

Bound and Scattering Solutions for a Delta Potential

Lecture 11

Physics 342
Quantum Mechanics I

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We understand that free particle solutions are meant to be combined into some sort of localized wave-packet. Now we can take piecewise potentials and construct stationary states, together with their time evolution – we expect to find both bound (discrete, normalizable) and scattering (continuous, finite at infinity) states, in general. Our first such potential will be the Dirac delta spike, so that almost everywhere, the potential is zero, and we basically have a boundary condition at the location of the spike.

11.1 Boundary Conditions

In electricity and magnetism, you have differential equations that come with particular boundary conditions. For example, the electrostatic potential satisfies $\nabla^2 V = -\frac{\rho}{\epsilon_0}$ in regions of space with charge density, and has an implicit boundary condition at spatial infinity (depending on gauge choice). It is often useful to cook up charge distributions that are not physically realizable in the interest of exactness. So, for example, sheets of charge have $\rho = \sigma \delta(z)$ (for a sheet of charge lying in the $z = 0$ plane), and these idealized sources introduce discontinuities in the potential. In this case, we have

$$\left. \frac{\partial V}{\partial n} \right|_{above} - \left. \frac{\partial V}{\partial n} \right|_{below} = -\frac{\sigma}{\epsilon_0}, \quad (11.1)$$

while the potential itself is continuous (the above is, of course, a manifestation of the discontinuity in the electric field). The issue never really comes up in “real life” since you cannot make an infinitesimally thin sheet of charge, so it’s a moot point. But still, good to know, and computationally useful.

In general, a mathematical problem, or mathematization of a physical problem, requires governing PDE structure, relating changes in time and space to sources (for example) and boundary conditions. For the wavefunction we have been discussing, there are some obvious and derivable boundary conditions that come up, again in the context of idealized potentials.

First, we require that the wavefunction be continuous – that’s reasonable if we are to interpret $|\Psi(x, t)|^2$ as a probability density – we’d like it if it didn’t matter if we approached an interval from the “left” or “right”. Continuity of the wavefunction and the potential directly implies continuity of the first derivative of $\Psi(x, t)$. But we want to use a discontinuous potential (a delta function, or a step function, or what have you). So what is the discontinuity in the first derivative given a discontinuous potential?

We can integrate over the discontinuity – suppose we have a potential that is discontinuous at the point x_0 , then if we integrate from $x_0 - \epsilon$ to $x_0 + \epsilon$, we have, from Schrödinger’s equation

$$-\frac{\hbar^2}{2m} \int_{x_0-\epsilon}^{x_0+\epsilon} \frac{d^2\psi}{dx^2} dx = \int_{x_0-\epsilon}^{x_0+\epsilon} E \psi(x) dx - \int_{x_0-\epsilon}^{x_0+\epsilon} V(x) \psi(x) dx. \quad (11.2)$$

The plan is to shrink the interval down until it encloses just x_0 , by sending $\epsilon \rightarrow 0$. Assuming that $\psi(x)$ itself is continuous, as suggested above, the first integral on the right will go to zero as $\epsilon \rightarrow 0$, so we neglect this term. The left-hand-side represents the discontinuity in the derivative of $\psi(x)$, and the relevant expression for the limit is

$$\left. \frac{d\psi(x)}{dx} \right|_{x_0-\epsilon}^{x_0+\epsilon} = \frac{2m}{\hbar^2} \int_{x_0-\epsilon}^{x_0+\epsilon} V(x) \psi(x) dx. \quad (11.3)$$

Now, as a model for the discontinuity, we’ll take two simple cases: $V(x) = \beta \delta(x - x_0)$ and $V(x) = \beta \theta(x - x_0)$, where¹

$$\theta(x) = \begin{cases} 0 & x < 0 \\ 1 & x > 0 \end{cases}. \quad (11.4)$$

For the delta function, the equation governing the derivative discontinuity (11.3) reads

$$\left. \frac{d\psi(x)}{dx} \right|_{x_0-\epsilon}^{x_0+\epsilon} = \frac{2m\beta}{\hbar^2} \psi(x_0) \quad (11.5)$$

¹Because the derivative of $\theta(x)$ “is” the delta function, and because the delta function is symmetric, when we need an expression for $\theta(0)$, we take $\theta(0) = \frac{1}{2}$.

so we find the discontinuity in the derivative (using the identifiers “left” for $x < x_0$ and “right” for $x > x_0$)

$$\left(\frac{d\psi_{right}}{dx} - \frac{d\psi_{left}}{dx} \right) \Big|_{x=x_0} = \frac{2m\beta}{\hbar^2} \psi(x_0) \quad (11.6)$$

For the step function, the integral on the right is easy – very close to x_0 , we have

$$\int_{x_0-\epsilon}^{x_0+\epsilon} \beta \theta(x-x_0) \psi(x) dx \approx \beta \epsilon \psi(x_0), \quad (11.7)$$

and the discontinuity in the derivative of ψ actually vanishes for $\epsilon \rightarrow 0$. Evidently, the discontinuity in the potential needs to be fairly severe to make much of a difference.

Nevertheless, discontinuity or no, we can use these two boundary conditions to set what will amount to constants of integration in the solution for the wave function. The procedure is identical to studying electromagnetic waves at the interface between two linear media (where the susceptibility is governed by precisely a step function) – we make an ansatz for the fields on “the left” and “right”, and then match the solutions at the interface. For this reason, the wavefunction matching is discussed in language very similar to that of monochromatic plane waves . . . light.

11.2 Delta Potential

As an example of how the boundaries can be used to set constants, consider a δ -function potential well (negative), centered at the origin. For $V(x) = -\alpha \delta(x)$, we have scattering solutions for $E > 0$, and bound states for $E < 0$.

11.2.1 Bound State

Let’s consider the bound state first: To the left and right of the origin, we are solving

$$-\frac{\hbar^2}{2m} \psi''(x) = -|E| \psi(x). \quad (11.8)$$

The solution, on either side, is a mixture of growing and decaying exponentials,

$$\psi_+(x) = A e^{\sqrt{\frac{2m|E|}{\hbar^2}} x} + B e^{-\sqrt{\frac{2m|E|}{\hbar^2}} x} \quad \psi_-(x) = C e^{\sqrt{\frac{2m|E|}{\hbar^2}} x} + D e^{-\sqrt{\frac{2m|E|}{\hbar^2}} x}, \quad (11.9)$$

with $\psi_+(x)$ on the right, $\psi_-(x)$ on the left. Now we can impose boundary conditions based solely on integrability – we cannot normalize exponentially growing solutions, so on the right, where $x > 0$, we set $A = 0$, and on the left, where $x < 0$, we set $D = 0$. This leaves us with

$$\psi_+(x) = B e^{-\sqrt{\frac{2m|E|}{\hbar^2}} x} \quad \psi_-(x) = C e^{\sqrt{\frac{2m|E|}{\hbar^2}} x}. \quad (11.10)$$

We want $\psi_+(x \rightarrow 0) = \psi_-(x \rightarrow 0)$ so that the wave function is continuous, and that tells us that $B = C$. Finally, we can normalize $\psi(x)$. When did we set the derivative discontinuity? The now-familiar story: Setting the boundary condition will impose a restriction on the allowed values of E , the state energy. From (11.6), we have

$$-B \sqrt{\frac{2m|E|}{\hbar^2}} - \left(B \sqrt{\frac{2m|E|}{\hbar^2}} \right) = -\frac{2m\alpha}{\hbar^2} B \quad (11.11)$$

so that $|E| = \frac{\alpha^2 m}{2\hbar^2}$, and of course, this is the magnitude, E itself is just

$$E = -\frac{\alpha^2 m}{2\hbar^2}. \quad (11.12)$$

What we have, then, is a single valid bound state. Going back to the wave function, we can normalize it easily:

$$\begin{aligned} \int_{-\infty}^{\infty} \psi(x)^2 dx &= \int_{-\infty}^0 \psi_-(x)^2 dx + \int_0^{\infty} \psi_+(x)^2 dx \\ &= 2B^2 \left(\frac{1}{2} \sqrt{\frac{\hbar^2}{2m|E|}} \right) \end{aligned} \quad (11.13)$$

so that

$$B = \frac{\sqrt{\alpha m}}{\hbar}. \quad (11.14)$$

The final solution, and it is the *only* solution for $E < 0$, is

$$\Psi(x, t) = \frac{\sqrt{\alpha m}}{\hbar} e^{-\frac{\alpha m|x|}{\hbar^2} + i \frac{\alpha^2 m t}{2\hbar^3}}. \quad (11.15)$$

The fact that we have only one bound state is an artifact of our potential.

11.2.2 Scattering States

If we take $E > 0$, then we recover the usual plane wave solutions,

$$\psi_-(x) = A e^{i\sqrt{\frac{2mE}{\hbar^2}}x} + B e^{-i\sqrt{\frac{2mE}{\hbar^2}}x} \quad \psi_+(x) = C e^{i\sqrt{\frac{2mE}{\hbar^2}}x} + D e^{-i\sqrt{\frac{2mE}{\hbar^2}}x} \quad (11.16)$$

Using our boundary conditions, we require that:

$$\psi_-(x=0) = \psi_+(x=0) \longrightarrow A + B = C + D \quad (11.17)$$

and

$$\left(\frac{d\psi_+}{dx} - \frac{d\psi_-}{dx} \right) \Big|_{x=0} = -\frac{2m\alpha}{\hbar^2} \psi(x=0) \quad (11.18)$$

$$i\sqrt{\frac{2mE}{\hbar^2}}(-C + D + A - B) = \frac{2m\alpha}{\hbar^2}(A + B).$$

Here, we appeal to your experience with monochromatic plane waves – we think of an incident, reflected, and transmitted wave, and these would correspond to the various terms in $\Psi_-(x, t)$ – written out, we have

$$\Psi(x, t) = \begin{cases} A e^{i\sqrt{\frac{2mE}{\hbar^2}}x - i\frac{E}{\hbar}t} + B e^{-i\sqrt{\frac{2mE}{\hbar^2}}x - i\frac{E}{\hbar}t} & x < 0 \\ C e^{i\sqrt{\frac{2mE}{\hbar^2}}x - i\frac{E}{\hbar}t} + D e^{-i\sqrt{\frac{2mE}{\hbar^2}}x - i\frac{E}{\hbar}t} & x > 0 \end{cases} \quad (11.19)$$

where we understand that the A and C terms represent waves traveling to the right, the B and D terms waves traveling to the left. Suppose we “send in” a plane wave from the left, then we have a reflected wave and a transmitted wave, so set $D = 0$. Our goal, as in E&M, is to relate the amplitudes of the reflected and transmitted waves to the amplitude of the incoming wave. We can do this with our boundary conditions – algebraically, we have to solve:

$$(A + B) = C \quad i\sqrt{\frac{2mE}{\hbar^2}}(A - B - C) = \frac{2m\alpha}{\hbar^2}(A + B) \quad (11.20)$$

for B and C in terms of A . Define $k = \frac{\sqrt{2mE}}{\hbar}$, then

$$B = \frac{i\frac{\alpha m}{k\hbar^2}}{1 - i\frac{\alpha m}{k\hbar^2}} A \quad C = \frac{1}{1 - i\frac{\alpha m}{k\hbar^2}} A \quad (11.21)$$

and, finally, define the combination $\frac{\alpha m}{k\hbar^2} \equiv \beta$, so we have

$$B = \frac{i\beta}{1 - i\beta} A \quad C = \frac{1}{1 - i\beta} A. \quad (11.22)$$

In electricity and magnetism, we talk about the “reflection” and “transmission” coefficients associated with monochromatic plane waves impinging on a surface. We can do the same thing here, define:

$$R \equiv \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1 + \beta^2} \quad T \equiv \frac{|C|^2}{|A|^2} = \frac{1}{1 + \beta^2}. \quad (11.23)$$

That’s handy, evidently, R and T are related to the percentage of probability that returns on the left, or heads on in to the right. Keep in mind that this is, in a sense, “per mode”. Plane wave solutions of the sort we currently have do not directly represent anything, since they are not normalizable. What we can, and will do is take a wave packet, send it in and look at how it scatters off of the delta function. That is a more physically realistic problem. Certainly, it is mathematically definable in terms of probability densities, which is a start.

11.3 Moving Gaussian Wave Packet

We studied the temporal evolution of a wavefunction that had a Gaussian shape at $t = 0$. But that evolution was dynamically uninteresting, since the expectation values of position and momentum were zero. The probability density decayed over time, but this only changed the variance associated with position, not its mean. If we want to “send in” a wave packet and have it interact with a scattering potential, we must have a wavefunction whose initial momentum is non-zero – then assuming no potential, the momentum will remain at that constant non-zero value.

How can we make a valid density that is normalizable and has some initial (expectation value of) momentum? We start by taking the initial density to be a Gaussian as before, but the wavefunction is *not* the density – in particular, we could multiply by $e^{i\bar{k}x}$ and $|\psi|^2$ is unchanged. The utility of this particular choice is obvious, the initial density is the same as the Gaussian, and the expectation value of position will be zero, but the derivative w.r.t. x will change. In particular, for

$$\bar{\psi}(x) = e^{i\bar{k}x} \left(\frac{2a}{\pi} \right)^{1/4} e^{-ax^2}, \quad (11.24)$$

we have:

$$\begin{aligned}
 1 &= \int_{-\infty}^{\infty} \bar{\psi}^* \bar{\psi} dx = 1 \\
 \langle x \rangle &= \int_{-\infty}^{\infty} \bar{\psi}^* x \bar{\psi} dx = 0 \\
 \langle p \rangle &= \int_{-\infty}^{\infty} \bar{\psi}^* \left(\frac{\hbar}{i} \frac{d}{dx} \right) \bar{\psi} dx = \hbar \bar{k},
 \end{aligned}
 \tag{11.25}$$

where the last relation is the usual de Broglie one. Now if we construct $\phi(k)$ for this initial waveform, and then $\Psi(x, t)$, we get

$$\phi(k) = \frac{1}{(2\pi a)^{1/4}} e^{-\frac{(k-\bar{k})^2}{4a}}
 \tag{11.26}$$

and

$$\Psi(x, t) = \left(\frac{2}{a\pi} \right)^{1/4} \frac{e^{-\frac{\hbar \bar{k}^2 t - 2m x (\bar{k} + i a x)}{4 a \hbar t - 2 i m}}}{\sqrt{\frac{1}{a} + \frac{2i \hbar t}{m}}},
 \tag{11.27}$$

and this has time-dependent expectation values:

$$\begin{aligned}
 \langle x \rangle &= \frac{\hbar \bar{k} t}{m} \\
 \langle p \rangle &= \hbar \bar{k} \\
 \langle H \rangle &= \frac{\hbar^2 (a + \bar{k}^2)}{2m}.
 \end{aligned}
 \tag{11.28}$$

The expectation value for x moves as we would expect, as $\langle p \rangle t / m$. The energy, similarly, is the “usual” value for a particle with speed p/m , but has the additional energy required just to have the particle around (the energy we computed when $\bar{k} = 0$).

Homework

Reading: Griffiths, pp. 68–76.

Problem 11.1

Show that the general solution

$$\Psi(x, t) = \int_{-\infty}^{\infty} \phi(k) \psi_k(x) e^{-\frac{i E_k}{\hbar} t} dk \quad (11.29)$$

satisfies $i \hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi(x, t)$ provided $\psi_k(x)$ satisfies $\hat{H} \psi_k(x) = E_k \psi_k(x)$. (This is just the continuum form of superposition – we use the function $\phi(k)$ to satisfy the initial condition $\Psi(x, 0) = \bar{\psi}(x)$).

Problem 11.2

For the traveling Gaussian solution in (11.27), we have (setting $k = \bar{k}$ to make the expressions cleaner):

$$\langle x^2 \rangle = \frac{1}{4a} + \frac{a \hbar^2 t^2}{m^2} + \frac{\hbar^2 k^2 t^2}{m^2} \quad (11.30)$$

use this, and any other expectation values (hint) you find useful, to compute σ_x^2 , σ_p^2 and the product $\sigma_x^2 \sigma_p^2$.

Problem 11.3

The delta well $V(x) = -\alpha \delta(x)$ has a bound state and a continuum of scattering states. We expect the totality of the stationary states to be mutually orthogonal – show that the bound state is orthogonal, in the usual function sense, to all of the scattering states, i.e. $\psi_b \cdot \psi_k = 0$ with:

$$\begin{aligned} \psi_b(x) &= \frac{\sqrt{m\alpha}}{\hbar} e^{-\frac{m\alpha|x|}{\hbar^2}} & E_b &= -\frac{m\alpha^2}{2\hbar^2} \\ \psi_k(x) &= \begin{cases} A \left(e^{ikx} + \frac{i\beta}{1-i\beta} e^{-ikx} \right) & x \leq 0 \\ \frac{A}{1-i\beta} e^{ikx} & x \geq 0 \end{cases} & E_k &= \frac{\hbar^2 k^2}{2m}, \end{aligned} \quad (11.31)$$

and $\beta \equiv \frac{m\alpha}{\hbar^2 k}$.