Equipment

- Load our full Python package on computer
- Discrete Finite Well.py & DiscretePIB.py
- Griffith’s text
- Moore’s text
- Printout of second computational reading.
- Printout of roster with what pictures I have

Check dailies

Things we’ve acquired so far and will use today:

Statistical Interpretation

\[ |\Psi(x,t)|^2 = \text{Probability Density} \]

\[ \langle Q(x,p) \rangle = \int \Psi_n^*(x,t)Q\left(x,\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi_n(x,t)dx \]

\[ \hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x} \]

Time-Independent Schrodinger Equation

\[ i\hbar \frac{\partial}{\partial t} \Psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x,t) + V(x)\Psi(x,t) \]

\[ \Psi_n(x,t) = \psi_n(x)\varphi_n(t) \]

\[ i\hbar \frac{\partial}{\partial t} \varphi_n(t) = E\varphi_n(t) \]

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

\[ \varphi_n(t) = e^{-\frac{E_n t}{\hbar}} \]

2.3 The Harmonic Oscillator

As you’re familiar from classical mechanics, \( V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2 \). Before launching into quantum mechanics, Griffiths extols the virtues of this potential: whether you’ve really got a potential of this form, or you’ve got most any complicated potential that has a local minimum (that is, a corresponding
force with a stable equilibrium point), for relatively small deviations from that minimum / equilibrium point, the Taylor Series approximation looks like this. So, it’s ubiquitous.

So the (time independent portion of the) Schrodinger Equation for this potential is

$$\psi_n(x)E = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_n(x) + \frac{1}{2} m a x^2 \psi_n(x)$$

Or in terms of operators,

$$\hat{H} \psi_n(x) = \frac{1}{2m} \left( \hat{p}^2 + (max)^2 \right) \psi_n(x)$$

With differential equations, you are free to take any zany approach to solve it, as long as you get the right answer in the end. He says there are two approaches, and we’ll take the “quicker and simpler (and a lot more fun)” one first.

### 2.3.1 Algebraic Method

The motivation for this approach is running with the hunch that the sum of these two terms squared should be the same as the product of two sums, not squared – this should factor. Throwing in an inspired constant factor, he defines

$$\hat{a}_+ \equiv \frac{1}{\sqrt{2m} \hbar \omega} (-i \hat{p} + max) \quad \text{and} \quad \hat{a}_- \equiv \frac{1}{\sqrt{2m} \hbar \omega} (i \hat{p} + max)$$

He argues through to the conclusion that the Schrodinger equation can indeed be written in terms of such factors (and we go on to see that it’s actually useful to do so.)

$$\hat{H} \psi_n(x) = \frac{1}{2m} \left( \hat{p}^2 + (max)^2 \right) \psi_n(x) = \hbar \omega (\hat{a}_+ \hat{a}_- - \frac{1}{2}) \psi_n(x) = \hbar \omega (\hat{a}_- \hat{a}_+ + \frac{1}{2}) \psi_n(x)$$

**Exercise:** plug in the expressions for \( \hat{a} \) and see that’s correct. Note: to make sure you do things correctly, need to actually write \( \hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x} \).

**Commutators:** Along the way, he introduces the notion of a “commutator”, a measure of just how badly operators don’t commute.

$$[x, \hat{p}] = i\hbar \quad \text{means} \quad \hat{x} \hat{p} \psi(x) - \hat{p} \hat{x} \psi(x) = i\hbar \psi(x)$$

And

$$[\hat{a}_-, \hat{a}_+] = 1 \quad \text{means} \quad \hat{a}_- \hat{a}_+ \psi(x) - \hat{a}_+ \hat{a}_- \psi(x) = \psi(x)$$

(Though cumbersome, I’m being using brackets to be explicit about the order of operations since these are operators rather than just functions or scalars.)

Note: Personally, I found these handy when simplifying some of the integrals I was going to do in the homework. They let me translate an integral of $$\psi^* \hat{x} \hat{p} \psi - i\hbar \psi^* \psi = \psi^* \hat{p} \hat{x} \psi$$.
Ladder Operators – stepping up, stepping down.

These operators get the name ‘raising’ and ‘lowering’ ‘ladder operators’ because when they act on a solution, they generate another solution with $\hbar\omega$ more or less energy. If not for this fact, these operators would have died an obscure death on someone’s pad of papers a few hours after they were first dreamt up. This is how they prove useful in solving the simple-harmonic oscillator’s Schrödinger equation.

Assert: if $\psi_n(x)$ is a solution to the simple harmonic oscillator Schrödinger equation, so is $c_n\psi_{n+1}(x) = \hat{a}_+\psi_n(x)$.

(proof for the $c_n$ is to remind us that even if $\psi_n$ happens to be normalized, $\psi_{n+1}$ isn’t necessarily)

Proof: First allow that is a solution to $\hbar\omega(\hat{a}_+\hat{a}_- + 1/2)\psi_n(x) = E_n\psi_n(x)$

Then $\hbar\omega(\hat{a}_+\hat{a}_- + 1/2)c_n\psi_{n+1}(x) = \hbar\omega(\hat{a}_+\hat{a}_- + 1/2)\psi_n(x) = \hat{a}_+\hbar\omega(\hat{a}_+\hat{a}_- + 1/2)\psi_n(x)$

But he’d proven that $\hat{a}_+\hat{a}_-\psi_n(x) = \psi_n(x) \Rightarrow \hat{a}_+\hat{a}_-\psi_n(x) = \psi_n(x) + \hat{a}_+\hat{a}_-\psi_n(x)$

So, we can rewrite this as $\hat{a}_+\hbar\omega(\hat{a}_+\hat{a}_- + 1/2)c_n\psi_{n+1}(x) = \hat{a}_+\psi_n(x)\hbar\omega + \hat{a}_+\hbar\omega(\hat{a}_+\hat{a}_- + 1/2)\psi_n(x) = \hat{a}_+\psi_n(x)\hbar\omega + \hat{a}_+E_n\psi_n(x)$

$\hat{a}_+\psi_n(x)(\hbar\omega + E_n) = c_n\psi_{n+1}(x)(\hbar\omega + E_n)$

So, indeed,

$\hbar\omega(\hat{a}_+\hat{a}_- + 1/2)c_n\psi_{n+1}(x) = E_n+\hbar\omega$ and $c_n\psi_{n+1}(x) = \hat{a}_+\psi_n(x)$.

Similarly, $c_d\psi_{n-1}(x) = \hat{a}_-\psi_n(x)$ is a solution with $E_{n-1} = E_n - \hbar\omega$.

So, if we can manage to figure out just one solution, then we can boot strap our way up and down to knowing all solutions.

He argues that, in spite of it’s being generally true that, for any $n$, there exists a solution $d_n\psi_{n-1}(x) = \hat{a}_-\psi_n(x)$, we also know that there must be a bottom to the physically realistic energies. He suggests that you bottom out with the trivial solution of 0.

$d_n\psi_{n-1}(x) = \hat{a}_-\psi_n(x) = \psi_n(x) = 0$.

Indeed, the constant 0 is a (boring) solution to the Schrödinger equation!

So, we can get our foot hold here, and work our way the ladder of states

$\hat{a}_-\psi_n(x) = 0$ where, again, $\hat{a}_- \equiv \frac{1}{\sqrt{2m\hbar\omega}}(ip + m\omega x) = \frac{1}{\sqrt{2m\hbar\omega}} \left( \hbar \frac{\partial}{\partial x} + m\omega x \right)$

Pause and consider: here’s where defining $a_+$ and $a_-$ has lead: rather than having to solve the differential equation
\[ \psi_n(x)E = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_n(x) + \frac{1}{2} m \omega^2 \psi_n(x) \]

We just have to solve
\[ \frac{1}{\sqrt{2m\hbar \omega}} \left( \hbar \frac{\partial}{\partial x} \psi_o(x) + m \omega \psi_o(x) \right) = 0 \]
and then bootstrap our way up using \( \psi_{n+1}(x) = \hat{a}_+ \psi_n(x) \).

Let’s do it!
\[
\frac{\partial \psi_o}{\partial x} = -\frac{m \omega}{\hbar} x \psi_o \\
\frac{1}{\psi_o} \frac{\partial \psi_o}{\partial x} = -\frac{m \omega}{\hbar} x \frac{\partial}{\partial x} \psi_o
\]
\[
\int \frac{1}{\psi_o} \frac{\partial \psi_o}{\partial x} = -\frac{m \omega}{\hbar} \int x \frac{\partial}{\partial x} \psi_o
\]
\[
\ln \left( \frac{\psi_o}{A} \right) = -\frac{m \omega}{\hbar} \frac{1}{2} x^2
\]
\[
\psi_o = Ae^{-\frac{m \omega}{2\hbar} x^2}
\]

For this solution, all that remains is to normalize.

**Daily Question Math:** Which integral from the back of the book does he use to evaluate the integral before equation 2.59? i.e. to normalize this wavefunction.

So we arrive at
\[
\psi_o = \left( \frac{m \omega}{\pi \hbar} \right)^{\frac{1}{4}} e^{-\left( \frac{m \omega}{2 \hbar} \right) x^2}
\]
Plugging this into the Schrodinger equation, we get the corresponding energy. We could plug it into the regular form, with the partial derivatives out for all to see, but we’ve built some specialized tools, and it pays to use them.
\[
E_n \psi_n = \hbar \omega (\hat{a}_+ \hat{a}_- + \frac{1}{2}) \psi_n
\]
\[
E_0 \psi_0 = \hbar \omega (\hat{a}_+ \hat{a}_- + \frac{1}{2}) \psi_0 = \hbar \omega (\hat{a}_+ \hat{a}_- \psi_0 + \frac{1}{2} \psi_0)
\]
But don’t forget that
\[
\hat{a}_- \psi_0(x) = 0
\]
which kills the first term, leaving just
\[
E_0 \psi_0 = \frac{1}{2} \hbar \omega \psi_0
\]
\[
E_0 = \frac{1}{2} \hbar \omega
\]
Now, while we don’t yet know the other wave functions (just how to get them) we do know their energies from having found that
\[
E_{n-1} = E_n - \hbar \omega \text{ or } E_{n-1} + \hbar \omega = E_n
\]
So,
\[ E_1 = \hbar \omega + E_0 = \hbar \omega + \frac{1}{2} \hbar \omega \]
\[ E_1 = \hbar \omega + E_1 = 2\hbar \omega + \frac{1}{2} \hbar \omega \]
\[ E_n = (n + \frac{1}{2}) \hbar \omega \]

**Normalization constants**

As for finding the wavefunctions, we can at least make normalizing them easy. We’ve got

\[ c_n \psi_{n+1} = \hat{a}_+ \psi_n \quad \text{or} \quad \psi_{n+1} = \frac{1}{c_n} \hat{a}_+ \psi_n \]

and \[ d_n \psi_{n-1} = \hat{a}_- \psi_n \quad \text{or} \quad \psi_{n-1} = \frac{1}{d_n} \hat{a}_- \psi_n \]

So, if we insist that

\[ 1 = \int |\psi_{n+1}|^2 \, dx = \int \left( \frac{1}{c_n} \hat{a}_+ \psi_n \right)^* \left( \frac{1}{c_n} \hat{a}_+ \psi_n \right) \, dx = \frac{1}{|c_n|^2} \int (\hat{a}_+ \psi_n)^* (\hat{a}_+ \psi_n) \, dx = \frac{1}{|c_n|^2} \int (\hat{a}_+ \hat{a}_- \psi_n) \, dx \]

Where the last equality comes from the general proof that he does between eqn’s 2.64 and 65)

Now, using the commutator \[ \hat{a}_- \hat{a}_+ \psi_n - \hat{a}_+ \hat{a}_- \psi_n = \psi_n \], we know

\[ \hat{a}_- \hat{a}_+ \psi_n = \hat{a}_+ \hat{a}_- \psi_n = \hat{a}_+ \hat{a}_- \psi_n = \hat{a}_+ \hat{a}_- \psi_n \]

And since \( \hbar \omega (n + \frac{1}{2}) \psi_n = E_n \psi_n = \hbar \omega (\hat{a}_+ \hat{a}_- + \frac{1}{2}) \psi_n \) clearly,

\[ n \psi_n = \hat{a}_- \hat{a}_+ \psi_n \]

So, \[ \hat{a}_- \hat{a}_+ \psi_n = (n+1) \psi_n \]

So, \[ |c_n|^2 = \int (\hat{a}_- \hat{a}_+ \psi_n)^* \psi_n \, dx = \int ((n+1) \psi_n)^* \psi_n \, dx = (n+1) \int (\psi_n)^* \psi_n \, dx = (n+1) \int |\psi_n|^2 \, dx \]

So, if \[ \int |\psi_n|^2 \, dx = 1 \] then \[ 1 = \int |\psi_{n+1}|^2 \, dx \] as long as \[ |c_n|^2 = (n+1) \]

Similarly, \[ 1 = \int |\psi_{n-1}|^2 \, dx \] if \[ |d_n|^2 = n \]

Boot strapping up from \( n = 0 \), we can then say that

\[ \psi_n(x) = \frac{1}{\sqrt{n}} (a_+ \psi_{n-1})(x) = \frac{1}{\sqrt{n!}} (a_+)^n \psi_0(x) \]

**Daily Question Math:** For the equation just after eq’n [2.64]: write out each term separately. Which term should use integration by parts? Show explicitly and mark which term goes to 0 and why.
Daily Question Math: Find the second excited state of the harmonic oscillator.

\[ \psi_{n+1}(x) = \hat{a}_+ \psi_n(x) \] 

so \( c_2 \psi_2(x) = \hat{a}_+ \psi_1(x) \), or \( \psi_2(x) = c_2 \hat{a}_+ \psi_1(x) \)

a. Sketch \( \psi_0 \), \( \psi_1 \), and \( \psi_2 \).

\[ \psi_0 = \left( \frac{m \omega}{\pi \hbar} \right)^{\frac{1}{4}} e^{-\left( \frac{m \omega}{2 \hbar} \right)x^2} = \left( \alpha \sqrt{\frac{2}{\pi}} \right)^{\frac{1}{2}} e^{-\alpha x^2} \]

\[ \psi_1 = \left( \frac{2}{\pi} \right)^{\frac{1}{2}} \sqrt{2} \alpha x e^{-\alpha x^2} \]

\[ \psi_2 = \left( \frac{2}{\pi} \right)^{\frac{1}{2}} \left( 4 \alpha x^2 - 1 \right) e^{-\alpha x^2} \]

b. Check the orthogonality of \( \psi_0 \), \( \psi_1 \), and \( \psi_2 \), by explicit integration. Hint: If you exploit the even-ness and odd-ness of the functions, there is only one integral left to do.

2. Starting Weekly HW (2.10-11 \( \psi_2 \)): For \( \psi_2 \) for the harmonic oscillator:

a. Compute \( <x> \), \( <p> \), \( <x^2> \), and \( <p^2> \) by explicit integration. Use the variable \( \xi \equiv \sqrt{m \omega / \hbar} x \) and the constant \( \alpha \equiv (m \omega / \pi \hbar)^{1/4} \).

b. Check the uncertainty principle for this state.

c. Compute \( <T> \) and \( <V> \) for these states without integration. Is their sum what you would expect?

Having developed handy rules in terms of \( a_+ \) and \( a_- \), even when we actually want to know about \( p \) and \( x \), it pays to do the work in terms of these.

Exercise: Combine \( \hat{a}_+ \equiv \frac{1}{\sqrt{2m \hbar \omega}} (-i \hat{p} + m \omega x) \) and \( \hat{a}_- \equiv \frac{1}{\sqrt{2m \hbar \omega}} (i \hat{p} + m \omega x) \) to get expressions for \( p \) and \( x \).

3. Starting Weekly HW (2.12): Find \( <x> \), \( <p> \), \( <x^2> \), \( <p^2> \), and \( <T> \), for the \( n \)th stationary state of the harmonic oscillator, using the method of example 2.5. Check that the uncertainty principle is satisfied.
**Discrete Schrödinger Equation**

_Starting Weekly Question:_ Exercises 1 & 2 of Implementing Discrete Schrödinger Eq’n handout

\[-\psi(x_{j-1}) + (2 + \tilde{v}(x_j))\psi(x_j) - \psi(x_{j+1}) = \varepsilon \psi(x_j)\]

1. Lay out all N equations in form suggestive of matrix

\[
\begin{pmatrix}
2 + \tilde{v}(x_1) & -1 \\
-1 & 2 + \tilde{v}(x_2) & -1 \\
& \ddots & \ddots \\
-1 & 2 + \tilde{v}(x_{N-1}) & -1 \\
& & -1 & 2 + \tilde{v}(x_N)
\end{pmatrix}
\begin{pmatrix}
\psi(x_1) \\
\psi(x_2) \\
\vdots \\
\psi(x_{N-1}) \\
\psi(x_N)
\end{pmatrix}
= \varepsilon
\begin{pmatrix}
\psi(x_1) \\
\psi(x_2) \\
\vdots \\
\psi(x_{N-1}) \\
\psi(x_N)
\end{pmatrix}
\]

Etc.

2. Written in matrix form

3. Have computer solve the matrix equation. It will find that there are N possible energies, and corresponding with each is a wave function, \( \psi(x) \). Of course, it won’t come up with an analytical expression for each wave function, rather, it will come up with, for each energy, a list of the wave function’s values at each discrete location, \( x_1, x_2, x_3, \ldots \)