A QUANTUM MECHANICS PRIMER:

An introduction to upper-division quantum mechanics using the particle-in-a-box

Brian Shotwell
Department of Physics, University of California, San Diego

The purpose of the following is to go over some basic concepts of quantum mechanics at an undergraduate level somewhere between lower-division and upper-division. Topics include bra/ket notation, states as elements of a physical vector space, operators, and time-evolution of states following the time-dependent Schrödinger Equation. It is for the student who has gone through an introductory sequence of physics that includes modern physics, but before the student has gone through an upper-division textbook at the level of Griffiths or similar. This student would probably be able to compute expectation values of a particle in a state described by its position-space wavefunction, $\psi(x)$, but might not know how $\psi(x)$ evolves over time, or is not familiar with more abstract representations of the state $|\psi\rangle$.

It is my experience that many lower-division courses in modern physics don't do an adequate job in introducing conceptual basics of Quantum Mechanics (QM). This leads to students who are asked to do too much in their upper-division (UD) course. Overwhelmed, these students succumb to "learning" QM by pattern-matching, praying that they see exam problems similar to example problems they've already seen before. It is hoped that this brief overview will help ease the transition into upper-division QM.

Frequently, axioms of quantum mechanics are introduced and then later applied to various applications/systems. Here I take a slightly different approach: topics are only introduced as needed to describe and generalize a very particular problem: the particle-in-a-box (PIB). Hopefully seeing the concepts arise organically will help motivate the material.

An alternative title to this would be "Linear Algebra in Quantum Mechanics." This title was ultimately not chosen because it is by no means a formal review. Instead, the intention is to be more impressionistic than comprehensive: it's designed to get students to realize their own misconceptions/preconceptions, generalize their understanding of QM via the language of linear algebra, familiarize themselves with notation and semantics, and learn the tools required to analyze other quantum-mechanical problems. It is with this background that they can be more active participants in their UD QM course.

Finally, I apologize if this work is superfluous. I wrote it because I've had a tough time directing students to a resource that I believed would help them in their upper-division QM course(s). Normally my suggestion is *Principles of Quantum Mechanics* by R. Shankar, but that's a bit too much to be used as a supplement to a first exposure to UD quantum. Unfortunately, the net result might be yet another person's ramblings on QM (which there are already way too many of).

Contents

Please send any comments, corrections, etc. to bshotwell@physics.ucsd.edu

1 Particle in a Box I: States & Operators

1.1 PIB Abstraction

1.1.1 Introduction / Motivation

Recall the following formula from your study of the "particle-in-a-box" (PIB), also called the "infinite potential well" or "infinite square well:"

$$\psi_n(x) = \begin{cases} \sqrt{\dfrac{2}{L}} \sin\left(\dfrac{n\pi x}{L}\right), & 0 < x < L \\ 0, & \text{otherwise} \end{cases} \qquad \left(\text{with energy } E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}\right) \tag{1}$$

These wavefunctions are those functions that "fit nicely" in a 1D box existing from $x = 0$ to $x = L$. You might equate "fit nicely" with "are solutions to Schrödinger's equation with appropriate boundary conditions." You probably solved problems similar to the following: given a wavefunction with $n = 2$, what is the probability that you'd find a particle somewhere between $x = 0$ and $x = L/3$? Oh, the answer isn't 1/3 like you expected? Guess quantum mechanics is weird then! ¯_(ツ)_/¯

The problem with these sorts of exercises is twofold:

1. They're oversimplified / too hypothetical.
2. These sorts of computations tell you little about understanding the principles of quantum mechanics that persist as you delve into the subject.

I don't have any remedy for (or issue with) number 1: PIB is largely a theoretical exercise, used to introduce students to quantum mechanical issues without the need for complicated mathematics. If you're not happy with PIB because it's too theoretical, then nothing written here is going to help much with that. What is dangerous though is number 2: students who come out of a lower-division introduction to quantum mechanics (QM) emerge with some common misconceptions about the subject that hinder their learning in an upper-division (UD) quantum mechanics class. In my opinion, these issues should be addressed before trying to tackle the material at the upper-division level so that students understand the point of what they're doing with the complicated mathematics before the end of the term.

In talking about PIB in a couple slightly different ways than what you might be used to, some ideas from linear algebra will inevitably arise. Hopefully you'll embrace this fact rather than recoil in fear! The linear algebra required is a small subset of what is covered in an upper-division math course on the subject. I've assumed the reader has taken a lower-division math class introducing linear algebra, including the calculation of eigenvalues and eigenvectors of a matrix, and how to perform some basic matrix algebra (for example, how to multiply a matrix and a column vector).

1.1.2 Allowed States

Consider the possible wavefunction $\psi_S(x)$ for a particle in a box. $\psi_S(x)$ is depicted in Figure 1 below [$\psi(x)$ on the vertical axis and x on the horizontal, assuming $L = 1$, and ignoring units]:

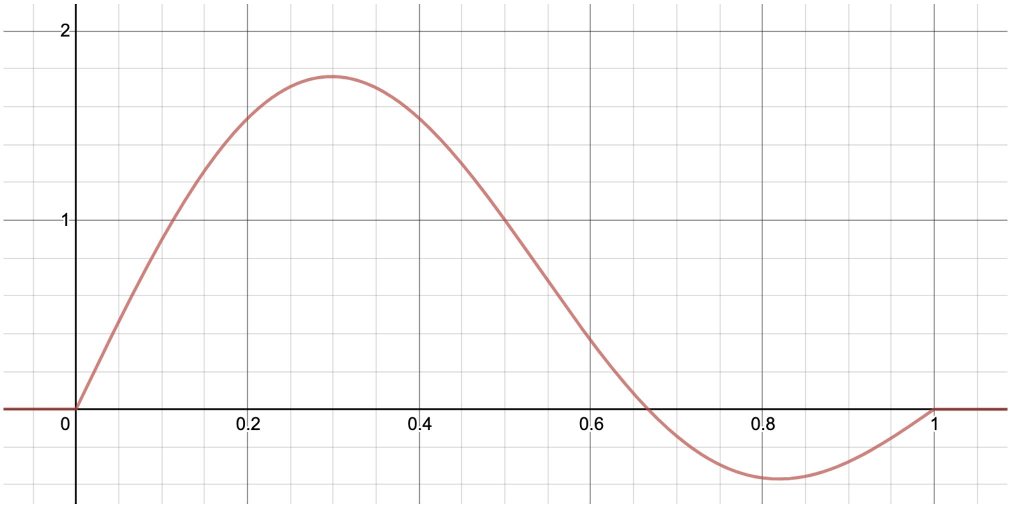

Figure 1: $\psi_S(x) \equiv [\psi_1(x) + \psi_2(x)]/\sqrt{2}$

Is this an allowed wavefunction? It doesn't have the form of the nice sine waves that you're used to seeing for this problem. Despite this fact, the answer is YES! This wavefunction is fine. It's the sum of equal parts $n = 1$ and $n = 2$, and it's just a snapshot at a particular time (the "S" in the name stands for "Sum"). In reality, if you were to plot this wavefunction over time, you'd see it sloshing back and forth between "mainly on the left" (what's shown above) and "mainly on the right." Chapter 2 will be dedicated to understanding the time-evolution of wavefunctions; this chapter is mainly focused on describing the state at any instant of time.

Here we arrive at the first of a few key generalizations about wavefunctions:

KEY POINT: If $\psi_1(x)$ and $\psi_2(x)$ are allowed wavefunctions, then so is $\psi_1(x) + \psi_2(x)$ (though unnormalized).

You might complain that this doesn't satisfy the Time-Independent Schrödinger Equation (TISE). In other words, if you take $\psi_S(x)$ and plug it into

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_S(x) \overset{?}{=} E\psi_S(x), \tag{2}$$

you'd get an equation that is not equal for all values of x between 0 and L. This is true. $\psi_S(x)$, although a perfectly fine wavefunction, *DOES NOT* satisfy the TISE. You've been lied to! Well, probably not, but it's a common misconception when first learning QM that all wavefunctions must be solutions to the TISE. In fact, that's not true. Only "special" ones.

Obviously the TISE doesn't tell the whole story with what's going on in QM. The Key Point above gives a hint as to what might be involved: linear algebra. It doesn't make much sense to cube a wavefunction (it wouldn't have the correct units, for example), but it's perfectly fine to take linear combinations of wavefunctions to get another wavefunction. This hints that the structure of quantum mechanics is that of a (physical) *vector space.*

Mathematicians sometimes use the word "vector" rather abstractly. You might be used to "vectors" as things with a magnitude and direction. Because of this, you might visualize a vector as an arrow in 2D or 3D (or similar). However, vectors in a vector space are more abstract than this. One example would be an additive model of *color.* In the "RGB" color model, you can represent any color as a certain amount of red, a certain amount of green, and a certain amount of blue. These three colors serve as the three basis vectors for a three-dimensional vector space of possible colors; each color is a vector in this vector space. Each color can be written as a linear combination of the three basis vectors.

As applied to PIB, each wavefunction is a "vector." The "special" wavefunctions $\psi_n(x)$ from Eq. (1) can serve as a basis for any possible wavefunction in the PIB. Why this is and how this works for a variety of problems are primary questions covered in any QM course.

There are a couple issues we'll have to mention at the onset that make QM a little different from (and more specialized than) a class in linear algebra:

1. The scalar field is the field of complex numbers (rather than real numbers, or rather than being left ambiguous, as is often the case in math classes).
2. Any two vectors that are different by an overall nonzero complex scalar are physically equivalent — in other words, if $\psi_2 = \lambda\psi_1$ for $\lambda \neq 0$ ($\lambda \in \mathbb{C}$), then ψ_1 and ψ_2 correspond to the same physical state. In your lower-division class, a consequence of this was the fact that you could take any unnormalized state and "normalize" it.

We'll discuss these issues and many others by looking at a specific example in the next section.

1.2 PIB as a 2-State System

We'll continue talking about the particle-in-a-box, but phrase it in terms of linear algebra. To do this, I'll make a huge simplification, and then talk about what happens when I relax that simplification in Sec. [1.3]. **The simplification that I'm going to assume is that the only values of n that the particle can have in the box are $n = 1$ and $n = 2$** (with energies E_1 and $E_2 = 4E_1$, respectively... remember that $E_n \propto n^2$).

You might ask, "what interesting thing(s) can we do with just two wavefunctions?" Well, the key point from the previous section opens some possibilities for us: we can combine two wavefunctions in lots of different ways to get a new one. This seems trivial, but (as we'll find out) the result of a measurement can depend crucially on how the wavefunctions are added!

It turns out that the best way to organize our thinking about wavefunctions is to use linear algebra, so a lot of what follows is applying linear algebra concepts to our 2-state PIB.

More generally, we need to focus on linear algebra because of the following: All the physical predictions of QM can be phrased in terms of a scalar product in the "Hilbert space," (to be defined in the next section), along with knowing the eigenfunctions of the measurement operators. This is very general, and applies to properties like spin/polarization where a position wavefunction alone does not fully describe the physical state.

1.2.1 From $\psi(x)$ to $|\psi\rangle$, Inner Product Spaces

$\psi_1(x)$ has a very particular shape to it, if you dissect the wavefunction as a function of position. **But it is the entire wavefunction that describes the state of a particle, and writing it in terms of position is one of many choices on how we want to look at it.**[1] It is the entire wavefunction $\psi_1(x)$ that has the energy E_1. It is the entire wavefunction that is a vector in the abstract vector space of allowed wavefunctions in the PIB. Therefore, we will stop calling this wavefunction $\psi_1(x)$, and start just calling it ψ_1. This is analogous to removing any reference to a basis when referring to a vector in Euclidean space: instead of saying that $\mathbf{A} = 4\hat{\mathbf{x}} + 3\hat{\mathbf{y}}$, we could just call it $\mathbf{A}$, which emphasizes the fact that the vector exists independently of how we describe it in terms of some basis. Maybe $\mathbf{A} = 5\hat{\mathbf{u}}$ for another basis $\{\hat{\mathbf{u}}, \hat{\mathbf{v}}\}$ — it doesn't really matter. It's still $\mathbf{A}$.

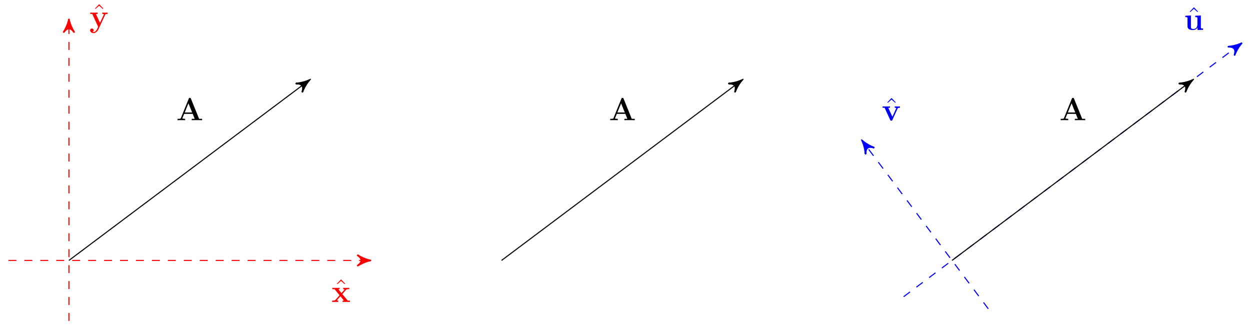

Figure 2: The vector **A** along with two different, superimposed coordinate systems. Note the vector itself does not change based on the coordinate system – only the components of the vector depend on the coordinate system.

Physicists like to emphasize the fact that the wavefunction is, in fact, a vector (in the abstract sense discussed in the last section). Rather than write an arrow above it or make it boldface, physicists do the following:

$$\text{“Physical Vector } \psi_1\text{”} \longrightarrow |\psi_1\rangle \tag{3}$$

$|\psi_1\rangle$ is called a "ket" (rhymes with Boba Fett). It represents a vector in "Hilbert Space," the abstract physical vector space that has wavefunctions as vectors. If our Hilbert space has a

---

[1] You could also talk about $\psi_1(k)$, the "momentum space" version of the wavefunction, by taking the Fourier transform of $\psi_1(x)$. This you'll learn how to do in an upper-division course.

small number of dimensions n, then we only need n vectors to serve as a basis that spans the space of all possible wavefunctions. In the case of our PIB with two states of energy E_1 and E_2, the vector space is two-dimensional, and we only need two vectors to span the space.[2] We can choose the vectors $|\psi_1\rangle$ and $|\psi_2\rangle$ for this, two wavefunctions with definite (and distinct) values of energy.

As a shorthand, physicists sometimes refer to a vector space with an ordered basis in terms of their "counter" label alone. So, replace $|\psi_1\rangle$ with $|1\rangle$ and replace $|\psi_2\rangle$ with $|2\rangle$. It's like a game of maximizing the amount of laziness / how much you get can away with redefining things until you get to as dense a language as possible.

Now that the basis vectors are chosen, because they're orthonormal, we can represent them with the following column vectors:

$$|1\rangle \text{ or } |\psi_1\rangle \longrightarrow \begin{pmatrix}1\\0\end{pmatrix} \quad \text{and} \quad |2\rangle \text{ or } |\psi_2\rangle \longrightarrow \begin{pmatrix}0\\1\end{pmatrix} \tag{4}$$

Why must $|\psi_n\rangle$ be orthonormal to do this? It'll take a few paragraphs to explain why. Let's go back to what orthonormal means in terms of an enumerated set of position-space wavefunctions:

$$\int_{-\infty}^{\infty} \psi_i^*(x)\psi_j(x)\,dx \overset{\text{if orthonormal}}{=} \delta_{ij} \equiv \begin{cases}1, & i=j\\ 0, & i\neq j\end{cases} \tag{5}$$

δ_{ij} defined in the equation is called the *Kronecker Delta* symbol (not to be confused with the Dirac delta function, which you'll learn about in UD QM or E&M).

Hilbert space is not just a vector space, it's an *inner product space* (a vector space with an inner product defined, which is a way of "multiplying" vectors to get a scalar out). If you have $\psi_i(x)$ and $\psi_j(x)$, and you want to take the inner product between them, then you may use the left side of Eq. (5). Remember, though, that $|\psi_i\rangle$ need not be represented by $\psi(x)$, In quantum mechanics, we write the inner product between two vectors (roughly speaking, the overlap between them) via "braket" notation (read as two words: "bra," which rhymes with saw, and "ket"). As an example of this, let's look at the inner product of $|1\rangle$ with either itself or $|2\rangle$:

$$\langle 1|1\rangle = \begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = 1 \qquad \langle 1|2\rangle = \begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = 0$$

The inner product of $|1\rangle$ with itself is 1, which is now how we'll keep track of a vector being "normalized." Now we see why, in order to represent the two vectors with the column vectors in Eq. (4), the vectors had to have been orthogonal, since the inner product $\langle 1|2\rangle$ is necessarily zero. This isn't too big a restriction: the states corresponding to different energies are

---

[2] If you're a linear algebra purist, you might complain that this is not a vector space in the strict sense, since there doesn't seem to be a zero vector. Our requirement that wavefunctions are normalized means that the zero vector is not a state of the system, and so we try to skirt this issue as much as possible. This is partially why we (sometimes) refer to this vector space as a "physical" vector space.

necessarily perpendicular and can serve as a basis.[3] Also, even if you have a basis that isn't orthonormal, you can make it orthonormal via a Gram-Schmidt process.

What is $\langle\psi|$? It's a "dual" vector to $|\psi\rangle$. People think of this a couple different ways, based on the following facts:[4]

- ⋆ Given an orthonormal basis for a vector space $\mathcal{V}$, there is a unique orthonormal basis for the dual vector space $\mathcal{V}^*$. Also, there is a unique bijection between these two bases. That is, each vector has its own unique "dual vector," and vice-versa. Therefore, $\langle\psi|$ is just another way of representing $|\psi\rangle$. The column vector representation of kets makes this particularly concrete: for every column vector, there is a row vector corresponding to it (take the complex conjugate, then the transpose of the column vector — the result is the dual vector).
- ⋆ The dual vector space is the space of all linear functions that will take as inputs vectors and spit out scalars. Again, the column vector representation of $|\psi\rangle$ illustrates this fact: what sort of object can you multiply with an $n \times 1$ column vector to get a scalar out? A $1 \times n$ row vector! The fact that we also take the complex conjugate will ensure that $\langle\psi|\psi\rangle$ is real (and must equal 1 to be properly normalized).

1.2.2 Complex Numbers, General States

Let's return to the two issues mentioned at the end of Sec. [1.1.2]: 1. (physical) states must be "normalized," and 2. linear combinations of states (with the scalar field being $\mathbb{C}$) are also states, after they're properly normalized.

Why are complex numbers used/required in Quantum Mechanics? There are lots of different answers to this question. For example, some people might say that it's because the time-dependent Schrödinger Equation has an i. Fine, but why write down an equation with an i in it in the first place? Personally, I find the best motivation comes from trying to explain the results of the Stern-Gerlach experiment. This is explained in detail in the first section of the first chapter of *Modern Quantum Mechanics* by J. J. Sakurai. One could make the argument that you could always describe complex numbers in terms of a collection of real numbers, and so the use of complex numbers is not absolutely required. Regardless, any attempt to describe QM in terms of real numbers alone would be needlessly clumsy, and so therefore we use complex numbers.

Complex numbers will be essential in describing the time-evolution of states, which is what we'll do in Chapter 2. For now, we just have to get used to how they work. For a

---

[3] This stems from the fact that the Hamiltonian is a Hermitian operator. These operators have special properties that we'll explore in Sec. [1.2.3]. Part of the reason for describing QM via linear algebra is to explain/prove general facts like this.

[4] Warning (notation): physicists and mathematicians differ over which vector is complex-conjugated in $\langle v_1|v_2\rangle$. The physicists' definition (used here, where it's $|v_1\rangle$ that is complex-conjugated) makes the interpretation in terms of matrices more apparent.

concrete example, all of the following are normalized states (i.e., $\langle\psi_i|\psi_i\rangle = 1$):

$$|\psi_a\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \quad |\psi_b\rangle = \begin{pmatrix}i\\0\end{pmatrix}, \quad |\psi_c\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}, \quad |\psi_d\rangle = \frac{1}{\sqrt{5}}\begin{pmatrix}-2i\\1\end{pmatrix} \tag{6}$$

What is $\langle\psi_d|$? Remember, it's the "conjugate-transpose" of $|\psi_d\rangle$:

$$\langle\psi_d| = \frac{1}{\sqrt{5}}\begin{pmatrix}+2i & 1\end{pmatrix}$$

$$\langle\psi_d|\psi_d\rangle = \left[\frac{1}{\sqrt{5}}\begin{pmatrix}+2i & 1\end{pmatrix}\right]\left[\frac{1}{\sqrt{5}}\begin{pmatrix}-2i\\1\end{pmatrix}\right] = \frac{1}{5}\Big[(+2i)(-2i)+(1)(1)\Big] = 1 \ \checkmark$$

Most lower-division courses try as hard as possible to remove any reference to complex numbers in quantum mechanics. That's why the states in Eq. (1) are real; they are actually only telling a part of the story. These states are *energy eigenstates* — states of definite energy — and for these states the total wavefunction $\Psi(x,t)$ factorizes into a real piece and a complex-phase piece: $\Psi(x,t) = \psi(x)e^{-iEt/\hbar}$.[5] [6] Not all wavefunctions have to have this property, though, and so it's misleading to say that we can just describe a wavefunction in terms of an entirely real wavefunction $\psi(x)$.

Is there a difference between the physical states $|\psi_a\rangle$ and $|\psi_b\rangle$ in Eq. (6)? Both are "normalized," and yet they don't seem exactly the same. These two states are off by an *overall phase*, which cannot be detected experimentally. Any two states $|\psi_i\rangle$ and $|\psi_j\rangle$ that are related by $|\psi_i\rangle = e^{i\theta}|\psi_j\rangle$ are only different by an overall phase (note $|\psi_b\rangle = e^{i\pi/2}|\psi_a\rangle$), which is unphysical (i.e., there is no measurement in "real life" that can detect the overall phase). However, the *relative phase* between two states *is* physical: there is a difference between the states $(|\psi_a\rangle + |\psi_c\rangle)/\sqrt{2}$ and $(|\psi_a\rangle - |\psi_c\rangle)/\sqrt{2}$. This is one essential ingredient to understanding why $\psi_S(x)$ (from Sec. [1.1.2]) changes over time. The specifics of this will follow from the Time-Dependent Schrödinger Equation, Eq. (27).

1.2.3 Operators and Measurements

One of the primary benefits of the linear algebra language is that it elucidates the role of "measurement" in quantum mechanics. **Any physical measurement (position of a particle, energy of a particle, spin of a particle, etc.) is represented with a (linear) Hermitian operator.** Given a basis, we can represent these operators as $n \times n$ matrices acting on $n \times 1$ column vectors, returning yet another $n \times 1$ column vector. A Hermitian operator satisfies $A = A^\dagger \equiv (A^*)^T = (A^T)^*$ ($A^\dagger$ is referred to as "A-dagger"): the operator is equal to its "conjugate-transpose." In terms of matrices, "conjugate" (the *) means take the complex-conjugate of each entry, and "transpose" (the ^{T}) means to swap A_{ij} with A_{ji}.

---

[5] This is covered in detail in the next chapter. For now, take it as given.

[6] There could also be an overall phase multiplying $\Psi(x,t)$ equal to $e^{i\phi_0}$. However, we have the freedom to choose the overall phase so that the wavefunction is real at $t = 0$. This is discussed in the next paragraph.

Here are some examples of Hermitian matrices that could possibly represent a physical observable in a 2-dimensional Hilbert space (such as our 2-state PIB):

$$\hat{A} = \begin{pmatrix} 5 & 0 \\ 0 & -8 \end{pmatrix}, \quad \hat{B} = \begin{pmatrix} 1 & i \\ -i & 0 \end{pmatrix}, \quad \hat{C} = \begin{pmatrix} 0 & 2+3i \\ 2-3i & 0 \end{pmatrix}, \quad \hat{D} = \begin{pmatrix} 1 & 2 \\ 2 & -2 \end{pmatrix} \tag{7}$$

You might want to note the following things:

- ⋆ There is a "hat" above the operator. This hat has nothing to do with unit vectors — it's telling the reader that the object is an operator. In other words, the object is not a number, but rather is designed to act on a state and return another state. Again, remember that an $n \times n$ matrix times an $n \times 1$ column vector gives another $n \times 1$ column vector.
- ⋆ The entries along the diagonal must be real. Entries A_{ij} on the off-diagonal ($i \neq j$) can have an imaginary component, but note $A_{ij} = A^*_{ji}$.
- ⋆ The components of the matrices depend on the choice of basis: if our column vectors in Eq. (4) corresponded not to $|1\rangle$ and $|2\rangle$, but rather to $(|1\rangle + |2\rangle)/\sqrt{2}$ and $(|1\rangle - |2\rangle)/\sqrt{2}$, then the matrices for $\hat{A}$, $\hat{B}$, $\hat{C}$, and $\hat{D}$ would have different entries. One of the problems at the end of this chapter suggests a few ways for how you might find these entries.

Hermitian matrices have a number of important properties. These properties are why they are so important/useful in quantum mechanics:

1. The eigenvalues of a Hermitian operator are real.
2. The eigenvectors of a Hermitian operator are complete (they span the vector space). In other words, for any Hermitian operator $\hat{A}$, any vector $|\psi\rangle$ (in the entire Hilbert space of possible wavefunctions) can be written as a linear combination of eigenvectors of $\hat{A}$. In other words, for any Hermitian operator $\hat{A}$ with eigenvectors $|\phi_i\rangle$, we can take any state $|\psi\rangle$ and write it as $|\psi\rangle = \Sigma_i c_i |\phi_i\rangle = c_1 |\phi_1\rangle + c_2 |\phi_2\rangle + c_3 |\phi_3\rangle + \cdots$.

Before applying this to quantum mechanics, let's just understand what point number 2 is saying above. Suppose you have the following (non-Hermitian) matrix Y (the "Y" is for yuck, or "y" would you try to use this as an operator):

$$Y = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$$

What are the eigenvectors of this matrix? They are the (nonzero) vectors $\mathbf{v}$ such that $Y\mathbf{v} = \lambda\mathbf{v}$ for some constant number λ. We'll get some practice finding eigenvalues/eigenvectors in Sec. [1.2.4] (in a few pages); eventually you'll be able to show that there is only one eigenvector, $\begin{pmatrix} 1 & 0 \end{pmatrix}^T = |1\rangle$ (remember, the "kets" are column vectors, so if I want to try and write it here in the middle of a paragraph I have to write it as a row vector, transposed). The span of the eigenvectors of Y is therefore the span of the single state $|1\rangle$. In other words, there's no way to write the state $|2\rangle$ in terms of the eigenvectors of Y! The eigenvectors of Y therefore *do not* span our 2-dimensional vector space (spanned by $|1\rangle$ and $|2\rangle$).

Our two facts lead directly to the following two axioms of quantum mechanics. *There is no proof of the following; things just sort of work out (meaning, QM has predictive power in analyzing the real world) if you take these "axioms" to be true:*

1. A physical measurement is represented by a Hermitian operator.
2. Suppose $|\psi\rangle = \Sigma_i c_i |\phi_i\rangle$, where $|\phi_i\rangle$ are the eigenvectors of the operator $\hat{A}$ with corresponding eigenvalues λ_i (assume all the λ_i's are distinct). Then the result of a measurement of $\hat{A}$ is λ_i with probability $|c_i|^2$. The physical state after the measurement is $|\phi_i\rangle$. Sometimes this is referred to as wavefunction "collapse" from $|\psi\rangle$ to $|\phi_i\rangle$, but some physicists think that this language is misleading since it suggests that the measurement is some discontinuous, nonlinear process.

The second point above says that, **if a physical measurement is performed to measure the value of operator $\hat{A}$, the value of the measurement is one of the eigenvalues of the operator. The state of the system after the measurement is the corresponding eigenvector.**

Let's see how this works in the PIB. The most important operator is the *Hamiltonian*, $\hat{H}$, which is an operator that measures the energy of the state. Again, assuming the 2-dimensional basis given by $|1\rangle$ and $|2\rangle$, the Hamiltonian operator has the following form:

$$\hat{H} = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} = \frac{\pi^2\hbar^2}{2mL^2}\begin{pmatrix} 1 & 0 \\ 0 & 4 \end{pmatrix} \tag{8}$$

How did I know that this was the Hamiltonian? Well, we already know that the basis vectors are states of definite energy, and so $\hat{H}|1\rangle = E_1|1\rangle$ and $\hat{H}|2\rangle = E_2|2\rangle$. The first equation gives the first column of $\hat{H}$, and the second equation gives the second column. Note that, since $|1\rangle$ and $|2\rangle$ are eigenvectors of the operator $\hat{H}$, the matrix corresponding to $\hat{H}$ is diagonal in this basis.

One way of writing operators in a basis-independent way is via the *outer product.* Notice that the Hamiltonian in Eq. (8) can be written as follows:

$$\hat{H} = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2| \tag{9}$$

The order of the bra and ket is reversed when comparing the outer product to what you've seen before with the inner product. An outer product is therefore an operator: it can act on a ket and return another ket. Let's verify that Eqs. (8) and (9) are saying the same thing. In other words, let's plug in the row-vector bras ($\langle 1|$ and $\langle 2|$) and column-vector kets ($|1\rangle$ and $|2\rangle$) into Eq. (9) to verify that we get the matrix in Eq. (8) for the energy eigenbasis:

$$\begin{aligned} \hat{H} &= E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2| \\ &= E_1\begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \end{pmatrix} + E_2\begin{pmatrix} 0 \\ 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \end{pmatrix} \\ &= E_1\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + E_2\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} \checkmark \end{aligned}$$

In general, any Hermitian operator with distinct[7] eigenvalues λ_n and orthonormal eigenvectors $|\mathbf{v}_n\rangle$ can be written in terms of outer products via

$$\hat{O} = \sum_n \lambda_n |\mathbf{v}_n\rangle \langle \mathbf{v}_n| \tag{10}$$

Notation: here, we are using "$\hat{H}$" to refer to either the abstract operator, *or* the specific representation of $\hat{H}$ in some basis (the matrix in Eq. (8)). Some books will refer to the latter as $(\hat{H})_{ij}$ to emphasize that we are writing down the $(i,j)^{\text{th}}$ component of $\hat{H}$ given a particular basis. Ditto for $|\psi\rangle$ vs. $(|\psi\rangle)_i$. Most books, though, aren't so particular / nitpicky, and it's up to the reader to infer which is meant. Furthermore, lots of times the "hat" is left off of the operator, especially if the operator is written out in matrix form. So, for example, you might see the Hamiltonian written as H instead of $\hat{H}$.

Semantics: you're going to see the following terms often in your study of QM:

- ⋆ *Eigenstates (of $\hat{A}$)*: the eigenvectors (i.e., physical states) of any operator $\hat{A}$.
- ⋆ *Energy eigenstates*: the eigenstates corresponding to the operator $\hat{H}$ (the Hamiltonian).
- ⋆ *Eigenkets*: A synonym for eigenstate.
- ⋆ *Stationary States*: A synonym for energy eigenstates.

1.2.4 An Example: back to $|\psi_S\rangle$, Expectation Values

Let's go back to the state $\psi_S(x)$ from Sec. [1.1.2], embracing the new notation that we've just developed. Define

$$|\psi_S\rangle \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{11}$$

This seems like we've removed any reference to the position, but there is a subtle reference: remember that relative phase is important. When we write the state $|\psi_S\rangle$ as in Eq. (11), we are assuming the relative phase between the two energy eigenstates is such that, if the wavefunction $\psi_S(x)$ were plotted, it would look like Figure 1. As we'll explore more in the next chapter, the wavefunction moves over time, and so at a later time the state will look like

$$|\psi_D\rangle \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{12}$$

The letter "D" is used for "difference," where $\psi_D(x) = [\psi_1(x) - \psi_2(x)]/\sqrt{2}$. This state has the wavefunction "more on the right" than on the left. Anyway, we'll focus mostly on just $\psi_S(x)$ in this section.

I want to analyze $|\psi_S\rangle$ in the context of two operators:

$$\hat{H} = \frac{\pi^2\hbar^2}{2mL^2} \begin{pmatrix} 1 & 0 \\ 0 & 4 \end{pmatrix}, \qquad \hat{L} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{13}$$

---

[7] You may wonder what happens if the eigenvalues are not distinct. In that case, Eq. (10) is still possible, but there is some freedom in the choice of the eigenvectors $\mathbf{v}_n$ because of the degeneracy.

$\hat{H}$ is the Hamiltonian operator constructed in the last section: it is the operator corresponding to the energy of any state living in this 2-dimensional Hilbert space. $\hat{L}$ is Hermitian, and so it can represent a physical operator, but we don't know what it could represent yet. We'll look at the properties of $\hat{L}$ in order to infer what it could be.

First, $\hat{H}$. What is the energy of the state $|\psi_S\rangle$? Well, remember "axiom 2" from the previous section: to find out the result of a measurement $\hat{A}$, we have to write our state in terms of the eigenvectors of $\hat{A}$. Then, we can read off the probabilities of the result of the measurement of $\hat{A}$ by reading off the squares of the coefficients $|c_i|^2$.

$$|\psi_S\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\end{pmatrix} + \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\end{pmatrix} \tag{14}$$

It appears that there is a 1/2 probability we would obtain E_1 and a 1/2 probability that we would obtain E_2 if we were to measure the energy of the state. The *expected value* of the energy of the state is therefore

$$\langle\hat{H}\rangle = E_{\text{avg}}\ (\text{or } \bar{E}) = \frac{1}{2}E_1 + \frac{1}{2}E_2 = \frac{1}{2}\Big[E_1 + (4E_1)\Big] = \frac{5}{2}E_1 = \frac{5\pi^2\hbar^2}{4mL^2}$$

$\langle\hat{H}\rangle$ is the expected value of the energy. There is another way to calculate the expected value of an operator: sandwich it between the bra and ket of the state:

$$\langle\hat{H}\rangle \equiv \langle\psi_S|\hat{H}|\psi_S\rangle = \frac{1}{2}\begin{pmatrix}1 & 1\end{pmatrix}\left[\frac{\pi^2\hbar^2}{2mL^2}\begin{pmatrix}1 & 0\\0 & 4\end{pmatrix}\right]\begin{pmatrix}1\\1\end{pmatrix} = \frac{\pi^2\hbar^2}{4mL^2}\begin{pmatrix}1 & 1\end{pmatrix}\begin{pmatrix}1\\4\end{pmatrix} = \frac{5\pi^2\hbar^2}{4mL^2} \tag{15}$$

This way of computing things is nice if you don't happen to know the coefficients c_i and/or the eigenvalues of your operator ahead of time.

This might remind you of calculations of energies from a lower-division class. In terms of position-space wavefunctions, you could also calculate the energy by "sandwiching" the operator in between $\psi^*(x)$ and $\psi(x)$ via

$$\langle\hat{H}\rangle = \int_{-\infty}^{\infty}\psi_S^*(x)\hat{H}\psi_S(x)\,dx = \int_{-\infty}^{\infty}\psi_S^*(x)\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right]\psi_S(x)\,dx \tag{16}$$

This is a perfectly valid way of finding the energy of the state $|\psi_S\rangle$, but hopefully you see that the calculation that we carried out was much simpler than writing out the entire wavefunction and carrying out the calculation of Eq. (16). This illustrates the utility of talking about states and operators a little more abstractly.

What happens if you measure the energy of the state? You will never get $(5/2)E_1$! You will either get E_1 or $4E_1$, with equal likelihood (since the state was "half $|1\rangle$" and "half $|2\rangle$"). Here's another warning about language: physicists will use E_{avg} and $\langle\hat{H}\rangle$ to mean the same thing, and they'll call it a variety of things: expected value / mean value of the energy, expected value / expectation value of the hamiltonian, etc. All of it means the same thing. However, you should keep in mind the following: **The Hamiltonian is the operator. The energy refers to either the expectation value of the Hamiltonian operator $\hat{H}$, or the result of a measurement of $\hat{H}$. If the state is an energy eigenstate, then these are the same, but in general they are not.**

Now, on to $\hat{L}$. As mentioned before, the matrix $\hat{L}$ is Hermitian, and so $\hat{L}$ can be a physical observable. Let's look at the expected value of $\hat{L}$ separately for the two states $|1\rangle$ and $|2\rangle$:

$$\langle 1|\hat{L}|1\rangle = \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0$$

$$\langle 2|\hat{L}|2\rangle = \begin{pmatrix} 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0$$

Hmmm... does this tell us anything? Yes: the expected value of $\hat{L}$, $\langle \hat{L} \rangle$, is 0 for either energy eigenstate $|1\rangle$ or $|2\rangle$. That doesn't mean that we'll necessarily get the value zero if we measure $\hat{L}$. It just means that, if we had several different copies of the PIB, each in the state $|1\rangle$, and we measured $\hat{L}$ a bunch of times, and then took the average of all these measurements, we'd get the value zero. By the way, having "several different copies" of a quantum system is often called having an *ensemble* of systems.

In general, the way you want to analyze a Hermitian operator is to look at its eigenvalues/eigenvectors. We need to find the eigenvectors of the matrix L (i.e., the vectors $\mathbf{v}$ such that $L\mathbf{v} = \lambda \mathbf{v}$). To do so, let's set up the eigenvalue/eigenvector equation

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix} \tag{17}$$

The eigenvalues of a Hermitian matrix are real, but that doesn't mean that the eigenvectors have to contain only real entries. In other words, since L is Hermitian, we know λ is a real number, but a and b can be complex numbers.

Equation (17) implies $b = \lambda a$ and $a = \lambda b$. Therefore, $a = \lambda(\lambda a) = \lambda^2 a$, and $\lambda = \pm 1$. We'll have to solve for the eigenvector $\begin{pmatrix} a & b \end{pmatrix}^T$ separately for each eigenvalue. First let's look at $\lambda_+ = +1$:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = (+1) \begin{pmatrix} a \\ b \end{pmatrix} \implies \begin{bmatrix} b = a \end{bmatrix} \implies \mathbf{v}_+ = \frac{e^{i\phi}}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \text{ is an eigenvector for } \lambda_+ = +1 \tag{18}$$

The eigenvector $\mathbf{v}_+$ defined in Eq. (18) can in general have any complex phase, hence the factor $e^{i\phi}$. Normally in quantum mechanics, we choose the complex phase to try to minimize the overall number of imaginary and/or negative numbers (so, let's set $\phi = 0$). Also, notice that the vector has been normalized (the factor of $1/\sqrt{2}$), so that it can represent a physical vector in the Hilbert space. $\mathbf{v}_-$ is similar, but with $b = -a = -1$ on the bottom entry (it's convention that it's the bottom entry that's gets the negative sign instead of the top entry... the two are off by an overall phase $\phi = \pi$). Overall then, the eigensystem of $\hat{L}$ is

$$\lambda_+ = +1, \text{ with } \mathbf{v}_+ = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \qquad \lambda_- = -1, \text{ with } \mathbf{v}_- = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$

Looking back on Eqs. (11) and (12), it appears that $|\psi_S\rangle$ is an eigenstate of $\hat{L}$ with eigenvalue $+1$, and $|\psi_D\rangle$ is an eigenstate with eigenvalue -1. If we definitely have the state $|\psi_S\rangle$ at a certain time, and measure $\hat{L}$ at that time, then we will measure the value $+1$ with 100% probability. However, just because we have the state at $|\psi_S\rangle$ at one moment doesn't mean that it will remain as $|\psi_S\rangle$ over time, and so *when* we perform the measurement will matter in what we get for the measurement.

For any general state, if we make a measurement of $\hat{L}$, we'll either be left with $|\psi_S\rangle$ (if we measure the value $+1$) or $|\psi_D\rangle$ (if we measure the value -1). By looking again at Figure 1, it appears that a positive measurement of $\hat{L}$ is correlated with the particle being more likely on the left hand side of the box, and a negative measurement with it being on the right. In fact, it was called "L" to refer to "Leftness." However, even if we take a general state $|\psi\rangle$, measure $\hat{L}$, and get $+1$, there is a lot we can't say:

1. We don't know that $|\psi\rangle$ was equal to $|\psi_S\rangle$ just before the measurement. Suppose the particle's wavefunction *just before* the measurement were $|\psi_{\text{before}}\rangle = c_S\,|\psi_S\rangle + c_D\,|\psi_D\rangle$. Then all we can infer with this measurement is that c_S was nonzero. In other words, $\langle\psi_S|\psi_{\text{before}}\rangle \neq 0$ (i.e., the overlap between $|\psi_{\text{before}}\rangle$ and $|\psi_S\rangle$ was nonzero).
2. We don't know that $|\psi\rangle$ will be equal to $|\psi_S\rangle$ a finite time after the measurement. While it's true that the particle is in the state $|\psi_S\rangle$ just after the measurement, it will evolve according to the Time-Dependent Schrödinger Equation, which will take the state of the particle away from $|\psi_S\rangle$ since it is not an energy eigenstate. This is what the entire next chapter is about.
3. We don't know that the particle was ever on the left side of the box! In fact, you have to learn to stop asking this question: the particle's state is described by the entire wavefuncton, and unless the whole wavefunction exists entirely on the left-side of the box, you can't say the particle is on the left side of the box.

1.3 Generalization to ∞ Dim.

Suppose the particle in a box had the three lowest energy states accessible. Then we have to consider $|3\rangle$ in our basis, and the Hilbert space is 3-dimensional. Any vector (i.e., state) we wish to describe can be written as

$$\begin{aligned} |\psi\rangle &= c_1\,|\psi_1\rangle + c_2\,|\psi_2\rangle + c_3\,|\psi_3\rangle \quad \text{(basis-independent)} \\ \psi(x) &= c_1\psi_1(x) + c_2\psi_2(x) + c_3\psi_3(x) \quad \text{(wavefunctions as functions of position)} \end{aligned} \tag{19}$$

Remember: these two equations are saying the same exact thing. It's just that the second happens to choose spatial position to represent the wavefunction, whereas the first equation is left general. The basis we're using for this vector space consists of three vectors: the three lowest energy eigenstates. In addition to this, though, there is a also a separate choice for how we represent each wavefunction. Another possibility for each $\psi_i(x)$ is to write it in terms of its Fourier Transform, $\psi_i(k)$.

It's clear how to generalize the previous sections if n is any finite number: just include the energy eigenstates up to and including n. But what if n is allowed to increase without bound? Then the Hilbert space is countably infinite – write down Eq. (19), but include an infinite number of terms. What is amazing is that, if you include *all* of the energy eigenstates (not just $|1\rangle$ and $|2\rangle$, but all the way up to infinity), then *any* wavefunction $\psi(x)$ that you can draw in between $x = 0$ and $x = L$ can be written as a sum of these energy eigenstates:

$$\psi(x) = c_1\psi_1(x) + c_2\psi_2(x) + c_3\psi_3(x) + \cdots = \sum_{n=1}^{\infty} c_n\psi_n(x) \tag{20}$$

This is known as *completeness* of the vector space. It may surprise you that we are able to reconstruct any (nice, reasonably well-behaved) function with just the collection of special functions $\sin(k_n x)$. The study of this and related facts is called Fourier analysis. Here, we just so happen to be looking at the completeness of just the energy eigenstates, but remember that the eigenstates of *any* Hermitian operator are complete!

For a concrete example of the completeness of the energy eigenstates, suppose you had the following "sawtooth" triangular wavefunction:

$$\psi_{\text{saw}}(x) = \begin{cases} Ax, & 0 < x < L \\ 0, & \text{otherwise} \end{cases} \tag{21}$$

To normalize the wavefunction we must choose $A = e^{i\phi}\sqrt{3}/L^{3/2}$ (and, for the sake of convenience, let's take $\phi = 0$ so that the wavefunction is initially real and nonnegative). It seems impossible, but we can actually write this function in terms of the energy eigenstates alone[8] (i.e., just the $\sin(\cdots)$ energy eigenstates $\psi_n(x)$). The answer for this example is

$$\psi_{\text{saw}}(x) = \sum_{n=1}^{\infty} c_n\psi_n(x), \quad \text{where} \quad c_n = \frac{-\sqrt{6}\cos(n\pi)}{n\pi} = (-1)^{n-1}\frac{\sqrt{6}}{n\pi} \tag{22}$$

The more terms we include in the sum, the better we approximate the wavefunction $\psi_{\text{saw}}(x)$. Actually, it would require an infinite amount of energy to get the state $\psi_{\text{saw}}(x)$, which you can confirm by doing the problem surrounding Eq. (26). This has to do with the fact that the wavefunction is not continuous at $x = L$. This is (one reason) why you had the requirement in your previous QM class that the wavefunction be continuous everywhere — the particle

---

[8] As for *how* to do this, Griffiths explains how in both his *Quantum Mechanics* and *Electrodynamics* UD textbooks. He calls it "Fourier's Trick."

would have infinite energy, otherwise.

For convenience, here is something you can copy-paste into desmos.com to see how the wavefunction looks depending on how many terms are included in the sum. The default in the following is to include terms up to and including $n = 5$, but try playing with it:

```
\left\{x<0:0,x>1:0,\sum_{n=1}^{5}(-1)^{n-1}\cdot
\frac{\sqrt{12}}{\pi\ n}\sin\left(n\cdot\pi\cdot x\right)\right\}
```

(I don't think Desmos will accept a copy-paste from a smartphone or tablet, so you'll have to do this from a computer). If copy-pasting isn't working from this .pdf file (a browser's rendering of a .pdf file sometimes will introduce spaces into the text where they shouldn't exist), try copying the text given on the following website:

https://bshotwell.physics.ucsd.edu/QuantumPrimerPlots.html

Look for the stuff under "The Sawtooth Wavefunction Psi_{saw}(x) with n terms included." The other things are for plots that we'll explore in Chapter 2.

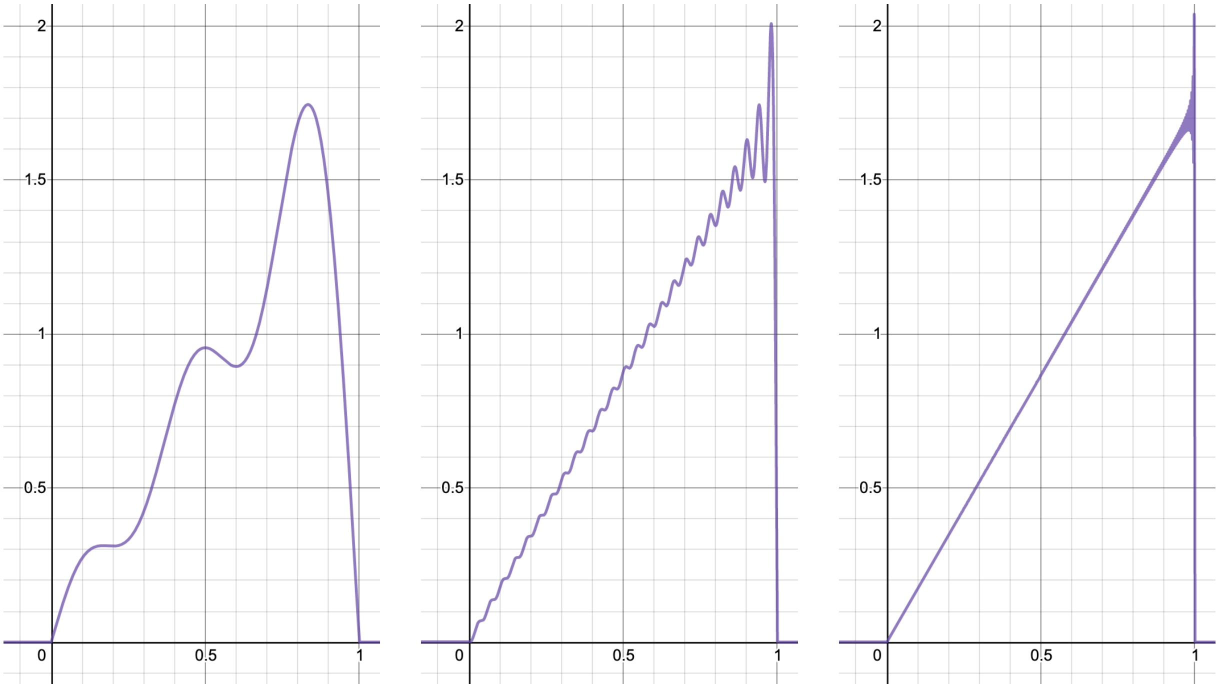

Figure 3: The "Sawtooth" wavefunction $\psi_{\text{saw}}(x)$ expressed as the sum of energy eigenstates via Eq. (22), including 5 terms (left), 50 terms (middle), and 500 terms (right).

1.4 Chapter 1 Exercises

1. Show that $\psi_S(x)$ *does not* satisfy Eq. (2), where

$$\psi_S(x) \equiv \frac{1}{\sqrt{2}}\Big[\psi_1(x) + \psi_2(x)\Big].$$

Because this is true, $\psi_S(x)$ is NOT a *stationary state.*

2. A general state in a 2-dimensional vector space can be written a couple different ways:

$$|\psi\rangle = \begin{pmatrix} a+bi \\ c+di \end{pmatrix} \quad OR \quad |\psi\rangle = \begin{pmatrix} \cos\theta \\ e^{i\phi}\sin\theta \end{pmatrix}$$

   (a) What is the condition on a, b, c, and d ($\in \mathbb{R}$) in order for $|\psi\rangle$ to be normalized?

   (b) Which way of describing the state do you think is better? Why?

3. Suppose you have the following kets:

$$|\psi_a\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} i \\ 1 \\ 1 \end{pmatrix}, \quad |\psi_b\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} 0 \\ 1 \\ -2i \end{pmatrix}$$

   Remember: If a number is multiplying a column vector, it's the same as multiplying each term in the column vector by that number.

   (a) For each wavefunction, find $|\psi_i|^2 = \langle\psi_i|\psi_i\rangle$. Is the wavefunction normalized?

   (b) Find $\langle\psi_a|\psi_b\rangle$ and $\langle\psi_b|\psi_a\rangle$. What is the relationship between the two?

4. Let

$$|\psi_A\rangle = \frac{1}{\sqrt{2}}\Big(|\psi_a\rangle + |\psi_b\rangle\Big) \quad \text{and} \quad |\psi_B\rangle = \frac{1}{\sqrt{2}}\Big(|\psi_a\rangle - |\psi_b\rangle\Big),$$

   where $|\psi_a\rangle$ and $|\psi_b\rangle$ are defined in Eq. (6). Are $|\psi_A\rangle$ and $|\psi_B\rangle$ the same physical state?

5. Our ability to represent operators in terms of matrices (given a basis) requires that all operators are *linear*. A linear operator $\hat{O}$ satisfies the following relationship:

$$\hat{O}\Big(\alpha|\psi_1\rangle + \beta|\psi_2\rangle\Big) = \alpha\hat{O}|\psi_1\rangle + \beta\hat{O}|\psi_2\rangle \tag{23}$$

   (true for any states $|\psi_1\rangle$ and $|\psi_2\rangle$ and any complex numbers α and β). Give an example of a nonlinear operator for our 2-dimensional PIB.

6. Define the operator $\hat{O}$ for the PIB as follows:

$$\hat{O} = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \tag{24}$$

   (a) Find the eigenvalues and corresponding eigenvectors of this matrix. One of these eigenvalues is positive and the other is negative — call the two eigenstates $|+\rangle$ and $|-\rangle$, respectively.

   (b) Write the state $|+\rangle$ in terms of $|1\rangle$ and $|2\rangle$.

   (c) Write the state $|\psi_S\rangle$ in terms of $|+\rangle$ and $|-\rangle$.

It turns out, if you start with a particle in the state $|\psi_S\rangle$ at time $t = 0$, then the state will look like one of these eigenvectors at time $t = T/4$ and the other at time $t = 3T/4$, where T is the period of the motion of the wavefunction (the amount of time it takes for the wavefunction to return to $|\psi_S\rangle$). As for which is which, we'll see how to do this in Chapter 2.

7. There's a shortcut to get the two eigenvalues of a 2×2 matrix A. It involves finding the trace of a matrix and the determinant of a matrix:

$$\begin{aligned}\operatorname{Tr} A &\equiv A_{11} + A_{22} = \lambda_1 + \lambda_2 \\ \operatorname{Det} A &\equiv A_{11}A_{22} - A_{12}A_{21} = \lambda_1\lambda_2\end{aligned}$$

   (a) Use these equations to find the eigenvalues of the matrix $\hat{D}$ in Eq. (7).

   (b) Find normalized eigenvectors for the two eigenvalues you found in part (a).

8. How many real numbers are required to completely describe a general 2×2 Hermitian matrix? What about a 3×3 matrix? Using these results, predict the number required for a general $n \times n$ Hermitian matrix.

9. Prove that the expectation value of a Hermitian operator is unchanged if the state changes by an overall phase.

10. Rewrite $\hat{L}$ [as defined in Eq. (13)] in terms of outer products of energy eigenkets. Your answer should have two terms – which term corresponds to the "1" in the upper-right corner of the matrix L?

11. $\hat{L}$ [as defined in Eq. (13)] takes $|0\rangle \to |1\rangle$ and $|1\rangle \to |0\rangle$. Knowing this, what would you expect the operator $\hat{L}^2$ to do? Confirm by computing the matrix L^2.

12. A *projection operator* is an operator $\hat{P}$ such that $\hat{P}^2 = \hat{P}$.

   (a) Show that the following operator is a projection operator by verifying that $P_1^2 = P_1$:

$$P_1 = |1\rangle\langle 1|$$

   Explain what you think this projection operator does. (in particular, why is the word "projection" useful in this description?)

   (b) As you may have already guessed, you can "project" onto any state of the system. Write down the projection operator corresponding to the operator that projects the state onto $|\psi_S\rangle$. Write this down both in terms of the outer product as well as a matrix in the energy eigenstate basis.

   (c) A projection operator doesn't have to project onto a single state — it could also project onto some subspace of your vector space. For example, take your vector space to be the 3-dimensional space spanned by $\{|1\rangle, |2\rangle, |3\rangle\}$ (as described at the beginning of Sec. [1.3]). Suppose you want to project onto the subspace spanned by just $\{|1\rangle, |2\rangle\}$ via

$$P = |1\rangle\langle 1| + |2\rangle\langle 2| = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{25}$$

Show that $|\psi_S\rangle\langle\psi_S| + |\psi_D\rangle\langle\psi_D|$ (where $|\psi_S\rangle = (|1\rangle + |2\rangle)/\sqrt{2}$ is still the sum of the first two energy eigenstates, and $|\psi_D\rangle$ is the difference) is the exact same projection operator by writing it out in matrix form and showing it equals the matrix on the right side of Eq. (25). Why do you think this is?

13. The operators $\hat{H}$ and $\hat{L}$ given in Eq. (13) were given in terms of the energy eigenbasis. Suppose, instead, we chose the basis formed by $|\psi_S\rangle$ and $|\psi_D\rangle$. That is, take

$$|\psi_S\rangle \longrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad |\psi_D\rangle \longrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

    (a) Give the 2×2 matrix for $\hat{L}$ in this basis. *Hint: it's diagonal. What two entries are required so that* $\hat{L}|\psi_S\rangle = +1|\psi_S\rangle$ *and* $\hat{L}|\psi_D\rangle = -1|\psi_D\rangle$?

    (b) The Hamiltonian is not diagonal in this basis, since the basis vectors are not energy eigenstates. Give the 2×2 matrix for $\hat{H}$ in this basis. Do this two ways:

        i. Find $\hat{H}|\psi_S\rangle$ (and similar for $\hat{H}|\psi_D\rangle$) by writing $|\psi_S\rangle$ in terms of $|1\rangle$ and $|2\rangle$, acting the hamiltonian on these eigenstates, and then writing $|1\rangle$ and $|2\rangle$ back in terms of $|\psi_S\rangle$ and $|\psi_D\rangle$.

        ii. Take the expression for $\hat{H}$ in terms of the outer product, Eq. (9), and rewrite the energy eigenstates appearing in this expression in terms of $\{|\psi_S\rangle, |\psi_D\rangle\}$.

14. The following problem concerns the commutativity of operators. We'll use the operators $\hat{H}$ and $\hat{L}$ for this (where the operators are defined in Eq. (13)).

    (a) Show that $\hat{H}\hat{L} \neq \hat{L}\hat{H}$ by writing out the matrices in the energy eigenbasis (i.e., in the basis where H is diagonal). For this reason, we say that these operators do not commute. Since $\hat{H}\hat{L}|\psi\rangle \neq \hat{L}\hat{H}|\psi\rangle$, it matters what order you perform the two measurements. Since operators multiply kets on the right hand side, you should think of $\hat{H}\hat{L}$ as meaning that the $\hat{L}$ measurement happens first, and then afterwards the $\hat{H}$ measurement acts on the result.

    (b) Show that $\hat{H}\hat{L}$ is not Hermitian. Of course, you could simply refer to the matrix $\hat{H}\hat{L}$ that you wrote out in part (a) to do this, but try to prove it independent of writing out components (i.e., don't write out the 2×2 matrix). This proof relies on the fact that the two operators do not commute. For this reason, you can't represent two consecutive noncommuting measurements as a single measurement.

15. The following question concerns the wavefunction $\psi_{\text{saw}}(x)$ introduced in Sec. [1.3].

(a) By setting the sum of the squares of the coefficients equal to one (with the coefficients defined by Eq. (22)), verify the following identity:

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}$$

(b) If a particle is in the state $\psi_{\text{saw}}(x)$, what is the probability that a measurement of the energy of the particle would be a value less than $10E_1$ (where E_1 is the energy of the lowest eigenstate of the PIB)?

(c) What is the probability that a measurement of the energy of the particle would be a value greater than $50E_1$?

(d) Confirm that the (theoretical) state $\psi_{\text{saw}}(x)$ actually has infinite energy by looking at the convergence of

$$\bar{E} \text{ or } \langle \hat{H} \rangle = \sum_{n=1}^{\infty} E_n |c_n|^2 \tag{26}$$

This is surprising considering you have a 60.8% chance of getting the ground state energy if you measure the energy of the state!

2 Particle in a Box II: Time-Evolution

The goal of this section is to solve for $\Psi(x,t)$ given $\psi(x) = \Psi(x,0)$ (equivalently, to solve for $|\Psi(t)\rangle$ given $|\Psi(0)\rangle$). You saw in the previous chapter that the Hamiltonian was the operator corresponding to the energy of the state. That's true, but we'll see in Sec. [2.1] that the Hamiltonian has another important interpretation. Stated informally, the Hamiltonian tells the state how it evolves in time. The formal statement is given by the Time Dependent Schrödinger Equation, Eq. (27).

In this chapter, we will use the conventional notation that capital Psi (i.e., $\Psi(x,t)$) has all time-dependence explicitly written out, and lower-case psi (i.e. $\psi(x)$) is a state at a particular time (often $t = 0$ by default).

2.1 General Time-Dependence

The Time-Dependent Schrodinger Equation (TDSE) is

$$\begin{gathered}\hat{H}\,|\Psi\rangle = i\hbar\frac{\partial}{\partial t}\,|\Psi\rangle \\ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t)\end{gathered} \tag{27}$$

The first equation is the general version, and the second equation is the equation as applied to the position basis (which you may have seen before in your lower-division course). The second results from the first because the Hamiltonian operator can be written as a kinetic energy piece (the second derivative operator) plus a potential energy piece (which depends only on position for many problems).

For the PIB, $V(x) = 0$, but for this section we'll leave $V(x)$ in to show the general result (which doesn't depend on the specific form of $V(x)$). The TDSE describes the time-evolution of any wavefunction. When we say that something is a possible wavefunction, it *must* satisfy the TDSE. A better way of thinking of it is that, given any initial wavefunction $\Psi(x, t = 0)$, the TDSE describes what that wavefunction will do over time.

Suppose the wavefunction $\Psi(x,t)$, which must satisfy Eq. (27), is also *separable*:

$$\Psi(x,t) \overset{!}{=} \psi(x)\Phi(t) \tag{28}$$

(the ! means "we require"). If this equation happens to be true, then you can show[9] that the two pieces $\psi(x)$ and $\Phi(t)$ satisfy the following two equations:

$$\begin{gathered}-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x) = E\psi(x) \\ \Phi(t) = e^{-iEt/\hbar}\end{gathered} \tag{29}$$

---

[9] A problem at the end of this chapter outlines how to do this, but it'll almost certainly be covered in detail in your UD QM course and it is not vital that you know the derivation right now.

In these equations, E is a constant independent of x and t. It has units of energy. These two facts strongly suggest that we interpret E as the energy of the wavefunction. The first line of Eq. (29) is the Time-Independent Schrödinger Equation. (Time-independent) Wavefunctions $\psi(x)$ that satisfy this equation are necessarily energy eigenstates. These states undergo a time evolution according to the following:

$$\Psi(x,t) = \psi(x) e^{-iEt/\hbar} \quad \text{(energy eigenstates)} \tag{30}$$

This was the claim made towards the end of Sec. [1.2.2]; we now see where it comes from.

If we combine this fact with the fact that the energy eigenstates form a complete basis, then we get the central result of this chapter:

$$\boxed{\Psi(x,t) = \sum_n C_n \, \psi_n(x) e^{-iE_n t/\hbar}} \quad \text{(any wavefunction)} \tag{31}$$

A general wavefunction does not split into a time-independent piece and a time-dependent piece, but it can always be written as a sum of such pieces, each of which is an energy eigenstate.

Remember one of the main points of the previous chapter: wavefunctions don't have to be represented with position-space wavefunctions. The form of Eq. (28) makes it look like the position basis is special, but it's not... all we really assumed was that the state factorizes into time-dependent piece times a time-independent state. The general version of Eq. (31) is

$$\boxed{|\Psi(t)\rangle = \sum_n C_n \, e^{-iE_n t/\hbar} \, |\psi_n\rangle} \tag{32}$$

As a reminder, the states $|\psi_n\rangle$ in Eq. (32) must be energy eigenstates, even though we can represent each eigenstate in terms of whatever basis is useful for the problem we're interested in.

The basis-independent versions of Eqs. (29) are

$$\begin{aligned} \hat{H} \, |\psi\rangle &= E \, |\psi\rangle \\ \Phi(t) &= e^{-iEt/\hbar} \end{aligned} \tag{33}$$

2.2 Time-Evolution of $|\psi_S\rangle$ in PIB

Suppose we start off with the state $|\psi\rangle = |\psi_S\rangle$ as depicted in Figure 1 at time $t = 0$. Then, according to Eq. (32), the state as a function of time is

$$|\Psi_S(t)\rangle \equiv \frac{1}{\sqrt{2}} \Big[\, |1\rangle \, e^{-iE_1 t/\hbar} + |2\rangle \, e^{-iE_2 t/\hbar} \Big]. \tag{34}$$

In principle, we are done, but perhaps it's worth exploring some properties of this wavefunction. It's the sum of two pieces, where the complex phase of each piece has a different angular velocity. The complex phase multiplying $|1\rangle$ has angular speed $\omega_1 = E_1/\hbar$, and the other complex phase (multiplying $|2\rangle$) has angular speed $\omega_2 = E_2/\hbar = 4\omega_1$.

The angular velocity of the two pieces are $\omega_2 = 4\omega_1$ and ω_1. Hence the overall wavefunction $\Psi(x,t)$ has oscillation frequency corresponding to angular velocity $\omega \equiv |\Delta\omega| = 3\omega_1$. In other words, after a total period

$$T = \frac{2\pi}{\omega} = \frac{2\pi}{3\omega_1} = \frac{2\pi\hbar}{3E_1} = \frac{4mL^2}{3\pi\hbar}, \tag{35}$$

the total wavefunction will return to its initial state. Why is this? Let's explain why three different ways.

2.2.1 Beat Frequency

It is a general property when adding together two waves of frequencies ω_1 and ω_2 that the frequency of the overall wave envelope is $|\Delta\omega| = |\omega_2 - \omega_1|$. This is known as the *beat frequency.* One example of this is an analog clock: it has an hour hand with angular frequency ω_0 (one revolution per 12 hours), and a minute hand with angular frequency $12\omega_0$ (one revolution per hour). How often does the minute hand line up with the hour hand? That is given by the beat frequency, $11\omega_0$. It happens 11 times every 12 hours, or once every 12/11 hours. If both the minute and hour hand start at 12:00 noon, then they'll line up again after $12/11 \approx 1.0909$ hours, or at approximately 1:05 and 27 sec (just after 1 o'clock).

Likewise, we have two contributions to the total wavefunction (the two terms in Eq. (34)), which are moving with two different angular frequencies (ω_1, and $\omega_2 = 4\omega_1$). Both complex phase pieces start out at 1... when do they line up again? It'll be after one period of the beat frequency. After this amount of time the two complex phases will be the same. This doesn't mean that they will be real numbers, but that they will have the same angle in the complex plane. This angle, as we'll see in the next section, is $2\pi/3$ for the "slow" term and $8\pi/3$ for the "fast" term. Note $e^{-8\pi i/3} = e^{-2\pi i}e^{-2\pi i/3} = e^{-2\pi i/3}$, and so these two phases are the same. There is zero relative phase between the two terms at this time. Remember the overall phase of $e^{-2\pi i/3}$ is unphysical, and so $e^{-2\pi i/3}|\psi_S\rangle$ is the same state as $|\psi_S\rangle$.

2.2.2 Race along a Circle

This is basically the same as the "beat frequency" discussed in the previous section, but done through a visual representation of the complex phase.

Two objects, a slow blue dot and a fast red box, are running around a circle over and over again. They both start at the same spot on the circle at $t = 0$ (on the right side of the unit circle) and move clockwise. The red box moves at four times the angular velocity of the blue dot. Suppose the time it takes the red dot to go once around the circle is T_2:

What is the first time $t > 0$ when the two objects line up again? We know it's sometime between T_2 and $1.5T_2$: at time $t = T_2$, the red box has undergone one full revolution, but it

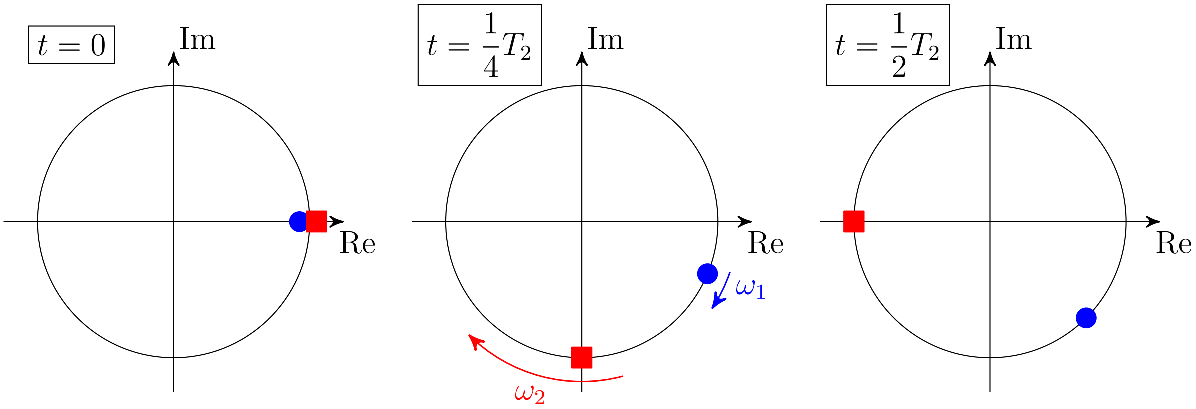

Figure 4: The phase of each component of $|\Psi_S(t)\rangle$ for three times. The blue circle corresponds to the term with energy E_1, and the red square corresponds to the term with energy $E_2 = 4E_1$. The red square has four times the angular speed as that of the blue circle.

has not yet "caught up" with the blue circle. At $t = 1.5T_2$ though, the red box has undergone one and a half full revolutions, and the blue circle has done $3/8$ of a full revolution, so the red square has already passed the blue circle. After thinking about it a while, you can convince yourself the two objects line up at $t = T_2 + T_2/3 = 4T_2/3$: the red square is 1/3rd of the way around its second revolution, and the blue circle is 1/3rd of the way along its journey in going across the bottom-left quadrant. At this time, both objects are at an angle $120° = 2\pi/3$ with respect to the real axis as measured clockwise.

$$\text{Note:} \quad \frac{4}{3}T_2 = \frac{4}{3}\cdot\frac{2\pi}{\omega_2} = \frac{4}{3}\cdot\frac{2\pi\hbar}{E_2} = \frac{8\pi\hbar}{3}\cdot\frac{2mL^2}{4\pi^2\hbar^2} = \frac{4mL^2}{3\pi\hbar} = T \checkmark \tag{36}$$

Obviously this guess-and-check method doesn't easily generalize, but it's worth seeing the complex phase in the complex plane.

2.2.3 Algebraic Calculation and $|\Psi_S(x,t)|^2$ over time

Another way to see how the beat frequency $\omega_2 - \omega_1$ arises is by taking Eq. (34), factoring out a $\exp(-i\omega_1 t)$, and rewriting the state with a different overall phase:

$$\begin{aligned} |\Psi_S(t)\rangle &= \frac{1}{\sqrt{2}}\left[|1\rangle\, e^{-i\omega_1 t} + |2\rangle\, e^{-i\omega_2 t}\right] \\ &= \frac{1}{\sqrt{2}}\, e^{-i\omega_1 t}\left[|1\rangle + |2\rangle\, e^{-i(\omega_2-\omega_1)t}\right] \\ &\cong \frac{1}{\sqrt{2}}\left[|1\rangle + |2\rangle\, e^{-i(\omega_2-\omega_1)t}\right] \end{aligned} \tag{37}$$

To get a sense of what this wavefunction looks like, let's look at the state and the probability density in the position basis. Define $\omega \equiv |\Delta\omega| = \omega_2 - \omega_1$:

$$\Psi_S(x,t) = \frac{1}{\sqrt{2}}\Big[\psi_1(x) + \psi_2(x)e^{-i\omega t}\Big] \tag{38}$$

Note the imaginary component is nonzero for almost all times. For example, after a quarter period ($t = T/4 = \pi/(2\omega)$),

$$\Psi_S(x, t = T/4) = \frac{1}{\sqrt{2}}\Big[\psi_1(x) + \psi_2(x)e^{-i\omega\left(\frac{\pi}{2\omega}\right)}\Big] = \frac{1}{\sqrt{2}}\Big[\psi_1(x) - i\psi_2(x)\Big]$$

Hopefully you can forgive the author of your Modern Physics textbook for making it appear as though the wavefunction $\psi(x)$ can always be real. In general it cannot for states that are not energy eigenstates, since the complex phase factors $\exp(-i\omega_n t)$ multiplying different eigenstates $|\psi_n\rangle$ have different phases.

You can get a sense of what the wavefunction is doing over time by looking at the probability density $|\Psi_S(x,t)|^2$. In addition to giving us a sense of "where" the particle is (roughly speaking), the quantity is strictly real (and nonnegative). Let's compute it for the state $\Psi_S(x,t)$ in Eq. (38):

$$\begin{aligned}
|\Psi_S(x,t)|^2 = \Psi_S^*(x,t)\Psi_S(x,t) &= \frac{1}{2}\Big[\psi_1^*(x) + \psi_2^*(x)e^{+i\omega t}\Big]\Big[\psi_1(x) + \psi_2(x)e^{-i\omega t}\Big] \\
&= \frac{1}{2}\Big[\psi_1(x)^2 + \psi_2(x)^2 + \psi_1(x)\psi_2(x)\Big(e^{+i\omega t} + e^{-i\omega t}\Big)\Big] \\
&= \frac{1}{2}\Big[\psi_1(x)^2 + \psi_2(x)^2 + 2\psi_1(x)\psi_2(x)\cos(\omega t)\Big]
\end{aligned} \tag{39}$$

Plug the explicit form of $\psi_1(x)$ and $\psi_2(x)$ (i.e., Eq. (1)) into Eq. (39) to get the following:

$$|\Psi_S(x,t)|^2 = \frac{1}{L}\left[\sin^2\left(\frac{\pi x}{L}\right) + \sin^2\left(\frac{2\pi x}{L}\right) + \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)\cos(\omega t)\right] \tag{40}$$

For convenience, here is something you can copy-paste into desmos.com to see how the probability density evolves over time (taking $L = 1$). Set the slider "t" to go from 0 to 1 (which is one full period), and have the step size be 0.01 or 0.001; as the animation goes from $t = 0$ to $t = 1$, you can get a sense of how the probability density moves over time. If copy-pasting isn't working from this .pdf file, the text is also here (again, this probably won't work from a tablet or smartphone, and you'll have to copy-paste from a computer).

```
\left\{x<0:0,x>1:0,\sin\left(\pi\cdot x\right)\cdot
\sin\left(\pi\cdot x\right)+
2\cdot\sin\left(\pi\cdot x\right)\cdot
\sin\left(2\cdot\pi\cdot x\right)\cdot
\cos\left(2\cdot\pi\cdot t\right)+
\sin\left(2\pi\cdot x\right)\cdot
\sin\left(2\pi\cdot x\right)\right\}
```

Recall the problem last chapter dealing with the operator "$\hat{O}$" (Eq. (24)) [if you haven't looked at and/or attempted this problem, you might want to now]. If you start with state $|\psi_S\rangle$ at $t = 0$ and wait a quarter of a period, you'll get the state $|+\rangle$, and if you want another half a period (so, $t = 3T/4$ overall), then you'll get the state $|-\rangle$. If you compare this with the animation showing $|\Psi_S(x,t)|^2$ over time, it appears that the operator $\hat{O}$ is measuring a kind of velocity of the wavefunction of the particle: a positive measurement of $\hat{O}$ (with corresponding state $|+\rangle$) corresponds to the probability density moving to the right, and a negative measurement of $\hat{O}$ (with corresponding state $|-\rangle$) corresponds to the probability density moving to the left.

It's dangerous to take the last paragraph too seriously: the operator $\hat{O}$ is not a definite measurement of the velocity of the wavefunction (or of the particle). The main reason for this is that the operator $\hat{O}$ is not the momentum operator. However, even if we forget about the momentum operator, we can explore another reason why there is a problem associating $\hat{O}$ with velocity. Pretend you have the state $|\psi_S\rangle$ (the state at $t = 0$), and then immediately measure $\hat{O}$. Because

$$|\psi_S\rangle = \left(\frac{1+i}{2}\right)|+\rangle + \left(\frac{1-i}{2}\right)|-\rangle\,,$$

the result of a measurement of $\hat{O}$ on $|\psi_S\rangle$ will be $|+\rangle$ with 50% probability and $|-\rangle$ with 50% probability. This runs counter to intuition for a couple of reasons: How could the wavefunction be moving to the left if in the state $|\psi_S\rangle$? (it seems to be as far left as it possibly could be.) Also, the wavefunction is momentarily "paused" when in the state $|\psi_S\rangle$, so you would expect the velocity at this time to be zero. In fact, you would *never* measure zero for the "velocity" with this interpretation!

2.3 Chapter 2 Exercises

1. This problem will focus on the steps required to get from Eq. (28) to Eq. (29):
   (a) Plug the ansantz [that is, Eq. (28)] into the TDSE, Eq. (27). Move all the terms to one side of the equation, divide by $\Psi(x,t) = \psi(x)\Phi(t)$, and simplify. You should be left with an equation where entire terms depend either only on x or only on t.
   (b) Based on part (a), you can write your equation as $f(x) + g(t) = 0$, where "$f(x)$" involves x and derivatives with respect to x but makes no reference to t (and similar for $g(t)$). If this equation is to be true for all x and all t, this means that $f(x)$ must equal a constant, and also that $g(t)$ must equal a constant. Explain why this must be true.
   (c) In part (b), you explained why $f(x) = E$ and $g(t) = -E$ (that is, the constants must be equal and opposite, since they must add up to zero). Solve the latter equation for $\Phi(t)$. Is your answer unique? Why can we just write it as in Eq. (29) (with no constant of integration)?
2. The analysis in Sec. [2.2] focused on $|\psi_S\rangle$, which at $t = 0$ is equal to $(|1\rangle + |2\rangle)/\sqrt{2}$.

Suppose, instead, that you have the state $|\psi_{23}\rangle$ at $t = 0$, defined by

$$|\psi_{23}\rangle \equiv \frac{1}{\sqrt{2}}\Big[\,|2\rangle - |3\rangle\,\Big]$$

(a) Find an expression for $|\Psi_{23}(t)\rangle$. What is the first time after $t = 0$ where the state is equal to $|\psi_{23}\rangle$?

(b) Find the wavefunction $\Psi_{23}(x, t)$ and the probability density $|\Psi_{23}(x, t)|^2$ in the position basis.

3. Suppose you had a state at time $t = 0$ comprised of an arbitrary linear combination of two distinct ($m \neq n$) eigenstates:

$$|\psi_{mn}\rangle = c_m\,|m\rangle + c_n\,|n\rangle$$

(as always, $|i\rangle$ refers to the i^{th} energy eigenstate of the PIB).

(a) Find $|\Psi_{mn}(t)\rangle$ and $\langle\Psi_{mn}(t)|$. Do not use the position basis.

(b) Find $\langle\Psi_{mn}(t)|\Psi_{mn}(t)\rangle$ and verify that it is independent of time. If the state $|\psi_{mn}\rangle$ (at $t = 0$) was normalized, what is the value of $\langle\Psi_{mn}|\Psi_{mn}\rangle$?

(c) Find the probability density (in the position basis), $|\Psi_{mn}(x, t)|^2$. You may use the basis wavefunctions $\psi_m(x)$ and $\psi_n(x)$ in your answer.

4. Given the state $|\psi_S\rangle$ at time $t = 0$, find $\langle\hat{L}\rangle$ as a function of time, where $\hat{L}$ is the "Leftness" operator defined in Eq. (13).

5. To see just how crazy a general wavefunction can get, we'll look at $\psi_{\text{saw}}(x)$ from last chapter. The overall wavefunction has an infinite number of terms, so let's define

$$\psi_{\text{saw}}^{(n\leq 5)}(x) = \sum_{n=1}^{5} c_n\psi_n(x), \quad \text{where} \quad c_n = \frac{-\sqrt{6}\cos(n\pi)}{n\pi} = (-1)^{n-1}\,\frac{\sqrt{6}}{n\pi}$$

Drawing inspiration from the Desmos input text following Eq. (40), create an animation that shows the time-evolution of $|\Psi_{\text{saw}}^{(n\leq 5)}(x, t)|^2$. The intention is NOT to solve for the probability density analytically – use a computer algebra system like Mathematica or similar to do the algebra, and then graph the result.[10]

---

[10] Obviously there are lots of ways you could choose to do this, but if you do use Mathematica, I would suggest using the "ComplexExpand[...]" function to simplify complex expressions. Also, if you want to output anything from Mathematica into Desmos, highlight the final output, copy it as "LaTeX," and paste it into Desmos.

3 Solutions to Exercises

I probably would have ignored the following advice when I was a student, but I'll put it here anyway: you will get more out of the exercises if you struggle with them for a bit first, before reading the solution.

3.1 Chapter 1 Solutions

1. Plug in $\psi_S(x)$ into Eq. (2), and write $\psi_S(x)$ in terms of $\psi_1(x)$ and $\psi_2(x)$:

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(\frac{1}{\sqrt{2}}\Big[\psi_1(x)+\psi_2(x)\Big]\right) &\overset{?}{=} E\left(\frac{1}{\sqrt{2}}\Big[\psi_1(x)+\psi_2(x)\Big]\right) \\ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left[\sin\left(\frac{\pi x}{L}\right)+\sin\left(\frac{2\pi x}{L}\right)\right] &\overset{?}{=} E\left[\sin\left(\frac{\pi x}{L}\right)+\sin\left(\frac{2\pi x}{L}\right)\right] \\ +\frac{\hbar^2\pi^2}{2mL^2}\left[\sin\left(\frac{\pi x}{L}\right)+4\sin\left(\frac{2\pi x}{L}\right)\right] &\neq E\left[\sin\left(\frac{\pi x}{L}\right)+\sin\left(\frac{2\pi x}{L}\right)\right] \end{aligned}$$

   There is no constant E for which the above equation is true for all $x \in [0, L]$. Therefore, the wavefunction $\psi_S(x)$ is not a solution to the T.I.S.E.

2. (a) The inner product $\langle\psi|\psi\rangle$ must equal 1 for the state to be normalized:

$$1 \overset{!}{=} \begin{pmatrix} a-bi & c-di \end{pmatrix}\begin{pmatrix} a+bi \\ c+di \end{pmatrix} = a^2+b^2+c^2+d^2 \implies \boxed{a^2+b^2+c^2+d^2=1} \tag{41}$$

   (b) Of course, this problem is subjective. However, I bet if you asked several physicists, the majority would say that the second representation is better (the one described with θ and ϕ). The reason for this is our desire to introduce the minimal number of parameters necessary to describe the state (2, vs. 4 with constraints). Notice how the state with $(a-d)$ appears to have 4 real degrees of freedom (d.o.f.). However, subjecting the state to the normalization condition Eq. (41) reduces this down to 3 d.o.f., and there is another redundancy due to the fact that the overall phase is irrelevant. The state with only θ and ϕ makes the fact that there are only 2 d.o.f. readily apparent: θ describes how much of the state is $|1\rangle$ vs. how much of it is $|2\rangle$, and ϕ describes the relative phase between the two. This is the minimal amount of information required to completely describe the state.

3. (a) The wavefunction $|\psi_i\rangle$ is normalized if $\langle\psi_i|\psi_i\rangle = 1$:

$$\langle\psi_a|\psi_a\rangle = \frac{1}{3}\begin{pmatrix} -i & 1 & 1 \end{pmatrix}\begin{pmatrix} i \\ 1 \\ 1 \end{pmatrix} = \frac{1}{3}\Big(1+1+1\Big) = 1 \checkmark$$

$$\langle\psi_b|\psi_b\rangle = \frac{1}{3}\begin{pmatrix} 0 & 1 & 2i \end{pmatrix}\begin{pmatrix} 0 \\ 1 \\ -2i \end{pmatrix} = \frac{1}{3}\Big(0+1+5\Big) = \frac{5}{3} \neq 1$$

Therefore, $|\psi_a\rangle$ is normalized but $|\psi_b\rangle$ is not. If the "$1/\sqrt{3}$" in $|\psi_b\rangle$ were replaced with $1/\sqrt{5}$, then $|\psi_b\rangle$ would be normalized.

(b) In general, $\langle\psi_a|\psi_b\rangle = \langle\psi_b|\psi_a\rangle^*$. For these particular states,

$$\langle\psi_a|\psi_b\rangle = \frac{1}{3}\begin{pmatrix}-i & 1 & 1\end{pmatrix}\begin{pmatrix}0\\1\\-2i\end{pmatrix} = \frac{1}{3}\Big(0+1-2i\Big) = \frac{1-2i}{3}$$

$$\langle\psi_b|\psi_a\rangle = \frac{1}{3}\begin{pmatrix}0 & 1 & +2i\end{pmatrix}\begin{pmatrix}i\\1\\1\end{pmatrix} = \frac{1}{3}\Big(0+1+2i\Big) = \frac{1+2i}{3} = \langle\psi_a|\psi_b\rangle^* \ \checkmark$$

4. Plugging in for $|\psi_a\rangle$ and $|\psi_b\rangle$,

$$|\psi_A\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1+i\\0\end{pmatrix} \quad \text{and} \quad |\psi_B\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1-i\\0\end{pmatrix}$$

$|\psi_A\rangle$ and $|\psi_B\rangle$ are off by an overall phase, and are therefore the same physical state.

5. There are an infinite number of answers to this question. One possibility is an operator which takes the state $|\psi\rangle$ into the state $|2\rangle\,|\langle 1|\psi\rangle|^2$. Let's plug this operator into both sides of Eq. (23), with $|\psi_1\rangle = |\psi_2\rangle = |1\rangle$:

$$\hat{O}\Big(\alpha|\psi_1\rangle + \beta|\psi_2\rangle\Big) = \hat{O}\Big[(\alpha+\beta)|1\rangle\Big] = |\alpha+\beta|^2|2\rangle$$
$$\alpha\hat{O}|\psi_1\rangle + \beta\hat{O}|\psi_2\rangle = \alpha|2\rangle + \beta|2\rangle = (\alpha+\beta)|2\rangle$$

In general these are not equal, and so the operator is not linear. For (counter)example, if $\alpha = 1$ and $\beta = i$, then $|\alpha+\beta|^2 = 2$, whereas $(\alpha+\beta) = 1+i$.

6. (a) Let's set up the eigenvalue/eigenvector equation as in Eq. (17):

$$\begin{pmatrix}0 & i\\-i & 0\end{pmatrix}\begin{pmatrix}a\\b\end{pmatrix} = \lambda\begin{pmatrix}a\\b\end{pmatrix}$$

This gives the two equations $bi = \lambda a$ and $-ia = \lambda b = -i\lambda^2 a \implies \lambda = \pm 1$. Solving each eigenvalue/eigenvector equation separately gives

$$\lambda_+ = +1, \text{ with } |+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} \qquad \lambda_- = -1, \text{ with } |-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix} \tag{42}$$

(b) Note we've already done this... the states $|+\rangle$ and $|-\rangle$ are already written in terms of $|1\rangle$ and $|2\rangle$ in Eq. (42). From this equation, we can read off the answer:

$$|+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} = \frac{1}{\sqrt{2}}|1\rangle - \frac{i}{\sqrt{2}}|2\rangle$$

(c) Let's solve this two different ways. There's the brute-force way, solving a system of equations by writing everything in terms of the energy eigenbasis (Solution #1), and the "elegant" way (Solution #2).

The second solution is "elegant" because it's a method that generalizes to different kinds of problems, utilizing the fact that the bases we work with are orthonormal. Do not ignore Solution #2, even if you understand / like Solution #1 better!

Solution #1:
Since we know what $|\psi_S\rangle$, $|+\rangle$, and $|-\rangle$ all look like in the energy eigenbasis, let's set up the equation relating the three in this basis:

$$\begin{gathered} |\psi_S\rangle = c_+ |+\rangle + c_- |-\rangle \\ \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = c_+\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} + c_-\frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix} \end{gathered} \tag{43}$$

This gives two equations for the two unknowns c_+ and c_-:

$$\begin{aligned} 1 &= c_+ + c_- \\ 1 &= -ic_+ + ic_- \end{aligned} \tag{44}$$

Take the first equation in Eqs. (44), multiply the equation by $-i$, and add it to the equation immediately following it:

$$\begin{aligned} -i + 1 = -2ic_+ \quad &\Longrightarrow \quad c_+ = \frac{1+i}{2} \\ &\Longrightarrow \quad c_- = \frac{1-i}{2} \end{aligned}$$

This gives

$$\boxed{|\psi_S\rangle = \left(\frac{1+i}{2}\right)|+\rangle + \left(\frac{1-i}{2}\right)|-\rangle}$$

Solution #2:
In this solution, we start with the relationship between $|\psi_S\rangle$, $|+\rangle$, and $|-\rangle$ (the first line of Eq. (43)), and multiply on the left by $\langle +|$ to get the coefficient c_+. Also, multiply by $\langle -|$ on the left to get the coefficient c_-. Note that, since $\{|+\rangle, |-\rangle\}$ constitutes an orthonormal basis, we know immediately $\langle +|+\rangle = 1$, $\langle -|-\rangle = 1$, and $\langle +|-\rangle = \langle -|+\rangle = 0$:

$$\begin{aligned} |\psi_S\rangle &= c_+ |+\rangle + c_- |-\rangle \\ \langle +|\psi_S\rangle &= c_+ \langle +|+\rangle + c_- \langle +|-\rangle = c_+ \\ c_+ = \langle +|\psi_S\rangle &= \frac{1}{2}\begin{pmatrix}1 & +i\end{pmatrix}\begin{pmatrix}1\\1\end{pmatrix} = \left(\frac{1+i}{2}\right) \\ \text{likewise, } c_- = \langle -|\psi_S\rangle &= \frac{1}{2}\begin{pmatrix}1 & -i\end{pmatrix}\begin{pmatrix}1\\1\end{pmatrix} = \left(\frac{1-i}{2}\right) \end{aligned} \tag{45}$$

therefore, again we see $\boxed{|\psi_S\rangle = \left(\frac{1+i}{2}\right)|+\rangle + \left(\frac{1-i}{2}\right)|-\rangle}$

7. Recall

$$D = \begin{pmatrix} 1 & 2 \\ 2 & -2 \end{pmatrix}$$

(a) The trace is $(1) + (-2) = -1$ and the determinant is $(1)(-2) - (2)(2) = -6$. So we are looking for two real numbers λ_1 and λ_2 such that

$$\lambda_1 + \lambda_2 = -1 \qquad \text{and} \qquad \lambda_1\lambda_2 = -6$$

This has solution $\boxed{\lambda_1 = -3}$ and $\boxed{\lambda_2 = +2}$ (which one is which doesn't matter).

(b) For $\lambda_1 = -3$,

$$\begin{pmatrix} 1 & 2 \\ 2 & -2 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} -3a \\ -3b \end{pmatrix} \implies \begin{cases} a + 2b = -3a \\ 2a - 2b = -3b \end{cases} \implies \boxed{\begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\sqrt{5}}\begin{pmatrix} 1 \\ -2 \end{pmatrix}}$$

Note the choice of eigenvector is not unique... all that matters is that $2a + b = 0$. I chose the overall normalization so that the state was normalized and so that the first entry was real and positive. This isn't required though – if you had -1 and $+2$ in the top and bottom entries of the column vector, that'd be perfectly fine. It's probably a good idea to get in the habit of normalizing each vector, though (hence the factor of $1/\sqrt{5}$). For $\lambda_2 = +2$,

$$\begin{pmatrix} 1 & 2 \\ 2 & -2 \end{pmatrix}\begin{pmatrix} c \\ d \end{pmatrix} = \begin{pmatrix} 2c \\ 2d \end{pmatrix} \implies \begin{cases} c + 2d = 2c \\ 2c - 2d = 2d \end{cases} \implies \boxed{\begin{pmatrix} c \\ d \end{pmatrix} = \frac{1}{\sqrt{5}}\begin{pmatrix} 2 \\ 1 \end{pmatrix}}$$

8. General 2×2 and 3×3 Hermitian matrices can be written as follows:

$$A_{2\times 2} = \begin{pmatrix} a_1 & a_2 + a_3 i \\ a_2 - a_3 i & a_4 \end{pmatrix} \quad \text{and} \quad B_{3\times 3} = \begin{pmatrix} b_1 & b_2 + b_3 i & b_5 + b_6 i \\ b_2 - b_3 i & b_4 & b_7 + b_8 i \\ b_5 - b_6 i & b_7 - b_8 i & b_9 \end{pmatrix}$$

A general 2×2 Hermitian matrix requires 4 real numbers, and a general 3×3 Hermitian matrix requires 9. It would appear then that a general $n \times n$ Hermitian matrix can be described with n^2 real numbers. In fact, this is not difficult to prove by induction: notice the addition of a new row (going from n to $n+1$) requires an additional $2n+1$ real numbers, and $n^2 + (2n+1) = (n+1)^2$.

9. First, observe the following:

$$\left(e^{i\phi}|\psi\rangle\right)^\dagger = \left(|\psi\rangle\right)^\dagger\left(e^{i\phi}\right)^\dagger = \langle\psi| e^{-i\phi}$$

Where you put the $\exp(-i\phi)$ doesn't really matter since it's just a number. However, it's important to note in general when you take the Hermitian conjugate of a product of operators that you switch the order. That is, $(AB)^\dagger = B^\dagger A^\dagger$. Also, for a number, taking the "dagger" is the same as just taking the complex conjugate (the transpose of a number is just the same number... the number is like a 1×1 matrix). Let's look at the expectation value of the operator $\hat{O}$ on the states $|\psi\rangle$ and $e^{i\phi}|\phi\rangle$

$$\langle\hat{O}\rangle_{|\psi\rangle} = \langle\psi|\hat{O}|\psi\rangle$$

$$\langle\hat{O}\rangle_{e^{i\phi}|\psi\rangle} = \Big(e^{i\phi}|\psi\rangle\Big)^\dagger \hat{O}\Big(e^{i\phi}|\psi\rangle\Big) = \langle\psi| e^{-i\phi}\hat{O}e^{i\phi}|\psi\rangle = \langle\psi| e^{-i\phi}e^{i\phi}\hat{O}|\psi\rangle = \langle\psi|\hat{O}|\psi\rangle \ \checkmark$$

Note that we were able to "commute" (switch the order of) $\exp(i\phi)$ and $\hat{O}$ since the former is just a number. If it were a matrix (a general operator), you cannot do this in general unless the two things you're swapping commute. By the way, a number in QM is sometimes referred to as a *c-number*, but this term is kind of outdated. It stands for "classical number," but you can also think of it as meaning "complex number."

10. $\hat{L}$, as defined in Eq. (13), is an operator that does the following:

$$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}0\\1\end{pmatrix} \quad\Longrightarrow\quad \hat{L}|1\rangle = |2\rangle$$

$$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}1\\0\end{pmatrix} \quad\Longrightarrow\quad \hat{L}|2\rangle = |1\rangle$$

In other words, the operator $\hat{L}$ takes $|1\rangle$ to $|2\rangle$ and $|2\rangle$ to $|1\rangle$. In terms of outer products, this statement is

$$\hat{L} = |2\rangle\langle 1| + |1\rangle\langle 2|$$

The "1" in the upper-right hand corner of the matrix L is the entry that takes $|2\rangle$ to $|1\rangle$. This is the term $|1\rangle\langle 2|$ in the outer product.

11. $L^2|1\rangle = L|0\rangle = |1\rangle$ and $L^2|0\rangle = L|1\rangle = |0\rangle$, and so we would expect $L^2 = \mathbb{1}_{2\times 2}$ (the identity matrix in two dimensions). If you multiply out the matrix, you can confirm this is true.

12. (a) $P_1^2 = \Big(|1\rangle\langle 1|\Big)\Big(|1\rangle\langle 1|\Big) = |1\rangle\langle 1|1\rangle\langle 1| = |1\rangle\langle 1| = P_1$ ✓ This projection operator "projects" onto the state $|1\rangle$ (i.e., it outputs only the part of the state that overlaps with $|1\rangle$).

    (b) Via the outer product, this is easy: $P = |\psi_S\rangle\langle\psi_S|$. Writing this out as matrices,

$$P = \frac{1}{2}\begin{pmatrix}1 & 1\end{pmatrix}\begin{pmatrix}1\\1\end{pmatrix} = \begin{pmatrix}1/2 & 1/2\\ 1/2 & 1/2\end{pmatrix}$$

    (c) In this 3-D space, $\langle\psi_S| = \begin{pmatrix}1 & 1 & 0\end{pmatrix}/\sqrt{2}$ and $\langle\psi_D| = \begin{pmatrix}1 & -1 & 0\end{pmatrix}/\sqrt{2}$:

$$|\psi_S\rangle\langle\psi_S| + |\psi_D\rangle\langle\psi_D| = \begin{pmatrix}1/2 & 1/2 & 0\\ 1/2 & 1/2 & 0\\ 0 & 0 & 0\end{pmatrix} + \begin{pmatrix}1/2 & -1/2 & 0\\ -1/2 & 1/2 & 0\\ 0 & 0 & 0\end{pmatrix} = \begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 0\end{pmatrix} \ \checkmark$$

    This is not too surprising, since $\{|\psi_S\rangle, |\psi_D\rangle\}$ & $\{|1\rangle, |2\rangle\}$ span the same subspace.

13. (a) Because the basis vectors $|\psi_S\rangle$ and $|\psi_D\rangle$ are eigenvectors of L, the matrix is diagonal. A diagonal matrix has its eigenvalues as entries (here, 1 and -1). The matrix L must be

$$L = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Note that, if $|\psi_D\rangle$ were instead the column vector $\begin{pmatrix} 1 & 0 \end{pmatrix}^T$ (with a 1 on the first entry rather than the second), then the -1 entry in L would instead go on the upper-left corner.

(b) i. Let's see the action of $\hat{H}$ on $|\psi_S\rangle$:

$$\begin{aligned}
\hat{H}\,|\psi_S\rangle &= \hat{H}\frac{1}{\sqrt{2}}\Big(\,|1\rangle + |2\rangle\,\Big) \\
&= \frac{1}{\sqrt{2}}\Big(E_1\,|1\rangle + E_2\,|2\rangle\,\Big) \\
&= \frac{1}{\sqrt{2}}\left[E_1\frac{1}{\sqrt{2}}\Big(\,|\psi_S\rangle + |\psi_D\rangle\,\Big) + E_2\frac{1}{\sqrt{2}}\Big(\,|\psi_S\rangle - |\psi_D\rangle\,\Big)\right] \\
&= \left(\frac{E_1+E_2}{2}\right)|\psi_S\rangle + \left(\frac{E_1-E_2}{2}\right)|\psi_D\rangle
\end{aligned}$$

Rewriting this equation in terms of matrices (in this new basis) gives

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \left(\frac{E_1+E_2}{2}\right)\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \left(\frac{E_1-E_2}{2}\right)\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} H_{11} \\ H_{21} \end{pmatrix} = \begin{pmatrix} \dfrac{E_1+E_2}{2} \\ \dfrac{E_1-E_2}{2} \end{pmatrix}$$

Likewise, acting $\hat{H}$ on $|\psi_D\rangle$ lets you solve for H_{12} and H_{22} (with a similar derivation to the above... work this out yourself to ensure you understand the above!). Overall, then, the hamiltonian in this basis is given by

$$H = \begin{pmatrix} \dfrac{E_1+E_2}{2} & \dfrac{E_1-E_2}{2} \\ \dfrac{E_1-E_2}{2} & \dfrac{E_1+E_2}{2} \end{pmatrix}$$

ii. The other suggestion for how to do this is via the outer product. This way is easier – simply take the Hamiltonian as expressed in Eq. (9) and write the energy eigenstates in terms of the new basis states:

$$\begin{aligned} H &= E_1 \left|1\right\rangle \left\langle 1\right| + E_2 \left|2\right\rangle \left\langle 2\right| \\ &= \frac{E_1}{2}\left[\Big(\left|\psi_S\right\rangle + \left|\psi_D\right\rangle\Big)\Big(\left\langle\psi_S\right| + \left\langle\psi_D\right|\Big)\right] + \frac{E_2}{2}\left[\Big(\left|\psi_S\right\rangle - \left|\psi_D\right\rangle\Big)\Big(\left\langle\psi_S\right| - \left\langle\psi_D\right|\Big)\right] \\ &= \left(\frac{E_1+E_2}{2}\right)\Bigg[\left|\psi_S\right\rangle\left\langle\psi_S\right| + \left|\psi_D\right\rangle\left\langle\psi_D\right|\Bigg] + \left(\frac{E_1-E_2}{2}\right)\Bigg[\left|\psi_S\right\rangle\left\langle\psi_D\right| + \left|\psi_D\right\rangle\left\langle\psi_S\right|\Bigg] \end{aligned}$$

These four terms (in the order they appear, left-to-right) give the values of H_{11}, H_{22}, H_{12}, and H_{21}, respectively.

14. (a) Multiply the two matrices both ways to show they aren't the same:

$$\hat{H}\hat{L} = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & E_1 \\ E_2 & 0 \end{pmatrix}$$
$$\hat{L}\hat{H} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} = \begin{pmatrix} 0 & E_2 \\ E_1 & 0 \end{pmatrix}$$

Because $E_1 \neq E_2$, these two matrices are not the same, and $\hat{H}\hat{L} \neq \hat{L}\hat{H}$.

(b) $(\hat{H}\hat{L})^\dagger = \hat{L}^\dagger\hat{H}^\dagger = \hat{L}\hat{H} \neq \hat{H}\hat{L}$, and so $\hat{H}\hat{L}$ is not Hermitian.

15. (a) This is a one-liner:

$$1 \overset{!}{=} \sum_{n=1}^{\infty} |c_n|^2 = \sum_{n=1}^{\infty}\left|(-1)^{n-1}\frac{\sqrt{6}}{n\pi}\right|^2 = \sum_{n=1}^{\infty}\frac{6}{n^2\pi^2} = \frac{6}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2} \implies \boxed{\sum_{n=1}^{\infty}\frac{1}{n^2} = \frac{\pi^2}{6}} \checkmark$$

(b) Only the lowest three energy eigenstates have energy less than $10E_1$ (note $E_3 = 9E_1$ and $E_4 = 16E_1$). Therefore, the probability a measurement of the energy will return a value less than $10E_1$ is the sum of the probabilities that the state is in one of the energy eigenstates $\left|1\right\rangle$, $\left|2\right\rangle$, or $\left|3\right\rangle$:

$$(\text{Prob})_{n\leq 3} = \sum_{n=1}^{3}|c_n|^2 = \frac{6}{\pi^2}\left(\frac{1}{1^2}+\frac{1}{2^2}+\frac{1}{3^2}\right) \approx \boxed{82.7\%}$$

(c) This is a similar calculation to that in part (b):

$$(\text{Prob})_{n\geq 8} = 1 - \sum_{n=1}^{7}|c_n|^2 = 1 - \frac{6}{\pi^2}\left(\frac{1}{1^2}+\frac{1}{2^2}+\cdots+\frac{1}{7^2}\right) \approx \boxed{8.1\%}$$

(d) Each new term we add in the definition for $\psi_{\text{saw}}(x)$ adds a constant amount of energy $(6/\pi^2)E_1$ to the state, and so the expected value of the energy diverges:

$$\bar{E} \text{ or } \langle\hat{H}\rangle = \sum_{n=1}^{\infty}E_n|c_n|^2 = \sum_{n=1}^{\infty}\left(n^2E_1\right)\left(\frac{6}{\pi^2 n^2}\right) \longrightarrow +\infty$$

This is perhaps not too surprising if you try graphing the state with a large number of terms (1000 or so) – the wavefunction seems to go a little crazy near $x = L$. Of course, this is because of the discontinuity in the wavefunction at this location.

3.2 Chapter 2 Solutions

1. (a) Guess the separable solution $\Psi(x,t) = \psi(x)\Phi(t)$:

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t) &= i\hbar\frac{\partial}{\partial t}\Psi(x,t) \\ -\frac{\hbar^2}{2m}\Phi(t)\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x)\Phi(t) &= i\hbar\psi(x)\frac{\partial}{\partial t}\Phi(t) \\ -\frac{\hbar^2}{2m}\Phi(t)\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x)\Phi(t) - i\hbar\psi(x)\frac{\partial}{\partial t}\Phi(t) &= 0 \\ \underbrace{-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2}{dx^2}\psi(x) + V(x)}_{\equiv f(x)} \underbrace{-\frac{i\hbar}{\Phi(t)}\frac{d}{dt}\Phi(t)}_{\equiv g(t)} &= 0 \end{aligned}$$

   (b) Let's focus, without loss of generality, on $f(x)$. It explicitly depends only on x and not on t. However, it can't depend on x: if it did, then so would $g(t)$ in order for the two terms to sum to zero. This is not true by assumption: g is a function only of t. Therefore, $f(x)$ must equal a constant.

   (c) Set $g(t) = -E$, and solve by separation of variables:

$$\frac{-i\hbar}{\Phi}\frac{d\Phi}{dt} = -E \implies \frac{d\Phi}{\Phi} = -\frac{iE}{\hbar}dt \implies \Phi(t) = \Phi(0)e^{-iEt/\hbar}$$

   The constant of integration, $\Phi(0)$, can be set to 1. The reason for this is that the overall multiplicative constant can be absorbed by $\psi(x)$, and set when the wavefunction is normalized.

2. (a) Tack on the energy-dependent complex phase for each piece:

$$\begin{aligned} |\Psi_{23}(t)\rangle &= \frac{1}{\sqrt{2}}\left[e^{-iE_2t/\hbar}|2\rangle - e^{-iE_3t/\hbar}|3\rangle\right] \\ &= \frac{1}{\sqrt{2}}\left[e^{-4iE_1t/\hbar}|2\rangle - e^{-9iE_1t/\hbar}|3\rangle\right] \\ &= \frac{1}{\sqrt{2}}e^{-4iE_1t/\hbar}\left[|2\rangle - e^{-5iE_1t/\hbar}|3\rangle\right] \\ &\cong \frac{1}{\sqrt{2}}\left[|2\rangle - e^{-5iE_1t/\hbar}|3\rangle\right] \end{aligned}$$

   The beat frequency and period are given by

$$\omega = |\Delta\omega| = \frac{5E_1}{\hbar} = \frac{5\pi^2\hbar}{2mL^2} \quad \text{and} \quad T = \frac{2\pi}{|\Delta\omega|} = \frac{4\pi mL^2}{5\pi^2\hbar} = \boxed{\frac{4mL^2}{5\pi\hbar}}$$

   (b) $|\Psi_{23}(t)\rangle$ and $|\Psi_{23}(x,t)|^2$ are basically given by Eqs. (38) and (40), but with beat frequency $\omega = \omega_3 - \omega_2$, ψ_1 replaced with ψ_2, and ψ_2 replaced with $-\psi_3$:

$$\begin{aligned} \Psi_{23}(x,t) &= \frac{1}{\sqrt{2}}\left[\psi_2(x) - \psi_3(x)e^{-i\omega t}\right] \\ |\Psi_{23}(x,t)|^2 &= \frac{1}{2}\left[\psi_2(x)^2 + \psi_3(x)^2 - 2\psi_2(x)\psi_3(x)\cos(\omega t)\right] \end{aligned}$$

3. (a) $|\Psi_{mn}(t)\rangle = c_m e^{-i\omega_m t}|m\rangle + c_n e^{-i\omega_n t}|n\rangle$ and $\langle\Psi_{mn}(t)| = \langle m| e^{+i\omega_m t}c_m^* + \langle n| e^{+i\omega_n t}c_n^*$.

   (b) Note $\langle m|n\rangle = \langle n|m\rangle = 0$ since we are told $m \neq n$:

   $$\begin{aligned}\langle\Psi_{mn}(t)|\Psi_{mn}(t)\rangle &= \Big(\langle m| e^{+i\omega_m t}c_m^* + \langle n| e^{+i\omega_n t}c_n^*\Big)\Big(c_m e^{-i\omega_m t}|m\rangle + c_n e^{-i\omega_n t}|n\rangle\Big)\\ &= |c_m|^2 + |c_n|^2 \checkmark \text{ (independent of time)}\end{aligned}$$

   If the wavefunction were initially normalized (as it should be it be called a proper wavefunction!), then $|c_m|^2 + |c_n|^2 = 1$. Therefore, the value of $\langle\Psi|\Psi\rangle$ remains 1 over time.

   (c) This is similar to the expression in part (b), except it doesn't quite simplify as nicely since we don't know the coefficients c_n nor c_m:

   $$\begin{aligned}\Psi_{mn}(x,t) &= c_m e^{-i\omega_m t}\psi_m(x) + c_n e^{-i\omega_n t}\psi_n(x)\\ |\Psi_{mn}(x,t)|^2 &= |c_m|^2\psi_m(x)^2 + |c_n|^2\psi_n(x)^2\\ &\qquad + \Big(c_m^* c_n e^{i(\omega_m-\omega_n)t} + c_m c_n^* e^{i(\omega_n-\omega_m)t}\Big)\psi_m(x)\psi_n(x)\end{aligned}$$

4. Although the wavefunction is initially an eigenstate of $\hat{L}$ (with eigenvalue 1), it is not in general after some time evolution. We know for a fact that after half a period the wavefunction is in the state $|\psi_D\rangle$, which is the eigenstate of $\hat{L}$ with eigenvalue -1, so our final answer had better be consistent with this fact.

   The strategy is to take the wavefunction at a general time $|\Psi_S(t)\rangle$, write the ket out as a column vector, and compute $\langle\hat{L}\rangle$ explicitly via matrices much like Eq. (15).

   The general wavefunction $|\Psi_S(t)\rangle$ was given in Eq. (37). We'll write it again here as a column vector in the energy eigenbasis:

   $$\begin{aligned}|\Psi_S(t)\rangle &= \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ e^{-i\omega t}\end{pmatrix}\\ \langle\hat{L}\rangle = \langle\Psi_S(t)|\hat{L}|\Psi_S(t)\rangle &= \frac{1}{2}\begin{pmatrix}1 & e^{+i\omega t}\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1\\ e^{-i\omega t}\end{pmatrix}\\ &= \frac{1}{2}\begin{pmatrix}1 & e^{+i\omega t}\end{pmatrix}\begin{pmatrix}e^{-i\omega t}\\ 1\end{pmatrix}\\ &= \frac{1}{2}\Big(e^{-i\omega t} + e^{+i\omega t}\Big) = \boxed{\cos(\omega t)}\end{aligned}$$

   Indeed, our answer is consistent with the fact that it starts out at 1 at $t = 0$, and is equal to -1 after half a period. Remember that the period here is given by Eq. (35).

5. It's surprising how chaotic the wavefunction gets with only 5 terms! Just imagine what 50 or 500 is like. The final Desmos input you can use to view the animation is a little too long to be printed here, but it can be found at the following link:

   https://bshotwell.physics.ucsd.edu/QuantumPrimerPlots.html