III. Solving Schrödinger's equation

We now attempt to actually start solving Schrödinger's equation in one or three dimensions. We start by writing it again (in one or three dimensions):

$$i\hbar\frac{\partial}{\partial t}\Psi\left(x,t\right)=\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V\left(x,t\right)\right]\Psi\left(x,t\right). \tag{3.1a}$$

$$i\hbar\frac{\partial}{\partial t}\Psi\left(\mathbf{r},t\right)=\left[-\frac{\hbar^2}{2m}\nabla^2+V\left(\mathbf{r},t\right)\right]\Psi\left(\mathbf{r},t\right) \tag{3.1b}$$

The first thing I want to note about these equations is that they are *linear*; that is, the wave function always appears to the first power. Suppose we have managed, somehow, to find two solutions, $\Psi_1\left(\mathbf{r},t\right)$ and $\Psi_2\left(\mathbf{r},t\right)$, to equation (3.1b), then it is easy to show that any linear combination of these functions is also a solution, *i.e.*, so also is the combination

$$\Psi\left(\mathbf{r},t\right)=c_1\Psi_1\left(\mathbf{r},t\right)+c_2\Psi_2\left(\mathbf{r},t\right) \tag{3.2}$$

where c_1 and c_2 are arbitrary complex constants. Obviously, this can be generalized to even more functions if we want to.

A. Solving Schrödinger's Equation in Free Space

We now attempt to actually start solving Schrödinger's equation in three dimensions for the case where there is no potential, so

$$i\hbar\frac{\partial}{\partial t}\Psi\left(\mathbf{r},t\right)=-\frac{\hbar^2}{2m}\nabla^2\Psi\left(\mathbf{r},t\right) \tag{3.3}$$

We already know some solutions of this equation; specifically,

$$\Psi\left(\mathbf{r},t\right)=e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t} \tag{3.4}$$

is known to satisfy Schrödinger's equation provided $\hbar\omega=\hbar^2\mathbf{k}^2/2m$. We can add up an arbitrary number of such solutions with different values of $\mathbf{k}$. Indeed, the most general solution would be to add up *all* values of $\mathbf{k}$, in which case the sum becomes an integral, and we therefore consider the solution[1]

$$\Psi\left(\mathbf{r},t\right)=\iiint\frac{d^3\mathbf{k}}{\left(2\pi\right)^{3/2}}c\left(\mathbf{k}\right)\exp\left(i\mathbf{k}\cdot\mathbf{r}-\frac{i\hbar\mathbf{k}^2}{2m}t\right) \tag{3.5}$$

[1] The factor of $\left(2\pi\right)^{3/2}$ in the denominator is a convenience, which makes our work a tiny bit simpler without changing the outcome. In one dimension it would be $\sqrt{2\pi}$.

Where $c(\mathbf{k})$ is an arbitrary complex function of **k**. This is an *enormous* number of solutions; indeed, as we will demonstrate in a moment, this actually represents *all* solutions. To check that it really is a solution, merely plug (3.5) back into (3.3) and check that the result is true. We find

$$-\frac{\hbar^2}{2m}\nabla^2\iiint\frac{d^3\mathbf{k}}{(2\pi)^{3/2}}c(\mathbf{k})\exp\left(i\mathbf{k}\cdot\mathbf{r}-\frac{i\hbar\mathbf{k}^2}{2m}t\right)=\iiint\frac{d^3\mathbf{k}}{(2\pi)^{3/2}}c(\mathbf{k})\frac{\hbar^2\mathbf{k}^2}{2m}\exp\left(i\mathbf{k}\cdot\mathbf{r}-\frac{i\hbar\mathbf{k}^2}{2m}t\right)$$
$$=i\hbar\frac{\partial}{\partial t}\iiint\frac{d^3\mathbf{k}}{(2\pi)^{3/2}}c(\mathbf{k})\exp\left(i\mathbf{k}\cdot\mathbf{r}-\frac{i\hbar\mathbf{k}^2}{2m}t\right)$$

(3.6)

The most general problem we can be given for a free particle is to be given the initial wave function $\Psi(\mathbf{r},t=0)=\psi(\mathbf{r})$ and then be asked to find the wave function at subsequent times. Setting $t = 0$ in (2.54), we see that

$$\psi(\mathbf{r})=\iiint\frac{d^3\mathbf{k}}{(2\pi)^{3/2}}c(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}} \tag{3.7}$$

Comparison with the Fourier transform (1.80) shows us that

$$c(\mathbf{k})=\tilde{\psi}(\mathbf{k})=\iiint\frac{d^3\mathbf{r}}{(2\pi)^{3/2}}\psi(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}} \tag{3.8}$$

We can perform the Fourier transform (3.8) for arbitrary wave function $\psi(\mathbf{r})$, and then plug the result back into (3.5). Of course, actually performing the integration analytically may be difficult, but often numerical methods will work even when it is difficult or impossible to do these integrals in closed form. Equations (3.5) and (3.8) can be easily generalized to an arbitrary number of dimensions.

As an example, suppose a particle of mass m in free one-dimensional space has initial wave function

$$\psi(x)=Nxe^{-Ax^2/2} \tag{3.9}$$

Where A and N are positive real constants. To find the solution of Schrödinger's equation (3.1a), we first find the constants $c(k)$ using a formula analogous to (3.8)

$$c(k)=\int\frac{dx}{\sqrt{2\pi}}e^{-ikx}\psi(x)=N\int\frac{dx}{\sqrt{2\pi}}x\exp\left(-\tfrac{1}{2}Ax^2-ikx\right) \tag{3.10}$$

This integral can be performed with the help of eq. (1.52):

$$\int_{-\infty}^{\infty}xe^{-Ax^2+Bx}dx=\sqrt{\frac{\pi}{A}}\frac{\partial}{\partial B}\left[\exp\left(\frac{B^2}{4A}\right)\right]=\frac{B\sqrt{\pi}}{2A^{3/2}}\exp\left(\frac{B^2}{4A}\right) \tag{3.11}$$

Making the substitutions $A\to\frac{1}{2}A$ and $B\to-ik$, you can easily complete the integral (3.10)

$$c(k) = -\frac{Nik}{A^{3/2}} \exp\left(-\frac{k^2}{2A}\right) \tag{3.12}$$

Plugging this into the one-dimensional version of (3.5), we then have

$$\Psi(x,t) = \int \frac{dk}{\sqrt{2\pi}} c(k) \exp\left(ikx - \frac{i\hbar k^2}{2m} t\right) = -\frac{Ni}{A^{3/2}\sqrt{2\pi}} \int k \exp\left(-\frac{k^2}{2A}\right) \exp\left(ikx - \frac{i\hbar k^2}{2m} t\right) dk,$$

$$\Psi(x,t) = -\frac{Ni}{A^{3/2}\sqrt{2\pi}} \int k \exp\left[-\left(\frac{1}{2A} + \frac{i\hbar t}{2m}\right) k^2 + ikx\right] dk \tag{3.13}$$

This integral is again of the type appearing in (3.11), except that the roles of x and k have been reversed, and this time we make the substitutions $A \to 1/2A + i\hbar t/2m$ and $B \to ix$, so we have

$$\begin{aligned} \Psi(x,t) &= -\frac{Ni}{A^{3/2}\sqrt{2\pi}} \frac{ix\sqrt{\pi}}{2(1/2A + i\hbar t/2m)^{3/2}} \exp\left[\frac{(ix)^2}{4(1/2A + i\hbar t/2m)}\right] \\ &= \frac{Nx}{(1 + i\hbar At/m)^{3/2}} \exp\left[-\frac{Ax^2}{2(1 + i\hbar At/m)}\right] \end{aligned} \tag{3.14}$$

It is obvious that (3.14) satisfies the boundary condition (3.9); it is less obvious that it satisfies the Schrödinger equation (3.1a).

B. The Time-independent Schrödinger equation

Superposition is a very useful method for solving a wide variety of problems. It is particularly useful in cases when the Schrödinger equation (3.1a) or (3.1b) has no explicit time dependence; that is, when V is independent of time. Suppose we are asked to find solutions of the equation

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r})\right] \Psi(\mathbf{r},t) \tag{3.15}$$

Let us seek solutions of the form

$$\Psi(\mathbf{r},t) = \psi(\mathbf{r}) \phi(t) \tag{3.16}$$

Plug this into (3.15), and then divide by both $\psi(\mathbf{r})$ and $\phi(t)$.

$$i\hbar \psi(\mathbf{r}) \frac{\partial}{\partial t} \phi(t) = \phi(t) \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r})\right] \psi(\mathbf{r})$$

$$\frac{i\hbar}{\phi(t)} \frac{\partial}{\partial t} \phi(t) = \frac{1}{\psi(\mathbf{r})} \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r})\right] \psi(\mathbf{r}) \tag{3.17}$$

Now, in (3.17), note that left side of the equation is independent of **r**, and the right side is independent of *t*. Since they are equal, they must both be independent of *both* **r** and *t*. We give this constant a name *E*, and write

$$\frac{i\hbar}{\phi(t)}\frac{d}{dt}\phi(t) = E = \frac{1}{\psi(\mathbf{r})}\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi(\mathbf{r}) \tag{3.18}$$

The left equality is relatively easy to solve. If you multiply both sides by *dt* and integrate, you will find[2]

$$\phi(t) = e^{-iEt/\hbar} \tag{3.19}$$

This is an equation for a wave with angular frequency $\omega = E/\hbar$, which allows us to identify *E* as the energy of the particle.

The right equality in equation (3.18) can be rewritten in what is known as the *time-independent Schrödinger equation* (in three dimensions) which is

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{3.20}$$

Of course, we still have to solve (3.20), which will depend on the particular form of $V(\mathbf{r})$. In general, there will be a list, generally an infinite list (sometimes discrete and sometimes continuous) of such solutions, which we denote with the index *n*, each with its own energy E_n, so that (3.20) should be written as

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi_n(\mathbf{r}) = E_n\psi_n(\mathbf{r}) \tag{3.21}$$

In general, we start with the (hard) problem of solving (3.21), then we substitute the resulting wave functions and (3.19) into (3.16), and finally take an arbitrary linear combination of the resulting solutions. So the most general solution of (3.15) will be

$$\Psi(\mathbf{r},t) = \sum_n c_n\psi_n(\mathbf{r})\exp(-iE_nt/\hbar) \tag{3.22}$$

We will leave the problem of finding the constants c_n for a general initial wave function $\Psi(\mathbf{r},t=0)$ to a later chapter. In general, however, we will treat Schrödinger's equation as solved as soon as we find the wave functions $\psi_n(\mathbf{r})$ and corresponding energies E_n.

What is the advantage of solving the time-independent Schrödinger equation (3.20) over simply solving the original Schrödinger equation? The primary advantage is that there is one less variable then in the original equation. The reduction of the number of variables is a vast advantage, and can often turn a seemingly intractable problem into a relatively simple one. For example, suppose we are working in one dimension, in which the time-independent Schrödinger equation takes the form

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[2] Technically, there is a constant of integration we have ignored here. This constant would become a multiplicative constant in equation (3.19). Ultimately, this multiplicative constant will be included when we use superposition to create the most general solution to (3.15), so there is no harm in momentarily leaving it out.

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi(x)=E\psi(x) \tag{3.23}$$

This is an *ordinary* differential equation, with no partial derivatives. Numerical methods for solving such ordinary differential equations are fast and highly accurate, so even if we *don't* manage to solve (3.23) analytically, we can effectively solve it numerically. As an additional advantage, (3.20) and (3.23) are both real equations, so when solving them we can set aside complex numbers and work with exclusively real functions.

C. Probability Current

In chapter II, section C, we claimed without proof that the normalization conditions (2.30) or (2.33) are preserved by the Schrödinger equation, (3.1a) or (3.1b). We will now demonstrate this, and discover an important new concept, the probability current. We start by taking the Schrödinger equation (3.1b) and multiplying by $\psi^*(\mathbf{r},t)$ on the left. We then take the complex conjugate of this equation.

$$i\hbar\Psi^*(\mathbf{r},t)\frac{\partial}{\partial t}\Psi(\mathbf{r},t)=\Psi^*(\mathbf{r},t)\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r},t)\right]\Psi(\mathbf{r},t) \tag{3.24a}$$

$$-i\hbar\Psi(\mathbf{r},t)\frac{\partial}{\partial t}\Psi^*(\mathbf{r},t)=\Psi(\mathbf{r},t)\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{r},t)\right]\Psi^*(\mathbf{r},t) \tag{3.24b}$$

We now subtract these two equations. Note that there will be a cancellation of the potential term; this cancellation occurs because $V(\mathbf{r},t)$ is real.

$$i\hbar\begin{bmatrix}\Psi^*(\mathbf{r},t)\dfrac{\partial}{\partial t}\Psi(\mathbf{r},t)\\ +\Psi(\mathbf{r},t)\dfrac{\partial}{\partial t}\Psi^*(\mathbf{r},t)\end{bmatrix}=\frac{\hbar^2}{2m}\left[\Psi(\mathbf{r},t)\nabla^2\Psi^*(\mathbf{r},t)-\Psi^*(\mathbf{r},t)\nabla^2\Psi(\mathbf{r},t)\right]. \tag{3.25}$$

We note that the left side of this equation is simply a time derivative of the probability density $\rho(\mathbf{r},t)=\Psi^*(\mathbf{r},t)\Psi(\mathbf{r},t)$. Also, the right side can be written in terms of a divergence, by noting that

$$\begin{aligned}\nabla\cdot\begin{bmatrix}\Psi(\mathbf{r},t)\nabla\Psi^*(\mathbf{r},t)\\ -\Psi^*(\mathbf{r},t)\nabla\Psi(\mathbf{r},t)\end{bmatrix}&=\left[\nabla\Psi(\mathbf{r},t)\right]\cdot\left[\nabla\Psi^*(\mathbf{r},t)\right]+\Psi(\mathbf{r},t)\nabla^2\Psi^*(\mathbf{r},t)\\ &\quad-\left[\nabla\Psi^*(\mathbf{r},t)\right]\cdot\left[\nabla\Psi(\mathbf{r},t)\right]-\Psi^*(\mathbf{r},t)\nabla^2\Psi(\mathbf{r},t)\\ &=\Psi^*(\mathbf{r},t)\nabla^2\Psi(\mathbf{r},t)-\Psi(\mathbf{r},t)\nabla^2\Psi^*(\mathbf{r},t)\end{aligned} \tag{3.26}$$

We now define the *probability current* $\mathbf{j}(\mathbf{r},t)$ by the equation

$$\mathbf{j}(\mathbf{r},t) \equiv \frac{\hbar}{2mi}\left[\Psi^*(\mathbf{r},t)\nabla\Psi(\mathbf{r},t) - \Psi(\mathbf{r},t)\nabla\Psi^*(\mathbf{r},t)\right] \tag{3.27}$$

Plugging this definition into (3.25) and using (3.26), we see that

$$i\hbar\frac{\partial}{\partial t}\rho(\mathbf{r},t) = -\frac{\hbar^2}{2m}\frac{2mi}{\hbar}\nabla\cdot\mathbf{j}(\mathbf{r},t)$$

$$\frac{\partial}{\partial t}\rho(\mathbf{r},t) + \nabla\cdot\mathbf{j}(\mathbf{r},t) = 0 \tag{3.28}$$

Equation (3.28) is a local version of conservation of probability. There is an identical equation in electromagnetism, where $\rho(\mathbf{r},t)$ is the charge density, and $\mathbf{j}(\mathbf{r},t)$ is electric current. To see more clearly that (3.28) is conservation of probability, integrate it over a volume *V*, which might represent all of space.

$$\frac{d}{dt}\iiint_V d^3\mathbf{r}\rho(\mathbf{r},t) = -\iiint_V d^3\mathbf{r}\nabla\cdot\mathbf{j}(\mathbf{r},t) \tag{3.29}$$

On the left side, the integral is the probability of a particle lying in the region *V*, as given by (2.32). On the right side, use Gauss's Law (1.23) to rewrite it as a surface integral.

$$\frac{d}{dt}P(\mathbf{r}\in V) = -\oiint_S \hat{\mathbf{n}}\cdot\mathbf{j}(\mathbf{r},t)\,dS \tag{3.30}$$

What (3.30) says is that the total probability of the particle lying in a given volume changes only due to the flow of the probability into or out of the surface of the region. In particular, if the volume *V* is all of space, and if the wave function is small at infinity, then the right hand side of (3.30) will vanish, and the total probability will remain a constant (equal to 1). So if the wave function is normalized as given by (2.33) is satisfied at one time, it will always be satisfied. Note that (3.27) and (3.28) can be trivially generalized to an arbitrary number of dimensions.

To get a better handle on probability current, consider for example the plane wave given by (3.4). The probability density at all places and times can be calculated trivially to be $\rho(\mathbf{r},t)=1$, which might lead one to mistakenly believe that there is no current flow at all. But the current density is *not* zero; indeed its value is

$$\begin{aligned}\mathbf{j}(\mathbf{r},t) &\equiv \frac{\hbar}{2mi}\left[e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega t}\nabla e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t} - e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t}\nabla e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t}\right] \\ &= \frac{\hbar i\mathbf{k}}{2mi}\left[e^{-i\mathbf{k}\cdot\mathbf{r}+i\omega t}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t} + e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t}\right] = \frac{\hbar\mathbf{k}}{m}\end{aligned} \tag{3.31}$$

Since $\hbar\mathbf{k}$ is the momentum of such a particle, this is just $\mathbf{p}/m$, the classical velocity, which means only that the resulting wave has its probability flowing at a steady rate, as we might expect.

D. Reflection from a Step Boundary

Consider a particle impacting from the left with energy E on a step boundary, as illustrated in Fig. 3-1, given by

$$V(x) = \begin{cases} 0 & \text{if } x < 0 \\ V_0 & \text{if } x > 0 \end{cases} \tag{3.32}$$

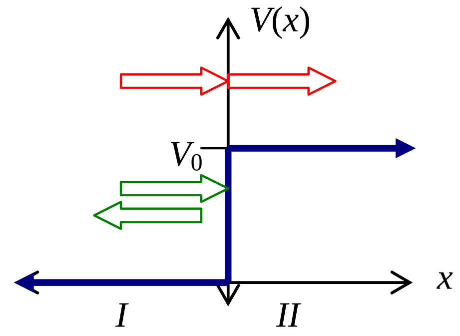

Figure 3-1: A particle approaches a step potential of magnitude V_0 from the left (region I). Classically, it will be reflected if it has insufficient energy to go over the step (green arrows) and will be reflected, while one that is above the step will be transmitted (red arrows).

Classically, the particle should continue onwards past the step if $E > V_0$, and it should be reflected back to the left if $E < V_0$. What happens quantum mechanically?

Since the potential is time independent, we will focus on the time-independent Schrödinger's equation (3.23). In the region $x < 0$, this is just

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_I(x) = E\psi_I(x) \tag{3.33}$$

where the Roman numeral I just denotes that we are in the region $x < 0$. This is just a free particle, and we already know solutions look something like e^{ikx}. If we plug this into equation (3.33), we find

$$\frac{\hbar^2 k^2}{2m} = E \tag{3.34}$$

This equation has two solutions, which I will call $\pm k$, where

$$k = \sqrt{2mE}/\hbar \tag{3.35}$$

The most general solution for this region will be linear combinations of the two solutions, which will look like

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} \tag{3.36}$$

Let's now solve the same equation in the region $x > 0$. Schrödinger's equation (3.23) in this region is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_{II}(x) = (E - V_0)\psi_{II}(x) \tag{3.37}$$

Let us assume for the moment that $E > V_0$. If we define

$$k' = \sqrt{2m(E - V_0)}/\hbar \tag{3.38}$$

then there are two solutions of the form $e^{\pm ik'x}$, so the general solution takes the form

$$\psi_{II}(x) = Ce^{ik'x} + De^{-ik'x} \tag{3.39}$$

We have solved Schrödinger's equation in regions I and II. What about the boundary? The potential is everywhere finite, and therefore, every term in Schrödinger's equation will be finite at $x = 0$. But Schrödinger's equation has a second derivative with respect to x. The second derivative can be finite only if the function and its first derivative are continuous, since derivatives are only defined for continuous functions. In other words, we must satisfy the boundary conditions

$$\begin{aligned} \psi_I(0) &= \psi_{II}(0) \\ \psi_I'(0) &= \psi_{II}'(0) \end{aligned} \tag{3.40}$$

Substituting in our expressions (3.36) and (3.39), this implies

$$\begin{aligned} A + B &= C + D \\ k(A - B) &= k'(C - D) \end{aligned} \tag{3.41}$$

It is worth stopping a moment to think about the significance of the four terms we have come up with, equations (3.36) and (3.39). To understand their meaning, look at the probability current for each of the four waves:

$$\begin{aligned} j_A &= |A|^2 \hbar k / m \\ j_B &= -|B|^2 \hbar k / m \\ j_C &= |C|^2 \hbar k' / m \\ j_D &= -|D|^2 \hbar k' / m \end{aligned} \tag{3.42}$$

Wave A has a positive current, which means it is moving to the right, and therefore it represents an incoming wave on the left. Wave B is a reflected wave, moving away to the left. Wave C represents the transmitted wave, moving off to the right. And what about D? It would represent a wave coming in from the right. Such a wave might exist, but we were asking specifically about a wave coming in from the left, so it is irrelevant to this problem, and we assume

$$D = 0 \tag{3.43}$$

We are now prepared to solve our simultaneous equations (3.41). If we solve them for B and C in terms of A, we find

$$\begin{aligned} C &= \frac{2k}{k + k'} A \\ B &= \frac{k - k'}{k + k'} A \end{aligned} \tag{3.44}$$

These two equations tell us the *magnitude* of the two waves, from which we can easily derive the relative size of the probability density. However, we are trying to figure out if the wave is reflected or transmitted, which is asking something about the *flow* of probability. In short, we want to know what fraction of the probability flowing *in* is reflected *back* and what fraction is transmitted forward. These two quantities are denoted R (for reflected) and T (for transmitted), and are given by

$$R \equiv \frac{|j_B|}{j_A} = \frac{|B|^2}{|A|^2} = \left(\frac{k-k'}{k+k'}\right)^2 ,$$
$$T \equiv \frac{j_C}{j_A} = \frac{|C|^2 k'}{|A|^2 k} = \frac{4kk'}{(k+k')^2} . \tag{3.45}$$

It is easy to demonstrate that $R+T=1$, which simply means that the wave is *certainly* either reflected or transmitted, as it must be. These equations can be rewritten in terms of E and V_0 with the help of (3.35) and (3.38) if desired.

One concern is that the wave functions we have found are *not* normalizable. The wave functions (3.36) and (3.39) do not diminish as they go to infinity. Of course, the same could be said of our plane wave solutions we found in section A. However, in section A, we were able to combine plane waves with different energies to form wave *packets* which we *could* normalize. The same is true here. Basically, this is possible because the wave solutions we found, (3.36) and (3.39), are not blowing up at infinity, and this made it relatively easy to combine them and make wave packets which do *not* grow without bounds at infinity.

We have solved the wave function *only* under the assumption that in (3.37), we have an energy E greater than the potential V_0. We need to reconsider the case when $E < V_0$, when classically the wave has insufficient energy to penetrate the barrier. To do so, we reexamine (3.37), which I trivially rewrite in the form

$$\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_{II}(x) = (V_0 - E)\psi_{II}(x) \tag{3.46}$$

We now define

$$\alpha = \sqrt{2m(V_0 - E)} \Big/ \hbar \tag{3.47}$$

Then the solutions of (3.46) will be exponentials of the form

$$\psi_{II}(x) = Ce^{-\alpha x} + De^{\alpha x} \tag{3.48}$$

It is time to consider the two solutions in more detail before moving onwards. The term C represents a wave that dies out in the region $x > 0$. In contrast, the term D results in a wave function that grows quickly; faster than any polynomial. As a consequence, it will be difficult to build wave packets out of the D term, because the wave grows so fast. Our conclusion is that the D term is non-physical, and we once again assume $D = 0$.

We now plug (3.36) and (3.48) (with $D = 0$) into the boundary conditions (3.40), which yields the simultaneous equations

$$A + B = C$$
$$ik(A - B) = -\alpha C \tag{3.49}$$

These equations can be solved for B and C in terms of the incoming wave A, which yields

$$B = \frac{-k + i\alpha}{k + i\alpha} A$$
$$C = \frac{2k}{k + i\alpha} A \tag{3.50}$$

Now it's time to figure out the probability of reflection and transmission. If you plug a wave function of the form $\psi(x) = Ce^{-\alpha x}$ into the formula for probability current, it is easy to see you just get $j_C = 0$, which makes the transmission probability zero. Hence we quickly find the reflection and transmission coefficients

$$R = \frac{|j_B|}{j_A} = \left|\frac{B}{A}\right|^2 = \frac{|-k + i\alpha|^2}{|k + i\alpha|^2} = \frac{k^2 + \alpha^2}{k^2 + \alpha^2} = 1,$$
$$T = \frac{j_C}{j_A} = 0 \tag{3.51}$$

Thus when the energy is insufficient to penetrate the barrier classically, it ends up being totally reflected, even though the wave function penetrates a short distance into the forbidden region. When E is less than V_0, when classical theory predicts penetration of the barrier, transmission *is* possible, even quantum mechanically, but there is also a possibility of reflection, as given in (3.45). There is even reflection when V_0 is negative; that is, when the potential barrier is negative. It would be as if you tried to run off a cliff, but instead reflected back! Figure 3-2 represents a sketch of the reflection probability as a function of E/V_0.

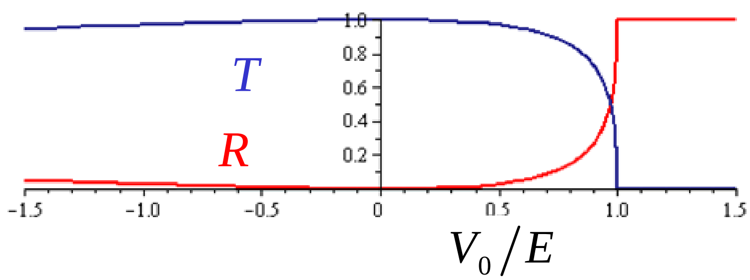

Figure 3-2: The probability of transmission (blue curve) and reflection (red curve) as a function of the size of the barrier. Note that there is *always* some reflection, except for the trivial case $V_0 = 0$. However, if the potential is larger than the energy, then the wave is completely reflected.

Note that in each of the cases we have studied, a free particle (section A) and a particle approaching a step barrier (this section), we found solutions for all possible energies. The reason this occurred is because in both cases, the energy of the particle was sufficient to get the particle out to infinity. In section E we will explore an alternative case, when the energy is assumed to be *less* than the energy at infinity. In such cases (called *bound states*), the wave function will vanish away at infinity, and the energy will turn out to only come in discrete possible values.

E. Bound States from a Double Delta potential

Let's turn our attention now to a different kind of problem, one where the particle's energy is less than the energy at infinity. Let's consider a particle of mass *m* in one dimension with potential

$$V(x) = -\lambda\left[\delta\left(x-\tfrac{1}{2}a\right)+\delta\left(x+\tfrac{1}{2}a\right)\right] \tag{3.52}$$

so that Schrödinger's equation takes the form

$$E\psi(x) = \left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \lambda\delta\left(x-\tfrac{1}{2}a\right) - \lambda\delta\left(x+\tfrac{1}{2}a\right)\right]\psi(x) \tag{3.53}$$

where *G* and λ are positive constants. In other words, the particle is free except at two points where the potential is negatively infinite, as sketched in Fig. 3-3. We will be seeking bound states with energy *E* < 0. According to classical physics, the particle will be stuck in one of the two infinitely narrow wells. What does quantum physics predict?

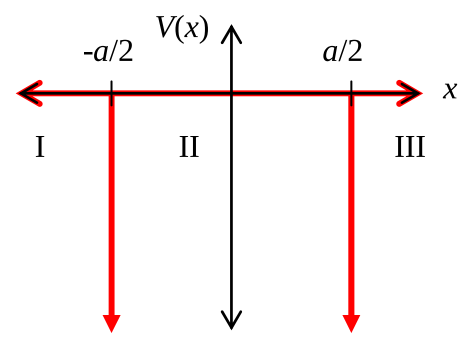

Figure 3-3: The potential is zero except at the two points $x = \pm\tfrac{1}{2}a$, where it is negatively infinite.

Away from the two delta functions, the particle is free, satisfying

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) \tag{3.54}$$

Keeping in mind that *E* is negative, we define

$$\beta \equiv \sqrt{-2mE}/\hbar \tag{3.55}$$

We then find that the solutions to (3.54) take the form $e^{\pm\beta x}$. However, there is no reason to believe that the form of the equation will *match* in the three regions marked I, II, and III in Figure 3-3, so the coefficients of the three waves will tend to be different. Furthermore, we don't want solutions which diverge at infinity, so in region III we reject waves that look like $e^{\beta x}$, and in region I we reject $e^{-\beta x}$. We therefore guess the solutions will take the form

$$\begin{aligned}\psi_I(x) &= Ae^{\beta x}\\ \psi_{II}(x) &= Be^{-\beta x}+Ce^{\beta x}\\ \psi_{III}(x) &= De^{-\beta x}\end{aligned} \tag{3.56}$$

What about boundary conditions? It is tempting to assume that the function and its derivative will be continuous, but this is not correct. To figure out what to do at the boundary, integrate (3.53) across one of the boundaries, say from $\tfrac{1}{2}a-\varepsilon$ to $\tfrac{1}{2}a+\varepsilon$. We find

$$E\int_{\frac{1}{2}a-\varepsilon}^{\frac{1}{2}a+\varepsilon}\psi(x)\,dx=-\frac{\hbar^2}{2m}\int_{\frac{1}{2}a-\varepsilon}^{\frac{1}{2}a+\varepsilon}\frac{d^2\psi(x)}{dx^2}dx-\lambda\int_{\frac{1}{2}a-\varepsilon}^{\frac{1}{2}a+\varepsilon}\psi(x)\begin{bmatrix}\delta\left(x-\frac{1}{2}a\right)\\+\delta\left(x+\frac{1}{2}a\right)\end{bmatrix}dx \qquad (3.57)$$

The first term on the right side is easy to evaluate, because the integral of the second derivative of a function is just the first derivative. The integral of a delta function is similarly easy to evaluate; it simply yields $\psi(x)$ at the boundary point $x=\frac{1}{2}a$. The other boundary point $x=-\frac{1}{2}a$ does not contribute, because it is not in the range of integration.

$$E\int_{\frac{1}{2}a-\varepsilon}^{\frac{1}{2}a+\varepsilon}\psi(x)\,dx=-\frac{\hbar^2}{2m}\left[\psi'_{III}\left(\tfrac{1}{2}a+\varepsilon\right)-\psi'_{II}\left(\tfrac{1}{2}a-\varepsilon\right)\right]-\lambda\psi\left(\tfrac{1}{2}a\right) \qquad (3.58)$$

Note that the derivative terms are evaluated using the appropriate functions in each range. Now, consider the limit as $\varepsilon\to 0$. The integrand on the left is finite, and the integral will become very small. So (3.58) becomes

$$\psi'_{III}\left(\tfrac{1}{2}a\right)-\psi'_{II}\left(\tfrac{1}{2}a\right)=-\frac{2m\lambda}{\hbar^2}\psi\left(\tfrac{1}{2}a\right) \qquad (3.59)$$

Now, spend a moment analyzing this equation. It says specifically that the derivative is *not* continuous at the boundary, it has a finite discontinuity there. However, a finite discontinuity implies that the *function* must at least be continuous, so we have

$$\psi_{II}\left(\tfrac{1}{2}a\right)=\psi_{III}\left(\tfrac{1}{2}a\right) \qquad (3.60)$$

This is fortunate, since otherwise in equation (3.59), we wouldn't know which function to use on the right side of the equation, but we see from (3.60) that it doesn't matter.

We can similarly integrate (3.58) across the boundary at $x=-\frac{1}{2}a$. This leads to two more boundary conditions.

$$\begin{gathered}\psi'_{II}\left(-\tfrac{1}{2}a\right)-\psi'_{I}\left(-\tfrac{1}{2}a\right)=-\frac{2m\lambda}{\hbar^2}\psi\left(-\tfrac{1}{2}a\right)\\ \psi_{II}\left(-\tfrac{1}{2}a\right)=\psi_{I}\left(-\tfrac{1}{2}a\right)\end{gathered} \qquad (3.61)$$

Let's write out equations (3.59), (3.60) and (3.61) in terms of our explicit wave functions (3.56). We find

$$\begin{aligned}Ae^{-\beta a/2}&=Be^{\beta a/2}+Ce^{-\beta a/2}\\ De^{-\beta a/2}&=Be^{-\beta a/2}+Ce^{\beta a/2}\\ -\frac{2m\lambda}{\hbar^2}Ae^{-\beta a/2}&=\beta\left[-Be^{\beta a/2}+Ce^{-\beta a/2}-Ae^{-\beta a/2}\right]\\ -\frac{2m\lambda}{\hbar^2}De^{-\beta a/2}&=\beta\left[-De^{-\beta a/2}+Be^{\beta a/2}-Ce^{\beta a/2}\right]\end{aligned} \qquad (3.62)$$

We have here four equations in four unknowns, which one would think would have a unique solution. Indeed, for a general value of the energy E (and corresponding parameter β), the unique solution to (3.62) is $A=B=C=D=0$. This however is an unacceptable solution. We want *non*-trivial solutions. To find them, we plug the first two equations into the latter two, which yields

$$\begin{aligned} \frac{m\lambda}{\hbar^2}\left[Be^{\beta a/2}+Ce^{-\beta a/2}\right]&=\beta Be^{\beta a/2} \\ \frac{m\lambda}{\hbar^2}\left[Be^{-\beta a/2}+Ce^{\beta a/2}\right]&=\beta Ce^{\beta a/2} \end{aligned} \tag{3.63}$$

Note that these equations are identical save for the interchange of the role of *B* and *C*. If either *B* or *C* vanish, then the other will as well, and the resulting solution is the trivial one. If they don't vanish, we can divide by either of them, and we can rewrite the two equations (3.63) as

$$\frac{B}{C}=\frac{C}{B}=e^{\beta a}\left[\frac{\hbar^2\beta}{m\lambda}-1\right] \tag{3.64}$$

Now, the only numbers that are their own reciprocal are ± 1, so substituting this in (3.64) and rearranging a bit, we must have

$$\frac{\hbar^2\beta}{m\lambda}=1\pm e^{-\beta a} \tag{3.65}$$

The left side of this equation is a simple line. The right side is two functions, one of which starts at 0, the other at 2, and then both asymptotically approach 1. It is easy to see, as illustrated in Fig. 3-4, that the linear function must cross the upper curve eventually, so there is always one solution β_+ to (3.65). The other curve crosses the line at $\beta=0$, but this turns out to lead to only a trivial solution to our equations. However, if λ is not too small, it is easy to show that there will be an additional crossing, which we denote β_-. In other words, we have

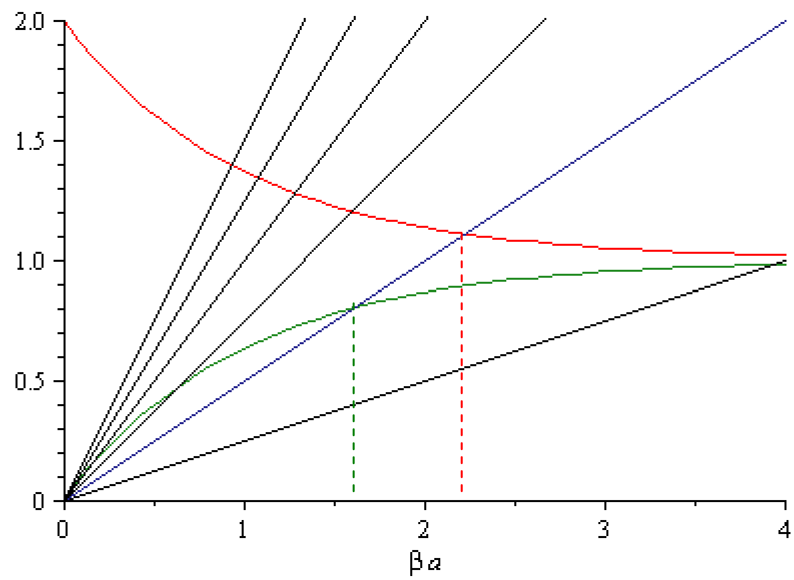

Figure 3-4: Graphical solution of eq. (3.65). We are trying to find where one of the straight lines crosses the red (for β_+) or green (for β_-) curves. The straight lines correspond to $\hbar^2/ma\lambda=0.25$, 0.50, 0.75, 1.00, 1.25, and 1.50 (bottom to top). The solutions for the $\hbar^2/ma\lambda=0.50$ (navy line) are $a\beta_+=2.2177$ and $a\beta_-=1.5936$ (dotted red and green lines respectively). Note that β_- will exist only if $\hbar^2/ma\lambda<1$.

one or two solutions to (3.65), which satisfy the two equations

$$\frac{\hbar^2\beta_+}{m\lambda} = 1 + e^{-\beta_+ a} \quad \text{and} \quad \frac{\hbar^2\beta_-}{m\lambda} = 1 - e^{-\beta_- a} \qquad (3.66)$$

The equation on the right can be shown to have solutions only if

$$\lambda > \frac{\hbar^2}{ma} \qquad (3.67)$$

The resulting energies are

$$E_\pm = -\frac{\hbar^2\beta_\pm^2}{2m} \qquad (3.68)$$

where the minus solution exists only if (3.67) is satisfied. These two energies are plotted in Fig. 3-5. Once we have the relevant value of β, we know $B = \pm C$, and we can get the other coefficients from the first two equations of (3.62). If we wish, we can then normalize the overall wave function. The final solution for $ma\lambda/\hbar^2 = 2$ are illustrated in Fig. 3-6. Note that one of the solutions is symmetric, and the other anti-symmetric across the origin. As we will later demonstrate, this is a general feature of problems where the potential is symmetric, $V(x) = V(-x)$.

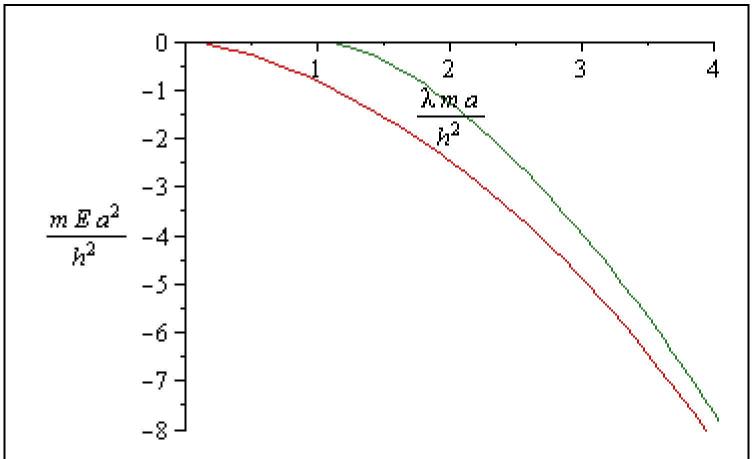

Figure 3-5: The energy $ma^2E/\hbar^2$ of the bound states for different values of $\lambda ma/\hbar^2$. Note that there is one solution (the plus or red solution) for $\lambda ma/\hbar^2 \le 1$; for $\lambda ma/\hbar^2 > 1$ there is also the minus (green) solution.

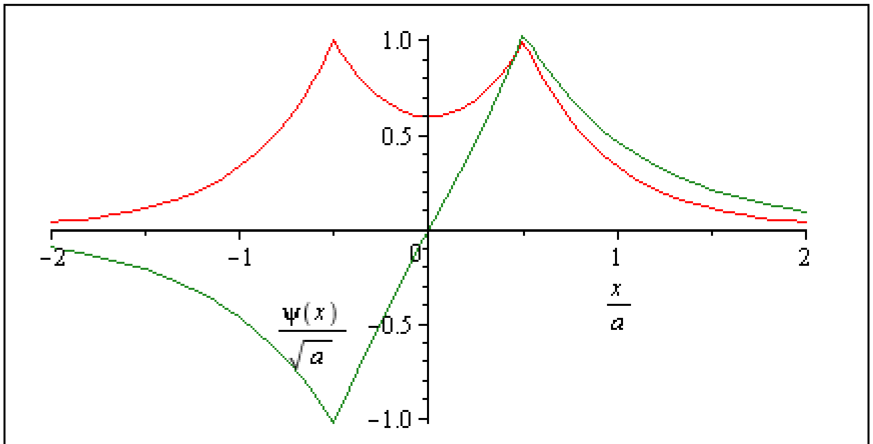

Figure 3-6: The plus (red) and minus (green) wave functions for $\lambda ma/\hbar^2 = 2$. Note that the plus solution is symmetric across the origin, and the minus is anti-symmetric. Note that in both cases, the wave function is continuous but its derivative is not.

In summary, in this case we have found that for the double delta function potential, there are bound states only for specific energies. The exact number of solutions depends on the depth of the attractive delta-function potentials; not surprisingly, the number increases as we increase λ. This is the general result for an attractive potential: the solutions will exist for only discrete energies. Often there will only be a finite number of such solutions, though we will find when the range of the attraction is long range enough, we will sometimes find an infinite number of energies.