

PHY 115A
Lecture Notes 2B:
Tunneling and Scattering
(Griffith's 2.5-2.6,9.1-9.2)

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Chapter 2

Tunneling and Scattering

2.26 Continuity of the Wave Function

Let's start with the case $V(x)$ is finite everywhere, then we start from the TISE:

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

Without loss of generality, we'll investigate continuity at $x = 0$, by integrating the TISE from $-\epsilon$ to $+\epsilon$:

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

We'll assume that we keep $\epsilon > 0$ here and everywhere below. By the fundamental theorem of calculus the LHS is:

$$\left. \frac{d\psi}{dx} \right|_{+\epsilon} - \left. \frac{d\psi}{dx} \right|_{-\epsilon} = \frac{2m}{\hbar^2} \int_{-\epsilon}^{+\epsilon} (V(x) - E) \psi(x) dx \quad (2.71)$$

In the limit $\epsilon \rightarrow 0$, the RHS vanishes since $V(x)$ is finite, so:

$$\lim_{\epsilon \rightarrow 0} \left(\left. \frac{d\psi}{dx} \right|_{+\epsilon} - \left. \frac{d\psi}{dx} \right|_{-\epsilon} \right) = 0$$

which is to say the derivative of the wave function is continuous, and so the wave function is continuous as well.

But what about infinite (or undefined) $V(x)$? Here we still insist that the wave function be continuous, as otherwise the state of a particle would be undefined at some point. But the derivative need not be continuous, as the $V(x)$ term in LHS in Equation 2.71 no longer vanishes in the limit $\epsilon \rightarrow 0$:

$$\lim_{\epsilon \rightarrow 0} \left(\left. \frac{d\psi}{dx} \right|_{+\epsilon} - \left. \frac{d\psi}{dx} \right|_{-\epsilon} \right) = \lim_{\epsilon \rightarrow 0} \frac{2m}{\hbar^2} \int_{-\epsilon}^{+\epsilon} V(x) \psi(x) dx \quad (2.72)$$

2.27 The Dirac Delta Function

The so-called “Dirac Delta Function” $\delta(x)$ is defined by it's behavior in an integral:

$$\int_{-\infty}^{+\infty} f(x) \delta(x) dx = f(0) \quad (2.73)$$

where it “picks out” the value of $f(x)$ at $x = 0$. It immediately follows (put $f(x) = 1$) that:

$$\int_{-\infty}^{+\infty} \delta(x) dx = 1 \quad (2.74)$$

Also, changing variables to make the substitutions clearer:

$$\int_{-\infty}^{+\infty} g(y) \delta(y) dy = g(0)$$

and putting $y = x - a$, we get:

$$\int_{-\infty}^{+\infty} g(x - a) \delta(x - a) dy = g(0)$$

and defining $f(x) \equiv g(x - a)$ we have:

$$\int_{-\infty}^{+\infty} f(x) \delta(x - a) dy = f(a) \quad (2.75)$$

The Dirac Delta Function isn't real a function at all, but it is often described as one:

$$\delta(x) = \begin{cases} 0, & x \neq 0 \\ \infty, & x = 0 \end{cases}$$

but such a definition shouldn't be taken too seriously. A better way to consider it is as a limit of perfectly reasonable functions with integral one, that get narrower and narrower around 0. Just as the limit of a series of rational numbers can be an irrational number, the δ -function is the limit of a sequence of integrable functions, but isn't itself square integrable. We could try:

$$\int_{-\infty}^{+\infty} \delta^2(x) dy = \delta(0) \quad (2.76)$$

but what are we to make of $\delta(0)$? At best, we could say it is in infinity. Mathematicians call the δ -function a generalized function or distribution. It only makes sense in the context of its defining integral equation above, and doesn't exist as a function on its own. If you think of what we actually do with wave functions (calculate integrals) this isn't really any limitation at all.

For $x \neq 0$, $\delta(x) = 0$ is well defined. But otherwise, just stick to its well defined properties (the numbered equations here) within integrals, and we will see the δ -function is extremely useful.

2.28 Bound State of the Delta Function Potential

We turn to the very useful example a delta function potential.

$$V(x) = -\alpha\delta(x) \quad (2.77)$$

Since we've agreed to never discuss the delta function at $x = 0$ outside of an integral, we will just say that $V(x)$ does not have a defined minimum, and so we are free to see if there are normalizable solution with $E < 0$.

Away from $x = 0$, where $\delta(x)$ is well defined, $V(x) = 0$ and the TISE is:

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x) = \kappa^2\psi(x), \quad \kappa \equiv \frac{\sqrt{-2mE}}{\hbar}.$$

which has general solutions:

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x}$$

But for the wave function to be well defined only:

$$\psi(x) = Ae^{-\kappa x}, \quad x > 0$$

and

$$\psi(x) = Be^{\kappa x}, \quad x < 0$$

are acceptable. From continuity of the wave function at $x = 0$, we conclude:

$$A = B$$

and write $\psi(x)$ as:

$$\psi(x) = \begin{cases} Be^{\kappa x} & x \leq 0 \\ Be^{-\kappa x} & x \geq 0 \end{cases}$$

We saw above that the presence of the δ -function means the wave function need not be continuous at $x = 0$, and in fact:

$$\lim_{\epsilon \rightarrow 0} \left(\frac{d\psi}{dx} \Big|_{+\epsilon} - \frac{d\psi}{dx} \Big|_{-\epsilon} \right) = \lim_{\epsilon \rightarrow 0} \frac{2m}{\hbar^2} \int_{-\epsilon}^{+\epsilon} V(x) (-\alpha \delta(x)) dx$$

The δ -function is well defined in the context of this integral, which can be evaluated as:

$$\lim_{\epsilon \rightarrow 0} \left(\frac{d\psi}{dx} \Big|_{+\epsilon} - \frac{d\psi}{dx} \Big|_{-\epsilon} \right) = \lim_{\epsilon \rightarrow 0} \left(-\frac{2m\alpha}{\hbar^2} \psi(0) \right) = -\frac{2m\alpha}{\hbar^2} \psi(0)$$

In our case:

$$\psi(0) = B$$

and:

$$\frac{d\psi}{dx} = \begin{cases} \kappa Be^{\kappa x} & x \leq 0 \\ -\kappa Be^{-\kappa x} & x \geq 0 \end{cases}$$

so:

$$\lim_{\epsilon \rightarrow 0} \left(\frac{d\psi}{dx} \Big|_{+\epsilon} - \frac{d\psi}{dx} \Big|_{-\epsilon} \right) = -\kappa B - \kappa B = -\frac{2m\alpha}{\hbar^2} B$$

or

$$\kappa = \frac{m\alpha}{\hbar^2}$$

or

$$E = -\frac{\hbar^2 \kappa^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}$$

Normalizing the wave function is left as an exercise, it yields:

$$|B|^2 = \kappa$$

2.29 Scattering States of the Delta Function Well

For the case that $E > 0$, we have the free particle TISE for $x < 0$:

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x) = -k^2\psi(x), \quad k \equiv \frac{\sqrt{2mE}}{\hbar}.$$

with general solution:

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

Similarly, for $x > 0$ the general solution is:

$$\psi(x) = Fe^{ikx} + Ge^{-ikx}$$

and so:

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x \leq 0 \\ Fe^{ikx} + Ge^{-ikx} & x \geq 0 \end{cases}$$

and:

$$\frac{d\psi}{dx} = \begin{cases} (iAk)e^{ikx} + (-iBk)e^{-ikx} & x \leq 0 \\ (iFk)e^{ikx} + (-iGk)e^{-ikx} & x \geq 0 \end{cases}$$

Continuity of $\psi(x)$ at $x = 0$ requires:

$$F + G = A + B$$

and from:

$$\lim_{\epsilon \rightarrow 0} \left(\frac{d\psi}{dx} \Big|_{+\epsilon} - \frac{d\psi}{dx} \Big|_{-\epsilon} \right) = -\frac{2m\alpha}{\hbar^2}\psi(0)$$

so:

$$\begin{aligned} ik(F - G - A + B) &= -\frac{2m\alpha}{\hbar^2}(A + B) \\ F - G &= (A - B) + i\frac{2m\alpha}{k\hbar^2}(A + B) \end{aligned}$$

Finally:

$$F - G = A(1 + 2i\beta) - B(1 - 2i\beta)$$

where:

$$\beta = \frac{m\alpha}{\hbar^2 k}$$

To measure scattering, let A represent the (known) incident wave and set

$$G = 0$$

so now we have two equations and two unknowns:

$$F = A + B$$

and:

$$F = A(1 + 2i\beta) - B(1 - 2i\beta)$$

Solving for F in terms of A :

$$\begin{aligned} F &= A(1 + 2i\beta) - (F - A)(1 - 2i\beta) \\ 2F(1 - i\beta) &= 2A \end{aligned}$$

and so:

$$F = \frac{A}{1 - i\beta}$$

similarly:

$$B = \frac{i\beta}{1 - i\beta}$$

The reflection coefficient is:

$$R = \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1 + \beta^2}$$

and:

$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \beta^2}$$

Notice that:

$$R + T = 1$$

Now let's look at what happens for:

$$V(x) = +\alpha\delta(x)$$

Nothing changes until we reach the boundary condition on the derivative, which becomes:

$$\lim_{\epsilon \rightarrow 0} \left(\frac{d\psi}{dx} \Big|_{+\epsilon} - \frac{d\psi}{dx} \Big|_{-\epsilon} \right) = +\frac{2m\alpha}{\hbar^2} \psi(0)$$

So we can read off the solutions for this case by putting $\beta \rightarrow -\beta$ in the solutions:
so the boundary conditions (keeping $G = 0$) become:

$$\begin{aligned} F &= A + B \\ F &= A(1 - 2i\beta) - B(1 + 2i\beta) \end{aligned}$$

2.30 Bound States of the Finite Square Well

Next we consider the finite square well potential:

$$V(x) = \begin{cases} -V_0, & -a \leq x \leq a \\ 0 & \text{otherwise} \end{cases}$$

As the potential is finite everywhere, we expect both ψ and $d\psi/dx$ to be continuous. The bound state potentials will have $-V_0 < E < 0$. For $x < -a$ and $x > a$, we encounter a familiar form of the TISE:

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2} \psi(x) = \kappa^2 \psi(x), \quad \kappa \equiv \frac{\sqrt{-2mE}}{\hbar}.$$

with the solutions

$$\psi(x) = Ae^{\kappa x}$$

for $x < -a$ and

$$\psi(x) = Be^{-\kappa x}$$

for $x > a$. Within the potential well at $-a \leq x \leq a$ we have:

$$\frac{d^2\psi}{dx^2} = -\frac{2m(V_0 + E)}{\hbar^2}\psi(x) = -k^2\psi(x), \quad k \equiv \frac{\sqrt{2m(V_0 + E)}}{\hbar}.$$

with general solution:

$$\psi(x) = C \sin(kx) + D \cos(kx)$$

At this point, we will save ourselves a lot of hassle by noting that $V(x)$ is even, and so the general solutions can be constructed as either even or odd solutions. (See Griffith's P2.1c). One major benefit of this, is that we need only establish continuity for $x \geq 0$ and we will automatically have it for $x \leq 0$.

Starting with the even solutions and $x \geq 0$, we write:

$$\psi(x) = \begin{cases} Be^{-\kappa x} & x > a \\ D \cos(kx) & 0 \leq x \leq a \end{cases}$$

and continuity implies:

$$Be^{-\kappa a} = D \cos(ka) \tag{2.78}$$

We see that the dimensionless quantities κa and ka are of interest, so it will simplify things to note that:

$$(ka)^2 + (\kappa a)^2 = \frac{-2mEa^2}{\hbar^2} + \frac{2m(E + V_0)a^2}{\hbar^2} = \frac{2mV_0a^2}{\hbar^2} \equiv z_0^2$$

The derivative is:

$$\frac{d\psi}{dx} = \begin{cases} -\kappa B e^{-\kappa x} & x > a \\ -kD \sin(kx) & 0 \leq x \leq a \end{cases}$$

which both must be continuous at $x = a$, so:

$$\begin{aligned} -\kappa B e^{-\kappa a} &= -kD \sin(ka) \\ \kappa B e^{-\kappa a} &= kD \sin(ka) \\ (\kappa a) B e^{-\kappa a} &= (ka) D \sin(ka) \end{aligned}$$

where we have multiplied by a so that the equation is in terms of the dimensionless constants ka and κa . Dividing by Equation 2.78 we obtain:

$$\begin{aligned} \kappa a &= (ka) \tan(ka) \\ \sqrt{z_0^2 - (ka)^2} &= (ka) \tan(ka) \\ \sqrt{z_0^2 - z^2} &= z \tan(z) \end{aligned}$$

where we have defined

$$z \equiv ka = \frac{\sqrt{2m(E + V_0)}a}{\hbar}$$

and so finally:

$$\sqrt{\left(\frac{z_0}{z}\right)^2 - 1} = \tan(z) \quad (2.79)$$

This is an equation with no known algebraic solution. It can be solved graphically or numerically. See Fig. 2.1. There are some interesting limiting cases to consider. When:

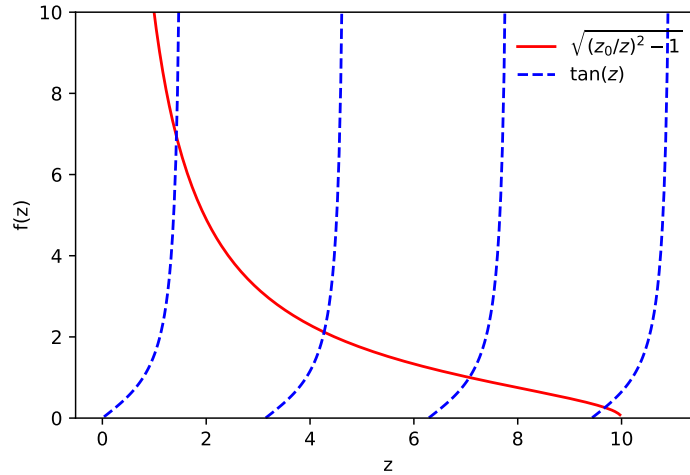


Figure 2.1: The allowed energies for the finite potential occur at the intersection of these curves.

$$z_0 < \frac{\pi}{2}$$

there is only one bound state (we haven't found the odd solutions yet, which is why this is $\pi/2$ and not π , as you might expect from the figure...) Recalling the definition for z_0 , this amounts to:

$$V_0 a^2 < \frac{\pi^2 \hbar^2}{8m}$$

which defines a shallow and narrow well.

Alternative, if z_0 is very large, then the intersection points are at:

$$z = \frac{n\pi}{2}, \quad n = 1, 3, 5, \dots$$

which means the allowed energies are:

$$E + V_0 = \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2}$$

which (relative to the bottom of the well) are the energies of the infinite square well.

2.31 Scattering States of the Finite Square Well

For $E > 0$, we have only free particle solutions, but with two different wave numbers, so we'll take:

$$k \equiv \frac{\sqrt{2mE}}{\hbar}, \quad \text{and} \quad k' \equiv \frac{\sqrt{2m(E + V_0)}}{\hbar}$$

with:

$$\frac{k'}{k} = \sqrt{\frac{E + V_0}{E}} \equiv \eta$$

and so:

$$k' = \eta k$$

Note that if this was an optics problem we would call η the refractive index. The piecewise general solution to the TISE is:

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < -a \\ Ce^{i\eta kx} + De^{-i\eta kx} & -a \leq x \leq a \\ Fe^{ikx} + Ge^{-ikx} & x > a \end{cases}$$

but we are going to write it this way instead:

$$\psi(x) = \begin{cases} Ae^{ik(x+a)} + Be^{-ik(x+a)} & x < -a \\ Ce^{i\eta kx} + De^{-i\eta kx} & -a \leq x \leq a \\ Fe^{ik(x-a)} + Ge^{-ik(x-a)} & x > a \end{cases}$$

which will make it much easier to evaluate at the boundaries ($x = \pm a$). We are free to do this because:

$$Ae^{ik(x+a)} = (Ae^{ika})e^{ikx}$$

where A is a constant we have not yet determined. The derivative is:

$$\frac{d\psi}{dx} = \begin{cases} ik(Ae^{ik(x+a)} - Be^{-ik(x+a)}) & x < -a \\ i\eta k(Ce^{i\eta kx} - De^{-i\eta kx}) & -a \leq x \leq a \\ ik(Fe^{ik(x-a)} - Ge^{-ik(x-a)}) & x > a \end{cases}$$

Define:

$$\alpha \equiv e^{i\eta ka}$$

and note that:

$$|\alpha|^2 = 1$$

which will be useful later. Now the four continuity equations are:

$$\begin{aligned} A + B &= C\alpha^* + D\alpha \\ A - B &= \eta(C\alpha^* - D\alpha) \\ C\alpha + D\alpha^* &= F + G \\ \eta(C\alpha - D\alpha^*) &= F - G \end{aligned}$$

The incoming waves are A and G . In principle, we can use two equations to eliminate the intermediate waves C and D . Then we can use the remaining two to calculate the outgoing waves B and F from the incoming waves A and G .

Note that the first two equations can be added to eliminate B :

$$A = \frac{(\eta + 1)\alpha^*}{2} C - \frac{(\eta - 1)\alpha}{2} D$$

But now let's make our lives a little easier and set $G = 0$. Then the last two equations become:

$$\begin{aligned}\alpha C + \alpha^* D &= F \\ \eta \alpha C - \eta \alpha^* D &= F\end{aligned}$$

Which we use to solve for C and D in terms of F :

$$C = \frac{\eta + 1}{2\eta} \alpha^* F$$

and:

$$D = \frac{\eta - 1}{2\eta} \alpha F$$

Plugging these back in to our expression for A :

$$\begin{aligned}A &= \frac{(\eta + 1)^2 (\alpha^2)^* - (\eta - 1)^2 \alpha^2}{4\eta} F \\ &= \frac{\eta^2 + 1}{2\eta} \frac{(\alpha^2)^* - \alpha^2}{2} + \frac{(\alpha^2)^* + \alpha^2}{2}\end{aligned}$$

Recalling our definition for α :

$$A/F = \cos(2\eta ka) - i \frac{\eta^2 + 1}{2\eta} \sin(2\eta ka)$$

and so the transmission is:

$$\frac{1}{T} = 1 + \frac{\eta^2 - 1}{4\eta^2} \sin^2(2\eta ka)$$

Notice that the transmission is one when either:

$$\eta = 1$$

which corresponds to no change in index of refraction, i.e. $V_0 = 0$. Or:

$$\sin^2(2\eta ka)$$

that is when:

$$2a \frac{\sqrt{2m(E + V_0)}}{\hbar} = n\pi$$

or:

$$E + V_0 = \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2}$$

which you may recognize as the allowed energies from the infinite potential well.

2.32 The WKB Approximation and the “Classical” Region

The inspiration for this approximation comes from the free particle, with wave function:

$$\psi(x) = A \exp(\pm i k x)$$

Consider a particle in a region where the potential V is constant, and $E > V$. Then the wave function is the same as the free particle but with:

$$k = \sqrt{2m(E - V)}/\hbar$$

We are going to try to extend this solution to the case that the potential is slowly varying. By slowly, we mean that $\psi(x)$ oscillates many times before the potential changes significantly. In this case, we anticipate that $\psi(x)$ will continue to oscillate, but the amplitude and phase will change slowly. We will therefore look for solutions of the form:

$$\Psi(x) = A(x) e^{i\phi(x)} \quad (2.80)$$

where:

$$A(x) \in \mathbb{R}, \quad \text{and} \quad \phi(x) \in \mathbb{R}$$

Our approximation is that $A(x)$ is slowly varying, in the sense that:

$$\left| \frac{1}{A} \frac{d^2 A}{dx^2} \right| \ll \left| \frac{1}{\psi} \frac{d^2 \psi}{dx^2} \right|$$

In a region where $E > V(x)$ we can write the SE as:

$$\frac{d^2 \psi}{dx^2} = -\frac{p^2(x)}{\hbar^2} \psi(x) \quad (2.81)$$

where

$$p(x) = \sqrt{2m(E - V(x))}$$

And so we can write our approximation as:

$$\left| \frac{A''}{A} \right| \ll \left| \frac{\psi''}{\psi} \right| = \frac{p^2(x)}{\hbar^2}$$

Returning to:

$$\psi(x) = A(x) e^{i\phi(x)}$$

we have:

$$\frac{d\psi}{dx} = (A' + i A \phi') e^{i\phi(x)}$$

and:

$$\begin{aligned} \frac{d^2 \psi}{dx^2} &= \{A'' + i A' \phi' + i A \phi'' + (A' + i A \phi') i \phi'\} e^{i\phi(x)} \\ &= \left\{ \left(A'' - A (\phi')^2 \right) + i (2 A' \phi' + A \phi'') \right\} e^{i\phi(x)} \\ -\frac{p^2}{\hbar^2} A &= \left(A'' - A (\phi')^2 \right) + i (2 A' \phi' + A \phi'') \end{aligned}$$

where in the last line we have used Equation 2.81. Since A and ϕ are real, this amounts to two equations (one for the real and one for the imaginary part):

$$-\frac{p^2}{\hbar^2} A = \left(A'' - A (\phi')^2 \right) \quad (2.82)$$

and

$$2A'\phi' + A\phi'' = 0 \quad (2.83)$$

We first solve Equation 2.83 by noting:

$$(A^2\phi')' = (2AA'\phi' + A^2\phi'') = A(2A'\phi' + A\phi'') = 0$$

So:

$$A^2\phi' = C^2$$

and:

$$A(x) = \frac{C}{\sqrt{\phi'}}$$

so we need only find $\phi(x)$ and we will have $A(x)$. That should come from solving Equation 2.83 which we write as:

$$(\phi')^2 = \frac{p^2}{\hbar^2} + \frac{A''}{A}$$

We cannot solve this in general, but we have already decided to make the approximation that $A(x)$ is varying slowly:

$$\left| \frac{A''}{A} \right| \ll \frac{p^2}{\hbar^2}$$

This approximation leads to:

$$\begin{aligned} (\phi')^2 &= \frac{p^2}{\hbar^2} \\ \frac{d\phi}{dx} &= \pm \frac{p}{\hbar} \end{aligned}$$

and so:

$$A(x) = \frac{C}{\sqrt{\phi'}} = \frac{C\sqrt{\hbar}}{\sqrt{p(x)}}$$

Integrating ϕ' we get:

$$\phi(x) = \pm \frac{i}{\hbar} \left(\int p(x) dx + D \right)$$

where D is a constant of integration. Assembling this all together we get:

$$\psi(x) = \frac{C\sqrt{\hbar}e^{\pm iD/\hbar}}{\sqrt{p(x)}} \exp\left(\pm \frac{i}{\hbar} \int p(x) dx\right)$$

which we can write as:

$$\psi(x) = \frac{C}{\sqrt{p(x)}} \exp\left(\pm \frac{i}{\hbar} \int p(x) dx\right) \quad (2.84)$$

where C here is a new complex constant. Notice that:

$$|\psi(x)|^2 = \frac{|C|^2}{p(x)}$$

2.33 Bound states of an Infinite Square Well with a Bumpy Bottom

Consider the example of the an infinite square well with some function $f(x)$ along the bottom (instead of $V(x) = 0$) for $0 < x < a$. The WKB approximation gives us the general solution:

$$\psi(x) = \frac{1}{\sqrt{p(x)}} \left(C e^{i\phi(x)} + D e^{-i\phi(x)} \right)$$

where we calculate:

$$\phi(x) = \frac{1}{\hbar} \int_0^x p(x) dx$$

Notice that we are free to choose the starting point for integration, and we need only take the postive version, since we've included $\pm\phi(x)$ in the general solution. Since $\phi(0) = 0$, and we must have $\psi(0) = 0$, then we have:

$$C + D = 0 \implies D = -C$$

and so:

$$\psi(x) = \frac{C}{\sqrt{p(x)}} \left(e^{i\phi(x)} + D e^{-i\phi(x)} \right) = \frac{i 2 C}{\sqrt{p(x)}} \sin(\phi(x))$$

which we can write as:

$$\psi(x) = \frac{C}{\sqrt{p(x)}} \sin(\phi(x))$$

by absorbing other factors into the constant C . Now we must also have:

$$\psi(x) = 0$$

which we requires that:

$$\phi(x) = n\pi$$

or:

$$\int_0^a p(x) dx = n\pi\hbar$$

Notice that for $V(x) = 0$ we have $p(x) = \sqrt{2mE}$ and so:

$$\int_0^a p(x) dx = \sqrt{2mE}a = n\pi\hbar$$

or:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2 m a^2}$$

2.34 Tunneling in the WKB Approximation

2.35 The Fourier Transform Revisited

Our inner product now extends between positive and negative infinity:

$$\langle \Psi, \phi \rangle \equiv \int_{-\infty}^{\infty} \Psi^*(x) \phi(x) dx \tag{2.85}$$

Our basis functions, which are now defined for any value of k ,

$$e_k = \frac{1}{\sqrt{2\pi}} \exp(ikx) \quad (2.86)$$

are still orthonormal, but the condition looks a bit different in the continuum case:

$$\langle e_k, e_{k'} \rangle = \delta(k - k')$$

See the appendix for more details on the Dirac delta function $\delta(x)$, which is zero everywhere but at $x = 0$, where it is infinite. It is the continuous version of δ_{nm} .

Our basis functions are also still complete. In the discrete case we have a complex Fourier coefficient for every integer n . Now we have a complex Fourier coefficient for any real value of k . In place of Fourier coefficients, we have instead a function of k which we call the Fourier transform: $\tilde{\Psi}(k)$. Instead of a sum over discrete terms, we now have to integrate over all values of k :

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\Psi}(k) \exp(ikx) dk. \quad (2.87)$$

Just as in the discrete case, we determine the Fourier transform from the inner product:

$$\tilde{\Psi}(k) = \langle e_k, \Psi \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x) \exp(-ikx) dx \quad (2.88)$$

Equation 2.88 is generally referred to as the *Fourier Transform*, while Equation 2.87 is referred to as the *Inverse Fourier Transform*.

2.36 The Fourier Transform in Quantum Mechanics

So far we have been considering the Fourier transform with respect to position x and wave-number k . A much more useful pair of variables for Quantum Mechanics turns out to be momentum p and position x . To relate p to k we need only apply the DeBroglie relation to the wavelength in the definition of the wavenumber:

$$k \equiv \frac{2\pi}{\lambda} = \frac{2\pi p}{h} = \frac{p}{\hbar}$$

We could therefore make the substitution $k \rightarrow p/\hbar$ (and $dk \rightarrow dp/\hbar$) in Equations 2.87 and 2.88. It turns out that a marginally more useful equation results if we make the normalization factors symmetric, by splitting the normalization factor of $1/\hbar$ across both equations with $1/\sqrt{\hbar}$ applied to each:

$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \tilde{\Psi}(p) \exp(ipx/\hbar) dp \quad (2.89)$$

$$\tilde{\Psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x) \exp(-ipx/\hbar) dx \quad (2.90)$$

The major benefit of this symmetric form is that the normalization of $\Psi(x)$ and $\tilde{\Psi}(p)$ in this case turns out to be the same:

$$\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = \int_{-\infty}^{\infty} |\tilde{\Psi}(p)|^2 dp = 1$$

Because we can always calculate $\Psi(x)$ from $\tilde{\Psi}(p)$ either one completely describes the quantum mechanical state. We call $\tilde{\Psi}(p)$ the momentum wave function. Whereas $|\Psi(x)|^2$ gives us the probability density for the quanton to be at position x , $|\tilde{\Psi}(p)|^2$ gives us the probability density for the quanton to have momentum p .