4	Wed. 9/24 Fri., 9/26	**2.5** Scattering from the Delta Potential (Q7.1, Q11) **Computational:** Time-Dependent Discrete Schro ***Science Poster Session**: Hedco7pm~9pm* **2.6** The Finite Square Well (Q 11.1-.4) beginning	**Daily 4.W** **Daily 4.F**
5	Mon. 9/29 Tues 9/30 Wed. 10/1 Fri. 10/3	**2.6** The Finite Square Well (Q 11.1-.4) continuing **Review** Ch 1 & 2 **Exam 1** (Ch 1 & 2)	**Daily 5.M** **Weekly 5** **Daily 5.W**

Equipment

- Load our full Python package on computer
- Comp 5: discrete Time-Dependent Schro
- Griffith's text
- Moore's text
- Printout of roster with what pictures I have

Check dailies

Announcements:

Daily 4.W Wednesday 9/24 **Griffiths 2.5** Scattering from the Delta Potential (Q7.1, Q11)

1. *Conceptual*: State the rules from Q11.4 in terms of mathematical equations. Can you match the rules to equations in Griffiths? If you can, give equation numbers.

7. *Starting Weekly, Computational*: Follow the instruction in the handout "Discrete Time-Dependent Schrodinger" to simulate a Gaussian packet's interacting with a delta-well.

2.5 The Delta-Function Potential

2.5.1 Bound States and Scattering States

1. *Conceptual*: Compare Griffith's definition of a bound state with Q7.1.
2. *Conceptual*: Compare Griffith's definition of tunneling with Q11.3.
3. *Conceptual*: Possible energy levels are quantized for what kind of states (bound, and/or unbound)? Why / why not?

Griffiths seems to bring up scattering states out of nowhere. By scattering does he just mean transmission and reflection?" Spencer

2.5.2 The Delta-Function

Recall from a few days ago that we'd encountered

$$2\frac{\sin\left((k-k_o)a\right)}{(k-k_o)} = \begin{cases} 0 & \text{for } k \neq k_o \\ 2a & \text{for } k = k_o \end{cases}$$

When we were dealing with the free particle, and we were planning on eventually sending the width of our finite well to infinity to arrive at the solution for the infinite well.

$$a \to \infty$$

In fact, the context of this relation was

$$\int_{-\infty}^{\infty} \tilde{\psi}_{k_o}^*(x)\Psi(x,0)_{particle}dx = \lim_{a\to\infty}\left(\sum_k \phi(k)\sqrt{\frac{1}{2\pi}}\left(2\frac{\sin((k-k_o)a)}{(k-k_o)}\right)\left(\frac{\pi}{a}\right)\right) = \phi(k_o)$$

In that limit, what we had our hands was

$$\int_{-\infty}^{\infty} \tilde{\psi}_{k_o}^*(x)\Psi(x,0)_{particle}dx = \int_{-\infty}^{\infty}\phi(k)\left(\lim_{a\to\infty}\sqrt{\frac{2}{\pi}}\frac{\sin((k-k_o)a)}{(k-k_o)}\right)dk = \phi(k_o)$$

In other words

$$\delta(k-k_o) = \lim_{a\to\infty}\sqrt{\frac{2}{\pi}}\frac{\sin((k-k_o)a)}{(k-k_o)}$$

Regardless of how you construct it, the thing about Dirac Delta functions is the effect they have on the integrals they're in. As in this case,

$$\int_{-\infty}^{\infty}\phi(k)\delta(k-k_o)dk = \phi(k_o)$$

It plucks out the integrand evaluated at just one single location.

2. *Starting Weekly HW*: (2.23)Evaluate the following integrals:

    a. $\int_{-3}^{+1}(x^3-4x^2+3x-2)\delta(x+1)dx$

    b. $\int_{0}^{\infty}[\cos(2x)+5]\delta(x-\pi)dx$

    c. $\int_{-3}^{+1}e^{(|x|+6)}\delta(x-4)dx$

We essentially derived such a beast and used it for relating the free particle's wave function and its 'density of states'.

Here, we're going to use it to define a potential well, so we can see the stark difference between *scattering* and *bound* states without the overhead of a particularly complicated potential.

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

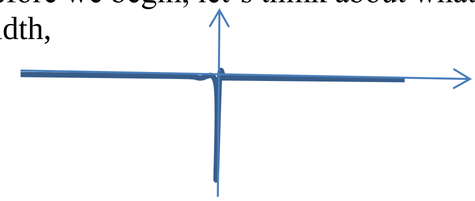
Defines a potential well at the origin of 'strength' α.

Schrodinger Equation

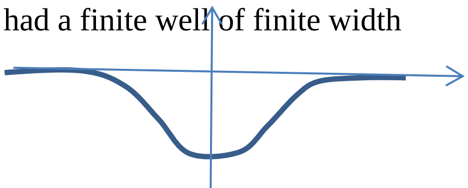
$$\psi_k(x)E_k = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_k(x) + V(x)\psi_k(x)$$

$$\psi_k(x)E_k = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_k(x) - \alpha\delta(x)\psi_k(x)$$

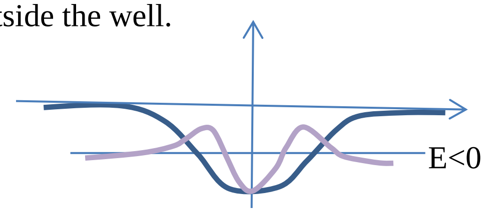
Before we begin, let's think about what we'd expect if instead of an infinite well of infinitesimal width,

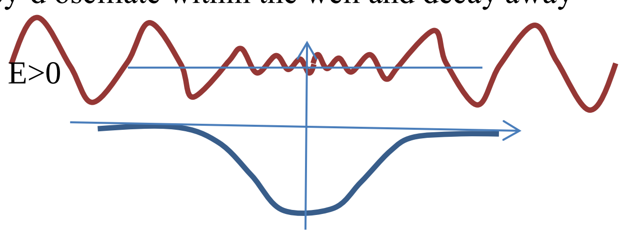


We had a finite well of finite width



We'd expect to see **bound** states for E < 0; they'd oscillate within the well and decay away outside the well.





We'd also expect to see **scattering** states for E>0; they'd oscillate outside the well with one amplitude and wavelength, and inside the well with smaller amplitude and shorter wavelength (as the kinetic energy would increase).

Bound States

Now imagine narrowing and deepening the well until there's simply no room *inside* it anymore. We'll consider the **bound** state first.

The well breaks up space into two free regions, to the left and right, so it makes sense to start out defining the wavefunction piecewise.

x<0

Anywhere to the left of the well,

$$\psi_k(x)E_k = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_k(x)$$

so the obvious solutions are

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

Plugging those in, we get the usual $k = \sqrt{2mE_k}/\hbar$.

However, if we are explicitly looking for *bound* states with $E_k<0$, then there's – sign hiding under the square root. Making that explicit,

$$E_k = -|E_k|$$

so

$$k = \sqrt{-2m|E_k|}/\hbar = i\sqrt{2m|E_k|}/\hbar$$

Defining

$$\kappa \equiv \sqrt{2m|E_k|}/\hbar,$$

then

$$k = i\kappa,$$

and plugging this back into our solutions to make the behavior more obvious,

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

So, we have exponential growth and decay.

Dead at infinity. The wavefunction needs to decay away to 0 at –infinity to be normalizable, so apparently, a = 0 since the first term won't do that for negative x.

$$\psi_{left}(x) = Be^{\kappa x}$$

x>0

On the other side of the well, the same reasoning must apply:

$$\psi_{right}(x) = Fe^{-\kappa x} + Ge^{\kappa x}$$

however, now to decay away to 0, it's *G* that must be 0 for positive x to take this to 0 at positive infinity.

$$\psi_{right}(x) = Fe^{-\kappa x}$$

Continuous

"Can we talk about why the wavefunction being continuous means that F=B for equation 2.122?"

Jessica

Now, we say that the wavefunction must be continuous, that is, approached from the left and the right, it must approach the same value in the middle:

$$\psi_{left}(0) = \psi_{right}(0)$$

$$Be^{\kappa 0} = Fe^{-\kappa 0}$$

$$B = F$$

So there wavefunction can be concisely written as

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

Now, *why* must the wavefunction be continuous in this way? The alternative is that it is essentially double valued at the joint between two regions, and given that the square of the thing is a probability density, having a double-valued probability makes no sense. (Note: this argument does not preclude it's differing by some phase since the phase cancels out when we square the wavefunction.) We'll return to the continuity condition later.

To polish off this wavefunction, we can normalize:

$$1 = \int_{-\infty}^{\infty} \psi^2(x)dx = \int_{-\infty}^{\infty} B^2 e^{-2\kappa|x|}dx = 2\int_{0}^{\infty} B^2 e^{-2\kappa|x|}dx = -\frac{2B^2}{2\kappa}\left(e^{-\infty} - e^{-0|}\right) = \frac{B^2}{\kappa} \Rightarrow B = \sqrt{\kappa}$$

As for finding that k value, we need one more condition to satisfy.

Derivative of wavefunction.

Griffiths suggests integrating Schrodinger's equation across the vanishingly-small width of the potential well to see what condition is on the derivative of the wavefunction.

$$\lim_{\varepsilon\to 0}\left(\int_{-\varepsilon}^{\varepsilon} \psi_k(x)\frac{2m}{\hbar^2}V(x)dx - \int_{-\varepsilon}^{\varepsilon} \psi_k(x)\frac{2m}{\hbar^2}E_k dx = \int_{-\varepsilon}^{\varepsilon} \frac{d^2\psi_k(x)}{dx^2}dx\right)$$

Sending the width of integration to 0, the middle term vanishes since it's something headed to 0 times a finite value;

$$\lim_{\varepsilon\to 0}\left(\int_{-\varepsilon}^{\varepsilon} \psi_k(x)\frac{2m}{\hbar^2}V(x)dx = \left.\frac{d\psi_k(x)}{dx}\right|_{-\varepsilon}^{\varepsilon}\right)$$

For a ***finite* potential**, the shrinking width of the left integral kills it too, and one's left with

$$\lim_{\varepsilon\to 0}\left(\left.\frac{d\psi_k(x)}{dx}\right|_{\varepsilon} - \left.\frac{d\psi_k(x)}{dx}\right|_{-\varepsilon} = 0\right)$$

Which would tell us that the derivative must be continuous.

However, for our *infinite* potential

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

$$-Be^{\kappa 0}\frac{2m}{\hbar^2}\alpha = \left(-B\kappa e^{-\kappa 0}\right) - \left(B\kappa e^{\kappa 0}\right)$$

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

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

So, returning to our energy relation,

$$\kappa \equiv \sqrt{2m|E_k|}/\hbar = \sqrt{-2mE_k}/\hbar \Rightarrow E_k = -\frac{\hbar^2\kappa^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}$$

For that matter, then our wavefunction is

$$\psi(x) = Be^{-\kappa|x|} = \sqrt{\kappa}e^{-\kappa|x|} = \frac{\sqrt{m\alpha}}{\hbar}e^{-\frac{m}{\hbar^2}\alpha|x|}$$

1. *Starting Weekly HW*: (2.27) Consider the double delta-function potential $V(x) = -\alpha[\delta(x+a)+\delta(x-a)]$, where α and a are positive constants.
    a. Sketch this potential.
    b. Write the schrodinger equation in each of the three regions.
    c. What is the solution to each of these differential equations?
    d. What are the boundary conditions?
    e. Does problem 2.1(c) apply here? Does it help?
    d. Write the possible solutions for ψ(x).
    e. How many bound states are there?

"Could we go over something similar to part d of number 2 on the weekly. I am not sure how to sew the boundary conditions together." Kyle B,

we also go over the symmetry of that delta potential? In addition as to why the middle region behave as hyperbolic functions rather than trigonometric. Jeremy,

Scattering States

Now, all this was assuming that the energies were negative. If we go back to the beginning and assume that they're *positive,* we should get the behavior of 'scattering states'.

$$\psi_{left}(x) = Ae^{ikx} + Be^{-ikx} \text{ and } \psi_{right}(x) = Fe^{ikx} + Ge^{-ikx}$$

Now, we apply our boundary conditions:

Dead at Infinity. Actually, we're going to defer this one, since we already know that a single energy state *isn't* normalizable, but a linear combination will be.

Continuous across the barrier.

$$\psi_{left}(0) = \psi_{right}(0)$$
$$A + B = F + G \quad \text{(a)}$$

Derivative's discontinuity across barrier.
Just a few moments ago, we'd integrated the Schrodinger equation across the barrier and quit generally arrived at

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

$$-\psi_k\frac{2m}{\hbar^2}\alpha = \left.\frac{d\psi_k}{dx}\right|_{\varepsilon} - \left.\frac{d\psi_k}{dx}\right|_{-\varepsilon}$$

So the derivative is discontinuous, there's kink in the function, at the well.

Plugging in our solution

$$-(A+B)\frac{2m}{\hbar^2}\alpha = ik(F-G)-ik(A-B)$$

Or

$$-(A+B)\frac{2m}{\hbar^2}\alpha = ik(F-G)-ik(A-B)$$

$$i(A+B)\left(\frac{2m}{k\hbar^2}\alpha\right) = (F-G)-(A-B)$$

$$(F-G) = A\left(1+i2\frac{m}{k\hbar^2}\alpha\right) - B\left(1-i2\frac{m}{k\hbar^2}\alpha\right) \qquad \text{(b)}$$

So, we have two equations relating the four unknowns and also the *k*'s.

This isn't as bad as it looks because forming some initial wave packet will determine the relative mixes of the components headed in different directions. However, we can get a bit further with just these two if we consider a specific scenario:

Scattering from Left
Classically, imagine a traveling wave coming from the left

Ae^{ikx} inbound

It would reflect and transmit at the barrier

Be^{-ikx} reflect and Fe^{ikx} transmit

So, in this scenario, G = 0.
Then our two relations simplify to

$$A+B=F \quad \text{And} \quad F = A\left(1+i2\frac{m}{k\hbar^2}\alpha\right) - B\left(1-i2\frac{m}{k\hbar^2}\alpha\right)$$

So we can, between these two relations express the amplitude of the *transmitted* and the *reflected* waves relative to that of the inbound wave

Substituting out B, we have

$$F = A\left(1+i2\frac{m}{k\hbar^2}\alpha\right)-(F-A)\left(1-i2\frac{m}{k\hbar^2}\alpha\right)$$

$$F\left(2-i2\frac{m}{k\hbar^2}\alpha\right) = A\left(1+i2\frac{m}{k\hbar^2}\alpha\right)+A\left(1-i2\frac{m}{k\hbar^2}\alpha\right)$$

$$F\left(2-i2\frac{m}{k\hbar^2}\alpha\right) = A2$$

$$F = A\frac{1}{\left(1-i\frac{m}{k\hbar^2}\alpha\right)} = A\frac{1+i\frac{m}{k\hbar^2}\alpha}{\left(1+\left(\frac{m}{k\hbar^2}\alpha\right)^2\right)}$$

Similarly,

$$A+B = A\left(1+i2\frac{m}{k\hbar^2}\alpha\right)-B\left(1-i2\frac{m}{k\hbar^2}\alpha\right)$$

$$B\left(2-i2\frac{m}{k\hbar^2}\alpha\right) = A\left(i2\frac{m}{k\hbar^2}\alpha\right)$$

$$B = A\frac{\left(i\frac{m}{k\hbar^2}\alpha\right)}{\left(1-i\frac{m}{k\hbar^2}\alpha\right)} = -A\frac{1}{\left(1+i\frac{k\hbar^2}{m\alpha}\right)} = -A\frac{\left(1-i\frac{k\hbar^2}{m\alpha}\right)}{\left(1+\left(\frac{k\hbar^2}{m\alpha}\right)^2\right)}$$

'Could we go over something similar to part d of number 2 on the weekly. I am not sure how to sew the

Kyle B, AHoN Hide response Post a response

Admin

I agree, could we also go over the symmetry of that delta potential? In addition as to why the middle region
than trigonometric.

Jeremy, Redlands, CA