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, than 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 $+\epsilon$:

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

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

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

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

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

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 $\epsilon \to 0$:

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

2.27 The Dirac Delta Function

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

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

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

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

Also, changing variables to make the subsitutions 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:

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

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:

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

but what are we to make of $\delta(0)$? At best, we could say it is in infinity. Mathematician's 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 it's 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.

$$V(x) = -\alpha\delta(x) \tag{2.77}$$

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:

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

which has general solutions:

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

But for the wave function to be well defined only:

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

and

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

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:

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

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

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

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:

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

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 $x < 0$:

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

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:

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

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:

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

similarlyy:

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

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:

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

So we can read off the solutions for this case by putting $\beta \to -\beta$ 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 The Finite Square Well

2.31 The WKB Approximation and the "Classical" Region

2.32 Tunneling in the WKB Approximation

2.33 The Fourier Transform Revisited

Our inner product now extends between positive and negative infinity:

$$\langle \Psi, \phi \rangle \equiv \int_{-\infty}^{\infty} \Psi^*(x)\phi(x)\,dx \tag{2.78}$$

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

$$e_k = \frac{1}{\sqrt{2\pi}} \exp(ikx) \tag{2.79}$$

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

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

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: $\widetilde{\Psi}(k)$. Instead of a sum over discrete terms, we now have to integrate over all values of k:

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{\Psi}(k) \exp(ikx)\, dk. \tag{2.80}$$

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

$$\widetilde{\Psi}(k) = \langle e_k, \Psi \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x) \exp(-ikx)\, dx \tag{2.81}$$

Equation 2.81 is generally referred to as the *Fourier Transform*, while Equation 2.80 is referred to as the *Inverse Fourier Transform*.

2.34 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 $k \to p/\hbar$ (and $dk \to dp/\hbar$)) in Equations 2.80 and 2.81. 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:

$$\Psi(x) \quad = \quad \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widetilde{\Psi}(p) \exp(ipx/\hbar)\, dp \tag{2.82}$$

$$\widetilde{\Psi}(p) \quad = \quad \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x) \exp(-ipx/\hbar)\, dx \tag{2.83}$$

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

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

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