\alpha}{2\sqrt{a}\hbar^2}$.)