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:

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

and

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

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 Bound States of the Finite Square Well

Next we consider the finite square well potential:

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

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:

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

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:

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

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:

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

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

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

and so finally:

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

(Interpretation, Limiting cases...)

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:

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

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:

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

but we are going to write it this way instead:

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

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:

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

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 know 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 at the allowed energies from the infinite potential well.

2.32 save...

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

Also, since:

$$(k'a)^2 - (ka)^2 = \frac{2mV_0a^2}{\hbar^2} \equiv z_0^2$$

it's related to our previous constant by:

$$n^2 - 1 = (z_0/z)^2$$

2.33 The WKB Approximation and the "Classical" Region

2.34 Tunneling in the WKB Approximation

2.35 The Fourier Transform Revisited

Our inner product now extends between positive and negative infinity:

$$\langle \Psi, \phi \rangle \equiv \int_{-\infty}^{\infty} \Psi^*(x)\phi(x)\, dx \tag{2.80}$$

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

$$e_k = \frac{1}{\sqrt{2\pi}} \exp(ikx) \tag{2.81}$$

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

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{\Psi}(k) \exp(ikx)\, dk. \tag{2.82}$$

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

$$\widetilde{\Psi}(k) = \langle e_k, \Psi \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x) \exp(-ikx)\, dx \tag{2.83}$$

Equation 2.83 is generally referred to as the *Fourier Transform*, while Equation 2.82 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 $k \to p/\hbar$ (and $dk \to dp/\hbar$)) in Equations 2.82 and 2.83. 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:

$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \widetilde{\Psi}(p) \exp(ipx/\hbar)\, dp \tag{2.84}$$

$$\widetilde{\Psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x) \exp(-ipx/\hbar)\, dx \tag{2.85}$$

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.