2.6 The Finite Square Well (Q 11.1-.4) beginning

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.F Friday 9/26 Griffiths 2.6 The Finite Square Well (Q 11.1-.4) beginning
1. Conceptual: What physical properties determine the number of bound states in a finite well?
2. Starting Weekly HW (2.34): Consider the “step” potentials:

\[ V(x) = \begin{cases} 
0, & \text{if } x \leq 0 \\
V_0, & \text{if } x > 0 
\end{cases} \]

\[ V(x) = \begin{cases} 
V_0, & \text{if } x \leq 0 \\
0, & \text{if } x > 0 
\end{cases} \]

a. Conceptual/Computational: In your DiscretePIB.py program, define a step potential (though it will be convenient to move the border to \( j = N/2 \) rather than 0). I suggest a height of \( V_0 \) around 0.05 so you can easily get some wave functions with energies below and some with energies above. So, define

```python
# step potential well
def V(j):
    V = 0
    if j > N/2:  # flipping inequality will flip which half of the space has the barrier
        V = 0.05  # barrier height
    return V
```

Run this for the first few wavefunctions so you can see the qualitative behavior. (This is due with conceptual questions.)

b. Show that the reflection coefficients for the two cases are equal when \( E > V_0 \).
   i. Start by doing the first case. How many regions are you using? What are your boundary conditions?
   ii. Write the Schrödinger equation in each region and solve. Solutions should be exponentials, not sines and cosines. You should be using \( k \) from equation 2.130 and \( l \) similar to (but not exactly) equation 2.148. Careful when defining these in terms of \( E \) and \( V_0 \).
   iii. Label your diagrams in part (h) with coefficients like in figure 2.15.
Assume wave enters from left. What goes to zero?
iv. Apply boundary conditions and calculate the reflection coefficient.
v. Repeat above for other case.
c. What happens when \( E < V_0 \)? Show calculation and comment on solution. Do only for the first case.

2.6 The Finite Square Well Potential

Conceptual: What physical properties determine the number of bound states in a finite well?

\[
V(x) = \begin{cases} 
-V_o & \text{for } -a \leq x \leq a \\
0 & \text{for } |x| > a 
\end{cases}
\]

Regions: Left \hspace{1cm} Middle \hspace{1cm} Right

Schrodinger Equation

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

\[
\psi_{kL}(x)E_k = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{kL}(x) \hspace{1cm} \psi_{kM}(x)E_k = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{kM}(x) - V_o\psi_{kM}(x) \hspace{1cm} \psi_{kR}(x)E_k = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{kR}(x)
\]

Bound States

1. Guess Solution

Before we guess it mathematically, it’s good to guess it conceptually, a drawing: exponentially decay away outside the well and sinusoidally oscillate within

\[
\psi_{kL}(x) = Be^{\alpha x} \hspace{1cm} \psi_{kM}(x) = C'e^{i\kappa x} + D'e^{-i\kappa x} \hspace{1cm} \psi_{kR}(x) = Fe^{-\alpha x}
\]

• Invoke Symmetry

While we could run with these three guesses, we can short-cut around some math by observing that the well is symmetric about 0, so the probability density must be also. That means that the wavefunction must be symmetric to within a sign; i.e., either
Symmetric:  
\( C' = D' \) and \( B = F \),

and of course,
\[
\psi_{kM}(x) = C'e^{ikx} + C'e^{-ikx} = 2C'e^{ikx} + e^{-ikx} = 2C' = C_S \cos(kx)
\]

\[
\psi_{s,x}(x) = \begin{cases} 
B'e^{kx} & \text{Left} \\
C_S \cos(kx) & \text{Middle} \\
B'e^{-kx} & \text{Right} 
\end{cases}
\]

or

Anti-Symmetric:  
\( C = -D \) and \( B = -F \),

and of course,
\[
\psi_{kM}(x) = C'e^{ikx} - C'e^{-ikx} = 2iC'e^{ikx} - e^{-ikx} = 2iC' = C_A \sin(kx)
\]

\[
\psi_{a,x}(x) = \begin{cases} 
B_A e^{kx} & \text{Left} \\
C_A \sin(kx) & \text{Middle} \\
-B_A e^{-kx} & \text{Right} 
\end{cases}
\]

Griffiths does the symmetric case, I’ll do the anti-symmetric.

2. Test Guess in Differential Equation

Left Solutions & Equation:  
Right Solutions & Equation:

\[
E_k \psi_{sL}(x) = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{sL}(x)
\]

\[
-|E_k| \psi_{sL}(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{sL}(x)
\]

plugging in \( \psi_{sL}(x) = Fe^{-\kappa x} \) gives the same result

\[
-|E_k| = -\frac{\hbar^2}{2m} \kappa^2 \Rightarrow \kappa = \sqrt{2m|E_k|/\hbar}
\]
Middle Solutions & Equation:

\[ E_k \psi_{LM}(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{LM}(x) - V_o \psi_{LM}(x) \]

\[ E_k C_A \sin(kx) = \frac{\hbar^2}{2m} k^2 C_A \sin(kx) - V_o C_A \sin(kx) \]

\[ V_o + E_k = \frac{\hbar^2}{2m} k^2 \]

\[ \frac{\sqrt{2m(V_o + E_k)}}{\hbar} = k \]

At this point, Griffiths defines \( \sqrt{2m(V_o + E_k)}/\hbar \equiv l \), but frankly the reason for doing so eludes me. We’re pretty used to calling this beast what it is, the wave number \( k \). And I’ll continue doing so, just be careful not to mistake it for the decay length \( \kappa \).

I agree, I am not sure why Griffiths decided to define \( z_0 = a/\hbar \sqrt{2mV_0} \), which are the equations before 2.156 on page 80 of the International Edition. Jeremy.

To make the equations look less cluttered; however, I think they make the physics less transparent, so I’m not doing that.

Something else that I want to point out, which is specific to this case, is that since \( E < 0 \), making the sign of the energy explicit, it’s easier to see that really we’ve got

\[ \sqrt{2m(V_o - |E_k|)}/\hbar = k \]

So, as usual, plugging the guessed solutions into the differential equations tells us something about one of the arbitrary constants: \( k \) for the middle region solution and \( \kappa \) for the outsides.

So, we have \( \sqrt{2m(V_o - |E_k|)}/\hbar = k \) and \( \kappa = \sqrt{2m|E_k|}/\hbar \)

It’s worth pointing out that, in terms of unknowns, we’ve just got the one, \( E_k \); if we knew that, we’d know both \( k \) and \( \kappa \).

3. Impose Boundary Conditions

a. Normalizable: \( \psi_{A,k}(\pm \infty) = 0 \) Already taken care of by our guess of exponential decay outside the well.

b. Wavefunction Continuous at boundaries:

\[ \psi_L(-a) = \psi_M(-a) \]

\[ \psi_M(a) = \psi_R(a) \]

\[ B_A e^{\kappa(-a)} = C_A \sin(k(-a)) \]

\[ B_A e^{\kappa a} = -C_A \sin(ka) \]

\[ C_A \sin(ka) = -B_A e^{-\kappa a} \text{ (same)} \]
c. Wavefunction’s Derivative Continuous at boundaries (given no delta potential)

\[
\begin{align*}
\frac{d}{dx}\psi_L(-a) &= \frac{d}{dx}\psi_M(-a) & \frac{d}{dx}\psi_M(a) &= \frac{d}{dx}\psi_R(a) \\
-kB_A e^{-\kappa x} &= -kC_A \cos(-ka) & kC_A \cos(ka) &= kB_A e^{-\kappa x} \text{ (same)}
\end{align*}
\]

So, at this moment, we have a grand total of four equations and five unknowns: \(E_k, k, \kappa, C_A, B_A\). We’ve got a choice of what algebra to do to do solve for some in terms of others. For completeness, my temptation is to impose the final ‘boundary condition’ – normalize the darn thing.

First, \(\psi_{A,k}(x) = \begin{cases} B_A e^{\kappa x} & \text{Left} \\ C_A \sin(ka) & \text{Middle} \\ -B_A e^{-\kappa x} & \text{Right} \end{cases} \)

Middle becomes \(\psi_{A,k}(x) = \begin{cases} B_A e^{\kappa x} & \text{Left} \\ -\left(\frac{B_A e^{-\kappa x}}{\sin(ka)}\right) \sin(ka) & \text{Middle} \\ -B_A e^{-\kappa x} & \text{Right} \end{cases} \)

\[
1 = \int_{-\infty}^{\infty} |\psi_{A,k}|^2 dx = \int_{-\infty}^{-a} |\psi_{A,k,L}|^2 dx + \int_{-a}^{a} |\psi_{A,k,M}|^2 dx + \int_{a}^{\infty} |\psi_{A,k,R}|^2 dx
\]

\[
1 = B_A^2 \int_{-\infty}^{-a} e^{2\kappa x} dx + B_A^2 \int_{-a}^{a} \left(\frac{e^{-2\kappa x}}{\sin^2(ka)}\right) \sin^2(ka) dx + B_A^2 \int_{a}^{\infty} e^{-2\kappa x} dx
\]

\[
1 = B_A^2 \left[ \frac{1}{2\kappa} \left( e^{-2\kappa a} - e^{-2\kappa b} \right) + \left( \frac{e^{-2\kappa a}}{\sin^2(ka)} \right) \int_{-a}^{a} \frac{1}{2} \cos(2kx) dx + \frac{1}{2\kappa} e^{-2\kappa b} - e^{-2\kappa b} \right]
\]

\[
1 = B_A^2 \left[ \frac{1}{\kappa} (e^{-2\kappa a}) + \left( \frac{e^{-2\kappa a}}{\sin^2(ka)} \right) \int_{-a}^{a} \frac{1}{2} (a - (-a)) + \frac{1}{2} \left( \sin(2ka) - \sin(2k(-a)) \right) \right]
\]

\[
1 = B_A^2 \left[ \frac{1}{\kappa} (e^{-2\kappa a}) + \left( \frac{e^{-2\kappa a}}{\sin^2(ka)} \right) \int_{-a}^{a} \frac{1}{4k} (\sin(2ka) + \sin(2ka)) \right]
\]

\[
1 = B_A^2 \left[ \frac{1}{\kappa} (e^{-2\kappa a}) + \left( \frac{e^{-2\kappa a}}{\sin^2(ka)} \right) \int_{-a}^{a} \frac{1}{2k} \sin(2ka) \right]
\]

\[
B_A = \frac{e^{\kappa a}}{\left( \frac{1}{\kappa} + \frac{2ka - \sin(2ka)}{2k \sin^2(ka)} \right)^{1/2}}
\]

4. Algebraic combinations of our equations to solve for our variables:
Solving for \(k, \kappa\)
"I am a little confused about about how we derives equation 2.156 can we go over this?"

Jessica

dividing equations 3.b and 3.c :

\[ C_A \sin (ka) = -B_A e^{-\alpha a}, \quad kC_A \cos (ka) = \kappa B_A e^{-\alpha a} \]

\[ k \tan (ka) = \kappa \]

But recall that the definitions of these two are \( \sqrt{2m(V_o - |E_k|)/\hbar} = k \) and \( \kappa = \sqrt{2m|E_k|}/\hbar \)

So,

\[ \sqrt{2m|E_k|}/\hbar \tan (a\sqrt{2m|E_k|}/\hbar) = \sqrt{2m(V_o - |E_k|)/\hbar} \]

\[ \tan (a\sqrt{2m|E_k|}/\hbar) = \sqrt{V_o - |E_k|} \]

\[ \tan (a\sqrt{2m|E_k|}/\hbar) = \sqrt{V_o - |E_k| - 1} \]

This analogous to Griffith’s equation 2.156 in terms of less compact, but more transparent variables.

Casting his equation in the same variables, you can see how the relation for the anti-symmetric solutions (which we’ve just found) differs from that for the symmetric solutions.

For Comparison: Symmetric: \( \tan (a\sqrt{2m(V_o - |E_k|)/\hbar}) = \sqrt{\frac{|E_k|}{V_o - |E_k|}} \)

Essentially, the roles of “\( z \) and \( z_o \)” are reversed.

In principle, this is the equation that solves for the allowed energies. In practice, it is a transcendental equation, so the allowed energies aren’t so easy to extract from this equation but if you knew your values for all the fixed parameters (\( a, m, V_o, \) and \( \hbar \)) it could be solved computationally. Griffiths plots the two functions and points out where they cross.

Aside from that sticky business, we’re done. We have our allowed energies, thus our \( k \) and \( \kappa \) values, thus our normalization constant. What more could we wish for?

**Scattering States**

Oh, right, that whole other family of solutions.

\( E > 0 \)

"What does Griffith’s mean when he says, "the well becomes transparent" after equation 2.169?"
In Japan, do they think of the wave coming from the right? This also brings up the question does the x-axis read positive on the left and negative on the right?"

**Kyle B.**

The choice does seem somewhat arbitrary; would it drastically alter anything if we visualize it coming from the other way?

**Bradley W**

Japan – Don’t know. The choice – no important difference. We could just as easily choose to imagine the wave coming from the right and headed to the left and get the same basic results with a few signs flipped to reflect the flip in our choice of direction. No bigger a deal than choosing a different coordinate system – the physics is the same.

1. **Guess Solution**

   By the usual convention, we’ll imagine a traveling wave inbound from the left, clearly some will get reflected back that way, some will transmit off to the right, and then something interesting may happen in the middle. So, we’ll build a guess accordingly:

   \[ \psi_k(x) = \begin{cases} 
   A e^{ikx} + B e^{-ikx} & \text{Left} \\
   C \sin(kx) + D \cos(kx) & \text{Middle} \\
   F e^{ikx} & \text{Right} 
   \end{cases} \]

   Now, it’s a bit of ‘inspiration’ that we choose to write the middle-region’s wavefunction this way, but here are a few excuses:

   1. that’s how we would have drawn it,
   2. this doesn’t actually limit the possibilities, if we guess wrong we’ll just get more awkward coefficients
   3. and it will help with the resonance phenomenon that, with Griffiths’ foresight, he sees coming.

3. **Conceptual:** How do we determine the number of scattering states?

   "I don't understand how to determine the number of scattering states, and I feel as though he glazes over the scattering states really fast. Could we go over the scattering states in class?"

   Trick question – it’s infinite.
2. Test Guess in Differential Equation

Left

\[ E_k \psi_{kl}(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{kl}(x) \]

Right

\[ E_k (A e^{ikx} + Be^{-ikx}) = \frac{\hbar^2}{2m} k^2 (A e^{ikx} + Be^{-ikx}) \]

\[ E_k = -\frac{\hbar^2}{2m} k^2 \Rightarrow k = \sqrt{2mE_k / \hbar} \]

Middle

\[ E_k \psi_{km}(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{km}(x) - V_o \psi_{km}(x) \]

\[ E_k (C \sin(k_m x) + D \cos(k_m x)) = \frac{\hbar^2}{2m} k_m^2 (C \sin(k_m x) + D \cos(k_m x)) - V_o (C \sin(k_m x) + D \cos(k_m x)) \]

\[ V_o + E_k = \frac{\hbar^2}{2m} k_m^2 \]

\[ \sqrt{2m(V_o + E_k) / \hbar} = k_m \]

3. Impose Boundary Conditions

4. Algebraic combinations of our equations to solve for our variables:
   Solving for k, k_m, and R and T
Daily 5.M Monday 9/29 Griffiths 2.6 The Finite Square Well (Q 11.1-.4) continuing

1. Conceptual: Can you come up with a “recipe” like the Q11 rules that will help with solving ANY 1D Schrödinger equation problem mathematically?
2. Conceptual: Are the following functions odd, even, or neither? Write a formula for each and plot to check yourself after you’ve given an answer.
   a. The fifth Hermite polynomial.
   b. The fourth excited state of the harmonic oscillator.
   c. \( e^{i/b} \)
   d. \( (x^5 + x^2) e^{-ax^2} \)
3. Conceptual: A particle is in a finite square well \( (V(x) \) given by eq. 2.145) with \( V_0 \) and \( a \) such that there are 11 bound states. The initial wave function of the particle is given by
   \[ \Psi(x,0) = A \left[ \frac{3}{7} \psi_1 + \frac{2}{11} \psi_3 + \frac{1}{3} \psi_4 \right] \]
   where \( \psi_1, \psi_3 \) and \( \psi_4 \) are stationary states.
   a. Find \( A \).
   b. What are the possible results of a measurement of Energy and what is the probability of measuring each one?
4. Starting Weekly, Computational: Modify your DiscretePIB.py program to handle the finite well instead. Here’s how: near the beginning add the lines

```python
#finite square well
def V(j):
    V = 0
    if j< N/3 or j > 2*N/3:  #well is central 1/3rd of simulated range
        V = 0.15  #barrier height
    return V
```
You can vary the width of the well and the height of the barriers on either side. This is essentially a finite well inside an infinite well (boundaries at \( j = 0 \) and \( j = N \)), which should work well as long as the wave functions die off well before reaching the simulations outer edges.

5. Starting Weekly HW (L7.57): Consider the following potential: \( V(x) = \begin{cases} 0, & x \leq 0 \\ V_0, & 0 < x < a \\ -\alpha V_0, & x \geq a \end{cases} \)
   a. Sketch this potential and comment on what you think will happen for \( E < V_0 \).
   b. Calculate the reflection coefficient.
6. "If we have time can we talk about simplifying the reflection coefficient for problem 5b on the weekly homework?" Jessica
7. "Is there a chance we could take some time out of lecture (or at the end of class) to get help on computational stuff? My code for #3 won’t work and I can’t figure out what it is from the handout alone." Casey P,
8. "I feel like there isn’t much to go over from the reading due monday and it really seems like it would be good to focus on stuff from the homework, specifically some computational and number 5 like Jessica suggested." Kyle B.
"If we were to have a potential well that was not symmetric such that the potential is greater on one side, would the solutions with E between the two V levels be considered a scattering state? Something similar to (6 from Daily 3.F 9/19).  

Spencer

Could we also go over in what cases we should be using k, κ and ℓ and if they should also include i?