Equipment
- Griffith’s text
- Moore’s text
- Printout of second computational reading.
- Printout of roster with what pictures I have

Announcement:
Food preferences for InStove

Check dailies

Time-Independent Schrodinger Equation

2.1 Stationary States

The Schrodinger equation

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

(Time Independent Schrodinger Equation)

is a new, exotic equation, who’s solutions have this new physical meaning

\[ \int_a^b |\Psi(x,t)|^2 \, dx = \left\{ \begin{array}{l} \text{probability of finding the particle} \\ \text{between a and b, at time t.} \end{array} \right\} \]

But mathematically, it’s just another partial differential equation waiting to be solved. So to solve it, we’ll take the same approach as generations of physicists had to solve the partial differential equations of classical physics – for waves, light, heat,…

Separation of Variables

In the Mandl reading, he systematically went through solving the differential equation for waves on a string. First, he crossed his fingers and hoped that individual solutions will have the form of a product of a time dependent function and a space dependent function. The proof will be in the pudding – if equations of that form can indeed solve the equation and satisfy given boundary conditions.

Faced with a new differential equation (Schrodinger’s equation) we’ll do the same.

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

Hope: \( \Psi_n(x,t) = \psi_n(x)\phi_n(t) \) (I subscript with an \( n \) to help us keep in mind that there may be a small or even infinite family of such solutions, and particular solutions that match specific boundary/initial conditions may be linear combinations of them.)

Plug in:
\[
\frac{i\hbar}{\partial t} \psi_n(x) \phi_n(t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_n(x) \phi_n(t) + V(x) \psi_n(x) \phi_n(t)
\]

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

Divide both sides by it

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

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

Now, if our guess leads us to this point, that the left hand side may be a function of \(t\) but not a function of \(x\) and it equals the right hand side which may be a function of \(x\) but not of \(t\). The only way that can be true is if neither side depends on either \(x\) or \(t\), that is, they equal a constant. With a bit of foresight, Griffith’s dubs it “E”.

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

So instead of one partial differential equation, we have two ordinary differential equations that share a common constant.

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

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

(Time independent Schrödinger Equation)

The equation on the left is trivial ‘what function is its own derivative times a constant? \(\phi_n(t) = e^{\alpha t}\)

Plug it in and you find that \(\alpha_n = \frac{E_n}{\hbar i} = -\frac{E_n}{\hbar}\)

So,

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

So,

\[
\Psi_n(x,t) = \psi_n(x) \phi_n(t) = \psi_n(x)e^{\frac{-E_n}{\hbar} t}
\]
1. Stationary States

While the wave function then has rather simple time dependence, the probability density has no time dependence:

\[
|\Psi_n(x,t)|^2 = \Psi_n^*(x,t)\Psi_n(x,t) = \psi_n^*(x)\phi_n^*(t)\psi_n(x)\phi_n(t) = \psi_n^*(x)e^{\frac{E_n}{\hbar}}\psi_n(x)e^{-\frac{E_n}{\hbar}} = \psi_n^*(x)\psi_n(x).
\]

Thus these states are known as “stationary states” since the corresponding probabilities are ‘stationary’ / not evolving in time.

**Daily Question: Conceptual:** What did Unit Q call a stationary state?

As you saw in the last chapter, the expectation value of x, and p, or any function thereof, has this form:

\[
\langle Q(x, p) \rangle = \int_a^b \Psi_n^*(x,t)Q\left(x, \frac{\hbar}{i}\partial_{\dot{r}}\right)\Psi_n(x,t)dx = \int_a^b \psi_n^*(x)\phi_n^*(t)Q\left(x, \frac{\hbar}{i}\partial_{\dot{r}}\right)\psi_n(x)\phi_n(t)dx
\]

\[
= \int_a^b \psi_n^*(x)Q\left(x, \frac{\hbar}{i}\partial_{\dot{r}}\right)\psi_n(x)\phi_n^*(t)\phi_n(t)dx = \int_a^b \psi_n^*(x)Q\left(x, \frac{\hbar}{i}\partial_{\dot{r}}\right)\psi_n(x)dx
\]

Which has no time dependence, so the expectation values are also time independent.

Of course, that means that their time derivatives are 0, \( \langle p \rangle = m\frac{d\langle x \rangle}{dt} = 0 \).

2. Hamiltonian

For example, in Chapter 1, Griffith rather off-handedly mentioned that the expectation value of kinetic energy is

\[
\langle T_n \rangle = \int_a^b \Psi_n^*(x,t)\left(-\frac{\hbar^2}{2m}\partial^2_x\right)\Psi_n^*(x,t)dx
\]

Rather obviously, the expectation value of the potential would be

\[
\langle V_n \rangle = \int_a^b \Psi_n^*(x,t)V(x)\Psi_n(x,t)dx
\]

So their sum would be the expectation value of the total energy (out of tradition denoted “H” for Hamiltonian – more specific than ‘total energy, it can be defined per degree of freedom)

\[
\langle H_n \rangle = \langle T_n \rangle + \langle V_n \rangle
\]

\[
\langle H_n \rangle = \int_a^b \Psi_n^*(x,t)\left(-\frac{\hbar^2}{2m}\partial^2_x + V(x)\right)\Psi_n(x,t)dx
\]

Then again, you probably recognize the right-hand side of the Schrödinger equation there, and we can substitute in the left-hand side instead

\[
\langle H_n \rangle = \int_a^b \Psi_n^*(x,t)\left(i\hbar\frac{\partial}{\partial t}\right)\Psi_n(x,t)dx
\]
But we’ve reasoned that \( \left( i\hbar \frac{\partial}{\partial t} \right) \Psi_n(x,t) = E_n \Psi_n(x,t) \).

So substituting that in,

\[
\langle H_n \rangle = \int_a^b \Psi_n^*(x,t) E_n \Psi_n(x,t) \, dx = E_n \int_a^b \Psi_n^*(x,t) \Psi_n(x,t) \, dx = E_n \int_a^b |\Psi_n(x,t)|^2 \, dx = E_n
\]

Thus the choice of naming the constant \( E \) in the first place – it’s the expectation value of the energy for the state which is time independent.

So, it’s the expectation value, but how broad is the distribution of energies you might measure for this state?

\[
\sigma_n = \sqrt{\langle H_n^2 \rangle - \langle H_n \rangle^2} = \sqrt{\langle H_n^2 \rangle - E_n^2}
\]

\[
\langle H_n \rangle^2 = \int_a^b \Psi_n^*(x,t) \hat{H}_n \Psi_n(x,t) \, dx = \int_a^b \Psi_n^*(x,t) \hat{H}_n \Psi_n(x,t) \, dx
\]

\[
\langle H_n \rangle^2 = E_n \int_a^b \Psi_n^*(x,t) \hat{H}_n \Psi_n(x,t) \, dx = E_n^2 \int_a^b |\Psi_n(x,t)|^2 \, dx = E_n^2
\]

\[
\sigma_n = \sqrt{E_n^2 - E_n^2} = 0.
\]

For these states, there is no spread. The energy is definite.

That’s why they’re often referred to as the ‘energy Eigen states’; they’re the states that have definite energy values.

3. Linear combination, Allowed Energy

Now, a specific solution to a differential equation, one that matches the boundary / initial conditions is a linear combination of the ‘generic’ solutions.

\[
\Psi(x,t) = \sum_n c_n \Psi_n(x,t) = \sum_n c_n \Psi_n(x) e^{-\frac{E_n}{\hbar} t}
\]

Daily Question: Conceptual: Equation 2.15 is related most closely to which of the “rules” from Unit Q?

Transition: All this has been said without getting specific about the potential energy function. To get any further, we need to do that – specify the functional form of the potential energy and see what kinds of spatial functions solve the time-independent Schrodinger equation for that.

2.2 The Infinite Square Well

"Where do the stationary states eqn. 2.35 come from?" Casey P

\[
V(x) = \begin{cases} 
0, & 0 \leq x \leq a \\
\infty, & \text{otherwise}
\end{cases}
\]
So, within the region, we simply have
\[ i\hbar \frac{\partial}{\partial t} \Psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x,t) \]
Quickly focusing on a separable solution,
\[ \Psi_n(x,t) = \psi_n(x) \phi_n(t) \]
We can adopt the results of the previous section, namely,
\[ \phi_n(t) = e^{-\frac{E_n t}{\hbar}} \] and so the differential equation we have to worry about is
\[ \psi_n(x)E = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_n(x) \]
What function equals the negative of its second derivative times a constant, sines and cosines for one thing (alternatively \(e^{ikx}\)’s). Since it’s a second order differential equation, we should have two independent solutions, sine and cosine will do the job.

So, we could say \( \psi_n(x) = A_n \sin(k_n x) + B_n \cos(k_n x) \).

Plugging back into the differential equation, we find that it works just great if
\[ E_n = \frac{\hbar^2 k_n^2}{2m} \]
**Boundary Conditions.**
As is traditional with differential equations, you next impose the boundary conditions. What is the boundary condition? As you’d expect classically, the chance of finding an object beyond an infinitely tall barrier is 0. Quantum mechanically, Moore had made an argument by rearranging the Schrodinger equation to focus on the relationship between a function’s value and its concavity:
\[ \frac{\frac{\partial^2 \psi_n(x)}{\partial x^2}}{\psi_n(x)} = \frac{2m}{\hbar^2} \{V(x) - E\} \]
In a region where \( V > E \), the ratio of concavity to the function’s value is positive – meaning that if the function is above the \( x \)-axis, it’s concave up. The two options are that either it arcs up, up and away as you go further in \( x \) – and so blows up toward infinity (clearly not a normalizable function, thus not a physically realistic wavefunction if allowed to proceed that way), or it arcs like an exponential decay and dies off as \( x \) goes to infinity. The strength of this arching scales with the difference between \( V \) and \( E \). In the case that \( V \) is infinite, the wave function dies immediately.

So, just outside the region \( 0 < x < a \), the wave function is 0. It makes no sense for the probability density to be discontinuous or multivalued at any point, even a boundary, so this will be our boundary condition – the wave functions have to be 0 at \( x = 0 \) and \( x = a \).

\[ \psi_n(0) = \psi_n(a) = 0 \]
Cosine fails this at \( x = 0 \), and sine satisfies it at \( x = a \) only if \( k_n = \frac{n\pi}{a} \) for \( n = 1,2,3,\ldots \)
Thus, the corresponding energies must be
\[ E_n = \frac{\hbar^2(n \pi / a)^2}{2m} \quad n = 1, 2, 3, \ldots \]
\[ \psi_n(x) = A_n \sin\left(\frac{n \pi x}{a}\right) \]

**Starting Weekly Question:** HW (2.4): Calculate \( <x> \), \( <x^2> \), \( <p> \), \( <p^2> \), \( \sigma_x \), and \( \sigma_p \), for the \( n \)th stationary state of the infinite square well. Check that the uncertainty principle is satisfied. Which state comes closest to the uncertainty limit?

In general then, given whatever initial conditions you have, the wavefunction would be a linear combination of these.
\[ \Psi(x,t) = \sum_n c_n \psi_n(x,t) = \sum_n c_n \psi_n(x) e^{-\frac{E_n}{\hbar} t} \]
\[ \Psi(x,t) = \sum_n c_n A_n \sin\left(\frac{n \pi x}{a}\right) e^{-\frac{E_n}{\hbar} t} \]

Taking a trivial example, let’s say that our ‘initial condition’ is that the wavefunction is simply a sine wave of a particular wavelength, that is, for some particular \( n \). Then, our solution has the form
\[ \psi_n(x,t) = A_n \sin\left(\frac{n \pi x}{a}\right) e^{-\frac{E_n}{\hbar} t} \]
And must be normalized to truly be a ‘wave function’ (that is, for its square to be a probability density.)

\[ 1 = \int_{-\infty}^{\infty} \left|\Psi(x,t)\right|^2 dx \quad \text{for} \quad \Psi_n(x,t) = \begin{cases} A_n \sin\left(\frac{n \pi x}{a}\right) e^{-\frac{E_n}{\hbar} t} & \text{for } 0 \leq x \leq a \\ 0 & \text{otherwise} \end{cases} \]
\[ 1 = \int_{0}^{a} A_n^2 \sin^2\left(\frac{n \pi x}{a}\right)dx = A_n^2 \int_{0}^{a} \sin^2\left(\frac{n \pi x}{a}\right)dx = A_n^2 \left[ \frac{a}{2} - \frac{1}{2} \sin\left(\frac{n \pi x}{a}\right) \right]_0^a = A_n^2 \frac{a}{2} \]
\[ A_n = A = \sqrt{\frac{2}{a}} \]
\[ \psi_n(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n \pi x}{a}\right) e^{-\frac{E_n}{\hbar} t} \quad \text{tada! The Stationary States} \]

"Where do the stationary states eqn. 2.35 come from?" **Casey P**

As Griffiths demonstrates, and you should have in the first day’s daily work,
\[
\int_0^a \Psi_m^*(x,t) \Psi_n(x,t) \, dx = \delta_{nm} = \begin{cases} 
1 & \text{if } n = m \\
0 & \text{otherwise}
\end{cases}.
\]

In that sense, these solutions form an ‘orthonormal set’. Since any other possible wavefunctions that fit in the infinite square well would have to be a linear combination of these,

\[
\Psi(x,t) = \sum_n c_n \Psi_n(x,t) = \sum_n c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right) e^{-\frac{iE_n t}{\hbar}}
\]

"Can we review Fourier series and explicitly tie them in to quantum?" **Bradley W**

Of course you’re familiar with a Taylor Series expansion – any (well-behaved) function can be expressed as a polynomial with appropriate coefficients (related to the function’s derivatives). There are other ‘basis sets’ of functions in to which some other function can be resolved. A “Fourier Series expansion” is a representation of some function as sum of sine and cosine (or equivalently, e^{ix}’s). The same basic idea – that any (well-behaved) function can be expressed as such a series. Fourier’s trick shows how to find the coefficients.

We can call it a ‘basis set.’

In fact, it is a ‘complete’ basis set in that all functions that respect the boundary conditions can be expressed as such a sum. I’m afraid that I’m not mathematician enough to know where to begin proving that Taylor or Fourier Series’ are “complete.”

For the particle in a Box, it happens that the stationary states are indeed sines, so the general notion that any solution is a linear combination of stationary states, a.k.a. Eigen states, is in this specific case, an example of Fourier Series. **However**, for more interesting potentials, the stationary states won’t be sines or cosines. But the general principle still holds: any solution is a linear combination of that system’s stationary states.

**Starting Weekly Question: (2.5):** A particle in the infinite square well has as its initial wave function:

\[\Psi(x,0) = A[\psi_1(x) + \psi_4(x)]\]

a. Normalize \(\Psi(x,0)\).

b. Find \(\Psi(x,t)\) and \(|\Psi(x,t)|^2\). Express the latter as a sinusoidal function of time, as in example 2.1. So simplify the result, use \(\omega = \pi^2 \hbar / 2ma^2\)

c. Compute \(\langle x \rangle\). Notice that it oscillates with time? What is the angular frequency of the oscillation? What is the amplitude?

d. Compute \(\langle p \rangle\). Hint: There is an easy way.

e. If you measured the energy of this particle, what values might you get, and what is the probability of getting each of them?

f. Find the expectation value of \(H\). How does it compare with the answer to e?

**Question:** "can we discuss Dirichlet's theorem?" **Jessica**

I also think that this would be good to go over in class. **Kyle B.**

Yes it would be helpful! **Jonathan**

A further explanation about Dirichlet's Theorem would be very helpful; Griffiths seemed to make this theorem too vague, unfortunately. **Jeremy.**
Fourier’s Trick:
Given that their orthonormal,
\[ \int_0^a \Psi_m^*(x,t)\Psi(x,t)\,dx = \sum_n \int_0^a \Psi_m^*(x,t)c_n\Psi_n(x,t)\,dx = \sum_n c_n \int_0^a \Psi_m^*(x,t)\Psi_n(x,t)\,dx = \sum_n c_n \delta_{nm} = c_m \]

**Question:** "Could we go over completeness and do an example similar to Example 2.2?"

**Spencer**

**Daily Question:** A particle in the infinite square well has the initial wave function
\[ \Psi(x,0) = \begin{cases} A, & 0 \leq x \leq a/2 \\ -A, & a/2 < x \leq a \end{cases} \]

**g.** Sketch \( \Psi(x,0) \) and determine the constant \( A \).

**h.** Find \( \Psi(x,t) \)

**i.** What is the probability that a measurement of the energy would yield the value \( E_1 \) (by these subscripts, I mean the corresponding energies according to eq’n 2.27, regardless of how you happened to number your wave functions)?

**j.** Find the expectation value of the energy. So, is this square-wave state physically achievable? It doesn’t converge – infinite energy. Not achievable. this is an example of our claim that the wavefunction can’t be discontinuous or multi-valued: that perfectly vertical line in the middle is impossible.

**Energies and their probabilities**

By the statistical interpretation, for any function of \( x \), including \( H \),
\[ \langle H \rangle = \int_a^b \Psi^*(x,t)\hat{H}\Psi(x,t)\,dx \]

\[ \langle H \rangle = \int \left[ \sum_m c_m^* \Psi_m^*(x,t) \right] \hat{H} \left[ \sum_n c_n \Psi_n(x,t) \right] \,dx = \sum_m \sum_n \hat{E}_m \Psi_m^*(x) \Psi_n(x) e^{iE_n t/\hbar - iE_m t/\hbar} \,dx = \sum_m \sum_n \hat{E}_m \Psi_m^*(x) \Psi_n(x) e^{iE_n t/\hbar - iE_m t/\hbar} \,dx \]

\[ = \sum_m \sum_n \hat{E}_m \Psi_m^*(x) \Psi_n(x) \,dx \int_0^a \Psi_m^*(x) \Psi_n(x) \,dx = \sum_m \sum_n \hat{E}_m \delta_{nm} \,dx = \sum_m \hat{E}_m \delta_{mm} \,dx = \hat{E}_m \,dx \]

\[ \langle H \rangle = \sum_n \hat{E}_n |c_n|^2 \]

So, comparing this with our discrete probability expressions from the beginning of Chapter 1, it’s pretty clear to identify the \( |c_n|^2 \) as the probability of each energy term: the probability of measuring each individual energy.
**Discrete Schrodinger Equation**

*Starting Weekly Question:* Exercises 1 & 2 of Implementing Discrete Schrodinger Eq’n handout

Question: "Can we talk about the Python code in the handout?" Mark T

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

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

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

Etc.

2. Written in matrix form

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

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, \(x_1, x_2, x_3, \ldots\)

**Friday**

Don’t forget your Discussion Prep – 8 a.m.