PHYS 4P51: Quantum Mechanics
Lecture Notes

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Last Updated: February 28, 2025
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1 Introduction

1.1 Course Outline

PHYS 4P51 is a quantum mechanics course at the 4th-year undergraduate level. It will be your last course in quantum mechanics before graduate school, and thus it should prepare you for graduate-level study and research.

My goal is that by the end of this course, you will gain a deep and intuitive understanding of the foundations of quantum theory, from the modern point of view of 21st-century theoretical physics – as it is currently understood by researchers in cutting-edge fields such as quantum foundations, quantum information, quantum computation, quantum field theory, and quantum gravity. Such an understanding will be absolutely crucial if you want to be a theorist, and will also be extremely useful if you want to be an experimentalist.

Before you begin this course, you should forget everything you learned about quantum mechanics before! We will re-learn quantum theory from scratch, developing it in an axiomatic and mathematically rigorous way from first principles. We will see that there is nothing mysterious about quantum mechanics, and obtain insight that will allow us to understand how it makes the universe works at the most fundamental level.

1.2 Exercises and Problems

Throughout these notes, you will find many **exercises** and **problems**.

- **Exercises** are usually just calculations. They are meant to verify that you understand how to calculate things, and they are usually simple and straightforward.

- **Problems** are usually proof-based. They are meant to verify that you understand the more abstract relations between the concepts we will introduce, and they often require some thought.

2 Non-Technical Overview

In this chapter, I will provide a non-technical overview of quantum physics, and how it compares to classical physics. I won't go into exactly who discovered what and in which year, because this is not a history course; this is a course about how the universe works. However, if you are interested in the history of quantum mechanics, there are many excellent websites and textbooks on the subject, and you are encouraged to look them up.

Instead, I will focus on two main goals in this chapter:

1. Introducing some of the fundamental experiments which illustrate why classical mechanics needs to be replaced with a more fundamental theory. This should also convince you that your classical intuition must be replaced with quantum intuition, which is what we will try to develop in this course.

2. Summarizing the fundamental properties of quantum mechanics and the differences between it and classical mechanics in non-technical terms, without going into the math. This should give you some idea of what we will study throughout this course in much more detail and with the full, uncensored mathematical framework.

2.1 The Failures of Classical Physics

2.1.1 Black-Body Radiation and the Ultraviolet Catastrophe

A *black body* is an object that absorbs all incoming light at all frequencies. It absorbs it and does not reflect it – therefore, it is black. More generally, it absorbs not just light, but all electromagnetic radiation. Black bodies also emit radiation, due to their heat. Electromagnetic radiation has a spectrum of wavelengths of different lengths. We are interested in predicting the amount of radiation emitted by the black body at each wavelength, which we will refer to as the black body's spectrum.

One can try to use classical physics to calculate this spectrum. It turns out that the amount of the radiation is inversely proportional to the wavelength[1]. This means that as the wavelength approaches zero, the amount of radiation approaches infinity! This is illustrated by the black curve in Figure 2.1. This result is called the *ultraviolet catastrophe*, since ultraviolet light has shorter wavelengths than visible light. Obviously, this does not fit well with experimental data, since when we measure the total radiation emitted from a black body, we most definitely do **not** measure it to be infinity!

[1] More precisely, the power emitted per unit area per unit solid angle per unit wavelength is proportional to $1/\lambda^4$ where λ is the wavelength... But fortunately, we don't need to be very precise here!

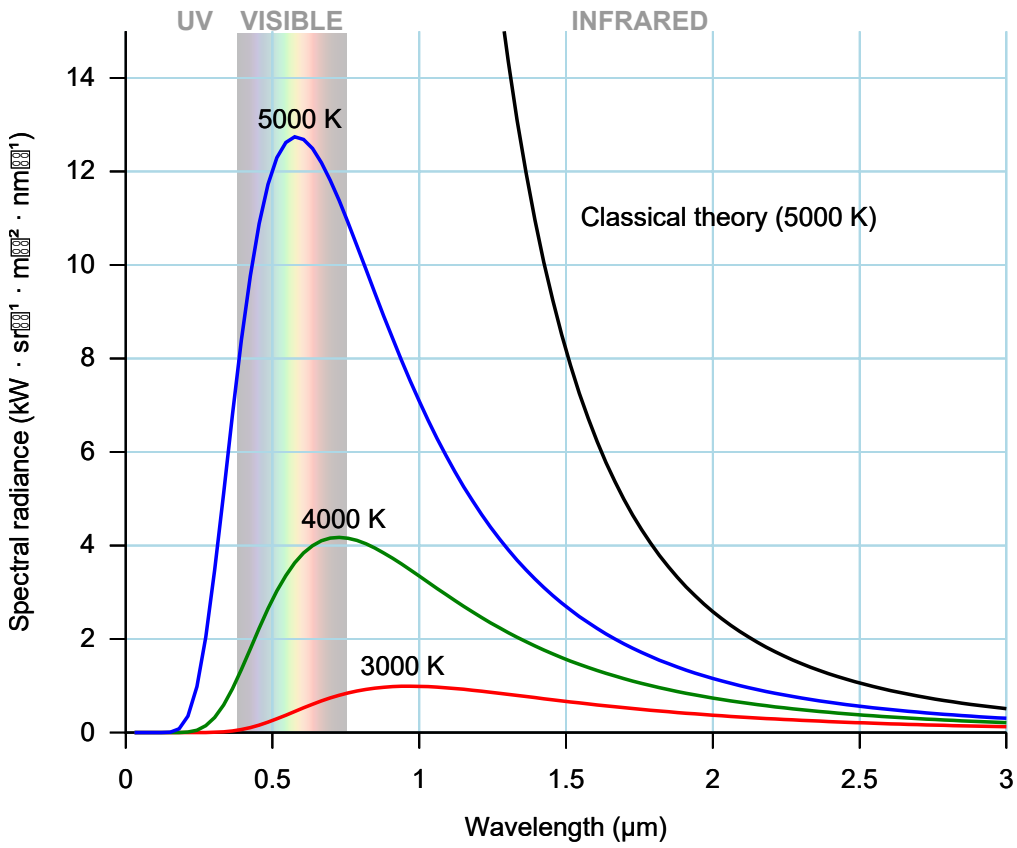

Figure 2.1: The electromagnetic spectrum of a black body. *Source: Wikipedia.*

To solve this problem, we must use quantum physics. If we assume that radiation can only be emitted in discrete "packets" of energy called *quanta*, we get the correct spectrum of radiation, which is compatible with experiment. The law describing the amount of radiation at each wavelength is called *Planck's law*. In Figure 2.1, we can see three different curves, calculated using Planck's law, giving the radiation spectrum at different temperatures (in Kelvin). You can see that the total amount of radiation is no longer infinite. The quanta of electromagnetic radiation are called *photons*.

2.1.2 The Photoelectric Effect

When light hits a material, it causes the material to emit electrons. This phenomenon is called the *photoelectric effect*. Using classical physics, and the assumption that light is a wave, we can make the following predictions:

- Brighter light should have more energy, so it should cause the emitted electrons to have more kinetic energy, and thus move faster.
- Light with higher frequency should hit the material more often, so it should cause a higher rate of electron emission, resulting in a larger electric current.

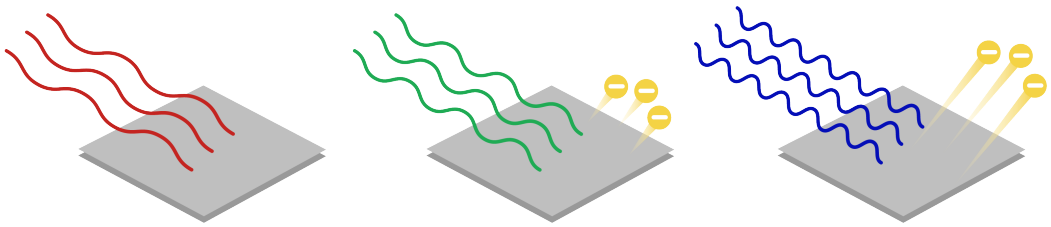

Figure 2.2: The photoelectric effect. *Source: Khan Academy.*

- Assuming there is a certain minimum energy needed to dislodge an electron from the material, sufficiently bright light of any frequency should cause electron emission.

However, what actually happens is the exact opposite:

- The kinetic energy of the emitted electrons increases with frequency, **not** brightness.
- The electric current increases with brightness, **not** frequency.
- Electrons are emitted only when the **frequency** of the light exceeds a certain threshold, regardless of how bright it is.

This is illustrated in Figure 2.2, where the red light does not cause any electrons to be emitted, but the green and blue lights do, since they have higher frequency. Furthermore, since the blue light has higher frequency than the green light, the kinetic energy of the emitted electrons is larger.

To explain this, we must again use quantum physics. Einstein proposed to use the same model that Planck suggested to solve the ultraviolet catastrophe, where light is made of discrete photons. Each photon has energy proportional to the frequency of the light, and brighter light of the same frequency simply has **more photons**, each photon still with the **same** amount of energy. This model fits the predictions perfectly.

So in Figure 2.2, making the red light brighter will increase the number of photons, but no matter how bright it is, the individual photons it's made of still do not have enough energy to dislodge an electron on their own. On the other hand, each individual photon of the green and blue lights has, on its own, enough energy to dislodge a photon, and even if the light is very dim, the electrons will still be emitted.

2.1.3 The Double-Slit Experiment

The previous two experiments may have convinced you that light is not a wave, but a particle. But is that really the case? The *double-slit experiment* shows that things are actually more complicated. In this experiment, a light beam hits a plate with two parallel slits. Most of the light is blocked by the plate, but some of it passes through the slits and hits a screen, creating a pattern of bright and dark bands.

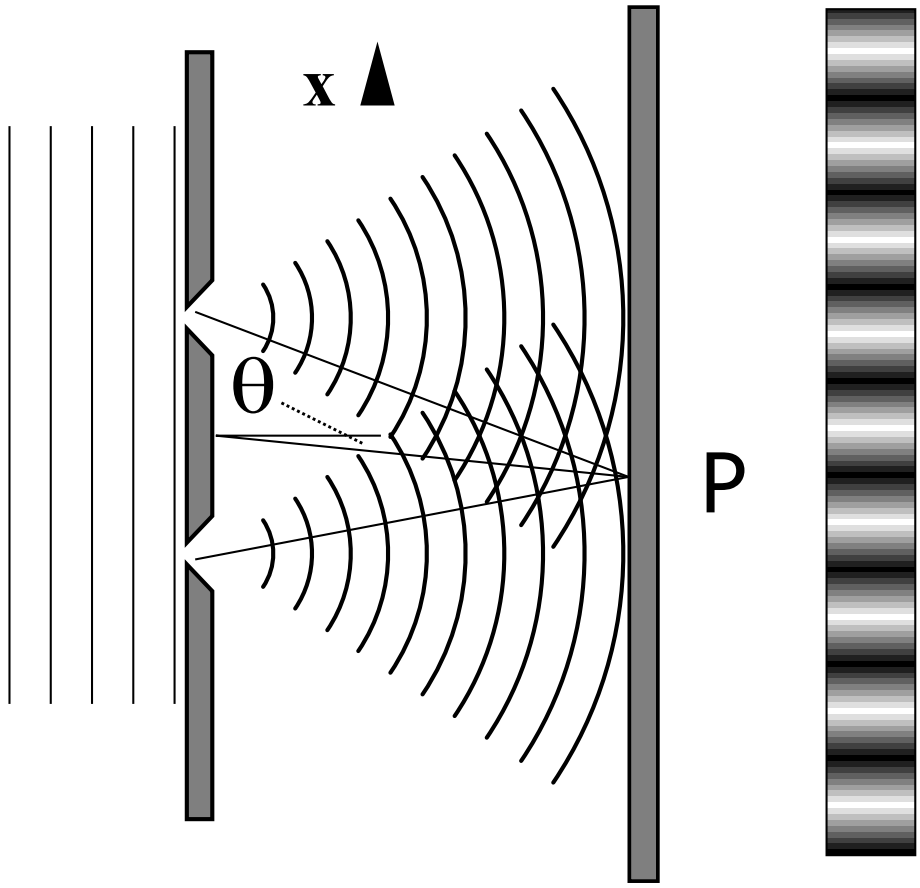

Figure 2.3: Light waves in the double-slit experiment. *Source: Wikipedia.*

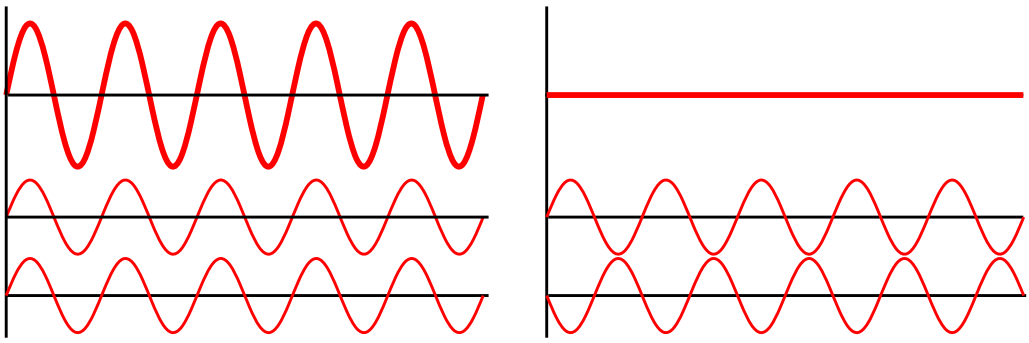

Figure 2.4: Constructive (left) and destructive (right) interference of two light waves. *Source: Wikipedia.*

This can be most naturally explained by assuming that light is not a particle, but a wave. Each of the slits becomes the origin of a new wave, as illustrated in Figure 2.3. Each of the

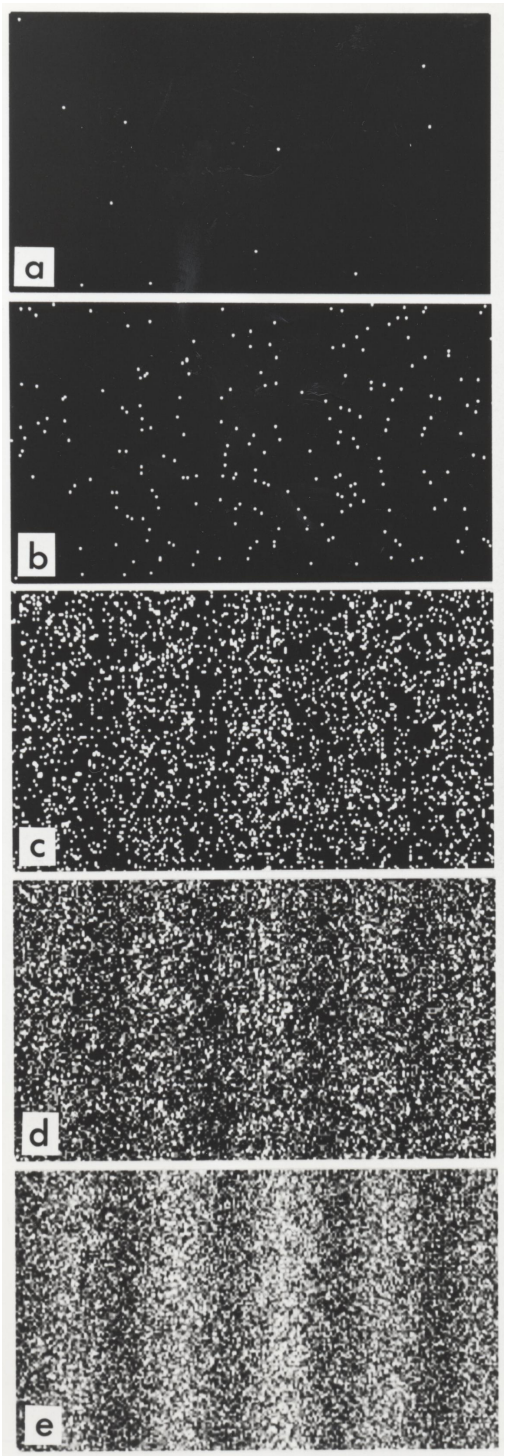

Figure 2.5: An interference pattern created by electrons in the double-slit experiment. Each image (from top to bottom) corresponds to a later point in time, after more electrons have accumulated. *Source: Wikipedia.*

two waves has crests and troughs. When a crest of one wave is at the same place as a crest of the other wave, they add up to create a crest with double the magnitude. This is called *constructive interference*. On the other hand, if a crest of one wave is at the same place as a trough of the other wave, they cancel each other. This is called *destructive interference*. See Figure 2.4 for an illustration. The pattern on the screen, as seen in Figure 2.3, is a consequence of this interference.

So the double-slit experiment seems to prove that light is a wave, in contradiction with black-body radiation and the photoelectric effect, which seem to prove that light is a particle. It turns out that, in fact, **both** are correct; the quantum nature of light has the consequence that it sometimes behaves like a classical wave, and other times like a classical particle. This is called *wave-particle duality*. Contrary to common misconception, this doesn't mean that light is "both a wave and a particle"; it simply demonstrates that the classical concepts of "wave" and "particle" are not the proper way to describe reality.

Okay, so light exhibits wave-particle duality. Maybe this makes sense. But matter, which is a tangible thing you can touch, is definitely made of particles, right? To check that, we can replace the beam of light with a beam of electrons. Since we think electrons are particles, not waves, we expect to find on the screen not an interference pattern, but just individual dots corresponding to the individual electron particles. And this is indeed what happens, except... If we run the experiment for some time, and let the electrons build up, then after a while we see that an interference pattern emerges nonetheless! This is shown in Figure 2.5.

What does this mean? It means that, in quantum physics, both light and matter exhibit wave-particle duality. In classical physics, the measurement of the position of the electron on the screen is deterministic; if we know the initial position and velocity of the electron, then we can predict exactly where the electron lands. In quantum physics, we instead have a probability distribution, which gives us the probability for the electron to be measured at each particular point on the screen. This probability distribution turns out to propagate in space like a wave, and interfere with itself constructively and destructively on the way as a wave does, which is what causes the interference pattern on the screen – it is actually a pattern of probabilities! In the end, the probability will be enlarged on some points of the screen and reduced on other points.

To clarify how the measurement of the positions of the electrons on the screen yields a probability distribution, consider instead a 6-sided die. If you roll the die just once or twice, you won't have much information about the probabilities to roll each number on the die. This is analogous to sending just a couple of electrons through the slits. What you need to do is to roll the die a large number of times, let's say 6,000 times. Then you count how many times the die rolled on each number. For example, if it rolled around 1,000 times on each number, then you know the die is fair; but if it rolled around 2,000 times on 6 and around 800 times on every other number, then you know the die is loaded. Similarly, we need to send a large number of electrons through the slits in order to determine the probability distribution for their positions on the screen. It turns out that the position of the electron is "loaded"!

As an aside, in 21st century terms, the precise answer to the question "is light a wave or a

particle?" turns out to be that both of them are different aspects of the same fundamental entity called the *quantum electromagnetic field*. This field propagates from place to place like a wave, but on the other hand, if you put enough energy into it, you can cause a *quantum excitation* in the field. It is this excitation that behaves like a particle.

Moreover, it turns out that **all** elementary particles are quantum fields, and thus all of them exhibit these two aspects. This is called *quantum field theory*. It neatly unites quantum mechanics with special relativity, and explains elementary particle physics in amazing accuracy – it is actually the most accurate theory in all of science! In this course we will focus on non-relativistic quantum mechanics, which is to quantum field theory as Newtonian physics is to special relativity. Quantum field theory is much more complicated, and is usually only taught at the graduate-school level.

2.1.4 The Stern-Gerlach Experiment

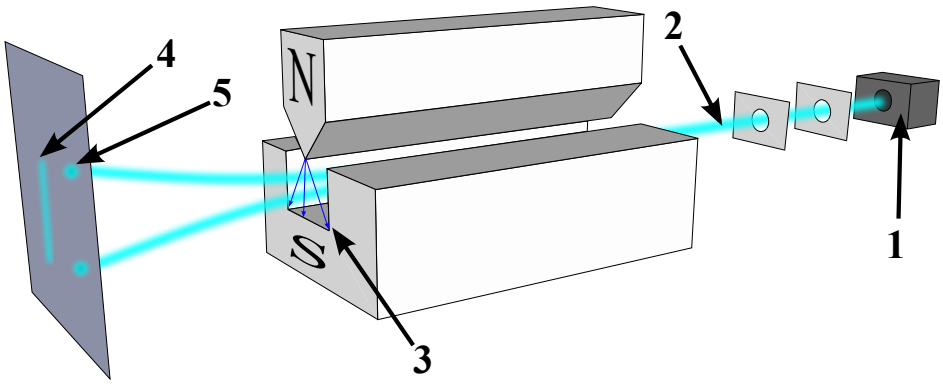

Figure 2.6: The Stern-Gerlach experiment. *Source: Wikipedia.*

In the *Stern-Gerlach experiment*, electrically neutral particles, such as silver atoms, are sent through an inhomogeneous magnetic field and into a screen. For reasons we won't go into (since they require some knowledge of electrodynamics), the magnetic field will deflect the particle up or down by an amount proportional to its angular momentum. According to classical physics, this angular momentum can have any value, and so we would expect to see

the particles hit every possible point along a **continuous** line on the screen. This is item (4) in Figure 2.6.

However, what actually happens when we perform the experiment is that the particles are deflected either up or down by the exact same amount each time, and hit only two specific **discrete** points on the screen. This is item (5) in Figure 2.6. To explain this, we must again use quantum physics. Quantum particles are not seen as classically spinning objects; instead they are said to have an **intrinsic** form of angular momentum called spin. For particles like electrons or silver atoms, a measurement of spin can only yield one of two options: "spin up" or "spin down".

The previous experiments we discussed showed us that something that is classically continuous – light, or more generally, electromagnetic radiation – is *quantized* in the quantum theory into discrete packets or quanta of energy called photons. Similarly, the Stern-Gerlach experiment tells us that another classically continuous thing, angular momentum, is also quantized in the quantum theory – into discrete spin. This seems to be a general property of most, but **not** all, quantum systems: something that in classical physics was continuous turns out to actually be discrete in quantum physics.

Finally, let me just mention that one can use spin to create *qubits*, or "quantum bits", where "spin up" represents a value of 0 and "spin down" represents a value of 1. Because spin is a quantum quantity, it satisfies all of the weird properties of quantum mechanics that we will discuss later. By taking advantage of these quantum properties, we can potentially do calculations faster with a quantum computer that uses qubits compared to a classical computer that uses classical bits.

2.2 Quantum vs. Classical Mechanics

Let us now summarize, in a non-technical way, the most important features of quantum mechanics and how they differ from their classical-mechanical counterparts.

1. **Quantum mechanics is, as far as we know, the exact and fundamental theory of reality.** Classical mechanics turns out to be just an approximation to this theory. This means that, in general, all modern theories of physics must be quantum theories if they intend to be fundamental. One important exception to that rule is general relativity, which we do not yet know how to describe as a quantum theory; if we did, we would call that theory *quantum gravity*. However, this is usually not a problem, since general relativity is mostly needed only when describing huge things like planets, stars, galaxies, and so on, in which case we do not need quantum mechanics since we are within the realm of validity of the classical approximation. In fact, this leads us to the next property:

2. **Quantum mechanics is the theory of the smallest things.** This includes elementary particles, atoms, and molecules. Since all big things are made of small things, quantum mechanics also describes humans, planets, galaxies, and the whole universe. However, this is exactly where the *classical limit* comes in; when many small quantum systems

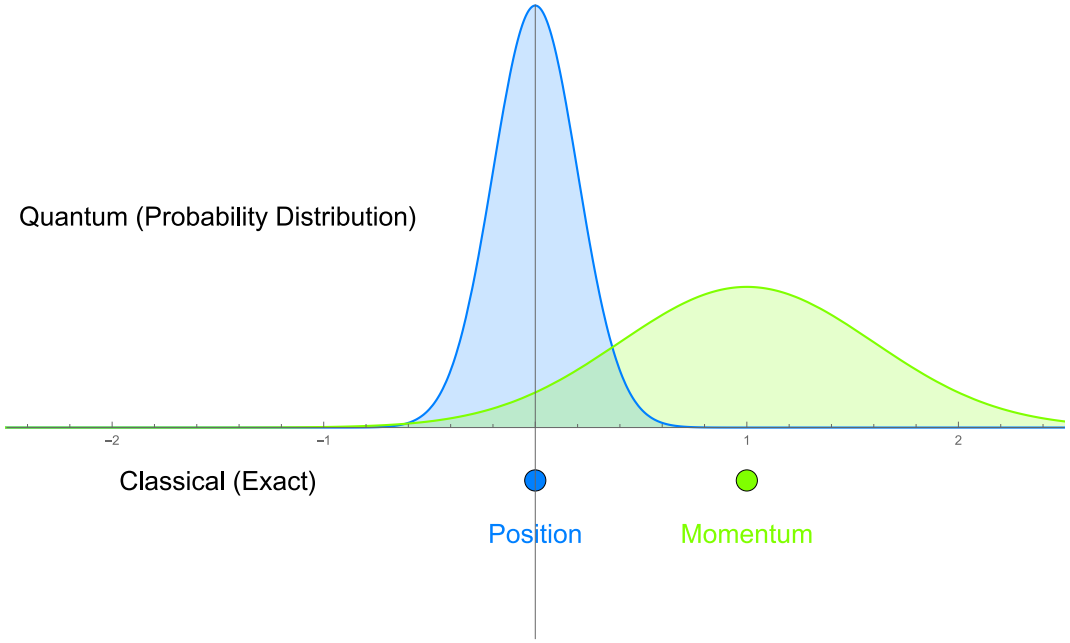

Figure 2.7: The uncertainty principle.

make up one big system, classical mechanics generally turns out to be a good enough description for all practical purposes. This is similar to how relativity is always the correct way to describe physics, but at low velocities, much smaller than the speed of light, Newtonian physics is a good enough approximation.

3. **Quantum mechanics usually involves discrete things.** This is in contrast with classical mechanics, which usually involves continuous things. In fact, continuous classical things generally turn out to be made of discrete quantum things. We saw an example of this when we discussed how light – a continuous electromagnetic field – is actually made of discrete photons. Similarly, we saw that angular momentum, which is continuous in the classical theory, is replaced by discrete spin in the quantum theory.

4. **Quantum mechanics is a probabilistic theory.** Classical mechanics, on the other hand, is a deterministic theory. For example, in classical mechanics, given a particle's exact position and momentum at any one time, we can (in principle) predict its position and momentum at any other time – with absolute certainty. However, in quantum mechanics, the most we can ever hope to know is the probability distribution to find the particle at a certain position or with a certain momentum. This is illustrated in Figure 2.7.

5. **Quantum mechanics allows for superposition of states.** In classical mechanics, the state of a particle is simply given by the exact values of its position and momentum. In contrast, in quantum mechanics the particle can – in fact, usually **must** – be in a *superposition* of possible positions and momenta. Each one of the possibilities in

the superposition has a probability assigned to it, and this is where the probability distribution in Figure 2.7 comes from.

6. **Quantum mechanics features uncertainty in measurements.** This is called the *uncertainty principle*. In classical mechanics, at least theoretically, we can precisely know both the position and momentum of the particle. However, in quantum mechanics, the more we know about the position, the less we know about the momentum – and vice versa. If the position probability distribution is narrow and concentrated at a certain region, meaning that there is low uncertainty in the position, then one can prove that the momentum probability distribution must be wide, meaning that there is high uncertainty in the momentum. The opposite is also true. This is again illustrated in Figure 2.7.

7. **Quantum mechanics has a stronger type of correlation called entanglement.** Classical mechanics also allows for correlation. For example, let's say I have two sealed envelopes with notes inside them, one with the number 0 and the other with the number 1. I give one to Alice and one to Bob. If Alice opens her envelope and sees the number 0, she can be sure that Bob has the envelope with the number 1, and vice versa. The results are clearly correlated. However, if we replace the notes with qubits – quantum bits which are in a superposition of 0 and 1 – then the envelopes are now correlated more strongly via *quantum entanglement*. We will discuss later in exactly what way quantum entanglement is stronger than classical correlation, but right now we will note that this fact is what gives quantum computers their power.

3 Mathematical Background

Quantum theory is the theoretical framework believed to describe all aspects of our universe at the most fundamental level. Mathematically, as we will see, it is relatively simple, although much more abstract than classical physics. However, conceptually, it is very hard to understand using the classical intuition we have from our daily lives. In these lectures we will learn to develop quantum intuition.

In this chapter we shall learn some basic mathematical concepts, focusing on complex numbers, linear algebra, and probability theory, which will be used extensively throughout the course. Even if the student is already familiar with these concepts, it is still a good idea to go over this chapter, since the unique notation commonly used in quantum mechanics is different than the notation used elsewhere in mathematics and physics.

3.1 Complex Numbers

Complex numbers are at the very core of the mathematical formulation of quantum theory. In this section we will give a review of complex numbers and present some definitions and results that will be used throughout the course.

3.1.1 Motivation

In real life, we only encounter *real numbers*. These numbers form a *field*, that is, a set of elements with well-defined operations of addition, subtraction, multiplication, and division. This field is denoted $\mathbb{R}$. Geometrically, we can imagine $\mathbb{R}$ as a 1-dimensional line, stretching from $-\infty$ to $+\infty$.

Unfortunately, it turns out that the field of real numbers has a serious flaw. One can write down completely reasonable-looking quadratic equations, with only real coefficient, which nonetheless have no solutions in $\mathbb{R}$. Consider the most general quadratic equation:

$$ax^2 + bx + c = 0, \qquad a, b, c \in \mathbb{R}. \tag{3.1}$$

One can easily prove (by completing the square) that there are two potential solutions, given by

$$x_\pm \equiv \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}. \tag{3.2}$$

Here, one solution corresponds to the choice $+$ and the other one to $-$. However, the square root $\sqrt{b^2 - 4ac}$ poses a problem, because the square of a real number is always non-negative[2]:

$$x^2 \geq 0, \qquad \forall x \in \mathbb{R}. \tag{3.3}$$

The number (and existence) of real solutions is thus determined by the sign of the expression inside the square root, called the *discriminant* $\Delta \equiv b^2 - 4ac$:

$$\begin{cases} \Delta > 0: & \text{two real roots } x_\pm = \dfrac{-b \pm \sqrt{\Delta}}{2a}, \\ \Delta = 0: & \text{one real root } x = -\dfrac{b}{2a}, \\ \Delta < 0: & \text{no real roots.} \end{cases} \tag{3.4}$$

It would be very convenient (not to mention more elegant) to have a field of numbers that is *algebraically closed*, meaning that every non-constant polynomial (and in particular, a quadratic polynomial) with coefficients in the field has a root in the field.

Since the problem stems from the fact that no real number can square to a negative number, let us simply extend our field with just one number, the *imaginary unit*, denoted[3] i, whose sole purpose is to square to a negative number. The most natural choice is for i to square to -1:

$$\mathrm{i}^2 \equiv -1. \tag{3.5}$$

[2] Here, $\forall$ means "for all".

[3] We use non-italic font exclusively for i in order to distinct it from i, which will be used for labels and variables. Of course, it is usually a wise idea not to have both i and i in the same equation in the first place, but sometimes that is unavoidable.

The new field created by extending $\mathbb{R}$ with i is the field of *complex numbers*, denoted $\mathbb{C}$. A general complex number is written

$$z = a + \mathrm{i}\, b, \qquad z \in \mathbb{C}, \qquad a, b, \in \mathbb{R}, \tag{3.6}$$

where a is called the *real part* and b is called the *imaginary part*, both real numbers.

Now, in the quadratic equation, having $\sqrt{\Delta}$ with a negative Δ is no longer a problem, since the number $\mathrm{i}\sqrt{-\Delta}$ squares to Δ:

$$\left(\mathrm{i}\sqrt{-\Delta}\right)^2 = \mathrm{i}^2\,(-\Delta) = (-1)\,(-\Delta) = \Delta. \tag{3.7}$$

Therefore, we conclude that **every** quadratic equation has a solution in the field of complex numbers[4]:

$$\begin{cases} \Delta > 0: & \text{two real roots } x_\pm = \dfrac{-b \pm \sqrt{\Delta}}{2a}, \\ \Delta = 0: & \text{one real root } x = -\dfrac{b}{2a}, \\ \Delta < 0: & \text{two complex roots } x_\pm = -\dfrac{b}{2a} \pm \mathrm{i}\,\dfrac{\sqrt{-\Delta}}{2a}. \end{cases} \tag{3.8}$$

As a matter of fact, this is a special case of the *fundamental theorem of algebra*: any polynomial of degree n with complex coefficients[5] has at least one, and at most n, unique complex roots[6]. The quadratic equation corresponds to the case $n = 2$.

Exercise 3.1.

A. Solve the quadratic equation

$$x^2 - 6x + 25 = 0. \tag{3.9}$$

B. Find the quadratic equation whose solutions are $z = 7 \pm 2\,\mathrm{i}$.

Problem 3.2. Above we saw that the equation $ax^2 + bx + c = 0$ with $a, b, c \in \mathbb{R}$ can either have two real solutions, one real solution, or two complex solutions that are conjugates of each other.

A. *Imaginary numbers*[7] are numbers of the form $\mathrm{i}\, b$ for $b \in \mathbb{R}$. What kind of equation has two imaginary solutions that are complex conjugates of each other?

B. What kind of equation has two imaginary solutions that are in general **not** complex conjugates of each other?

[4] Note that real numbers are a special case of complex numbers, so the two real roots are also two complex roots.

[5] Again, real numbers are a special case of complex numbers, so the coefficients can be all real.

[6] Or equivalently, it has exactly n not necessarily unique complex roots, accounting for possible degeneracy/multiplicity. For example, for $\Delta = 0$ the quadratic equation has two degenerate roots, or one root of multiplicity 2.

[7] Sometimes also called *purely imaginary numbers*.

C. What kind of equation has two arbitrary complex solutions that are in general not complex conjugates of each other?

Note: In all of the above, don't just find a specific equation that has this property – find a **family** of equations with arbitrary parameters of certain types.

3.1.2 Operations on Complex Numbers

Complex numbers can be added and multiplied with other complex numbers. There is really nothing special about these operations, except that it is customary to group the imaginary parts (i.e. anything that is a multiple of i) together and turn i^2 into -1 in the final result:

$$(a + \mathrm{i}\, b) + (c + \mathrm{i}\, d) = (a + c) + \mathrm{i}\,(b + d)\,, \tag{3.10}$$

$$(a + \mathrm{i}\, b)\,(c + \mathrm{i}\, d) = (ac - bd) + \mathrm{i}\,(ad + bc)\,. \tag{3.11}$$

Next, note that the two solutions to a quadratic equation with $\Delta < 0$ are the same, up to the sign of i. That is, if we replace i with $-\mathrm{i}$ in one of the solutions, we get the other solution. Such numbers are called *complex conjugates*, and the process of replacing i with $-\mathrm{i}$ is called *complex conjugation*. The complex conjugate of z is denoted z^*:

$$z = a + \mathrm{i}\, b \quad \Longrightarrow \quad z^* = a - \mathrm{i}\, b. \tag{3.12}$$

Of course, the conjugate of the conjugate is the original number:

$$(z^*)^* = z. \tag{3.13}$$

This means that the complex conjugation operation is an *involution*, that is, its own inverse.

Complex conjugation allows us to write a general formula for the real or imaginary parts of a complex number, denoted $\mathrm{Re}\, z$ and $\mathrm{Im}\, z$ respectively:

$$\mathrm{Re}\, z \equiv \frac{z + z^*}{2}, \qquad \mathrm{Im}\, z \equiv \frac{z - z^*}{2\,\mathrm{i}}. \tag{3.14}$$

You can check that if $z = a + \mathrm{i}\, b$ then we get $\mathrm{Re}\, z = a$ and $\mathrm{Im}\, z = b$, as expected.

Exercise 3.3. What are the real and imaginary parts of $4 - 7\,\mathrm{i}$? What is its complex conjugate?

Problem 3.4. If a number is the complex conjugate of itself, can you say anything interesting about that number? What about if a number is minus the complex conjugate of itself?

3.1.3 The Complex Plane and Real 2-Vectors

Recall that the field of real numbers $\mathbb{R}$ is geometrically a line. The space $\mathbb{R}^n$ is an n-dimensional space which is home to *real n-vectors*, that is, ordered lists of n real numbers of the form $(v_1, \ldots, v_n)$. In particular, $\mathbb{R}^2$ is geometrically a plane, with vectors of the form (x, y).

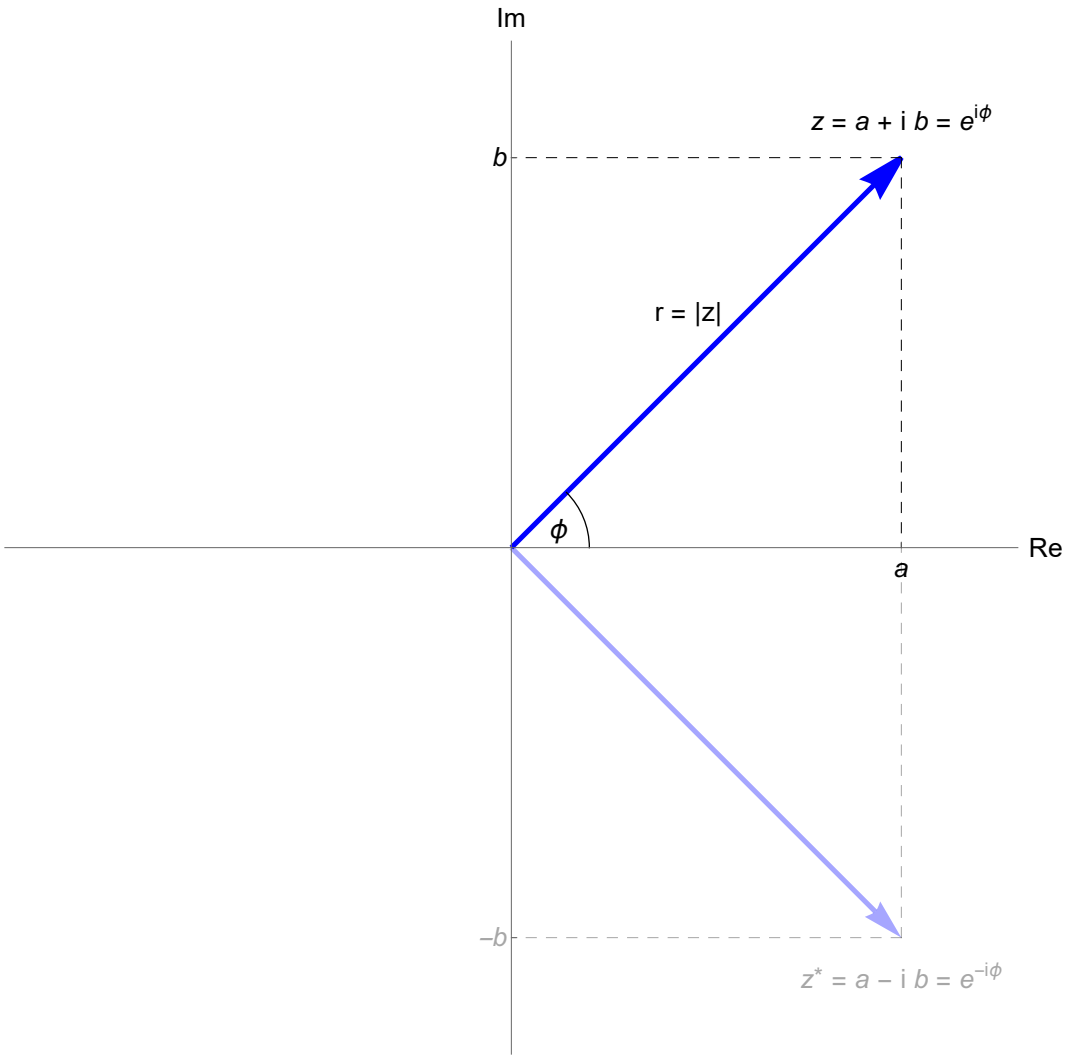

Figure 3.1: The complex plane, with a complex number $z = a + \mathrm{i}\, b$ and its conjugate $z^* = a - \mathrm{i}\, b$. Also shown is the polar representation of both numbers (see Section 3.1.4).

The *complex plane* $\mathbb{C}$ is similar to $\mathbb{R}^2$, except that instead of the x and y axes we have the real and imaginary axes respectively. The real unit 1, which squares to $+1$, defines the positive direction of the real axis, while the imaginary unit i, which squares to -1, defines the positive direction of the imaginary axis. This is illustrated in Figure 3.1.

Since $\mathbb{C}$ is a plane, we can define vectors on it, just like on $\mathbb{R}^2$. A real 2-vector (a, b) is an arrow in $\mathbb{R}^2$ which points from the origin $(0, 0)$ to the point that is a steps in the direction of the x axis and b steps in the direction of the y axis. A complex number $z = a + \mathrm{i}\, b$ is similarly an arrow in $\mathbb{C}$ which points from the origin 0 to the point that is a steps along the real axis and b steps along the imaginary axis.

The complex conjugate $z^* = a - \mathrm{i}\, b$ is obtained by replacing i with $-\mathrm{i}$. Since i defines the

direction of the imaginary axis, this is equivalent to flipping the imaginary axis. In other words, z^* is the reflection of z along the real axis, as shown in Figure 3.1.

From the Pythagorean theorem, we know that the magnitude (or length) of the real 2-vector (a, b) is $\sqrt{a^2 + b^2}$. The *magnitude* or *absolute value* $|z|$ of the complex number $z = a + \mathrm{i}\, b$ is also $\sqrt{a^2 + b^2}$. (Inspect Figure 3.1 to see how the Pythagorean theorem fits in.) Furthermore, since z^* is just a reflection of z, they both have the same magnitude. A convenient way to calculate the magnitude of either z or z^* it to multiply them with each other:

$$|z|^2 = |z^*|^2 \equiv z^* z = (a + \mathrm{i}\, b)\,(a - \mathrm{i}\, b) = a^2 - \mathrm{i}^2\, b^2 = a^2 + b^2, \tag{3.15}$$

so

$$|z| = |z^*| = \sqrt{a^2 + b^2}. \tag{3.16}$$

For an abstract complex number (where we don't necessarily know the explicit values of the real and imaginary parts) one can also write

$$|z| = |z^*| = \sqrt{(\mathrm{Re}\, z)^2 + (\mathrm{Im}\, z)^2}. \tag{3.17}$$

We note that there is an *isomorphism* between complex numbers and real 2-vectors. An isomorphism between two spaces is a mapping between the spaces that can be taken in either direction (i.e. is invertible), and preserves the structure of each space. The isomorphism between $\mathbb{C}$ and $\mathbb{R}^2$ is given by:

$$a + \mathrm{i}\, b \longleftrightarrow (a, b)\,. \tag{3.18}$$

We have already seen that the norm operation is preserved. Similarly, addition of complex numbers

$$(a + \mathrm{i}\, b) + (c + \mathrm{i}\, d) = (a + c) + \mathrm{i}\,(b + d)\,. \tag{3.19}$$

maps into addition of 2-vectors

$$(a, b) + (c, d) = (a + c, b + d)\,. \tag{3.20}$$

Exercise 3.5. Let $z = 5 + 6\,\mathrm{i}$ and $w = 7 + 8\,\mathrm{i}$.

A. Calculate z^*, w^*, $|z|$, $|w|$, $z + w$, $z - w$, $|z + w|$, $|z - w|$, and zw.

B. Find the 2-vectors isomorphic to z and w.

Problem 3.6. Let the vector $\mathbf{v} \equiv (a, b) \in \mathbb{R}^2$ be isomorphic to the complex number $z \equiv a + \mathrm{i}\, b \in \mathbb{C}$. Show explicitly that the following operations on $\mathbf{v}$ map to equivalent operations on z:

1. Multiplication of $\mathbf{v}$ by a real number $\lambda \in \mathbb{R}$.
2. Reflection of $\mathbf{v}$ with respect to the x axis.
3. Reflection of $\mathbf{v}$ with respect to the y axis.

4. Reflection of **v** with respect to the both axes.

Formulate the equivalent operations on z in terms of z itself, **without** using a, b, $\operatorname{Re} z$, or $\operatorname{Im} z$.

3.1.4 Polar Coordinates and Complex Phases

A vector in $\mathbb{R}^2$ can be converted from Cartesian coordinates (x, y) to *polar coordinates* (r, ϕ). The r coordinate is the magnitude of the vector, and the ϕ coordinate is the angle that the vector makes with respect to the x axis. The relation between the coordinate systems is given by

$$x = r\cos\phi, \qquad y = r\sin\phi, \tag{3.21}$$

$$r = \sqrt{x^2 + y^2}, \qquad \phi = \arctan\frac{y}{x}. \tag{3.22}$$

This simply follows from the definitions of $\cos\phi$ and $\sin\phi$, since the vector creates a right triangle with the x axis (see Figure 3.1). For example, the vector $(x, y) = \left(1, \sqrt{3}\right)$ in Cartesian coordinates corresponds to $r = 2$ and $\phi = \pi/3$.

x and y can be any real numbers, but r must be non-negative and ϕ must be in the range $(-\pi, \pi]$ (in radians) where $\phi = 0$ corresponds to the x axis. However, there is a subtlety here: the range of the arctan function is $(-\pi/2, \pi, 2)$, so ϕ needs to be further adjusted according to the quadrant. One can instead use a more complicated definition that automatically takes the quadrant into account:

$$\phi = \begin{cases} \arctan(\frac{y}{x}) & \text{if } x > 0, \\ \arctan(\frac{y}{x}) + \pi & \text{if } x < 0 \text{ and } y \geq 0, \\ \arctan(\frac{y}{x}) - \pi & \text{if } x < 0 \text{ and } y < 0, \\ +\frac{\pi}{2} & \text{if } x = 0 \text{ and } y > 0, \\ -\frac{\pi}{2} & \text{if } x = 0 \text{ and } y < 0, \\ \text{undefined} & \text{if } x = 0 \text{ and } y = 0. \end{cases} \tag{3.23}$$

This function is sometimes called atan2 (x, y), and it is implemented in most programming languages. Note that ϕ is undefined at the origin since a vector of length zero does not point in any direction.

Given that complex numbers are isomorphic to real 2-vectors, we should be able to write complex numbers in polar coordinates as well. Looking at (3.21), and replacing x and y with a and b, we see that

$$z = a + \mathrm{i}\, b = r\left(\cos\phi + \mathrm{i}\sin\phi\right). \tag{3.24}$$

We can write this more compactly using *Euler's formula*:

$$\mathrm{e}^{\mathrm{i}\phi} = \cos\phi + \mathrm{i}\sin\phi \quad \Longrightarrow \quad z = r\,\mathrm{e}^{\mathrm{i}\phi}. \tag{3.25}$$

This is illustrated in Figure 3.1. In this context, the angle ϕ is called the *complex phase*. It is of extreme importance in quantum mechanics, as we shall see.

Exercise 3.7. Write $2\,\mathrm{i} - 3$ in polar coordinates.

Problem 3.8. Prove, using Euler's formula, that $\left|\mathrm{e}^{\mathrm{i}\,\phi}\right| = 1$, that is, the magnitude of the complex number $\mathrm{e}^{\mathrm{i}\,\phi}$ is 1. If $z = r\,\mathrm{e}^{\mathrm{i}\,\phi}$, what is $|z|$?

Problem 3.9. Prove Euler's formula.

3.2 Linear Algebra

The most important and fundamental mathematical structure in quantum theory is the *Hilbert space*, a type of complex vector space. In this section we will define Hilbert spaces and learn about many important concept and results from linear algebra that apply to them.

3.2.1 Complex Vector Spaces

A real n-vector is an ordered list of n real numbers. Analogously, a *complex n-vector* is an ordered list of n complex numbers. For example, a complex 2-vector with two complex components Ψ_1 and Ψ_2 is written as:

$$|\Psi\rangle \equiv \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}. \tag{3.26}$$

The notation $|\Psi\rangle$ is **unique to quantum mechanics**, and it is called *bra-ket notation* or sometimes *Dirac notation*. In this notation, we write a straight line $|$ and an angle bracket $\rangle$, and between them, a label. We will usually denote a general vector with the label Ψ; this label, and its lowercase counterpart ψ, are very commonly used in quantum mechanics. However, we can use whatever label we want to describe our vector – including letters, numbers, symbols, or even whole words and sentences, for example:

$$|A\rangle\,, |\beta\rangle\,, |3\rangle\,, |\clubsuit\rangle\,, |\text{Bob}\rangle\,, |\text{Schrödinger's Cat Is Alive}\rangle\,, \ldots \tag{3.27}$$

This is a great advantage of the bra-ket notation, as it allows us to be very descriptive in the labels we choose for our vectors – which we can't do with the notation $\mathbf{v}$ or $\vec{v}$ commonly used for vectors in mathematics and physics.

A *vector space* $\mathcal{V}$ over a field[8] $\mathbb{F}$ is a set of vectors equipped with two operations: *addition of vectors* and *multiplication of vector by scalar*, where a *scalar* is any number from the field $\mathbb{F}$. Vector addition must satisfy the following conditions:

1. *Closed* – the sum of two vectors is another vector in the same space:

$$\forall\, |\Psi\rangle\,, |\Phi\rangle \in \mathcal{V}: \qquad |\Psi\rangle + |\Phi\rangle \in \mathcal{V}. \tag{3.28}$$

[8]The field is usually taken to be $\mathbb{R}$ or $\mathbb{C}$. Naturally, for a complex vector space, it will be $\mathbb{C}$.

2. *Commutative* – the order of vectors doesn't matter:

$$\forall \left|\Psi\right\rangle, \left|\Phi\right\rangle \in \mathcal{V}: \qquad \left|\Psi\right\rangle + \left|\Phi\right\rangle = \left|\Phi\right\rangle + \left|\Psi\right\rangle. \tag{3.29}$$

3. *Associative* – if three vectors are added, it doesn't matter which two are added first:

$$\forall \left|\Psi\right\rangle, \left|\Phi\right\rangle, \left|\Theta\right\rangle \in \mathcal{V}: \qquad \Big(\left|\Psi\right\rangle + \left|\Phi\right\rangle\Big) + \left|\Theta\right\rangle = \left|\Psi\right\rangle + \Big(\left|\Phi\right\rangle + \left|\Theta\right\rangle\Big). \tag{3.30}$$

4. *Identity vector* or *zero vector* – there is a (unique) vector[9] 0 which, when added to any vector, does not change it:

$$\exists 0 \in \mathcal{V}: \qquad \forall \left|\Psi\right\rangle \in \mathcal{V}: \qquad \left|\Psi\right\rangle + 0 = \left|\Psi\right\rangle. \tag{3.31}$$

5. *Inverse vector* – for every vector there exists another (unique) vector such that the two vectors sum to the zero vector:

$$\forall \left|\Psi\right\rangle \in \mathcal{V}: \qquad \exists \Big(-\left|\Psi\right\rangle\Big) \in \mathcal{V}: \qquad \left|\Psi\right\rangle + \Big(-\left|\Psi\right\rangle\Big) = 0. \tag{3.32}$$

Furthermore, multiplication by a scalar must satisfy the following conditions:

1. *Closed* – the product of a vector and a scalar is a vector in the same space:

$$\forall \alpha \in \mathbb{F}, \qquad \forall \left|\Psi\right\rangle \in \mathcal{V}: \qquad \alpha \left|\Psi\right\rangle \in \mathcal{V}. \tag{3.33}$$

2. *Associative* – if two scalars are multiplied by a vector, it doesn't matter whether we first multiply the two scalars or we first multiply one of the scalars with the vector:

$$\forall \alpha, \beta \in \mathbb{F}, \qquad \forall \left|\Psi\right\rangle \in \mathcal{V}: \qquad (\alpha\beta)\left|\Psi\right\rangle = \alpha\left(\beta\left|\Psi\right\rangle\right). \tag{3.34}$$

3. *Distributive* over addition of scalars:

$$\forall \alpha, \beta \in \mathbb{F}, \qquad \forall \left|\Psi\right\rangle \in \mathcal{V}: \qquad (\alpha + \beta)\left|\Psi\right\rangle = \alpha\left|\Psi\right\rangle + \beta\left|\Psi\right\rangle. \tag{3.35}$$

4. *Distributive* over addition of vectors:

$$\forall \alpha \in \mathbb{F}, \qquad \forall \left|\Psi\right\rangle, \left|\Phi\right\rangle \in \mathcal{V}: \qquad \alpha\left(\left|\Psi\right\rangle + \left|\Phi\right\rangle\right) = \alpha\left|\Psi\right\rangle + \alpha\left|\Phi\right\rangle. \tag{3.36}$$

5. *Identity scalar* or *unit scalar* – there is a (unique) scalar 1 which, when multiplied by any

[9] Note that here we are using a slight abuse of notation by denoting the zero vector as the **number** 0, instead of using bra-ket notation. The reason is that $|0\rangle$ already has a special common meaning in quantum mechanics, as we will see later; in the context of that special meaning, $|0\rangle$ is **not** the zero vector.

vector, does not change it:

$$\exists 1 \in \mathbb{F}: \qquad \forall |\Psi\rangle \in \mathcal{V}: \qquad 1\,|\Psi\rangle = |\Psi\rangle\,. \tag{3.37}$$

We now define a 2-dimensional *complex vector space*, which we denote $\mathbb{C}^2$, as the space of complex 2-vectors over $\mathbb{C}$, with addition of vectors given by

$$|\Psi\rangle \equiv \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} \in \mathbb{C}^2, \qquad |\Phi\rangle \equiv \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} \in \mathbb{C}^2 \quad \Longrightarrow \quad |\Psi\rangle + |\Phi\rangle = \begin{pmatrix} \Psi_1 + \Phi_1 \\ \Psi_2 + \Phi_2 \end{pmatrix}, \tag{3.38}$$

and multiplication of vector by scalar given by

$$|\Psi\rangle \equiv \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} \in \mathbb{C}^2, \qquad \lambda \in \mathbb{C} \quad \Longrightarrow \quad \lambda\,|\Psi\rangle = \begin{pmatrix} \lambda\Psi_1 \\ \lambda\Psi_2 \end{pmatrix}. \tag{3.39}$$

The n-dimensional complex vector space $\mathbb{C}^n$ is defined analogously. In this course, we will mostly focus on $\mathbb{C}^2$ for simplicity, in particular when giving explicit examples.

Exercise 3.10. Let

$$|\Psi\rangle \equiv \begin{pmatrix} 3+\mathrm{i} \\ -9 \end{pmatrix}, \qquad |\Phi\rangle \equiv \begin{pmatrix} \mathrm{i}-1 \\ -10\,\mathrm{i} \end{pmatrix}, \qquad \alpha = 7\,\mathrm{i} - 2, \qquad \beta = -4 - 8\,\mathrm{i}\,. \tag{3.40}$$

Calculate $\alpha\,|\Psi\rangle + \beta\,|\Phi\rangle$.

Problem 3.11. Check that the addition and multiplication as defined above indeed satisfy all of the required conditions for a vector space. You can do this just for $\mathbb{C}^2$, for simplicity.

3.2.2 Dual Vectors, Inner Products, Norms, and Hilbert Spaces

A *dual vector* is defined by writing the vector as a row instead of a column, and replacing each component with its complex conjugate. We denote the dual vector of $|\Psi\rangle$ as follows:

$$\langle\Psi| = \begin{pmatrix} \Psi_1^* & \Psi_2^* \end{pmatrix}. \tag{3.41}$$

In terms of notation, there is now an opposite angle bracket $\langle$ on the left of the label, and the straight line $|$ is on the right. Addition and multiplication by a scalar are defined as for vectors, simply replacing columns with rows. However, you may **not** add vectors and dual vectors together – adding a row to a column is undefined!

If we are given a dual vector, we can take **its** dual to get a "normal" (column) vector. In this case, the operation of taking the dual involves writing the vector as a column instead of a row and taking the complex conjugates of the components. This means that the operation of taking the dual is an involution – taking the dual of a vector twice gives back the same vector, since $(z^*)^* = z$.

Using dual vectors, we may define the *inner product*. This product allows us to take a vector and a dual vector and produce a (complex) number out of them, similarly to the dot product of real vectors[10]. Importantly, the inner product only works for one vector and one dual vector, **not** for two vectors or two dual vectors. To calculate it, we multiply the components of both vectors one by one and add them up:

$$\langle \Psi | \Phi \rangle = \begin{pmatrix} \Psi_1^* & \Psi_2^* \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} = \Psi_1^* \Phi_1 + \Psi_2^* \Phi_2. \tag{3.42}$$

In bra-ket notation, vectors $|\Psi\rangle$ are called *"kets"* and dual vectors $\langle \Psi|$ are called *"bras"*. Then the notation for $\langle \Psi | \Phi \rangle$ is called a *"bra(c)ket"*.

We define the *norm-squared* of a vector by taking its inner product with its dual ("squaring" it):

$$\|\Psi\|^2 \equiv \langle \Psi | \Psi \rangle = \begin{pmatrix} \Psi_1^* & \Psi_2^* \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} = |\Psi_1|^2 + |\Psi_2|^2, \tag{3.43}$$

where the magnitude-squared of a complex number z was defined in Section 3.1.3 as $|z|^2 \equiv z^* z$. Then we can define the *norm* as the square root of the norm-squared:

$$\|\Psi\| \equiv \sqrt{\|\Psi\|^2} = \sqrt{\langle \Psi | \Psi \rangle}. \tag{3.44}$$

Observe how taking the dual of a vector generalizes taking the complex conjugate of a number, and taking the norm of a vector generalizes taking the magnitude of a number; indeed, for 1-dimensional vectors, these operations are the same!

A vector space with an inner product is called a *Hilbert space*, provided it is also a *complete metric space*[11] and that the inner product satisfies the same properties (which you will derive in problems 3.13, 3.14, and 3.15) as the standard inner product on $\mathbb{C}^n$. In particular, $\mathbb{C}^n$ itself is a Hilbert space, but there are many other Hilbert spaces, some of them much more abstract. The usual notation for a general Hilbert space is $\mathcal{H}$.

[10] The dot product of the real vectors $\mathbf{v} \equiv (v_1, v_2)$ and $\mathbf{w} \equiv (w_1, w_2)$ in $\mathbb{R}^2$ is defined as $\mathbf{v} \cdot \mathbf{w} \equiv v_1 w_1 + v_2 w_2$. In principle, this definition **does** secretly involve a dual (row) vector and a (column) vector, but since we do not need to take the complex conjugate, we don't really need to worry about dual vectors. However, it is important to note that in real vector spaces with curvature, such as those used in general relativity, the dot product must be replaced with a more complicated inner product which involves the metric, and it again becomes crucial to distinguish vectors from dual vectors – which in this context are also called contravariant and covariant vectors respectively.

[11] A vector space is a *complete metric space* if whenever an infinite series of vectors $|\Psi_i\rangle$ *converges absolutely*, that is, the series of the norms of the vectors converges:

$$\sum_{i=0}^{\infty} \|\Psi_i\| < \infty, \tag{3.45}$$

then the series of the vectors themselves converges as well, to some vector $|\Psi\rangle$ in the Hilbert space:

$$\sum_{i=0}^{\infty} |\Psi_i\rangle = |\Psi\rangle\,. \tag{3.46}$$

Exercise 3.12. Let

$$|\Psi\rangle \equiv \begin{pmatrix} 7+7\,\mathrm{i} \\ -7-2\,\mathrm{i} \end{pmatrix}, \qquad |\Phi\rangle \equiv \begin{pmatrix} -2-7\,\mathrm{i} \\ \mathrm{i} \end{pmatrix}. \tag{3.47}$$

Calculate $\langle\Psi|$, $\langle\Phi|$, $\|\Psi\|$, $\|\Phi\|$, $\langle\Psi|\Phi\rangle$, and $\langle\Phi|\Psi\rangle$.

Problem 3.13. Prove that the norm-squared $\|\Psi\|^2$ is always non-negative, and it is zero if and only if $|\Psi\rangle$ is the zero vector, that is, the vector whose components are all zero. In other words, the inner product is *positive-definite*. As a corollary, explain why we must take the complex conjugate of the components when we convert a vector to a dual vector. (What would have happened if we didn't?)

Problem 3.14. Prove that $\langle\Phi|\Psi\rangle = \langle\Psi|\Phi\rangle^*$, that is, if we swap the order of vectors in the inner product we get the complex conjugate of the original product. Thus, unlike the dot product, the inner product on $\mathbb{C}^n$ is not symmetric. However, it is *conjugate-symmetric*, and in particular, the magnitude of the inner product remains the same, since $|z| = |z^*|$.

Problem 3.15. Prove that if $\alpha, \beta \in \mathbb{C}$ and $|\Psi\rangle, |\Phi\rangle, |\Theta\rangle \in \mathbb{C}^n$ then

$$\langle\Psi|\left(\alpha\,|\Phi\rangle + \beta\,|\Theta\rangle\right) = \alpha\langle\Psi|\Phi\rangle + \beta\langle\Psi|\Theta\rangle, \tag{3.48}$$

that is, the inner product is *linear* in its second argument.

3.2.3 Orthonormal Bases

An *orthonormal basis* of $\mathbb{C}^n$ is a set of n non-zero vectors $\{|B_1\rangle, \ldots, |B_n\rangle\}$ – which we will usually denote $|B_i\rangle$ for short, with the implication that $i \in \{1, \ldots, n\}$ – such that:

1. They *span* $\mathbb{C}^n$, which means that any vector $|\Psi\rangle \in \mathbb{C}^n$ can be written **uniquely** as a *linear combination* of the basis vectors, that is, a sum of the vectors $|B_i\rangle$ multiplied by some complex numbers $\lambda_i \in \mathbb{C}$:

   $$|\Psi\rangle = \sum_{i=1}^{n} \lambda_i\,|B_i\rangle\,. \tag{3.49}$$

   This property ensures that the basis can be used to define any single vector in the space $\mathbb{C}^n$, not just part of that space.
   As a simple example, in $\mathbb{R}^3$ the vector $\hat{\mathbf{x}} \equiv (1,0,0)$ pointing along the x axis and the vector $\hat{\mathbf{y}} \equiv (0,1,0)$ pointing along the y axis span the xy plane, but **not** all of $\mathbb{R}^3$. To get a basis for all of $\mathbb{R}^3$, we must add an appropriate third vector, such as the vector $\hat{\mathbf{z}} \equiv (0,0,1)$ pointing along the z axis. (But other vectors, such as $(1,2,3)$, would work as well.)

2. They are *linearly independent*, in that if the zero vector is a linear combination of the basis

vectors, then the coefficients in the linear combination must all be zero:

$$\sum_{i=1}^{n} \lambda_i |B_i\rangle = 0 \quad \Longrightarrow \quad \lambda_i = 0, \qquad \forall i. \tag{3.50}$$

Linear independence means (as you will show in Problem 3.17) that no vector in the set can be written as a linear combination of the other vectors in the set. If we could have done so, then that vector would have been redundant, and we would have needed to remove it in order to obtain a basis.
As a simple example, the set composed of $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $(1, 2, 0)$ is linearly dependent, since $(1, 2, 0) = \hat{\mathbf{x}} + 2\hat{\mathbf{y}}$, but the set $\{\hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}\}$ is linearly independent.

3. They are all *orthogonal* to each other, that is, the inner product of any two **different** vectors evaluates to zero:

$$\langle B_i | B_j \rangle = 0, \qquad \forall i \neq j. \tag{3.51}$$

4. They are all *unit vectors*, that is, they have a norm (and norm-squared) of 1:

$$\|B_i\|^2 = \langle B_i | B_i \rangle = 1, \qquad \forall i. \tag{3.52}$$

In fact, properties 3 and 4 may be expressed more compactly as:

$$\langle B_i | B_j \rangle = \delta_{ij} = \begin{cases} 0 & \text{if } i \neq j, \\ 1 & \text{if } i = j, \end{cases} \tag{3.53}$$

where δ_{ij} is called the *Kronecker delta*. If this combined property is satisfied, we say that the vectors are *orthonormal*[12].

These requirements become much simpler in $n = 2$ dimensions. An orthonormal basis for $\mathbb{C}^2$ is a set of 2 non-zero vectors $|B_1\rangle, |B_2\rangle$ such that:

1. They span $\mathbb{C}^2$, which means that any vector $|\Psi\rangle \in \mathbb{C}^2$ can be written as a linear combination of the basis vectors:

$$|\Psi\rangle = \lambda_1 |B_1\rangle + \lambda_2 |B_2\rangle, \tag{3.54}$$

for a unique choice of $\lambda_1, \lambda_2 \in \mathbb{C}$.

2. They are linearly independent, which means that we cannot write one in terms of a scalar times the other, i.e.:

$$|B_1\rangle \neq \lambda |B_2\rangle, \qquad \lambda \in \mathbb{C}. \tag{3.55}$$

3. They are orthonormal to each other, that is, the inner product between them evaluates

[12] Actually, bases don't have to be orthonormal in general, but in quantum mechanics they always are, for reasons that will become clear later.

to zero and both of them have unit norm:

$$\langle B_1|B_2\rangle = 0, \tag{3.56}$$

$$\|B_1\|^2 = \langle B_1|B_1\rangle = 1, \qquad \|B_2\|^2 = \langle B_2|B_2\rangle = 1. \tag{3.57}$$

A very important basis, the *standard basis* of $\mathbb{C}^2$, is defined as:

$$|1_1\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |1_2\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{3.58}$$

We similarly define the standard basis of $\mathbb{C}^n$ for any n in the obvious way.

Problem 3.16. Show that the standard basis vectors satisfy the properties above.

Problem 3.17. Show that linear independence means that no vector in the basis can be written as a linear combination of the other vectors in the basis.

Problem 3.18. Any basis which is orthogonal but not orthonormal, that is, does **not** satisfy property 4, can be made orthonormal by *normalizing* each basis vector, that is, dividing it by its norm:

$$|B_i\rangle \mapsto \frac{|B_i\rangle}{\|B_i\|}. \tag{3.59}$$

Show that if an orthogonal but not orthonormal basis satisfies properties 1-3, then it still satisfies them after normalizing it in this way.

Exercise 3.19. Consider the complex vector

$$|\Psi\rangle \equiv \begin{pmatrix} 1+\mathrm{i} \\ 2+2\,\mathrm{i} \end{pmatrix}. \tag{3.60}$$

Normalize $|\Psi\rangle$ and find another complex vector $|\Phi\rangle$ such that the set $\{|\Psi\rangle, |\Phi\rangle\}$ is a basis of $\mathbb{C}^2$ (i.e. satisfies all of the properties above).

Problem 3.20. Find an orthonormal basis of $\mathbb{C}^3$ which is **not** the standard basis or a scalar multiple of the standard basis. Show that it is indeed an orthonormal basis.

3.2.4 Matrices and the Adjoint

A *matrix* in n dimensions is an $n \times n$ array[13] of (complex) numbers. In $n = 2$ dimensions we have

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \qquad A_{11}, A_{12}, A_{21}, A_{22} \in \mathbb{C}. \tag{3.61}$$

[13] In fact, matrices don't have to be square, they can have a different number of rows and columns, that is, $n \times m$ where $n \neq m$; but non-square matrices are generally not of much interest in quantum mechanics.

A matrix can act on a vector to produce another vector. If it's a ket (a vertical/column vector), the result is another ket. If it's a bra (a horizontal/row dual vector), the result is another bra.

If the matrix acts on a ket, then it must act **from the left**, and the element at **row** i of the resulting ket is obtained by taking the inner product of **row** i of the matrix with the ket:

$$A|\Psi\rangle = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} = \begin{pmatrix} A_{11}\Psi_1 + A_{12}\Psi_2 \\ A_{21}\Psi_1 + A_{22}\Psi_2 \end{pmatrix}. \tag{3.62}$$

If the matrix acts on a bra, then it must act **from the right**, and the element at **column** i of the resulting bra is obtained by taking the inner product of **column** i of the matrix with the bra:

$$\langle\Psi| A = \begin{pmatrix} \Psi_1^* & \Psi_2^* \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} \Psi_1^* A_{11} + \Psi_2^* A_{21} & \Psi_1^* A_{12} + \Psi_2^* A_{22} \end{pmatrix}. \tag{3.63}$$

Note that the dual vector $\langle\Psi| A$ is **not** the dual of the vector $A|\Psi\rangle$, as you can see by taking the dual of (3.62). However, we can define the *adjoint* of a matrix by transposing rows into columns and then taking the complex conjugate of all the components:

$$A^\dagger = \begin{pmatrix} A_{11}^* & A_{21}^* \\ A_{12}^* & A_{22}^* \end{pmatrix}, \tag{3.64}$$

where the notation † for the adjoint is called *dagger*. Then the vector dual to $A|\Psi\rangle$ is $\langle\Psi| A^\dagger$, as you will check in Problem 3.22. Actually, taking the adjoint of a matrix is exactly the same operation as taking the dual of a vector! The only difference is that for a matrix we have n columns to transpose into rows, while for a vector we only have one. Therefore, we have

$$|\Psi\rangle^\dagger = \langle\Psi|, \qquad \langle\Psi|^\dagger = |\Psi\rangle, \tag{3.65}$$

and we get the following nice relation:

$$(A|\Psi\rangle)^\dagger = \langle\Psi| A^\dagger. \tag{3.66}$$

The *identity matrix*, which we will write simply as 1, is:

$$1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{3.67}$$

Acting with it on any vector or dual vector does not change it: $1|\Psi\rangle = |\Psi\rangle$.

Problem 3.21. To rotate (real) vectors in $\mathbb{R}^2$ by an angle θ, we take their product with the (real) *rotation matrix*:

$$R(\theta) \equiv \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}. \tag{3.68}$$

A. Calculate the matrix $R(\pi/3)$.

B. Write down the vector resulting from rotating $(-5, 9)$ by $\pi/3$ radians, in both Cartesian and polar coordinates.

C. Repeat (B) for rotating a general 2-vector (x, y) by a general angle θ.

D. Find the mapping between rotations of 2-vectors in $\mathbb{R}^2$ and rotations of complex numbers in $\mathbb{C}$, and explain what is the analogue of the rotation matrix in terms of complex numbers.

Problem 3.22. Show that the vector dual to $A|\Psi\rangle$ is indeed $\langle\Psi|A^\dagger$.

Exercise 3.23. Let

$$A \equiv \begin{pmatrix} 1+5\,\mathrm{i} & 2 \\ 3-7\,\mathrm{i} & 4+8\,\mathrm{i} \end{pmatrix}, \qquad \langle\Psi| \equiv \begin{pmatrix} \mathrm{i}-2 & \mathrm{i}-3 \end{pmatrix}. \tag{3.69}$$

Calculate $A|\Psi\rangle$ and $\langle\Psi|A^\dagger$ separately, and then check that they are the dual of each other.

Problem 3.24. Show that $\left(A^\dagger\right)^\dagger = A$. This means that the adjoint operation is an involution, exactly like complex conjugation and taking the dual of a vector. In fact, all three are the exact same operation. By choosing an appropriate matrix, explain how taking the complex conjugate of a number is a special case of taking the adjoint of a matrix.

Problem 3.25. Show that the action of a matrix on a vector is *linear*, that is,

$$A(\alpha|\Psi\rangle + \beta|\Phi\rangle) = \alpha A|\Psi\rangle + \beta A|\Phi\rangle. \tag{3.70}$$

3.2.5 The Outer Product

We have seen that vectors and dual vectors may be combined to generate a complex number using the inner product. We can similarly combine a vector and a dual vector to generate a matrix, using the *outer product*. Given

$$\langle\Psi| \equiv \begin{pmatrix} \Psi_1^* & \Psi_2^* \end{pmatrix}, \qquad |\Phi\rangle \equiv \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}, \tag{3.71}$$

we define the outer product as the matrix whose component at row i, column j is given by multiplying the component at row i of $|\Phi\rangle$ with the component at column j of $\langle\Psi|$:

$$|\Phi\rangle\langle\Psi| = \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} \begin{pmatrix} \Psi_1^* & \Psi_2^* \end{pmatrix} = \begin{pmatrix} \Psi_1^*\Phi_1 & \Psi_2^*\Phi_1 \\ \Psi_1^*\Phi_2 & \Psi_2^*\Phi_2 \end{pmatrix}. \tag{3.72}$$

Note how when taking an inner product the straight lines | face each other: $\langle\Psi|\Phi\rangle$, while when taking an outer product the angle brackets $\rangle\langle$ face each other. This shows some of the elegance of the Dirac notation! A bra-ket is an inner product, while a ket-bra is an outer product.

We can assign a rank to scalars, vectors, and matrices:

- Scalars have rank 0 since they have $n^0 = 1$ component,
- Vectors have rank 1 since they have $n^1 = n$ components,
- Matrices have rank 2 since they have n^2 components.

Then the inner product reduces the rank of the vectors from 1 to 0, while the outer product increases the rank from 1 to 2.

Exercise 3.26. Calculate the outer product $|\Psi\rangle\langle\Phi|$ for

$$|\Psi\rangle = \begin{pmatrix} 1 \\ 2+\mathrm{i} \end{pmatrix}, \qquad |\Phi\rangle = \begin{pmatrix} 3-\mathrm{i} \\ 4\,\mathrm{i} \end{pmatrix}. \tag{3.73}$$

Remember that when writing the dual vector, the components are complex conjugated!

3.2.6 The Completeness Relation

Let us write the vector $|\Psi\rangle$ as a linear combination of basis vectors:

$$|\Psi\rangle = \sum_{i=1}^{n} \lambda_i \, |B_i\rangle \, . \tag{3.74}$$

Taking the inner product of the above equation with $\langle B_j|$ and using the fact that the basis vectors are orthonormal,

$$\langle B_i|B_j\rangle = \delta_{ij} = \begin{cases} 0 & \text{if } i \neq j, \\ 1 & \text{if } i = j, \end{cases} \tag{3.75}$$

we get:

$$\langle B_j|\Psi\rangle = \sum_{i=1}^{n} \lambda_i \langle B_j|B_i\rangle = \sum_{i=1}^{n} \lambda_i \delta_{ij} = \lambda_j, \tag{3.76}$$

since all of the terms in the sum vanish except the one with $i = j$. Therefore, the coefficients λ_i in (3.74) are given, for any vector $|\Psi\rangle$ and for any basis $|B_i\rangle$, by

$$\lambda_i = \langle B_i|\Psi\rangle. \tag{3.77}$$

Now, since λ_i is a scalar, and multiplication by a scalar is commutative (unlike the inner and outer products!), we can move it to the right in (3.74):

$$|\Psi\rangle = \sum_{i=1}^{n} |B_i\rangle \, \lambda_i. \tag{3.78}$$

We haven't actually **done** anything here; where to write the scalar, on the left or right of the vector, is completely arbitrary – it's just conventional to write it on the left. Then, replacing λ_i

with $\langle B_i|\Psi\rangle$ as per (3.77), we get

$$|\Psi\rangle = \sum_{i=1}^{n} |B_i\rangle\langle B_i|\Psi\rangle. \tag{3.79}$$

To make this even more suggestive, let us add parentheses:

$$|\Psi\rangle = \left(\sum_{i=1}^{n} |B_i\rangle\langle B_i|\right)|\Psi\rangle. \tag{3.80}$$

Note that what we did here is go from a **vector** $|B_i\rangle$ times a **complex number** $\langle B_i|\Psi\rangle$ to a **matrix** $|B_i\rangle\langle B_i|$ times a **vector** $|\Psi\rangle$, for each i. The fact that these two different products are actually equal to one another (as you will prove in Problem 3.28) is not at all trivial, but it is one of the main reasons we like to use bra-ket notation! The notation now suggests (see Problem 3.29) that

$$\sum_{i=1}^{n} |B_i\rangle\langle B_i| = 1, \tag{3.81}$$

where $|B_i\rangle\langle B_i|$ is the outer product defined above, and the 1 on the right-hand side is the identity matrix. This extremely useful result is called the *completeness relation*.

In $\mathbb{C}^2$, we simply have

$$|B_1\rangle\langle B_1| + |B_2\rangle\langle B_2| = 1. \tag{3.82}$$

Exercise 3.27. Given the basis

$$|B_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad |B_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \tag{3.83}$$

first show that it is indeed an orthonormal basis, and then show that it satisfies the completeness relation given by (3.82).

Problem 3.28. A. Provide a rigorous proof that, for any three vectors $|A\rangle, |B\rangle, |C\rangle \in \mathbb{C}^n$ and for any dimension n, the following equality is satisfied:

$$|A\rangle\langle B|C\rangle = \Big(|A\rangle\langle B|\Big)|C\rangle. \tag{3.84}$$

In other words, the product ket-bra-ket is *associative*. On the left-hand side we have a vector $|A\rangle$ time a scalar $\langle B|C\rangle$ (which is the result of an inner product), while on the right-hand side we have a matrix $|A\rangle\langle B|$ (which is the result of an outer product) times a vector $|C\rangle$, but the two sides are nonetheless equal.

B. Use the associative property to prove that

$$|\Psi\rangle = \sum_{i=1}^{n} |B_i\rangle\langle B_i|\Psi\rangle = \left(\sum_{i=1}^{n} |B_i\rangle\langle B_i|\right)|\Psi\rangle. \tag{3.85}$$

Problem 3.29. Importantly, we didn't "divide (3.80) by $|\Psi\rangle$" to get (3.81)! You can't do that with matrices and vectors. Instead, (3.81) follows from the fact that any matrix A which satisfies $|\Psi\rangle = A\,|\Psi\rangle$ for **every** vector $|\Psi\rangle$ must necessarily be the identity matrix. Prove this.

3.2.7 Representing Vectors in Different Bases

Let us consider a complex n-vector defined as follows:

$$|\Psi\rangle \equiv \begin{pmatrix} \Psi_1 \\ \vdots \\ \Psi_n \end{pmatrix}, \qquad \Psi_i \in \mathbb{C}. \tag{3.86}$$

Given an orthonormal basis $|B_i\rangle$, we have seen that we can write $|\Psi\rangle$ as a linear combination of the basis vectors:

$$|\Psi\rangle = \sum_{i=1}^{n} \lambda_i\,|B_i\rangle\,. \tag{3.87}$$

The coefficients $\lambda_i \in \mathbb{C}$ depend on $|\Psi\rangle$ and on the basis vectors, as we showed in (3.77):

$$\lambda_i \equiv \langle B_i|\Psi\rangle \quad \Longrightarrow \quad |\Psi\rangle = \sum_{i=1}^{n} |B_i\rangle\langle B_i|\Psi\rangle \tag{3.88}$$

With these coefficients, we can *represent* the vector $|\Psi\rangle$ in the basis $|B_i\rangle$. This representation will be a vector of the same dimension n, with the components being the coefficients $\lambda_i = \langle B_i|\Psi\rangle$, and will be denoted as follows:

$$|\Psi\rangle\Big|_B \equiv \begin{pmatrix} \langle B_1|\Psi\rangle \\ \vdots \\ \langle B_n|\Psi\rangle \end{pmatrix} = \begin{pmatrix} \lambda_1 \\ \vdots \\ \lambda_n \end{pmatrix}. \tag{3.89}$$

We say that λ_i are the *coordinates* of $|\Psi\rangle$ with respect to the basis $|B_i\rangle$.

The correct way to understand the meaning of a vector is as an **abstract** entity, like an arrow in space, which does not depend on any particular basis – it is just there. However, if we want to do concrete calculations with a vector, we must somehow represent it numerically. This is done by choosing a basis and writing down the coordinates of the vector in that basis.

Therefore, whenever we define a vector using its components – as we have been doing throughout this chapter – there is always a specific basis in which the vector is represented, with the components being the coordinates in this basis. If no particular basis is explicitly specified, it is implied that it is the standard basis. But no representation is better than the other; we usually choose whatever basis is most convenient to work with. In quantum mechanics, we often choose a basis defined by some physical observable, as we will see below.

Exercise 3.30. Let a vector $|\Psi\rangle$ be represented in the standard basis as

$$|\Psi\rangle \equiv \begin{pmatrix} 1-9\,\mathrm{i} \\ 7\,\mathrm{i}-2 \end{pmatrix}. \tag{3.90}$$

Find its representation $|\Psi\rangle\,\big|_B$ in terms of the orthonormal basis

$$|B_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad |B_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{3.91}$$

Problem 3.31. Prove that the inner product (and thus also the norm) is independent of the choice of basis. That is, for any two vectors $|\Psi\rangle$ and $|\Phi\rangle$ and any two bases $|B_i\rangle$ and $|C_i\rangle$,

$$\langle\Psi|\Phi\rangle\Big|_B = \langle\Psi|\Phi\rangle\Big|_C. \tag{3.92}$$

3.2.8 Change of Basis

Let the representation of a vector $|\Psi\rangle$ in the basis $|B_i\rangle$ be

$$|\Psi\rangle\Big|_B = \begin{pmatrix} \langle B_1|\Psi\rangle \\ \vdots \\ \langle B_n|\Psi\rangle \end{pmatrix} = \sum_{i=1}^{n} |B_i\rangle\langle B_i|\Psi\rangle. \tag{3.93}$$

Given a different basis $|C_i\rangle$, we have a different representation

$$|\Psi\rangle\Big|_C = \begin{pmatrix} \langle C_1|\Psi\rangle \\ \vdots \\ \langle C_n|\Psi\rangle \end{pmatrix} = \sum_{i=1}^{n} |C_i\rangle\langle C_i|\Psi\rangle. \tag{3.94}$$

To find a relation between the two representations, we use the completeness relation, (3.81):

$$\sum_{j=1}^{n} |B_j\rangle\langle B_j| = 1. \tag{3.95}$$

Inserting it in the middle of the inner product representing the coordinates $\langle C_i|\Psi\rangle$, we get that for all i

$$\langle C_i|\Psi\rangle = \langle C_i|\left(\sum_{j=1}^{n} |B_j\rangle\langle B_j|\right)|\Psi\rangle = \sum_{j=1}^{n}\langle C_i|B_j\rangle\langle B_j|\Psi\rangle. \tag{3.96}$$

Again, the Dirac notation proves to be pretty convenient! This relation can be expressed in matrix form as follows:

$$\begin{pmatrix} \langle C_1|\Psi\rangle \\ \vdots \\ \langle C_n|\Psi\rangle \end{pmatrix} = \begin{pmatrix} \langle C_1|B_1\rangle & \cdots & \langle C_1|B_n\rangle \\ \vdots & \ddots & \vdots \\ \langle C_n|B_1\rangle & \cdots & \langle C_n|B_n\rangle \end{pmatrix} \begin{pmatrix} \langle B_1|\Psi\rangle \\ \vdots \\ \langle B_n|\Psi\rangle \end{pmatrix}, \tag{3.97}$$

or in other words,

$$|\Psi\rangle\Big|_C = P_{C\leftarrow B}\,|\Psi\rangle\Big|_B, \tag{3.98}$$

where the *change-of-basis matrix* from $|B_i\rangle$ to $|C_i\rangle$, denoted $P_{C\leftarrow B}$, is defined as

$$P_{C\leftarrow B} \equiv \begin{pmatrix} \langle C_1|B_1\rangle & \cdots & \langle C_1|B_n\rangle \\ \vdots & \ddots & \vdots \\ \langle C_n|B_1\rangle & \cdots & \langle C_n|B_n\rangle \end{pmatrix}. \tag{3.99}$$

Exercise 3.32. Consider the two bases

$$|B_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad |B_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}, \tag{3.100}$$

$$|C_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \mathrm{i} \end{pmatrix}, \qquad |C_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -\mathrm{i} \\ -1 \end{pmatrix}. \tag{3.101}$$

A. The vector $|\Psi\rangle$ is represented in the standard basis as

$$|\Psi\rangle = \begin{pmatrix} -3 \\ 2+\mathrm{i} \end{pmatrix}. \tag{3.102}$$

Find its representations in the bases $|B_i\rangle$ and $|C_i\rangle$.

B. Find the change-of-basis matrix $P_{C\leftarrow B}$. Calculate $P_{C\leftarrow B}\,|\Psi\rangle\,\big|_B$ and verify that the result is equal to the expression you obtained in (A) for $|\Psi\rangle\,\big|_{C_i}$.

3.2.9 Multiplication and Inverse of Matrices

The *matrix product* of two matrices is another matrix. The element of that matrix at row i, column j is calculated by taking the inner product of row i of the left matrix with column j of the right matrix:

$$AB = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}\begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} = \begin{pmatrix} A_{11}B_{11}+A_{12}B_{21} & A_{11}B_{12}+A_{12}B_{22} \\ A_{21}B_{11}+A_{22}B_{21} & A_{21}B_{12}+A_{22}B_{22} \end{pmatrix}. \tag{3.103}$$

Observe that the action of a matrix on a vector, and the inner and outer products of vectors, are all just special cases of matrix multiplication – where a ket is a matrix with only one column, and a bra is a matrix with only one row!

Given a matrix A, if there exists another matrix A^{-1} such that

$$A^{-1}A = AA^{-1} = 1, \tag{3.104}$$

then the matrix A is called *invertible* and A^{-1} is called its *inverse matrix*. Note that $\left(A^{-1}\right)^{-1} = A$, so the operation of taking the inverse is an involution. Sometimes matrices do not have an inverse; such matrices are called *singular*.

Exercise 3.33. Calculate the products AB and BA where:

$$A \equiv \begin{pmatrix} -1 & 3 \\ -6\,\mathrm{i} & 2\,\mathrm{i}-1 \end{pmatrix}, \qquad B \equiv \begin{pmatrix} 9-8\,\mathrm{i} & 7 \\ 4\,\mathrm{i} & -2\,\mathrm{i} \end{pmatrix}. \tag{3.105}$$

Problem 3.34. Find a general formula for the inverse of a 2×2 matrix by taking

$$A \equiv \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \qquad A^{-1} \equiv \begin{pmatrix} e & f \\ g & h \end{pmatrix}, \tag{3.106}$$

and solving for e, f, g, h in terms of a, b, c, d.

Exercise 3.35. Find the inverse of the matrix

$$A \equiv \begin{pmatrix} 1 & 2-4\,\mathrm{i} \\ -\,\mathrm{i} & -2 \end{pmatrix}. \tag{3.107}$$

You can use the formula you found in Problem 3.34.

Problem 3.36. Show that $(AB)^\dagger = B^\dagger A^\dagger$ and $(AB)^{-1} = B^{-1}A^{-1}$ for any two matrices A and B.

Problem 3.37. Matrix multiplication is not commutative in general. That is, for two arbitrary matrices A and B, it is not in general true that $AB = BA$. Find an example of two matrices which commute, and an example of two matrices which do not commute. In each case, show that they indeed commute or don't commute.

Problem 3.38. Show that multiplying by a scalar $\lambda \in \mathbb{C}$ is the same as multiplying by a matrix with all of its elements equal to zero except for the elements on the diagonal, which are all equal to λ:

$$\lambda A = \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix} A. \tag{3.108}$$

This is also known as a *scalar matrix*.

Problem 3.39. Given two bases $|B_i\rangle$ and $|C_i\rangle$, show that the change-of-basis matrix $P_{B\leftarrow C}$ is the inverse of the change-of-basis matrix in the other direction, $P_{C\leftarrow B}$.

3.2.10 Matrices Inside Inner Products

Since $A|\Phi\rangle$ is itself a vector, we may calculate the inner product of that vector with the dual vector $\langle\Psi|$, which as usual gives us a complex number:

$$\begin{aligned}\langle\Psi|A|\Phi\rangle &= \begin{pmatrix} \Psi_1^* & \Psi_2^* \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} \\ &= \Psi_1^* A_{11}\Phi_1 + \Psi_2^* A_{21}\Phi_1 + \Psi_1^* A_{12}\Phi_2 + \Psi_2^* A_{22}\Phi_2.\end{aligned}$$

If we take the dual of $A|\Phi\rangle$ we get $\langle\Phi|A^\dagger$, as you proved in Problem 3.22. Thus, inverting the order of the inner product, we get

$$\begin{aligned}\langle\Phi|A^\dagger|\Psi\rangle &= \begin{pmatrix} \Phi_1^* & \Phi_2^* \end{pmatrix} \begin{pmatrix} A_{11}^* & A_{21}^* \\ A_{12}^* & A_{22}^* \end{pmatrix} \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} \\ &= \Psi_1 A_{11}^*\Phi_1^* + \Psi_2 A_{21}^*\Phi_1^* + \Psi_1 A_{12}^*\Phi_2^* + \Psi_2 A_{22}^*\Phi_2^*.\end{aligned}$$

This is, of course, the complex conjugate of $\langle\Psi|A|\Phi\rangle$, since inverting the order of the inner product results in the complex conjugate. In other words, we have the relation

$$\langle\Psi|A|\Phi\rangle^* = \langle\Phi|A^\dagger|\Psi\rangle. \tag{3.109}$$

Taking the complex conjugate reverses the order of the inner product, and also replaces the matrix with its adjoint.

Exercise 3.40. Calculate the inner product $\langle\Psi|A|\Phi\rangle$ where

$$|\Psi\rangle = \begin{pmatrix} 5+2\,\mathrm{i} \\ -3\,\mathrm{i} \end{pmatrix}, \qquad A = \begin{pmatrix} 9 & 8\,\mathrm{i} \\ 6\,\mathrm{i} & 5-4\,\mathrm{i} \end{pmatrix}, \qquad |\Phi\rangle = \begin{pmatrix} 3+4\,\mathrm{i} \\ 2 \end{pmatrix}. \tag{3.110}$$

3.2.11 Eigenvalues and Eigenvectors

If the matrix A, acting on the (non-zero) vector $|\Psi\rangle$, results in a scalar multiple of $|\Psi\rangle$:

$$A|\Psi\rangle = \lambda|\Psi\rangle, \qquad \lambda \in \mathbb{C}, \tag{3.111}$$

then we call $|\Psi\rangle$ an *eigenvector* of A and λ its *eigenvalue*. Note that $|\Psi\rangle$ cannot be the zero vector, but λ can be zero.

For example, if

$$A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{3.112}$$

then it's easy to see that

$$|\Psi\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{3.113}$$

is an eigenvector with eigenvalue $+1$ and

$$|\Phi\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{3.114}$$

is an eigenvector with eigenvalue -1:

$$A|\Psi\rangle = |\Psi\rangle, \qquad A|\Phi\rangle = -|\Phi\rangle. \tag{3.115}$$

Exercise 3.41. The matrix

$$A \equiv \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix} \tag{3.116}$$

has two eigenvectors. Find them and their corresponding eigenvalues.

Problem 3.42. Prove that, if $|\Psi\rangle$ is an eigenvector of a matrix A, then $\alpha|\Psi\rangle$ is also an eigenvector of A for any $\alpha \in \mathbb{C}$, and it has the same eigenvalue.

3.2.12 Hermitian Matrices

A matrix A is called *Hermitian* if it's equal to its adjoint:

$$A = A^\dagger. \tag{3.117}$$

Thus, it is sometimes also referred to as a *self-adjoint* matrix. For such a matrix, we have that

$$\langle\Psi|A|\Phi\rangle^* = \langle\Phi|A|\Psi\rangle. \tag{3.118}$$

A Hermitian matrix is analogous to a real number, since $z = z^*$ implies that z is real.

The eigenvalues of a Hermitian matrices must all be real. To see this, let λ be an eigenvalue of the Hermitian matrix A with the eigenvector $|\Psi\rangle$:

$$A|\Psi\rangle = \lambda|\Psi\rangle. \tag{3.119}$$

Then we can take the inner product of both sides with $\langle\Psi|$:

$$\langle\Psi|A|\Psi\rangle = \langle\Psi|\lambda|\Psi\rangle = \lambda\langle\Psi|\Psi\rangle = \lambda\||\Psi\rangle\|^2, \tag{3.120}$$

where were able to move λ out of the inner product because it's just a number. From (3.118), we have:

$$\langle\Psi|A|\Psi\rangle = \langle\Psi|A|\Psi\rangle^*, \tag{3.121}$$

so $\langle\Psi|A|\Psi\rangle$ is real. Since $\||\Psi\rangle\|^2$ is also real – and non-zero, since $|\Psi\rangle$ is an eigenvector, so by definition it cannot be the zero vector – we conclude that λ must be real.

Now, let $|\Psi\rangle$ and $|\Phi\rangle$ be two eigenvectors of A corresponding to different eigenvalues λ and

μ respectively:

$$A\,|\Psi\rangle = \lambda\,|\Psi\rangle\,, \qquad A\,|\Phi\rangle = \mu\,|\Phi\rangle\,, \qquad \lambda \neq \mu. \tag{3.122}$$

Let us take the inner product of the first equation with $\langle\Phi|$ and of the second equation with $\langle\Psi|$:

$$\langle\Phi|A|\Psi\rangle = \langle\Phi|\lambda|\Psi\rangle = \lambda\langle\Phi|\Psi\rangle, \tag{3.123}$$

$$\langle\Psi|A|\Phi\rangle = \langle\Psi|\mu|\Phi\rangle = \mu\langle\Psi|\Phi\rangle. \tag{3.124}$$

From (3.118), the first equation is the complex conjugate of the second equation. Since λ must be real – as we just proved – we get

$$\mu\langle\Psi|\Phi\rangle = (\lambda\langle\Phi|\Psi\rangle)^* = \lambda\langle\Psi|\Phi\rangle. \tag{3.125}$$

Seeing that $\lambda \neq \mu$ by our assumption, this equation can only be true if

$$\langle\Psi|\Phi\rangle = 0. \tag{3.126}$$

In other words, eigenvectors of a Hermitian matrix corresponding to different eigenvalues are orthogonal. Now, since an eigenvector multiplied by a scalar is still an eigenvector, the eigenvectors $|\Psi\rangle$ and $|\Phi\rangle$ can be divided by their norms, so that they are not only orthogonal but also orthonormal.

Moreover, one can prove that for any Hermitian matrix A in $\mathbb{C}^n$, there is an orthonormal basis of $\mathbb{C}^n$ consisting of eigenvectors of A. Such a basis is called an *orthonormal eigenbasis*. The proof requires some slightly more advanced tools from linear algebra, so we won't write it here. However, this theorem is extremely important in quantum theory. As we will see, Hermitian matrices represent physical observables in quantum theory, and their eigenvalues correspond to the possible values obtained by performing measurements on these observables. The fact that there is an orthonormal basis of eigenvectors will prove very useful for studying observables in quantum theory.

Problem 3.43. Let A and B be Hermitian matrices. Under what conditions is the product AB Hermitian?

Exercise 3.44. Consider the matrix

$$A \equiv \begin{pmatrix} 0 & 2\,\mathrm{i} \\ c & 0 \end{pmatrix}. \tag{3.127}$$

A. Find the value of c for which A is a Hermitian matrix.

B. Find the eigenvalues of A with the value of c that you found in (A).

C. Find an orthonormal eigenbasis of A with the value of c that you found in (A). Show that it is indeed orthonormal.

Problem 3.45. Find the most general 2×2 Hermitian matrix by demanding that $A = A^\dagger$ and finding conditions on the components of A.

3.2.13 Unitary Matrices

A matrix U is called *unitary* if its adjoint is also its inverse:

$$U^{-1} = U^\dagger \quad \Longrightarrow \quad UU^\dagger = U^\dagger U = 1. \tag{3.128}$$

A unitary matrix is analogous to a complex number with norm 1, since such a number satisfies $z^*z = zz^* = |z|^2 = 1$.

Acting with a unitary matrix on two vectors preserves their inner product. To see this, consider a unitary matrix U and two vectors $|\Psi\rangle$ and $|\Phi\rangle$. If we act with U on both vectors, we get $U|\Psi\rangle$ and $U|\Phi\rangle$. Taking the bra of the ket $U|\Psi\rangle$, we obtain

$$(U|\Psi\rangle)^\dagger = \langle\Psi| U^\dagger. \tag{3.129}$$

If we take the inner product of $U|\Psi\rangle$ and $U|\Phi\rangle$, we get

$$\langle\Psi|U^\dagger U|\Phi\rangle = \langle\Psi|\Phi\rangle, \tag{3.130}$$

since $U^\dagger U = 1$. Therefore, the inner product of these two vectors is the same before and after acting on them with U.

Now, let λ be an eigenvalue of the unitary matrix U with the eigenvector $|\Psi\rangle$:

$$U|\Psi\rangle = \lambda|\Psi\rangle. \tag{3.131}$$

Taking the adjoint of both sides, we get

$$\langle\Psi| U^\dagger = \langle\Psi|\lambda^*. \tag{3.132}$$

Multiplying both equations together, we have

$$\langle\Psi| U^\dagger U|\Psi\rangle = \langle\Psi|\lambda^*\lambda|\Psi\rangle. \tag{3.133}$$

On the left-hand side $U^\dagger U = 1$, and on the right-hand side $\lambda^*\lambda = |\lambda|^2$, so

$$\langle\Psi|\Psi\rangle = |\lambda|^2\langle\Psi|\Psi\rangle \quad \Longrightarrow \quad \|\Psi\|^2 = |\lambda|^2\|\Psi\|^2. \tag{3.134}$$

Since $|\Psi\rangle$ is an eigenvector, it is not the zero vector, and $\|\Psi\|^2 \neq 0$. Hence, we conclude that the eigenvalues of a unitary matrix must all have magnitude 1. This means that they lie on the unit circle of the complex plane, and are of the form $z = e^{i\phi}$ for some $\phi \in \mathbb{R}$.

As with Hermitian matrices, eigenvectors of a unitary matrix corresponding to different eigenvalues are orthogonal (you will prove this in Problem 3.48), and you can always find an orthonormal eigenbasis of eigenvectors of a unitary matrix.

Problem 3.46. Find the most general 2×2 unitary matrix by demanding that $U^{-1} = U^\dagger$ or $UU^\dagger = U^\dagger U = 1$ and finding conditions on the components of U.

Problem 3.47. Find three 2×2 matrices that are both Hermitian and unitary (other than the identity matrix).

Problem 3.48. Prove that eigenvectors of a unitary matrix corresponding to different eigenvalues are orthogonal.

Problem 3.49. Prove that the columns of a unitary matrix, treated as kets, form an orthonormal basis on $\mathbb{C}^n$. Then prove that the same is true for the rows of a unitary matrix, treated as bras.

3.2.14 Normal Matrices

A normal matrix is a matrix A which satisfies $A^\dagger A = AA^\dagger$. Observe that a normal matrix is analogous to a complex number z, since such a number trivially satisfies $z^* z = zz^*$. It is easy to see that Hermitian matrices, which satisfy $A^\dagger = A$, and unitary matrices, which satisfy $A^\dagger = A^{-1}$, are both special cases of normal matrices.

If A is normal and all of its eigenvalues are real, then it is Hermitian. If A normal and all of its eigenvalues have unit magnitude, then it is unitary. Furthermore, it turns out that the condition that the matrix has an orthonormal eigenbasis applies not just to Hermitian and unitary matrices, but in general to any normal matrix; in fact, it is true **if and only if** the matrix is normal.

Problem 3.50. Let A and B be normal matrices. Under which condition are both AB and $A + B$ also normal?

3.2.15 Representing Matrices in Different Bases

In Section 3.2.7 we saw that vectors are abstract entities which can have different representations in different bases. The same is true for matrices. Consider a matrix A and a basis $|B_i\rangle$. Inserting the completeness relation (3.81) **twice**, one time on each side of A, we get:

$$\begin{aligned} A &= \left(\sum_{i=1}^{n} |B_i\rangle\langle B_i| \right) A \left(\sum_{j=1}^{n} |B_j\rangle\langle B_j| \right) \\ &= \sum_{i=1}^{n} \sum_{j=1}^{n} |B_i\rangle\langle B_i|A|B_j\rangle\langle B_j| \\ &= \sum_{i=1}^{n} \sum_{j=1}^{n} \left(A_{ij}\right)_B |B_i\rangle\langle B_j|, \end{aligned}$$

where[14]

$$\left(A_{ij}\right)_B \equiv \langle B_i|A|B_j\rangle \in \mathbb{C}, \qquad i, j \in \{1, \ldots, n\} \tag{3.135}$$

are the *coordinates* of A in the basis $|B_i\rangle$.

[14]Note that we could move $\left(A_{ij}\right)_B$ to the left since it is a scalar.

We have obtained a sum over outer products of the form $|B_i\rangle\langle B_j|$. Recall that the outer product of two vectors is a matrix; thus $|B_i\rangle\langle B_j|$ can be thought of as "basis matrices", in analogy with basis vectors. The representation of A in terms of a linear combination of these "basis matrices" is called the *outer product representation* of A, and it is very useful in quantum theory. We can also write this representation in matrix form as

$$(A)_B = \begin{pmatrix} \langle B_1|A|B_1\rangle & \cdots & \langle B_1|A|B_n\rangle \\ \vdots & \ddots & \vdots \\ \langle B_n|A|B_1\rangle & \cdots & \langle B_n|A|B_n\rangle \end{pmatrix}. \tag{3.136}$$

In another basis $|C_i\rangle$, the matrix A will have the representation

$$(A)_C = \sum_{i=1}^{n}\sum_{j=1}^{n} \left(A_{ij}\right)_C |C_i\rangle\langle C_j| = \begin{pmatrix} \langle C_1|A|C_1\rangle & \cdots & \langle C_1|A|C_n\rangle \\ \vdots & \ddots & \vdots \\ \langle C_n|A|C_1\rangle & \cdots & \langle C_n|A|C_n\rangle \end{pmatrix}, \tag{3.137}$$

where now the coordinates $\left(A_{ij}\right)_C$ are given by

$$\left(A_{ij}\right)_C \equiv \langle C_i|A|C_j\rangle \in \mathbb{C}, \qquad i,j \in \{1,\ldots,n\}. \tag{3.138}$$

Inserting the completeness relation (3.81) into the coordinates twice, similarly to what we did above, we get

$$\begin{aligned} \langle C_i|A|C_j\rangle &= \langle C_i| \left(\sum_{k=1}^{n} |B_k\rangle\langle B_k|\right) A \left(\sum_{\ell=1}^{n} |B_\ell\rangle\langle B_\ell|\right) |C_j\rangle \\ &= \sum_{k=1}^{n}\sum_{\ell=1}^{n} \langle C_i|B_k\rangle\langle B_k|A|B_\ell\rangle\langle B_\ell|C_j\rangle. \end{aligned}$$

Problem 3.51. Show that this relation can be written in matrix form as follows:

$$\begin{pmatrix} \langle C_1|A|C_1\rangle & \cdots & \langle C_1|A|C_n\rangle \\ \vdots & \ddots & \vdots \\ \langle C_n|A|C_1\rangle & \cdots & \langle C_n|A|C_n\rangle \end{pmatrix} =$$

$$= \begin{pmatrix} \langle C_1|B_1\rangle & \cdots & \langle C_1|B_n\rangle \\ \vdots & \ddots & \vdots \\ \langle C_n|B_1\rangle & \cdots & \langle C_n|B_n\rangle \end{pmatrix} \begin{pmatrix} \langle B_1|A|B_1\rangle & \cdots & \langle B_1|A|B_n\rangle \\ \vdots & \ddots & \vdots \\ \langle B_n|A|B_1\rangle & \cdots & \langle B_n|A|B_n\rangle \end{pmatrix} \begin{pmatrix} \langle B_1|C_1\rangle & \cdots & \langle B_1|C_n\rangle \\ \vdots & \ddots & \vdots \\ \langle B_n|C_1\rangle & \cdots & \langle B_n|C_n\rangle \end{pmatrix},$$

and thus the relation between the representations of A in different bases is given by

$$(A)_C = P_{C\leftarrow B}\,(A)_B\,P_{B\leftarrow C}, \tag{3.139}$$

where

$$P_{C\leftarrow B} \equiv \begin{pmatrix} \langle C_1|B_1\rangle & \cdots & \langle C_1|B_n\rangle \\ \vdots & \ddots & \vdots \\ \langle C_n|B_1\rangle & \cdots & \langle C_n|B_n\rangle \end{pmatrix} \tag{3.140}$$

is the change-of-basis matrix (3.99), and $P_{B\leftarrow C} = P_{C\leftarrow B}^{-1}$. This is analogous to the relation between vectors in different bases, $|\Psi\rangle\Big|_C = P_{C\leftarrow B}\,|\Psi\rangle\Big|_B$.

Problem 3.52. Let U be a unitary matrix and let $|B_i\rangle$ be an orthonormal basis.

A. Prove that $|C_i\rangle \equiv U\,|B_i\rangle$ is also an orthonormal basis.

B. Prove that U has the outer product representation

$$U = \sum_{i=1}^{n} |C_i\rangle\,\langle B_i|\,. \tag{3.141}$$

C. Conversely, prove that if $|B_i\rangle$ and $|C_i\rangle$ are two **arbitrary** orthonormal bases, then the matrix U **defined** by (3.141) is unitary.

3.2.16 Diagonalizable Matrices

A diagonal matrix is a matrix with all of its elements equal to zero except for the elements on the diagonal, for example:

$$D = \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix}. \tag{3.142}$$

A matrix A is called *diagonalizable* if there exists an invertible matrix P such that the matrix $P^{-1}AP$ is diagonal. In quantum theory, we are mostly concerned with the case where P is also a unitary matrix, such that $P^\dagger AP$ is diagonal. It turns out that a matrix A is diagonalizable by a unitary matrix P if and only if A is normal. This means, in particular, that both Hermitian and unitary matrices are diagonalizable in such a way.

Let A be a normal matrix with an orthonormal eigenbasis $|B_i\rangle$ with corresponding eigenvalues λ_i:

$$A\,|B_i\rangle = \lambda_i\,|B_i\rangle\,, \qquad \forall i. \tag{3.143}$$

Now, consider the change-of-basis matrix (3.99), this time from the eigenbasis $|B_i\rangle$, which is orthonormal to the standard basis $|1_i\rangle$:

$$P_{1\leftarrow B} \equiv \begin{pmatrix} \langle 1_1|B_1\rangle & \cdots & \langle 1_1|B_n\rangle \\ \vdots & \ddots & \vdots \\ \langle 1_n|B_1\rangle & \cdots & \langle 1_n|B_n\rangle \end{pmatrix}. \tag{3.144}$$

Note that each eigenvector $|B_i\rangle$ is represented in the standard basis $|1_i\rangle$ as follows:

$$|B_i\rangle\Big|_1 = \begin{pmatrix} \langle 1_1|B_i\rangle \\ \vdots \\ \langle 1_n|B_i\rangle \end{pmatrix}, \qquad \forall i. \tag{3.145}$$

Hence, the columns of $P_{1\leftarrow B}$ are in fact the eigenvectors $|B_i\rangle$ themselves, as expressed in the standard basis:

$$P_{1\leftarrow B} = \begin{pmatrix} |B_1\rangle & \cdots & |B_n\rangle \end{pmatrix}. \tag{3.146}$$

Let us denote $P \equiv P_{1\leftarrow B}$ for short. Then

$$\begin{aligned} AP &= A \begin{pmatrix} |B_1\rangle & \cdots & |B_n\rangle \end{pmatrix} \\ &= \begin{pmatrix} A|B_1\rangle & \cdots & A|B_n\rangle \end{pmatrix} \\ &= \begin{pmatrix} \lambda_1|B_1\rangle & \cdots & \lambda_n|B_n\rangle \end{pmatrix}. \end{aligned}$$

How did we get this? Remember that in Section 3.2.9 we said that the element of the matrix AP at row i, column j is calculated by taking the inner product of row i of A with column j of P. But column j of P is just $|B_j\rangle$. The product $A|B_i\rangle$ is another ket, whose rows are obtained by taking the inner product of each row of A with $|B_i\rangle$ respectively. The last equality follows from (3.143).

Next, we write the full matrix and decompose it into two matrices:

$$AP = \begin{pmatrix} \lambda_1\langle 1_1|B_1\rangle & \cdots & \lambda_n\langle 1_1|B_n\rangle \\ \vdots & \ddots & \vdots \\ \lambda_1\langle 1_n|B_1\rangle & \cdots & \lambda_n\langle 1_n|B_n\rangle \end{pmatrix} = \begin{pmatrix} \langle 1_1|B_1\rangle & \cdots & \langle 1_1|B_n\rangle \\ \vdots & \ddots & \vdots \\ \langle 1_n|B_1\rangle & \cdots & \langle 1_n|B_n\rangle \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_n \end{pmatrix}. \tag{3.147}$$

You should calculate the product on the right-hand side (even just for $n = 2$ or $n = 3$) to convince yourself that this decomposition is indeed correct. Now, if we define a new diagonal matrix, with the eigenvalues on the diagonal:

$$D \equiv \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_n \end{pmatrix}, \tag{3.148}$$

then we can write (3.147) as

$$AP = PD. \tag{3.149}$$

Finally, we multiply by P^{-1} from the left to get

$$P^{-1}AP = D. \tag{3.150}$$

Exercise 3.53. Diagonalize the following matrix:

$$A = \begin{pmatrix} 1 & 3 \\ 3 & 1 \end{pmatrix}. \tag{3.151}$$

Problem 3.54. Prove that the change-of-basis matrix $P \equiv P_{1\leftarrow B}$ as defined above, with $|B_i\rangle$ an orthonormal eigenbasis, is unitary. This means that we can also write $P^\dagger AP = D$, since $P^{-1} = P^\dagger$ for unitary matrices.

Problem 3.55. Show that if A is a normal matrix then it has the outer product representation

$$A = \sum_{i=1}^{n} \lambda_i |B_i\rangle \langle B_i|, \tag{3.152}$$

where $|B_i\rangle$ is an orthonormal eigenbasis and λ_i are the eigenvalues of the eigenvectors $|B_i\rangle$.

3.2.17 The Cauchy-Schwarz Inequality

The *Cauchy-Schwarz inequality* states that for any two vectors $|\Psi\rangle$ and $|\Phi\rangle$, we have

$$|\langle\Psi|\Phi\rangle| \leq \||\Psi\rangle\| \, \||\Phi\rangle\|. \tag{3.153}$$

To prove it, consider an orthonormal basis $|B_i\rangle$ such that[15]

$$|B_1\rangle \equiv \frac{|\Phi\rangle}{\||\Phi\rangle\|}. \tag{3.154}$$

[15]Such a basis can always be generated using a method called the *Gram-Schmidt process*, which we will not describe here.

Then, using the completeness relation (3.81), we find:

$$\begin{aligned}
\|\Psi\|^2 \|\Phi\|^2 &= \langle\Psi|\Psi\rangle \|\Phi\|^2 \\
&= \langle\Psi| \left(\sum_{i=1}^{n} |B_i\rangle\langle B_i| \right) |\Psi\rangle \|\Phi\|^2 \\
&= \langle\Psi| \left(|B_1\rangle\langle B_1| + \sum_{i=2}^{n} |B_i\rangle\langle B_i| \right) |\Psi\rangle \|\Phi\|^2 \\
&= \langle\Psi| \left(\frac{1}{\|\Phi\|^2} |\Phi\rangle\langle\Phi| + \sum_{i=2}^{n} |B_i\rangle\langle B_i| \right) |\Psi\rangle \|\Phi\|^2 \\
&= \left(\frac{1}{\|\Phi\|^2} \langle\Psi|\Phi\rangle\langle\Phi|\Psi\rangle + \sum_{i=2}^{n} \langle\Psi|B_i\rangle\langle B_i|\Psi\rangle \right) \|\Phi\|^2 \\
&= \left(\frac{1}{\|\Phi\|^2} |\langle\Psi|\Phi\rangle|^2 + \sum_{i=2}^{n} |\langle\Psi|B_i\rangle|^2 \right) \|\Phi\|^2 \\
&= |\langle\Psi|\Phi\rangle|^2 + \sum_{i=2}^{n} |\langle\Psi|B_i\rangle|^2 \|\Phi\|^2 \\
&\geq |\langle\Psi|\Phi\rangle|^2 .
\end{aligned}$$

Taking the square root, we obtain (3.153).

Problem 3.56. Explain each step in the proof above.

Exercise 3.57. Check this inequality explicitly for three pairs of vectors of your choice.

Problem 3.58. Find a condition that is equivalent to an **equality** in the Cauchy-Schwarz inequality. That is, find an "if and only if" statement for $|\langle\Psi|\Phi\rangle| = \|\Psi\| \|\Phi\|$ involving properties of $|\Psi\rangle$ and $|\Phi\rangle$. Prove the statement in **both directions**.

3.3 Probability Theory

3.3.1 Random Variables and Probability Distributions

A *random variable* X is a function which assigns a real value to each possible outcome of an experiment or process. Sometimes these values will be the actual measured value in some way: for example, the value of the random variable X for rolling a 6-sided die will simply be the number on the die. Other times, the value of the random variable will be just a numerical label assigned to each outcome: for example, for a coin toss we can assign 1 to heads and 0 to tails (but we can also assign any other numbers, if we want).

These examples were of *discrete* random variables, but we can also have *continuous* random variables, such as the position of a particle along a line, which in principle can take any real value. For simplicity, we will focus on discrete random variables here.

A (discrete) *probability distribution* assigns a probability to each value of a random variable. We denote by $P(X = x)$ the probability that the random variable X will have the value x. A *probability* is a number between 0 and 1, which denotes how likely it is (in percentage) for the value to occur, so 0 means this value **never** occurs and 1 (= 100%) means this value **always** occurs.

The probabilities for all the possible values must sum to 1, because if for example they only sum to 0.9, this means that in 10% of the cases the random variable has **no value**, which doesn't really make sense. Also, if $P(X = x) = 0$ then there must be at least one other possible value that X can take, since it will never evaluate to x, and if $P(X = x) = 1$ then there cannot be any other possible values that X can take, since it always evaluates to x.

For example, for the coin toss we have

$$P(X = 0) = \frac{1}{2}, \qquad P(X = 1) = \frac{1}{2}, \tag{3.155}$$

and for the 6-sided die roll we have

$$P(X = 1) = \frac{1}{6}, \qquad P(X = 2) = \frac{1}{6}, \qquad P(X = 3) = \frac{1}{6}, \tag{3.156}$$

$$P(X = 4) = \frac{1}{6}, \qquad P(X = 5) = \frac{1}{6}, \qquad P(X = 6) = \frac{1}{6}. \tag{3.157}$$

Note how the probabilities sum to 1 in each case. Of course, we could also say that maybe the coin toss results in heads only 49.9% of the time, and tails another 49.9% of the time, and the remaining 0.2% is the probability for the coin to balance perfectly on its edge... But usually we ignore subtleties like this and assume we have **idealized** coins. Similarly, we could also have a *loaded coin* which lands on heads more or less frequently than it lands on tails, but usually we assume that the coins are fair unless stated otherwise. The same discussion applies for dies, with any number of sides: they are, by default, assumed to be idealized and fair.

These probability distributions are *uniform*, since they assign the same probability to each value of X. However, probability distributions need not be uniform. A simple example is a loaded coin, which perhaps has

$$P(X = 0) = \frac{1}{3}, \qquad P(X = 1) = \frac{2}{3}. \tag{3.158}$$

As a more interesting example, if we toss **two** fair coins X_1 and X_2 and define a random variable to be the sum of the results, $X \equiv X_1 + X_2$, then we can get any of the following 4 outcomes:

$$0 + 0 = 0, \qquad 0 + 1 = 1, \qquad 1 + 0 = 1, \qquad 1 + 1 = 2. \tag{3.159}$$

The probability for each outcome is

$$\frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}, \tag{3.160}$$

but the outcome 1 appears twice; thus

$$P(X=0)=\frac{1}{4},\qquad P(X=1)=\frac{1}{2},\qquad P(X=2)=\frac{1}{4}. \tag{3.161}$$

Of course, the probabilities still sum to 1.

Exercise 3.59. Calculate the probability distribution for the sum of two rolls of a 6-sided die. This is known to players of role-playing games (such as Dungeons & Dragons) as a "2d6", where we define ndN to be the sum of n rolls of an N-sided die.

3.3.2 Conditional Probability

Consider two random variables, X and Y. Let X have N possible values x_i, $i \in \{1,\ldots,N\}$ and let Y have M possible values y_i, $i \in \{1,\ldots,M\}$. Then the *joint probability* to get $X = x_i$ **and** $Y = y_j$ at the **same time**, for some specific choice of i and j, is denoted

$$P\left(X=x_i \cap Y=y_j\right), \tag{3.162}$$

where $\cap$ means[16] "and". Furthermore, we have

$$\sum_{j=1}^{M} P\left(X=x_i \cap Y=y_j\right) = P\left(X=x_i\right), \tag{3.163}$$

because the total probability to get $X = x_i$ is the sum of all the different probabilities that involve $X = x_i$ plus something else. To illustrate this, consider the following random variables:

$$X = \text{whether you pass or fail this course,} \tag{3.164}$$

$$Y = \text{whether you did or did not do all the homework.} \tag{3.165}$$

There are in total 4 different combinations, and their probabilities must sum to 1. Maybe the probabilities are as follows:

$$P(\text{pass} \cap \text{did homework}) = 40\%, \tag{3.166}$$

$$P(\text{pass} \cap \text{didn't do homework}) = 20\%, \tag{3.167}$$

$$P(\text{didn't pass} \cap \text{did homework}) = 10\%, \tag{3.168}$$

$$P(\text{didn't pass} \cap \text{didn't do homework}) = 30\%. \tag{3.169}$$

Then clearly the total probability that you pass (whether or not you did the homework) is $40\% + 20\% = 60\%$, and the total probability that you do not pass is $10\% + 30\% = 40\%$. This is exactly what (3.163) means.

[16] More precisely, $\cap$ means the intersection of two sets, where one is the set of events for which $X = x_i$ and the other is the set of events for which $Y = y_j$.

However, what you really want to know is the probability that you pass given that you did the homework vs. the probability that you pass given that you did not do the homework. This is called *conditional probability*. The probability for outcome X **given** outcome Y is denoted $P(X|Y)$, where $|$ is read as "given that". It is related to $P(X \cap Y)$ as follows:

$$P(X|Y) = \frac{P(X \cap Y)}{P(Y)}. \tag{3.170}$$

In other words, it is the probability that both X and Y happened, divided by the probability for Y to happen. Let us calculate:

$$P(\text{pass} \mid \text{did homework}) = \frac{40\%}{40\% + 10\%} = 80\%, \tag{3.171}$$

$$P(\text{pass} \mid \text{didn't do homework}) = \frac{20\%}{20\% + 30\%} = 40\%. \tag{3.172}$$

So you better do all the homework, because that doubles your chances of passing the course!

Exercise 3.60. There are six more conditional probabilities that we did not calculate here. Calculate them. What do you learn from the results?

Exercise 3.61. A test for COVID-19 has[17] a 1% chance of **false positive**, i.e. the result is positive but the patient **isn't** actually sick, and a 1% chance of **false negative**, i.e. the result is negative but the patient **is** actually sick. Assume that 0.1% of the population is actually sick.

A. Fill in the blanks in the following table:

	Sick	Healthy	Total
Actual status		99.9%	100%
Positive test	0.099%		1.098%
Negative test	0.001%	98.901%	

(3.173)

B. Given that you tested positive, what is the conditional probability that you actually have COVID-19?

C. Given that you tested negative, what is the conditional probability that you actually don't have COVID-19?

D. Which result should you trust, a positive one or a negative one?

3.3.3 Expected Values

The *expected value* (or *expectation value* or *mean*) $\langle X \rangle$ of a random variable X is the average over all the possible values X can take, weighted by their assigned probabilities:

$$\langle X \rangle \equiv \sum_{i=1}^{N} P(X = x_i)\, x_i, \tag{3.174}$$

[17] FYI: This exercise is not based on any real data!

where N is the total number of possible outcomes, x_i is the value of outcome number i, and $P(X = x_i)$ is the probability to get x_i. In the example of the coin toss, we have:

$$\langle X \rangle = \frac{1}{2} \cdot 0 + \frac{1}{2} \cdot 1 = \frac{1}{2} = 0.5, \tag{3.175}$$

and for the 6-sided die roll, we have:

$$\langle X \rangle = \frac{1}{6} \cdot 1 + \frac{1}{6} \cdot 2 + \frac{1}{6} \cdot 3 + \frac{1}{6} \cdot 4 + \frac{1}{6} \cdot 5 + \frac{1}{6} \cdot 6 = \frac{7}{2} = 3.5. \tag{3.176}$$

Observe that the expected value in both cases is not an actual value the random variable can take! This is often the case with discrete random variables.

We will now prove that the expected value is linear:

$$\langle \alpha X + \beta Y \rangle = \alpha \langle X \rangle + \beta \langle Y \rangle, \qquad \alpha, \beta \in \mathbb{R}. \tag{3.177}$$

This can be broken down into two rules:

$$\langle \alpha X \rangle = \alpha \langle X \rangle, \qquad \langle X + Y \rangle = \langle X \rangle + \langle Y \rangle. \tag{3.178}$$

The first rule is easy to prove:

$$\begin{aligned} \langle \alpha X \rangle &= \sum_{i=1}^{N} P(\alpha X = \alpha x_i)(\alpha x_i) \\ &= \alpha \sum_{i=1}^{N} P(X = x_i) x_i. \end{aligned}$$

To prove the second part, let X have N possible values x_i and let Y have M possible values y_i, as in the previous section. Then in calculating $\langle X + Y \rangle$ we need to sum over both N and M, to ensure we take all possible combinations of X and Y into account. Using (3.163), we get:

$$\begin{aligned} \langle X + Y \rangle &= \sum_{i=1}^{N} \sum_{j=1}^{M} P(X = x_i, Y = y_j)(x_i + y_j) \\ &= \sum_{i=1}^{N} \left(\sum_{j=1}^{M} P(X = x_i, Y = y_j) \right) x_i + \sum_{j=1}^{M} \left(\sum_{i=1}^{N} P(X = x_i, Y = y_j) \right) y_j \\ &= \sum_{i=1}^{N} P(X = x_i) x_i + \sum_{j=1}^{M} P(Y = y_j) y_j \\ &= \langle X \rangle + \langle Y \rangle, \end{aligned}$$

as we wanted to prove.

Exercise 3.62. Calculate the expected value for the sum of two coin tosses and for a 2d6 roll (the sum of two 6-sided dies). First, do it by defining one random variable for the sum,

calculating the probabilities, and then using the definition of the expected value. Then, do it by considering just one coin or one 6-sided die respectively, and use (3.177). Compare your results.

3.3.4 Standard Deviation

The *standard deviation*[18] measures how far the outcomes are expected to be from the expected value. To calculate the standard deviation, we take the expected value of $(X - \langle X \rangle)^2$, that is, the square of the difference between the **actual** value of X and its **expected** value $\langle X \rangle$. Then, we take the square root of the result to obtain the standard deviation ΔX:

$$\Delta X \equiv \sqrt{\left\langle (X - \langle X \rangle)^2 \right\rangle}. \tag{3.179}$$

To simplify this, first we note that

$$(X - \langle X \rangle)^2 = X^2 - 2X \langle X \rangle + \langle X \rangle^2 . \tag{3.180}$$

In this formula, X^2 is a random variable (whose values are the squares of the values of X), but $\langle X \rangle$ is just a **number**, not a random variable. Since it is a number, we can treat it as a random variable that only returns one value with 100% probability, which means that

$$\langle \langle X \rangle \rangle = \langle X \rangle . \tag{3.181}$$

So, by (3.177), we have:

$$\begin{aligned} \left\langle (X - \langle X \rangle)^2 \right\rangle &= \langle X^2 \rangle - 2 \langle X \rangle \langle X \rangle + \langle X \rangle^2 \\ &= \langle X^2 \rangle - \langle X \rangle^2 . \end{aligned}$$

Therefore, the standard deviation can be written as follows:

$$\Delta X = \sqrt{\langle X^2 \rangle - \langle X \rangle^2}. \tag{3.182}$$

This form is easier to do calculations with. For example, for the coin toss we have from before

$$\langle X \rangle = \frac{1}{2}, \tag{3.183}$$

and we also calculate:

$$\langle X^2 \rangle = \frac{1}{2} \cdot 0^2 + \frac{1}{2} \cdot 1^2 = \frac{1}{2}, \tag{3.184}$$

[18] By the way, the square of the standard deviation is called the *variance*, but it will not interest us in this course.

which gives us

$$\Delta X = \sqrt{\frac{1}{2} - \frac{1}{4}} = \frac{1}{2}. \tag{3.185}$$

This makes sense, as the two actual values of the outcomes, 0 and 1, lie exactly $1/2$ away from the expected value $\langle X \rangle = 1/2$ in each direction. So they each "deviate" from it by $1/2$.

For the die roll, we have from before

$$\langle X \rangle = \frac{7}{2}, \tag{3.186}$$

and we also calculate:

$$\langle X^2 \rangle = \frac{1}{6}\left(1^2 + 2^2 + 3^2 + 4^2 + 5^2 + 6^2\right) = \frac{91}{6}, \tag{3.187}$$

which gives us

$$\Delta X = \sqrt{\frac{91}{6} - \frac{49}{4}} = \sqrt{\frac{35}{12}} \approx 1.7. \tag{3.188}$$

Exercise 3.63. Calculate the standard deviation for the sum of two coin tosses and for a 2d6 roll.

3.3.5 Normal (Gaussian) Distributions

The *normal* (or *Gaussian*) *distribution* is depicted in Figure 3.2. Unlike the distributions we have considered so far, it is continuous; but we won't worry about that right now. The shape of the distributions is a "bell curve", centered on some mean (or expected) value μ (equal to 0 in the plot) and with a standard deviation σ. The values of μ and σ can be any real numbers.

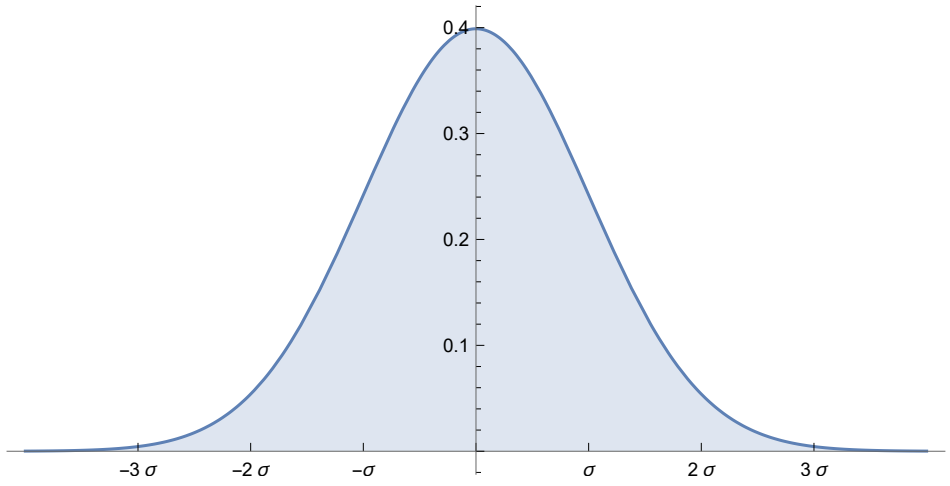

Figure 3.2: The normal (or Gaussian) distribution.

The *"68-95-99.7 rule"* tells us the fraction of outcomes which lie within 1, 2 and 3 standard deviations of the mean:

- Roughly 68% of the outcomes lie between -1σ and $+1\sigma$,
- Roughly 95% of outcomes lie between -2σ and $+2\sigma$,
- Roughly 99.7% of outcomes lie between -3σ and $+3\sigma$.

The normal distribution is the most common probability distribution you will encounter in this course, and in physics and math in general. The reason for that is that there is a theorem, the *central limit theorem*, which states that whenever we take the sum of independent random variables, the probability distribution of the sum will gradually start to look like a normal distribution. As we add more and more variables, the sum will get closer and closer to a normal distribution.

This can already be seen in the case of the die rolls. For a 1d6 roll we have a uniform distribution, as depicted in Figure 3.3. For a 2d6 roll, we get a triangular distribution centered at the mean value of 7, as depicted in Figure 3.4. When solving Exercise 3.59, you found that the probability for each possible combination of die rolls is $\frac{1}{6} \cdot \frac{1}{6} = \frac{1}{36}$, but as for the sum of the rolls, the outcomes 2 and 12 appear only once (corresponding to 1+1 and 6+6 respectively), while the outcome 7 appears six times (corresponding to 1+6, 2+5, 3+4, 4+3, 5+2, and 6+1) and thus has a probability of $6/36 = 1/6$, and so on.

For a 3d6 roll, the sum of three rolls of a 6-sided die, as depicted in Figure 3.5, we see that the probability distribution is starting to obtain the signature "bell" shape of the normal distribution. Its mean value is 10.5, as you can calculate (3×3.5). We will get closer and closer to a normal distribution as we increase the number of dice, that is, the n in nd6. In the limit $n \to \infty$, we will **precisely** obtain a normal distribution, but even for small values of n, the approximation is already close enough for most practical purposes.

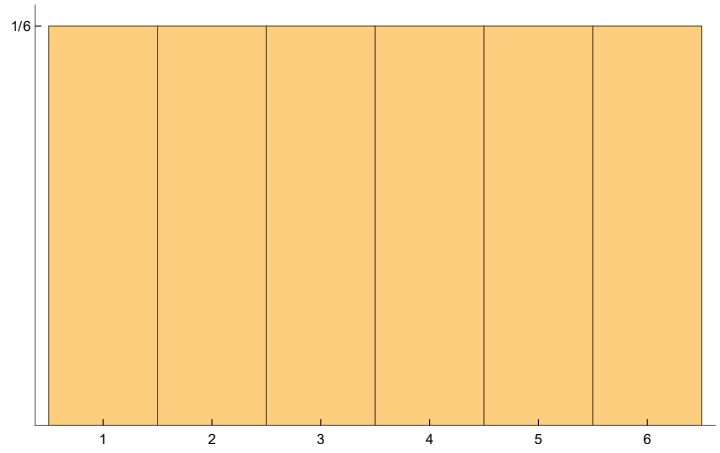

Figure 3.3: The distribution of results for one roll of a 6-sided die, also known as 1d6. It is a uniform distribution.

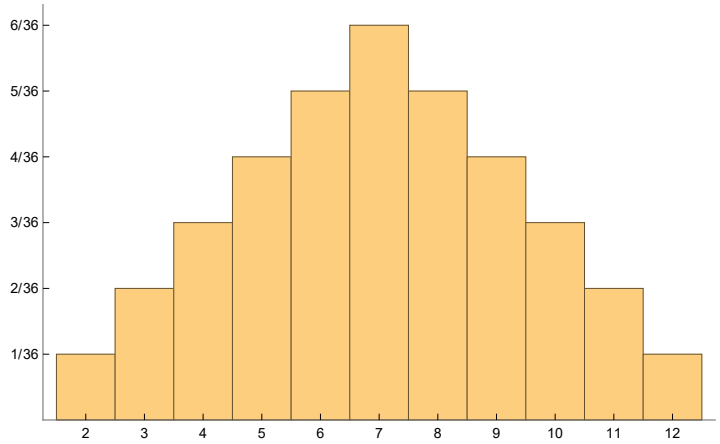

Figure 3.4: The distribution of results for the sum of two rolls of a 6-sided die, also known as 2d6. It is triangular.

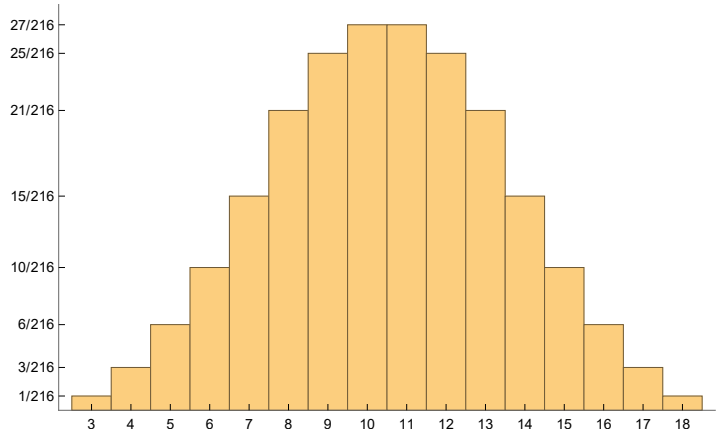

Figure 3.5: The distribution of results for the sum of three rolls of a 6-sided die, also known as 3d6. It is starting to obtain the "bell" shape of a normal distribution.

Exercise 3.64. Plot the probability distributions of the sum of n coin tosses, from $n = 1$ and up to a value of n large enough for the distribution to start looking like a normal distribution.

Problem 3.65. Write a computer program (I recommend using either Mathematica or Python) that will generate a plot of the probability distribution for an nds roll with an arbitrary number of rolls n and an arbitrary number of sides s (where $s = 2$ corresponds to a coin). It should also plot the continuous normal distribution (with the correct mean and standard deviation) over the discrete distribution, to check how closely they match. Generate some plots using your program, and use them to demonstrate the central limit theorem for different values of n and s.

Problem 3.66. A wizard can cast one of two spells on a dragon.

- For **Psychic Ray**, the dragon makes a saving throw: it rolls a d20, and if it gets 8 or higher, it succeeds. If the saving throw fails, the spell does 10d8 points of psychic damage. If the saving throw succeeds, the damage is reduced by 50%.
- For **Fiery Missile**, the wizard rolls a d20, and if the result is 9 or higher, the attack hits. If the attack misses, no damage will be done. If the attack hits, the spell will do 6d6+8d10 points of fire damage. However, the wizard is not sure if the dragon is resistant to fire or not; there is a probability of 30% that it is resistant, in which case the damage is reduced by 50%.

Which spell will do more damage on average?

4 The Foundations of Quantum Theory

Now that we have obtained the required mathematical tools, we can finally present quantum theory! This theory provides the correct fundamental framework for virtually all of known physics. We will see that its fundamental ingredients are Hilbert spaces with states and operators. These universal ingredients are then used to create particular models describing specific physical systems.

In this chapter, we will work exclusively with **discrete** quantum systems, which are based on **finite-dimensional** Hilbert spaces. These are much simpler than **continuous** quantum systems, which are based on **infinite-dimensional** Hilbert spaces. In particular, the math is much simpler – just linear algebra, without any calculus. However, it turns out that finite-dimensional Hilbert spaces are sufficient to define all of the fundamental concepts in quantum theory, and derive almost all of the most important results.

4.1 Axiomatic Definition

4.1.1 Dimensionless and Dimensionful Constants

Consider the *fine-structure constant*, which represents the strength of the electromagnetic interaction:

$$\alpha \approx 0.0073. \tag{4.1}$$

This constant is not specified in any particular units, such as meters or second; it is a **pure number**. We call such a constant *dimensionless*.

In contrast, some constants in physics are *dimensionful*. This means that their numerical value depends on the system of units we use. For example, the speed of light c has the following

values in different systems of units:

$$\begin{aligned} c &\approx 3.0 \times 10^8 \,\text{meters/second} \\ &\approx 1.1 \times 10^7 \,\text{miles/minute} \\ &\approx 170 \,\text{astronomical units/day} \\ &\approx 3.5 \times 10^{-5} \,\text{parsecs / hour} \\ &\approx 1 \,\text{light year / year.} \end{aligned}$$

What this means is that the numerical value of the speed of light does not have any physical meaning whatsoever[19]! It is merely a consequence of choosing to work with one system of units and not the other. But units are human constructs; the universe could not care less what units humans choose to measure things with. Therefore, none of the numbers written above have any actual meaning.

The numerical values of **dimensionless** constants are the only numbers that have a physical meaning, as they do not depend on the system of units. However, keep in mind that they are still, unavoidably, just parameters that are defined by humans in a certain way. There's nothing special about the number $\alpha \approx 0.0073$ itself; we could also define another parameter $\beta \equiv 2\alpha$ and use that in our equations instead. So don't try to do numerology[20] with the specific value of α! What is important here is not the numerical value itself, but the fact that it is independent of the choice of units.

For this reason, it is most natural to work in *Planck units*, where:

$$c = G = \hbar = \frac{1}{4\pi\varepsilon_0} = k_B = 1. \tag{4.2}$$

Here c is the speed of light, G is the *gravitational constant* used in Newtonian gravity, $\hbar$ is the *(reduced) Planck constant* used in quantum mechanics, $1/4\pi\varepsilon_0$ is the *Coulomb constant* used in electromagnetism, and k_B is the *Boltzmann constant* used in statistical mechanics.

All of these are **dimensionful** constants, which means we don't really care about their numerical values – so we might as well just set them to 1. This allows us to simply remove them from our equations. For example, instead of writing $\sqrt{\hbar G/c^3}$ – also known as the *Planck length* – we just write 1, and this allows us to write the equation $A = \hbar G\gamma\sqrt{j\,(j+1)}/c^3$ as $A = \gamma\sqrt{j\,(j+1)}$. Much simpler, right[21]?

Planck units are commonly used when doing research in theoretical physics, because they make equations simpler, more elegant, and less cluttered. However, sometimes we get numerical results that we wish to convert to real-world units such as kilograms and meters.

[19] Indeed, in modern SI units the speed of light is **defined** to be 299,792,458 meters per second, and this definition is used to measure the length of a meter – not the other way around.

[20] Interestingly, in the past some physicists tried to claim that α equals exactly $1/137$, but more precise measurements revealed that this is not actually the case. Still, you will often see it written as $1/137$ for that historical reason.

[21] This is the equation for the eigenvalues of the area operator in loop quantum gravity. We will learn about operators in the next section.

To do this, all we need to do is to find the combination of the constants in (4.2) that has the desired units. For example, if we know that our pure number represents length, then we can multiply it by the Planck length $\sqrt{\hbar G/c^3} \approx 1.6 \times 10^{-35}$ meters to find its value in meters.

Since this course is taught by a theorist, we will use Planck units exclusively. This means that unlike in a traditional quantum mechanics course, $\hbar$ will not appear in any of our equations!

Exercise 4.1. Calculate your age, height, mass, and body temperature in Planck units. For this, you will have to find combinations of the dimensionful constants we set to 1 in (4.2) that give you the desired units, as we did for the Planck length.

4.1.2 Hilbert Spaces, States, and Operators

Recall that in Section 3.2.2 we defined a Hilbert space as a vector space with an inner product that is also a complete metric space with respect to that inner product. Quantum theory can be defined **axiomatically** using the theory of Hilbert spaces. In this chapter we will list a total of seven fundamental axioms, plus an eighth axiom that may or may not be fundamental.

The System Axiom: A *system* in quantum theory is the mathematical representation of a physical system (such as a particle) as a Hilbert space. The type and dimension of the Hilbert space will depend on the particular system. Note that the dimension of the Hilbert space is **unrelated** to the dimension of spacetime.

In the finite-dimensional case, for example when the system involves spin, the Hilbert space will usually be $\mathbb{C}^n$ for some n, such as $\mathbb{C}^2$, which was used in most of the examples above and will continue to be used below. In the infinite-dimensional case, for example when the system involves position and momentum (which are, in general, continuous and not discrete) the Hilbert space it will usually be a space of functions, which is much more complicated.

The State Axiom: A *state* of a quantum system is a vector with unit norm in the system's Hilbert space, that is, a vector $|\Psi\rangle$ which satisfies

$$\||\Psi\rangle\| = \sqrt{\langle\Psi|\Psi\rangle} = 1. \tag{4.3}$$

States represent the different configurations the system can have. It is important to stress that **only** unit vectors can represent states. If for some reason we have a vector with non-unit norm, we must normalize it (divide it by its norm) to obtain a unit vector, which can then represent a state.

Another important aspect of states is that they are only defined **up to a complex phase**. This means that, if the vector $|\Psi\rangle$ represents a state, then all vectors of the form $e^{i\phi}|\Psi\rangle$ for $\phi \in \mathbb{R}$ represent the **same**[22] state as $|\Psi\rangle$. Note that adding a phase to a vector does not change the

[22] Actually, the more precise definition is that a state is a *ray* in a Hilbert space. Rays are defined as *equivalence classes* of vectors such that a vector $|\Psi\rangle$ is equivalent to $\lambda|\Psi\rangle$ for any scalar $\lambda \in \mathbb{C}$. The scalar can be separated into a polar representation, $\lambda = re^{i\phi}$, as we discussed in Section 3.1.4. The r part stretches the magnitude of the vector by a factor of r, and the $e^{i\phi}$ part (the phase) rotates it by ϕ radians. Any vector in the same equivalence class represents the **same** state, so multiplying the vector by a scalar will not change the state it represents, whatever

norm, since

$$\left\|e^{i\phi}\Psi\right\| = \sqrt{\left(e^{i\phi}|\Psi\rangle\right)^{\dagger} e^{i\phi}|\Psi\rangle} = \sqrt{\langle\Psi| e^{-i\phi} e^{i\phi}|\Psi\rangle} = \sqrt{\langle\Psi|\Psi\rangle} = \|\Psi\|. \tag{4.4}$$

The Operator Axiom: An *operator* on a Hilbert space is a linear transformation which takes a vector and outputs another vector. By "linear" we mean that the operator A satisfies

$$A\left(|\Psi\rangle + |\Phi\rangle\right) = A|\Psi\rangle + A|\Phi\rangle, \qquad A\left(\lambda|\Psi\rangle\right) = \lambda A|\Psi\rangle, \tag{4.5}$$

where $|\Psi\rangle$ and $|\Phi\rangle$ are vectors and λ is a scalar. In the discrete case, operators are just matrices on $\mathbb{C}^n$. In the continuous case, where the vectors are actually functions, the operators will be derivatives acting on the functions[23]. In quantum theory, operators transform states into other states, and they represent an action performed on the system, such as a measurement, a transformation, or an evolution in time.

4.1.3 Hermitian Operators and Observables

An operator corresponding to a Hermitian matrix[24] is a *Hermitian operator*. Above you have proved some interesting properties of these operators. In particular, their eigenvalues are real, and there is an orthonormal basis consisting of their eigenvectors (a.k.a. an eigenbasis).

The Observable Axiom: In quantum theory, Hermitian operators correspond to *observables*, that is, properties of the system that can be measured. The eigenvalues of these operators, which are real as for all Hermitian operators, exactly correspond to all the different possible outcomes of the measurement. The mapping is one-to-one and onto (a.k.a. a *bijection*), meaning that each eigenvalue corresponds to exactly one measurement outcome and vice versa. This makes sense because we always measure real numbers; there are no measurement devices that measure complex numbers!

Examples of observables are position, momentum, angular momentum, energy, and spin (which is intrinsic angular momentum, as we learned in Section 2.1.4). All of these may be represented as Hermitian operators on an appropriate Hilbert space.

4.1.4 Probability Amplitudes

Let the state of a quantum system be $|\Psi\rangle$. Once we have chosen a Hermitian operator to represent our observable, we may obtain an orthonormal basis of states $|B_i\rangle$ corresponding

the magnitude and phase are. However, it is conventional to choose states to be represented specifically by a unit vector from the equivalence class, since otherwise we would have to normalize vectors to 1 all the time. This is also the reason we only use orthonormal bases in quantum theory.

[23] In it interesting to note that there is often still a sense in which operators and states in a continuous Hilbert space have the equivalent of indices and elements. You will learn about this in more advanced courses on quantum mechanics, especially quantum field theory.

[24] In an infinite-dimensional Hilbert space, where we don't necessarily have a matrix representation, a Hermitian operator is defined using the property that it is self-adjoint.

to the eigenvectors of that operator. In quantum mechanics, these eigenvectors are called *eigenstates*.

The Probability Axiom: The inner product $\langle B_i|\Psi\rangle$ is called the *probability amplitude* to measure the eigenvalue λ_i corresponding to the eigenstate $|B_i\rangle$, given the state $|\Psi\rangle$. When we take the magnitude-squared of a probability amplitude, we get the corresponding probability. Thus

$$|\langle B_i|\Psi\rangle|^2 \tag{4.6}$$

is the probability to measure the eigenvalue λ_i corresponding to the eigenstate $|B_i\rangle$, given the state $|\Psi\rangle$. This is also known as the *Born rule*.

The first four axioms that we presented here simply defined the meaning of systems, states, operators, and observables in mathematical terms. The Probability Axiom, on the other hand, has to do with the relations between these mathematical structures. One can thus justifiably ask: why would this be a probability in the first place?

Unfortunately, since this is an axiom, it cannot be derived from anything more fundamental, such as other axioms. However, at the very least, we can verify that it indeed behaves exactly like a probability is expected to. This follows from the fact that

$$\begin{aligned}
\sum_{i=1}^{n} |\langle B_i|\Psi\rangle|^2 &= \sum_{i=1}^{n} \langle B_i|\Psi\rangle^* \langle B_i|\Psi\rangle \\
&= \sum_{i=1}^{n} \langle\Psi|B_i\rangle\langle B_i|\Psi\rangle \\
&= \langle\Psi| \left(\sum_{i=1}^{n} |B_i\rangle\langle B_i| \right) |\Psi\rangle \\
&= \langle\Psi|\Psi\rangle \\
&= 1,
\end{aligned}$$

where we used the following:

- Taking the complex conjugate of an inner product switches the order of the vectors,
- The completeness relation (3.81),
- All quantum states have a norm (and thus also norm-squared) of 1.

What does this mean? The number $|\langle B_i|\Psi\rangle|^2$ for each value of i from 1 to n corresponds to each of the n possible outcomes of a measurement. We know that it must be non-negative, because it is a magnitude of a complex number. Also, when taking the sum of all such numbers, we get 1. In other words, the numbers $|\langle B_i|\Psi\rangle|^2$ behave like probabilities: they are real numbers between 0 and 1, which always sum to 1. Why they actually represent probabilities is a question that has no good answer except that this is just how quantum theory works, and it can be verified experimentally.

One might wonder why we bothered mentioning the probability amplitudes $\langle B_i|\Psi\rangle$, which are complex numbers, instead of just directly calculating the probabilities $|\langle B_i|\Psi\rangle|^2$. It turns out that the fact that probability amplitudes are complex numbers is an essential part of what makes quantum mechanics different from classical mechanics. In fact, you can even think of quantum mechanics as a generalization of classical probability theory where probabilities are allowed to be complex numbers.

We could write down a classical theory which assigns probabilities to each measurement outcome; but since probabilities must be real non-negative numbers, when they are added the result is always a higher probability. Therefore, classical probabilities interfere only **constructively**. In quantum theory, on the other hand, one does not add probabilities, but probability amplitudes; and as we will see, they can interfere with one another both constructively **and** destructively, just as we discussed in Section 2.1.3.

If the probability amplitudes for two events have opposite complex phases (for example, one is positive and one is negative) they can even cancel each other out completely – so that neither event happens, since their total probability amplitude (and thus also probability) is zero! This, of course, can never happen with classical probability.

Exercise 4.2. In the Hilbert space $\mathbb{C}^2$, consider the Hermitian operator

$$\sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{4.7}$$

Find its eigenstates (make sure they are normalized to 1!) and eigenvalues. Then, calculate the probability to measure each of the eigenvalues given that the system is in the state

$$|\Psi\rangle \equiv \frac{1}{\sqrt{10}} \begin{pmatrix} 1 \\ 3 \end{pmatrix}. \tag{4.8}$$

Verify that the probabilities sum to 1.

4.1.5 Superposition

Consider an observable represented by a Hermitian operator with an orthonormal basis of eigenstates $|B_i\rangle$. As with any basis, we may write the state vector $|\Psi\rangle$ as a linear combination of the basis eigenstates $|B_i\rangle$:

$$|\Psi\rangle = \sum_{i=1}^{n} |B_i\rangle\langle B_i|\Psi\rangle. \tag{4.9}$$

Remember that each coefficient $\langle B_i|\Psi\rangle$ is the probability amplitude to measure the eigenvalue corresponding to the eigenstate $|B_i\rangle$ given that the system is in the state $|\Psi\rangle$. So this is a sum over the basis states $|B_i\rangle$, corresponding to the possible measurement outcomes, with a probability amplitude attached to each of these outcomes, which depends on the state $|\Psi\rangle$.

Such a linear combination of states[25] is called a *superposition*.

The concept of superposition is responsible for many of the weird properties of quantum mechanics, as we will soon see. Importantly, superposition is **not** an axiom, but simply an (almost trivial) mathematical property of vectors in Hilbert spaces. This means that superposition follows automatically from the previous axioms; it is not something that needs to be introduced separately.

You will often hear people (including physicists, if they are being sloppy) say that superposition means that "the system is in multiple states at the same time". For example, it is frequently said about particles – which can be in a superposition of eigenstates corresponding to different outcomes for the measurement of their position – that "the particle is in multiple places at the same time". However, this is a common misconception – or at the very least, an overly literal interpretation of the math.

The fact that a state $|\Psi\rangle$ can be written in a superposition of eigenstates $|B_i\rangle$ doesn't mean that the system is actually "in" all of these different states at once. The system is, in fact, in only **one** state: the state $|\Psi\rangle$. This state can be represented in the eigenbasis $|B_i\rangle$, and doing this reveals the probability to measure each of the eigenvalues. However, one can always find[26] an orthonormal basis where $|\Psi\rangle$ itself is one of the basis states – and often, this can be an eigenbasis corresponding to another observable of the system. In that basis, the system will **not** be in a superposition – it will just be in the state $|\Psi\rangle$, with a probability amplitude of $\langle\Psi|\Psi\rangle = 1$!

So instead of saying that "the system is in all of the states $|B_1\rangle, \ldots, |B_n\rangle$ at once", it is more precise to say that the system is currently in the state $|\Psi\rangle$, and a measurement of the observable with the eigenbasis $|B_i\rangle$ could yield different outcomes, with the probability amplitude for outcome number i given by the *projection*[27] of $|\Psi\rangle$ on $|B_i\rangle$, calculated by taking the inner product $\langle B_i|\Psi\rangle$. It sounds less cool and mysterious, but it is more accurate and less prone to confusion and misinterpretation.

Of course, this description is too technical for the average person, which is why physicists usually choose to just say, incorrectly, that "the system is in multiple states at the same time". But now that you actually know the math of quantum theory, you should be able to understand the correct definition of superposition! I will let you digest all of this for now, and in Section 4.2.4 we will discuss an analogy, using a concrete quantum system, that should help you understand this better.

Exercise 4.3. Consider again the Hermitian operator from Exercise 4.2,

$$\sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{4.10}$$

[25] More generally, a superposition is any linear combination of states. The states don't have to be basis eigenstates and the coefficients don't have to be probability amplitudes – but they usually are.

[26] Using the Gram-Schmidt process mentioned in Footnote 15.

[27] In $\mathbb{R}^n$, the projection of $\mathbf{v}$ on $\mathbf{w}$ (or $\mathbf{w}$ on $\mathbf{v}$) is given by the dot product $\mathbf{v} \cdot \mathbf{w}$. Projections in $\mathbb{C}^n$ generalize this concept, with the inner product replacing the dot product.

Write down an example of a state $|\Psi\rangle$ which corresponds to a probability of $1/3$ to measure the eigenvalue $+1$ and a probability of $2/3$ to measure the eigenvalue -1.

Exercise 4.4. A quantum system described by the Hilbert space $\mathbb{C}^3$ has an observable corresponding to a Hermitian operator A with the matrix representation

$$A \equiv \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix}. \tag{4.11}$$

A. Find its eigenvalues and their corresponding eigenstates. Make sure the states are normalized to 1.

B. Find three **different** states such that a measurement of the observable A will produce the lowest eigenvalue with probability $1/7$, the highest eigenvalue with probability $2/7$, and the middle eigenvalue with probability $4/7$. When we say different states, we mean that the vectors that represent them cannot be scalar multiples of each other; recall from Footnote 22 that such vectors are in the same equivalence class, and thus represent the same state. Make sure the states are normalized to 1.

C. Write the state

$$|\Psi\rangle \equiv \frac{1}{\sqrt{15}} \begin{pmatrix} 1 \\ -2 \\ 3 - \mathrm{i} \end{pmatrix} \tag{4.12}$$

as a superposition of eigenstates of A, and calculate the probabilities to measure each eigenvalue of A given that the system is in the state $|\Psi\rangle$. Verify that the probabilities sum to 1.

4.1.6 Inner Products with Matrices, and the Expectation Value

Consider a Hermitian operator A with an orthonormal basis of n eigenstates $|B_i\rangle$ and n eigenvalues λ_i. To remind you, this means that

$$A\,|B_i\rangle = \lambda_i\,|B_i\rangle\,, \qquad \langle B_i|B_j\rangle = \delta_{ij}, \tag{4.13}$$

where δ_{ij} is the Kronecker delta, which we defined in (3.53):

$$\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j, \\ 1 & \text{if } i = j. \end{cases} \tag{4.14}$$

Then we have, for any $i, j \in \{1, \ldots, n\}$:

$$\begin{aligned}\langle B_i|A|B_j\rangle &= \langle B_i|\left(A|B_j\rangle\right)\\ &= \langle B_i|\lambda_j|B_j\rangle\\ &= \lambda_j\langle B_i|B_j\rangle\\ &= \lambda_j\delta_{ij}.\end{aligned}$$

Let us also recall the completeness relation (3.81):

$$\sum_{i=1}^{n}|B_i\rangle\langle B_i| = 1. \tag{4.15}$$

Now, let $|\Psi\rangle$ be the state of the system. Then:

$$\begin{aligned}\langle\Psi|A|\Psi\rangle &= \langle\Psi|\left(\sum_{i=1}^{n}|B_i\rangle\langle B_i|\right)A\left(\sum_{j=1}^{n}|B_j\rangle\langle B_j|\right)|\Psi\rangle\\ &= \sum_{i=1}^{n}\sum_{j=1}^{n}\langle\Psi|B_i\rangle\langle B_i|A|B_j\rangle\langle B_j|\Psi\rangle\\ &= \sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_j\delta_{ij}\langle\Psi|B_i\rangle\langle B_j|\Psi\rangle.\end{aligned}$$

When taking the sum over j, the Kronecker delta δ_{ij} is always 0 except when $j = i$. Therefore the sum over j always reduces to just one element, the one where $j = i$. We get:

$$\begin{aligned}\langle\Psi|A|\Psi\rangle &= \sum_{i=1}^{n}\lambda_i\langle\Psi|B_i\rangle\langle B_i|\Psi\rangle\\ &= \sum_{i=1}^{n}\lambda_i\langle\Psi|B_i\rangle\langle\Psi|B_i\rangle^*\\ &= \sum_{i=1}^{n}\lambda_i\left|\langle\Psi|B_i\rangle\right|^2,\end{aligned}$$

where in the second line we used the fact that switching the order of the vectors in the inner product is equivalent to taking the complex conjugate.

Recall that $|\langle\Psi|B_i\rangle|^2$ is the probability to measure the eigenvalue λ_i associated with the eigenstate $|B_i\rangle$ given the state $|\Psi\rangle$. Therefore, this is a sum of the possible values of the measurement of A, weighted by their probabilities. But this exactly the expected value for the measurement of A, as we defined in (3.174). For this reason, we sometimes simply write $\langle A\rangle$ (the usual notation for the expected value) instead of $\langle\Psi|A|\Psi\rangle$, as long as it is clear that the expected value is taken with respect to the state $|\Psi\rangle$. If we want to specify the state explicitly, we can also use the notation

$$\langle A\rangle_\Psi \equiv \langle\Psi|A|\Psi\rangle. \tag{4.16}$$

Note that the terms "expected value" and "expectation value" are often used interchangeably, but the former seems to be more popular in classical probability theory while the latter is more popular in quantum theory.

Exercise 4.5. Calculate $\langle A \rangle_\Psi$ where

$$A \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{4.17}$$

for the following three states:

$$|\Psi_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \tag{4.18}$$

$$|\Psi_2\rangle = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \tag{4.19}$$

$$|\Psi_3\rangle = \frac{1}{\sqrt{13}} \begin{pmatrix} 3 \\ 2 \end{pmatrix}. \tag{4.20}$$

Exercise 4.6. Calculate $\langle A \rangle_\Psi$ for A and $|\Psi\rangle$ as defined in Exercise 4.4:

$$A \equiv \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \qquad |\Psi\rangle \equiv \frac{1}{\sqrt{15}} \begin{pmatrix} 1 \\ -2 \\ 3 - \mathrm{i} \end{pmatrix}. \tag{4.21}$$

Then, calculate the expected value explicitly as defined in (3.174), using the probabilities you calculated in part (C) of Exercise 4.4, and verify that you get the same result.

4.1.7 Summary For Discrete Systems

To summarize, here are the axioms of quantum theory we formulated so far. Here we formulate them specifically for discrete systems with finite-dimensional Hilbert spaces:

1. **The System Axiom:** Discrete physical systems are represented by complex n-dimensional Hilbert spaces $\mathbb{C}^n$, where n depends on the specific system.

2. **The State Axiom:** The states of the system are represented by unit n-vectors in the system's Hilbert space, up to a complex phase.

3. **The Operator Axiom:** The operators on the system, which act on states to produce other states, are represented by $n \times n$ matrices in the system's Hilbert space.

4. **The Observable Axiom:** Physical observables in the system are represented by Hermitian operators on the system's Hilbert space. The eigenvalues of the observable (which are always real, since it's Hermitian) represent its possible measured values.

The eigenstates of the observable can be used to form an orthonormal eigenbasis of the Hilbert space.

5. **The Probability Axiom:** For any observable, the probability amplitude to measure the eigenvalue corresponding to the eigenstate $|B_i\rangle$, given that the system is in the state $|\Psi\rangle$, is the inner product $\langle B_i|\Psi\rangle$. The probability is given by the magnitude squared of the amplitude, $|\langle B_i|\Psi\rangle|^2$.

We also discussed two important consequences of these axioms:

- **Superposition:** Any state $|\Psi\rangle$ can be written as a linear combination of the eigenstates $|B_i\rangle$ of an observable, with the probability amplitudes $\langle B_i|\Psi\rangle$ as coefficients:

$$|\Psi\rangle = \sum_{i=1}^{n} |B_i\rangle\langle B_i|\Psi\rangle. \tag{4.22}$$

- **Expectation Value:** If the system is in the state $|\Psi\rangle$, the expectation value for the measurement of the observable A is given by $\langle\Psi|A|\Psi\rangle$.

There are some more axioms that we will add later, but first let us discuss a concrete example of a physical quantum systems and see these axioms in action.

Problem 4.7. Are these axioms enough to actually do physics? If not, what do you think is missing and why?

4.2 Two-State Systems, Spin $1/2$, and Qubits

So far in this chapter, we discussed quantum theory in an abstract way. However, a theory of physics is useless without a concrete mapping between the theory and reality. The simplest non-trivial[28] quantum system is described by a 2-dimensional Hilbert space, and is thus called a *two-state system*. All such system can also be used as *qubits*, or quantum bits – where one state (doesn't matter which one) corresponds to 0 and the other state corresponds to 1. Let us now describe such systems in detail.

4.2.1 The Pauli Matrices

Let us introduce the *Pauli matrices*:

$$\sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y \equiv \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4.23}$$

As the notation suggests, each matrix is associated with a spatial axis: x, y, and z. These three matrices have the following properties (here i stands for x, y, or z):

[28] 1-dimensional Hilbert spaces are of course simpler, but they are trivial, since there is only one state the system can be in, with probability 1.

- They are Hermitian: $\sigma_i^\dagger = \sigma_i$. This means they can represent observables.
- They are unitary: $\sigma_i^\dagger = \sigma_i^{-1}$. This means they can represent transformations.
  - Since they are both Hermitian and unitary, they are their own inverse: $\sigma_i = \sigma_i^\dagger = \sigma_i^{-1}$. This means that $\sigma_i^2 = 1$. A matrix which is its own inverse is called *involutory*.
- They have two eigenvalues: $+1$ and -1.
  - The eigenstates of σ_x are:

$$|+x\rangle \equiv |+\rangle \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad |-x\rangle \equiv |-\rangle \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{4.24}$$

  - The eigenstates of σ_y are:

$$|+y\rangle \equiv |+\mathrm{i}\rangle \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \mathrm{i} \end{pmatrix}, \qquad |-y\rangle \equiv |-\mathrm{i}\rangle \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix}. \tag{4.25}$$

  - The eigenstates of σ_z are:

$$|+z\rangle \equiv |0\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |-z\rangle \equiv |1\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{4.26}$$

    where, confusingly, $|0\rangle$ corresponds to the eigenvalue $+1$ and $|1\rangle$ corresponds to the eigenvalue -1 (but that is the standard convention).
- Since the Pauli matrices are normal, the eigenstates of each matrix form an orthonormal eigenbasis of $\mathbb{C}^2$. As you can see, the eigenstates of σ_z are just the standard basis.
- The eigenstates of σ_x and σ_z are related to each other as follows:

$$|+\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle + |1\rangle\right), \qquad |-\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle - |1\rangle\right), \tag{4.27}$$

$$|0\rangle = \frac{1}{\sqrt{2}} \left(|+\rangle + |-\rangle\right), \qquad |1\rangle = \frac{1}{\sqrt{2}} \left(|+\rangle - |-\rangle\right). \tag{4.28}$$

- A useful mnemonic is as follows: for each n, the state $|n\rangle$ has the number n in the bottom component (excluding the factor of $1/\sqrt{2}$ if it exists). So the states $|\pm\rangle$ have ± 1 in the bottom component, the states $|\pm \mathrm{i}\rangle$ have $\pm \mathrm{i}$ in the bottom component, and the states $|0\rangle$ and $|1\rangle$ have 0 and 1 in the bottom component respectively.

Problem 4.8. Prove that σ_x, σ_y and σ_z are Hermitian.

Problem 4.9. Prove that σ_x, σ_y and σ_z are unitary.

Problem 4.10. Consider the real vector space of 2×2 Hermitian matrices. This is a vector space where **the vectors are Hermitian matrices** and the scalars are real numbers. Don't get confused: in an **abstract** vector space, anything can be a "vector" – including numbers, matrices, tensors of higher rank, functions, and even weirder stuff.

A. Show that the real vector space of 2×2 Hermitian matrices satisfies all of the conditions in our definition of a vector space in Section 3.2.1.

B. Show that the set $\{1, \sigma_x, \sigma_y, \sigma_z\}$, composed of the identity matrix 1 and the three Pauli matrices, is a basis of the real vector space of 2×2 Hermitian matrices. (Since we haven't defined an inner product on this space, you don't need to show that the basis is orthonormal.)

4.2.2 Spin $1/2$

Recall that in Section 2.1.4 we saw that, in the Stern-Gerlach experiment, the measurement of angular momentum of a particle had only one of two discrete results: "spin up" (if the particle is deflected up) or "spin down" (if the particle is deflected down).

More generally, in quantum theory, every particle has a property called *spin*, which is a half-integer s:

$$s \in \left\{0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots\right\}. \tag{4.29}$$

The measurement of intrinsic angular momentum of a particle of spin s, in any direction, always returns one of the results in the set

$$\{-s, -s+1, \ldots, s-1, s\}. \tag{4.30}$$

Note that this set always contains $2s+1$ values. Thus:

- A particle of spin 0 always has intrinsic angular momentum 0;
- A particle of spin $1/2$ has intrinsic angular momentum $-1/2$ or $+1/2$;
- A particle of spin 1 has intrinsic angular momentum -1, 0, or $+1$;
- A particle of spin $3/2$ has intrinsic angular momentum $-3/2$, $-1/2$, $+1/2$, or $+3/2$;
- and so on.

The particles in the Stern-Gerlach experiment have spin $1/2$, where "spin up" corresponds to intrinsic angular momentum $+1/2$ and "spin down" corresponds to $-1/2$. Since these particles have exactly two possible states, spin up and down, they can be represented as a two-state quantum system.

The Pauli matrix σ_i is a Hermitian operator, and thus it should correspond to an observable. That observable is **twice** the spin in the i direction, since the Pauli matrices have eigenvalues

± 1, but the spin should be $\pm 1/2$. It is thus customary to define

$$S_x \equiv \frac{1}{2}\sigma_x, \qquad S_y \equiv \frac{1}{2}\sigma_y, \qquad S_z \equiv \frac{1}{2}\sigma_z, \tag{4.31}$$

such that S_i is a Hermitian operator corresponding to spin $\pm 1/2$ along the i direction. You can check that S_i have the same eigenstates as σ_i, but they correspond to the eigenvalues $\pm 1/2$ instead of ± 1.

In Problem 4.10 you proved that the set $\{1, \sigma_x, \sigma_y, \sigma_z\}$ forms a basis for the real vector space of 2×2 Hermitian matrices. This means that any Hermitian operator on the Hilbert space $\mathbb{C}^2$ can be written as a linear combination of these 4 matrices. Since Hermitian operators correspond to observables, this means that **every possible observable** in $\mathbb{C}^2$ can be written in terms of the Pauli matrices and the identity matrix.

In particular, given a unit vector $\mathbf{v} \in \mathbb{R}^3$ pointing in an arbitrary direction in space (the real space, not the Hilbert space!)

$$\mathbf{v} \equiv (x, y, z), \qquad \sqrt{x^2 + y^2 + z^2} = 1, \tag{4.32}$$

we can represent the measurement of intrinsic angular momentum along that direction as the Hermitian operator (on the Hilbert space, $\mathbb{C}^2$)

$$S_{\mathbf{v}} \equiv xS_x + yS_y + zS_z = \frac{1}{2}\begin{pmatrix} z & x - \mathrm{i}\, y \\ x + \mathrm{i}\, y & -z \end{pmatrix}, \tag{4.33}$$

which has the spin up and spin down eigenstates

$$|\uparrow\rangle \equiv \frac{1}{\sqrt{2\,(1+z)}}\begin{pmatrix} 1+z \\ x + \mathrm{i}\, y \end{pmatrix}, \qquad |\downarrow\rangle \equiv \frac{1}{\sqrt{2\,(1-z)}}\begin{pmatrix} 1-z \\ -x - \mathrm{i}\, y \end{pmatrix}. \tag{4.34}$$

So we learn that, for a spin $1/2$ particle, the measurement of intrinsic angular momentum along **any** direction in space always yields one of exactly two possible results – spin up, $+1/2$, or spin down, $-1/2$ – with the probability amplitudes calculated using the Hermitian operator $S_{\mathbf{v}}$.

Exercise 4.11. Show that the eigenstates $|\uparrow\rangle$ and $|\downarrow\rangle$ indeed correspond to the eigenstates of S_x, S_y, and S_z – except the state $|1\rangle$ (the $-1/2$ eigenstate of S_z), which results in a division by zero in the bottom component.

Exercise 4.12. A spin-$1/2$ particle is in the state

$$|\Psi\rangle \equiv \frac{1}{\sqrt{10}}\begin{pmatrix} 1 \\ 3 \end{pmatrix}. \tag{4.35}$$

A. What are the probabilities to measure spin up or down in the x direction?

B. What are the probabilities to measure spin up or down in the y direction?

C. What are the probabilities to measure spin up or down in the z direction?

D. What are the probabilities to measure spin up or down in the direction of the unit vector $\left(\frac{1}{3}, \frac{2}{3}, \frac{2}{3}\right)$?

E. What are the expectation values for a measurement of spin in each of the directions specified in (A)–(D)? (Make sure you are using S_i and not σ_i for this calculation!)

Problem 4.13.

A. Let us define the *matrix commutator* (or *operator commutator*):

$$[A, B] \equiv AB - BA. \tag{4.36}$$

*S*how that the spin-1/2 operators S_i have the *commutation relations*:

$$\left[S_x, S_y\right] = \mathrm{i}\, S_z, \qquad \left[S_y, S_z\right] = \mathrm{i}\, S_x, \qquad \left[S_z, S_x\right] = \mathrm{i}\, S_y. \tag{4.37}$$

B. Show that the commutation relations (4.37) can be written compactly as

$$\left[S_i, S_j\right] = \mathrm{i} \sum_{k=1}^{3} \epsilon_{ij}{}^{k} S_k, \tag{4.38}$$

where the indices i, j, k take the values $\{1, 2, 3\}$ corresponding to $\{x, y, z\}$, and $\epsilon_{ij}{}^{k}$ is the *Levi-Civita symbol*, defined as

$$\epsilon_{ij}{}^{k} \equiv \begin{cases} +1 & \text{if } (i, j, k) \text{ is an even permutation of } (1, 2, 3)\,, \\ -1 & \text{if } (i, j, k) \text{ is an odd permutation of } (1, 2, 3)\,, \\ 0 & \text{otherwise.} \end{cases} \tag{4.39}$$

By *even permutation* or *odd permutation* we mean that the permutation involves exchanging elements an even or odd number of times. For example, $(1, 3, 2)$ is an odd permutation, because we exchanged elements once: $2 \leftrightarrow 3$. However, $(3, 1, 2)$ is an even permutation, because we exchanged elements twice: $2 \leftrightarrow 3$ and then $1 \leftrightarrow 3$.

C. The *matrix anti-commutator* (or *operator anti-commutator*) is defined as follows:

$$\{A, B\} \equiv AB + BA. \tag{4.40}$$

Show that the spin-1/2 operators S_i have the *anti-commutation relation*

$$\left\{S_i, S_j\right\} = \frac{1}{2}\delta_{ij}, \tag{4.41}$$

where δ_{ij} is the Kronecker delta (times the identity matrix 1).

4.2.3 Qubits

A *classical bit* can be in one of two states: 0 or 1. A *quantum bit*, or *qubit* for short, is instead in a **superposition** of two states, denoted $|0\rangle$ and $|1\rangle$:

$$|\Psi\rangle = a\,|0\rangle + b\,|1\rangle\,, \qquad |a|^2 + |b|^2 = 1, \tag{4.42}$$

where $a, b \in \mathbb{C}$ are the probability amplitudes:

$$a \equiv \langle 0|\Psi\rangle, \qquad b \equiv \langle 1|\Psi\rangle. \tag{4.43}$$

Since the system has two states, it can be represented by the Hilbert space $\mathbb{C}^2$, and it is conventional to choose $|0\rangle$ and $|1\rangle$ to be the vectors in the standard basis, which in this case is called the *computational basis*:

$$|0\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |1\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{4.44}$$

Any two-state quantum system can serve as a qubit. In fact, even systems with more than two states can be used, as long as two of these states can be decoupled (separated) from the rest. Some examples include:

- Any spin 1/2 particle, such as an electron, where $|0\rangle$ and $|1\rangle$ are the eigenstates of the spin operator along the z direction, S_z, so they represent spin up and spin down, respectively, along that direction.
- The number of particles (doesn't matter what kind of particles) in a system, where $|0\rangle$ corresponds to a state with no particles (a *vacuum*) and $|1\rangle$ corresponds to a state with exactly one particle.
- The *polarization* of a photon, where $|0\rangle$ is horizontal and $|1\rangle$ is vertical polarization. (In classical electromagnetism, an electromagnetic wave is composed of oscillating electric and magnetic fields, and the polarization is the direction of the electric field.)

Qubits are used in quantum computers as the basic units of computations, just like bits in classical computers. Since so many different systems can be represented mathematically in the same way, we can build quantum computers in many different ways. We will discuss quantum computers (from the theoretical point of view) in more details later.

4.2.4 The Meaning of Superposition

In Section 4.1.5 we discussed the concept of superposition, and we emphasized that it is inaccurate to describe a system in a superposition of two states as being "in both states at once". Similarly, it is a common misconception that quantum computers are powerful because

qubits, which are in a superposition of $|0\rangle$ and $|1\rangle$, and in some way "both 0 and 1 at the same time" and this allows the quantum computer to "calculate all the possibilities at once". That would have been awesome, but unfortunately that is **not** how quantum computers work! We will see how they really work later in this course.

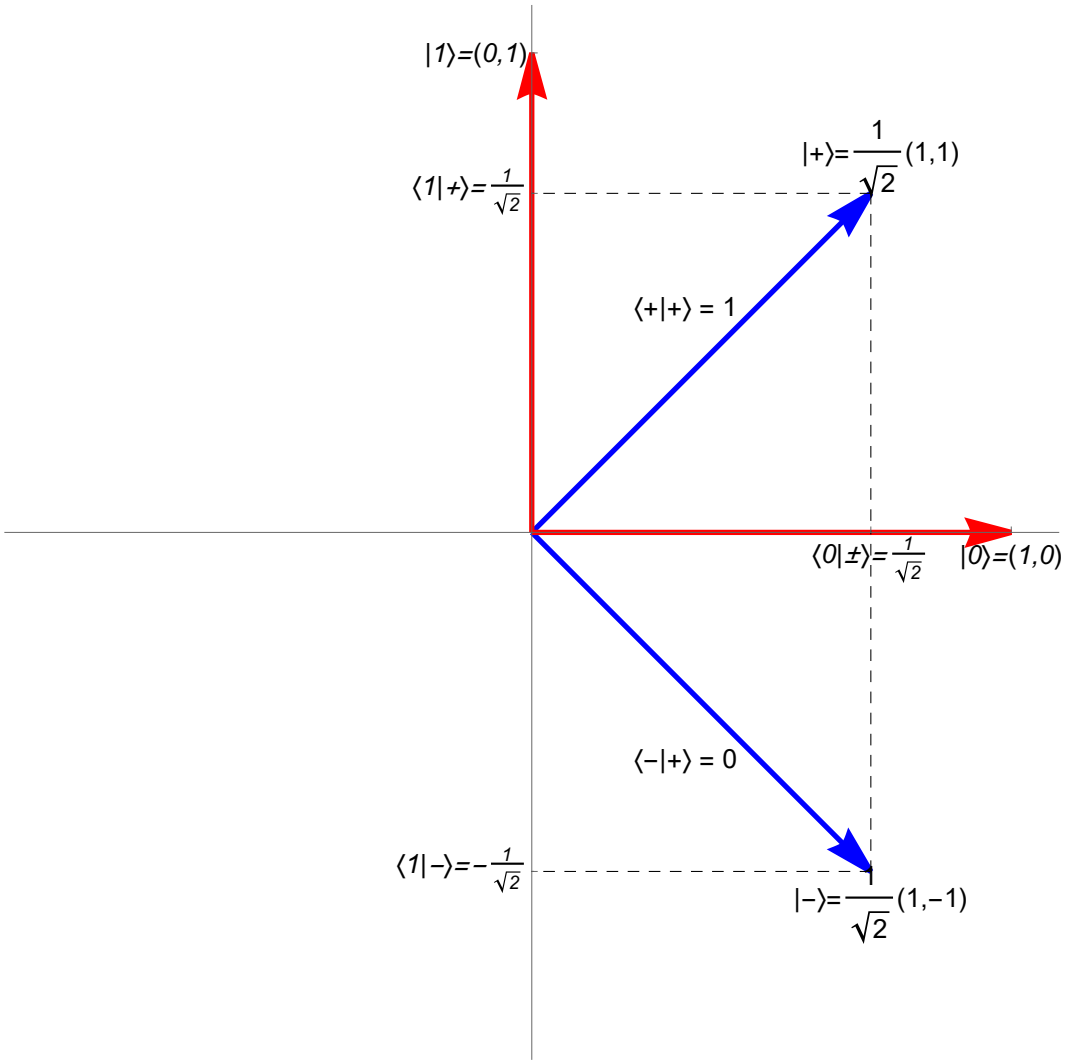

Figure 4.1: The eigenbasis $\{|0\rangle, |1\rangle\}$, in red, and the eigenbasis $\{|+\rangle, |1\rangle\}$, in blue. A qubit in the state $|+\rangle$ is in a superposition of $|0\rangle$ and $|1\rangle$, but this does not mean it is in the states $|0\rangle$ and $|1\rangle$ "at the same time" – it is only in one state, $|1\rangle$.

Now that we are familiar with a concrete quantum system, we can use it to illustrate further the meaning of superposition. Let us consider, as a simple example, a qubit in the state $|+\rangle$ (the eigenstate of spin $+1/2$ in the x direction):

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = \frac{1}{\sqrt{2}}\left(\begin{pmatrix}1\\0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\right) = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}. \tag{4.45}$$

For simplicity, let us forget for a second that we are dealing with complex vectors, and imagine that they are vectors in $\mathbb{R}^2$, since that is much easier to visualize; see Figure 4.1. As vectors in $\mathbb{R}^2$, the state $|0\rangle = (1, 0)$ points east and the eigenstate $|1\rangle = (0, 1)$ points north. This does **not** mean that $|+\rangle$ is "pointing both north and east at the same time". It does not, in fact, point in either of these directions; instead, it points in a third direction, namely north-east.

In other words, if we just look at the vector represented by $|+\rangle$, without considering any particular basis, it is just a vector pointing in **one** particular direction, and in this direction only. The superposition only exists if we insist to represent $|+\rangle$ in this particular eigenbasis, but there can be another eigenbasis, e.g. the eigenbasis composed of $|+\rangle$ itself along with $|-\rangle$, in which $|+\rangle$ is **not** in a superposition.

What this means is that a state only appears to be in a superposition when we choose a particular observable and represent that state as a superposition of eigenstates with respect to that observable. But the system itself is still in the same state, regardless of which eigenbasis we choose. The projections of the state of the system on the basis eigenstates give us the probability amplitudes relevant to that measurement; for example, in Figure 4.1 we see that the probability amplitudes to measure $|0\rangle$ or $|1\rangle$ are both $1/\sqrt{2}$. However, in the basis consisting of $|+\rangle$ and $|-\rangle$, we instead have that the probability amplitude to measure $|+\rangle$ is 1 and the probability amplitude to measure $|-\rangle$ is 0.

In the specific case where the qubit is the spin of a spin-1/2 particle, we know that if the qubit is in the state $|+\rangle$, this means that a measurement of spin along the x axis will yield spin up with probability 1. We can say, if we want, that the system is in a state of spin up along the x axis, and this defines the state uniquely. We also see that, in this basis, the system is not in a superposition; it is just one state.

However, in the basis corresponding to measurement of spin along the z axis, we may write the state as a superposition, $|+\rangle = (|0\rangle + |1\rangle) / \sqrt{2}$. This doesn't mean that the qubit is in both the states $|0\rangle$ and $|1\rangle$ "at the same time"; it means that it is in a state where a measurement of spin along the z axis will yield spin up or spin down with equal probability.

If being in the superposition $(|0\rangle + |1\rangle) / \sqrt{2}$ doesn't mean that the qubit is **both** $|0\rangle$ **and** $|1\rangle$ at the same time, perhaps it could mean that the qubit is **either** $|0\rangle$ **or** $|1\rangle$, but we just don't know which one it is, and when we perform a measurement we will discover which state it was in all along? Unfortunately, that interpretation doesn't work either. Theories where the system is in only one particular unknown ("hidden") state, but we only discover which one after we measure it, are called *hidden variable theories*. They are mostly thought to be incorrect, since they violate a theorem called Bell's theorem, which we will learn about in Section 4.3.6.

Some theories of hidden variables that are compatible with Bell's theorem do exist, but most physicists don't believe they could replace quantum mechanics, because they are complicated, contrived, and *non-local*; the latter means that they allow faster-than-light or instantaneous communication[29]. Indeed, some non-local hidden variable theories, such as *de Broglie–Bohm*

[29]This doesn't necessarily mean the theory allows us to send information faster than light. The components of the system can communicate with each other faster than light, but not necessarily in a way that we can actually control or make use of. We will discuss this in more detail in Section 4.3.6.

theory, require all of the particles in the universe to be able to instantaneously communicate with each other at all times!

So in conclusion, being in a superposition of two states doesn't mean being in **both** the first state **and** the second state, but also doesn't mean being in **either** the first state **or** the second state. Instead, we must conclude that the terms "and" and "or" are classical terms that can only be used in a classical theory; superposition is a new quantum term, which simply does not have any classical analogue.

Compare this with our discussion of wave-particle duality in Section 2.1.3. This duality doesn't mean that light is "**both** a wave **and** a particle", and it also doesn't mean that light is "**either** a wave **or** a particle". What it really means is that the classical concepts of "wave" and "particle" are not the proper way to describe reality. Similarly, it turns out that the classical terms "and" and "or" cannot be used to describe reality at the deepest level; for that, we need to introduce quantum superposition.

4.3 Composite Systems and Quantum Entanglement

4.3.1 The Tensor Product

So far, we have only considered single, isolated physical systems, described by a single Hilbert space. What if we have more than one system, such as a collection of particles? This calls for a new axiom:

The Composite System Axiom: Given two physical quantum systems represented by two Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ respectively, the *tensor product* of the two spaces, denoted

$$\mathcal{H}_A \otimes \mathcal{H}_B, \tag{4.46}$$

is another Hilbert space, representing the *composite system* which combines the two original systems. The dimension of the composite Hilbert space is the product of the dimensions of the individual spaces:

$$\dim\left(\mathcal{H}_A \otimes \mathcal{H}_B\right) = \dim \mathcal{H}_A \cdot \dim \mathcal{H}_B. \tag{4.47}$$

For example, the dimension of $\mathbb{C}^m \otimes \mathbb{C}^n$ is mn.

Given a state $|\Psi_A\rangle$ in $\mathcal{H}_A$ and a state $|\Psi_B\rangle$ in $\mathcal{H}_B$, we can use the tensor product to form a new state in $\mathcal{H}_A \otimes \mathcal{H}_B$:

$$|\Psi_A\rangle \otimes |\Psi_B\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B. \tag{4.48}$$

However, **not all states** in $\mathcal{H}_A \otimes \mathcal{H}_B$ are necessarily of this form; this fact will prove essential soon, when we discuss entanglement. Furthermore, if $|A_i\rangle$, $i \in \{1, \ldots, m\}$ is an orthonormal basis of $\mathcal{H}_A$ and $|B_j\rangle$, $j \in \{1, \ldots, n\}$ is an orthonormal basis of $\mathcal{H}_B$, then

$$|A_i\rangle \otimes |B_j\rangle, \qquad i \in \{1, \ldots, m\}, \qquad j \in \{1, \ldots, n\}, \tag{4.49}$$

is an orthonormal basis of $\mathcal{H}_A \otimes \mathcal{H}_B$. Note that there are mn basis states in total, since the

dimension of the composite Hilbert space is mn.

The tensor product is linear. This means that for $\lambda \in \mathbb{C}$, $|\Psi_A\rangle \in \mathcal{H}_A$, and $|\Psi_B\rangle \in \mathcal{H}_B$ we have

$$\lambda \left(|\Psi_A\rangle \otimes |\Psi_B\rangle \right) = \Big(\lambda \, |\Psi_A\rangle \Big) \otimes |\Psi_B\rangle = |\Psi_A\rangle \otimes \Big(\lambda \, |\Psi_B\rangle \Big) , \tag{4.50}$$

for $|\Psi_A\rangle , |\Phi_A\rangle \in \mathcal{H}_A$ and $|\Theta_B\rangle \in \mathcal{H}_B$ we have

$$\Big(|\Psi_A\rangle + |\Phi_A\rangle \Big) \otimes |\Theta_B\rangle = |\Psi_A\rangle \otimes |\Theta_B\rangle + |\Phi_A\rangle \otimes |\Theta_B\rangle , \tag{4.51}$$

and for $|\Psi_A\rangle \in \mathcal{H}_A$ and $|\Theta_B\rangle , |\Omega_B\rangle \in \mathcal{H}_B$ we have

$$|\Psi_A\rangle \otimes \Big(|\Theta_B\rangle + |\Omega_B\rangle \Big) = |\Psi_A\rangle \otimes |\Theta_B\rangle + |\Psi_A\rangle \otimes |\Omega_B\rangle . \tag{4.52}$$

In particular, notice from (4.50) that scalars commute with the tensor product, so we can move them in or out of the product as we see fit – just as, until now, we have been moving scalars in and out of inner and outer products. Importantly, the tensor product itself is **not** commutative:

$$|\Psi_A\rangle \otimes |\Psi_B\rangle \neq |\Psi_B\rangle \otimes |\Psi_A\rangle . \tag{4.53}$$

The order matters, since the **first** state must come from the **first** Hilbert space, and the **second** state must come from the **second** Hilbert space – which may be a completely different space with completely different states. For example, in the tensor product $\mathbb{C}^2 \otimes \mathbb{C}^3$ the first state must be represented by a 2-vector while the second state must be represented by a 3-vector – so they cannot be interchanged.

Now, if O_A is an operator on $\mathcal{H}_A$ and O_B is an operator on $\mathcal{H}_B$, then $O_A \otimes O_B$ is an operator on $\mathcal{H}_A \otimes \mathcal{H}_B$, which is defined such that each operator acts only on the state coming from the same space as that operator:

$$\Big(O_A \otimes O_B \Big) \Big(|\Psi_A\rangle \otimes |\Psi_B\rangle \Big) = \Big(O_A \, |\Psi_A\rangle \Big) \otimes \Big(O_B \, |\Psi_B\rangle \Big) . \tag{4.54}$$

In other words, the **first** operator in the product $O_A \otimes O_B$ acts only on the **first** state in the product $|\Psi_A\rangle \otimes |\Psi_B\rangle$, and the **second** operator in the product $O_A \otimes O_B$ acts only on the **second** state in the product $|\Psi_A\rangle \otimes |\Psi_B\rangle$. This **has** to be the case, since e.g. in the tensor product $\mathbb{C}^2 \otimes \mathbb{C}^3$ the first operator must be represented by a 2×2 matrix and act on 2-vectors while the second operator must be represented by a 3×3 matrix and act on 3-vectors. Note that, as for the tensor product of states, not all operators in $\mathcal{H}_A \otimes \mathcal{H}_B$ are necessarily of this form.

If we have two bras $\langle \Psi_A| \in \mathcal{H}_A$ and $\langle \Psi_B| \in \mathcal{H}_B$, their tensor product $\langle \Psi_A| \otimes \langle \Psi_B|$ is a bra in $\mathcal{H}_A \otimes \mathcal{H}_B$, and the inner product of this bra with a ket of the form $|\Phi_A\rangle \otimes |\Phi_B\rangle$ in $\mathcal{H}_A \otimes \mathcal{H}_B$ is

defined by taking the inner products of each bra with the ket from the same space:

$$\Big(\langle\Psi_A| \otimes \langle\Psi_B|\Big)\Big(|\Phi_A\rangle \otimes |\Phi_B\rangle\Big) = \langle\Psi_A|\Phi_A\rangle\langle\Psi_B|\Phi_B\rangle. \tag{4.55}$$

The **first** bra acts only on the **first** ket and the **second** bra acts only on the **second** ket. Once again, the inner product **must** work this way, since for example in $\mathbb{C}^2 \otimes \mathbb{C}^3$ we can only take the inner product of 2-vectors with 2-vectors and 3-vectors with 3-vectors – the inner product of a 2-vector with a 3-vector is undefined.

Similarly, if we have two operators $O_A, P_A \in \mathcal{H}_A$ and two operators $O_B, P_B \in \mathcal{H}_B$, then the composite operator $O_A \otimes O_B \in \mathcal{H}_A \otimes \mathcal{H}_B$ acts on the composite operator $P_A \otimes P_B \in \mathcal{H}_A \otimes \mathcal{H}_B$ in the only way that makes sense, with each operator acting on the operator from the same space:

$$\Big(O_A \otimes O_B\Big)\Big(P_A \otimes P_B\Big) = O_A P_A \otimes O_B P_B. \tag{4.56}$$

Finally, above we stated the Composite System Axiom for two quantum systems, but we can use it recursively to define the composite Hilbert space of any number of systems: just take the tensor product of all the Hilbert spaces together,

$$\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C \otimes \dots \tag{4.57}$$

Everything we defined above still applies, with the obvious generalizations.

Problem 4.14. Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be two Hilbert spaces. Find an isomorphism between the composite Hilbert spaces $\mathcal{H}_A \otimes \mathcal{H}_B$ and $\mathcal{H}_B \otimes \mathcal{H}_A$.

Problem 4.15. Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be two Hilbert spaces, let A be an operator in $\mathcal{H}_A$, and let B be an operator in $\mathcal{H}_B$.

A. Construct an operator in $\mathcal{H}_A \otimes \mathcal{H}_B$ which acts as A does on the states of $\mathcal{H}_A$, but leaves the states of $\mathcal{H}_B$ unchanged.

B. Construct an operator in $\mathcal{H}_A \otimes \mathcal{H}_B$ which acts as B does on the states of $\mathcal{H}_B$, but leaves the states of $\mathcal{H}_A$ unchanged.

C. Show that the two operators you constructed commute by calculating their commutator as defined in (4.36).

4.3.2 Vectors and Matrices in the Composite Hilbert Space

Consider the tensor product $\mathbb{C}^m \otimes \mathbb{C}^n$. Since the dimension of this Hilbert space is mn, and since in any finite-dimensional Hilbert space we know how to represent states as vectors and operators as matrices of the same dimension as the Hilbert space (as discussed in Sections 3.2.7 and 3.2.15 respectively), we conclude that states in $\mathbb{C}^m \otimes \mathbb{C}^n$ can be represented as mn-vectors and operators in $\mathbb{C}^m \otimes \mathbb{C}^n$ can be represented as $mn \times mn$ matrices. In other words, $\mathbb{C}^m \otimes \mathbb{C}^n$ is isomorphic to $\mathbb{C}^{mn}$.

Explicitly, for two states represented by the vectors[30]

$$|\Psi\rangle \equiv \begin{pmatrix} \Psi_1 \\ \vdots \\ \Psi_m \end{pmatrix} \in \mathbb{C}^m, \qquad |\Phi\rangle \equiv \begin{pmatrix} \Phi_1 \\ \vdots \\ \Phi_n \end{pmatrix} \in \mathbb{C}^n, \tag{4.58}$$

we define the tensor product as follows:

$$|\Psi\rangle \otimes |\Phi\rangle \equiv \begin{pmatrix} \Psi_1 |\Phi\rangle \\ \vdots \\ \Psi_m |\Phi\rangle \end{pmatrix} = \begin{pmatrix} \Psi_1 \begin{pmatrix} \Phi_1 \\ \vdots \\ \Phi_n \end{pmatrix} \\ \vdots \\ \Psi_m \begin{pmatrix} \Phi_1 \\ \vdots \\ \Phi_n \end{pmatrix} \end{pmatrix} = \begin{pmatrix} \Psi_1\Phi_1 \\ \vdots \\ \Psi_1\Phi_n \\ \vdots \\ \Psi_m\Phi_1 \\ \vdots \\ \Psi_m\Phi_n \end{pmatrix} \in \mathbb{C}^{mn}. \tag{4.59}$$

For example:

$$\begin{pmatrix} 1 \\ 2 \end{pmatrix} \otimes \begin{pmatrix} 3 \\ 4 \end{pmatrix} = \begin{pmatrix} 1 \cdot \begin{pmatrix} 3 \\ 4 \end{pmatrix} \\ 2 \cdot \begin{pmatrix} 3 \\ 4 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 1 \cdot 3 \\ 1 \cdot 4 \\ 2 \cdot 3 \\ 2 \cdot 4 \end{pmatrix} = \begin{pmatrix} 3 \\ 4 \\ 6 \\ 8 \end{pmatrix}. \tag{4.60}$$

Similarly, for two operators represented by the matrices[31]

$$A \equiv \begin{pmatrix} A_{11} & \cdots & A_{1m} \\ \vdots & \ddots & \vdots \\ A_{m1} & \cdots & A_{mm} \end{pmatrix} \in \mathbb{C}^{m\times m}, \qquad B \equiv \begin{pmatrix} B_{11} & \cdots & B_{1n} \\ \vdots & \ddots & \vdots \\ B_{n1} & \cdots & B_{nn} \end{pmatrix} \in \mathbb{C}^{n\times n}, \tag{4.61}$$

[30] Note that before we used the subscript to indicate which space the state belongs to, but now the subscript is instead a vector index.

[31] Here, $\mathbb{C}^{n\times n}$ denotes the space of $n \times n$ complex matrices.

we define the tensor product as follows[32]:

$$
\begin{aligned}
A \otimes B &\equiv \begin{pmatrix} A_{11}B & \cdots & A_{1m}B \\ \vdots & \ddots & \vdots \\ A_{m1}B & \cdots & A_{mm}B \end{pmatrix} \\
&= \begin{pmatrix} A_{11}\begin{pmatrix} B_{11} & \cdots & B_{1n} \\ \vdots & \ddots & \vdots \\ B_{n1} & \cdots & B_{nn} \end{pmatrix} & \cdots & A_{1m}\begin{pmatrix} B_{11} & \cdots & B_{1n} \\ \vdots & \ddots & \vdots \\ B_{n1} & \cdots & B_{nn} \end{pmatrix} \\ \vdots & \ddots & \vdots \\ A_{m1}\begin{pmatrix} B_{11} & \cdots & B_{1n} \\ \vdots & \ddots & \vdots \\ B_{n1} & \cdots & B_{nn} \end{pmatrix} & \cdots & A_{mm}\begin{pmatrix} B_{11} & \cdots & B_{1n} \\ \vdots & \ddots & \vdots \\ B_{n1} & \cdots & B_{nn} \end{pmatrix} \end{pmatrix} \\
&= \begin{pmatrix} A_{11}B_{11} & \cdots & A_{11}B_{1n} & \cdots & A_{1m}B_{11} & \cdots & A_{1m}B_{1n} \\ \vdots & \ddots & \vdots & & \vdots & \ddots & \vdots \\ A_{11}B_{n1} & \cdots & A_{11}B_{nn} & \cdots & A_{1m}B_{n1} & \cdots & A_{1m}B_{nn} \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ A_{m1}B_{11} & \cdots & A_{m1}B_{1n} & \cdots & A_{mm}B_{11} & \cdots & A_{mm}B_{1n} \\ \vdots & \ddots & \vdots & & \vdots & \ddots & \vdots \\ A_{m1}B_{n1} & \cdots & A_{m1}B_{nn} & \cdots & A_{mm}B_{n1} & \cdots & A_{mm}B_{nn} \end{pmatrix} \in \mathbb{C}^{mn \times mn}.
\end{aligned}
$$

For example:

$$
\begin{aligned}
\begin{pmatrix} 0 & 1 \\ 2 & 0 \end{pmatrix} \otimes \begin{pmatrix} 3 & 0 \\ 0 & 4 \end{pmatrix} &= \begin{pmatrix} 0 \cdot \begin{pmatrix} 3 & 0 \\ 0 & 4 \end{pmatrix} & 1 \cdot \begin{pmatrix} 3 & 0 \\ 0 & 4 \end{pmatrix} \\ 2 \cdot \begin{pmatrix} 3 & 0 \\ 0 & 4 \end{pmatrix} & 0 \cdot \begin{pmatrix} 3 & 0 \\ 0 & 4 \end{pmatrix} \end{pmatrix} \\
&= \begin{pmatrix} 0 \cdot 3 & 0 \cdot 0 & 1 \cdot 3 & 1 \cdot 0 \\ 0 \cdot 0 & 0 \cdot 4 & 1 \cdot 0 & 1 \cdot 4 \\ 2 \cdot 3 & 2 \cdot 0 & 0 \cdot 3 & 0 \cdot 0 \\ 2 \cdot 0 & 2 \cdot 4 & 0 \cdot 0 & 0 \cdot 4 \end{pmatrix} \\
&= \begin{pmatrix} 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 4 \\ 6 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 \end{pmatrix}.
\end{aligned}
$$

[32]Note that the tensor product of vectors is a special case of the tensor product of matrices, with the vectors treated as single-column matrices.

Exercise 4.16. For the specific $|\Psi\rangle$, $|\Phi\rangle$, A, and B we used above:

$$|\Psi\rangle \equiv \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \qquad |\Phi\rangle \equiv \begin{pmatrix} 3 \\ 4 \end{pmatrix}, \tag{4.62}$$

$$A \equiv \begin{pmatrix} 0 & 1 \\ 2 & 0 \end{pmatrix}, \qquad B \equiv \begin{pmatrix} 3 & 0 \\ 0 & 4 \end{pmatrix}, \tag{4.63}$$

calculate

$$\Big(A \otimes B\Big)\Big(|\Psi\rangle \otimes |\Phi\rangle\Big). \tag{4.64}$$

Do so in two ways:

1. Directly in the composite Hilbert space[33] $\mathbb{C}^2 \otimes \mathbb{C}^2 \simeq \mathbb{C}^4$ using the 4×4 matrix and 4-vector found above.
2. Separately in each of the component spaces using the two 2×2 matrices and the two 2-vectors (acting with the first matrix on the first vector and the second matrix on the second vector), and then calculating the tensor product of the results.

Then compare your results and verify that they are the same.

Problem 4.17.

A. Prove that the tensor product preserves the adjoint operation on both vectors and matrices. That is,

$$\Big(|\Psi\rangle \otimes |\Phi\rangle\Big)^\dagger = \langle\Psi| \otimes \langle\Phi|, \qquad (A \otimes B)^\dagger = A^\dagger \otimes B^\dagger. \tag{4.65}$$

B. Prove that the tensor product of two Hermitian operators is Hermitian, and the tensor product of two unitary operators is unitary.

Problem 4.18. Consider the tensor product $\mathbb{C}^m \otimes \mathbb{C}^n$ for arbitrary m and n. Show that the standard basis of $\mathbb{C}^m \otimes \mathbb{C}^n$ is obtained by taking the tensor products of the standard basis states of $\mathbb{C}^m$ and $\mathbb{C}^n$.

Exercise 4.19. Calculate the tensor product

$$|+\rangle \otimes |-\rangle \otimes |0\rangle, \tag{4.66}$$

where $|+\rangle$ and $|-\rangle$ are the $+1$ and -1 eigenstates of σ_x respectively, and $|0\rangle$ is the $+1$ eigenstate of σ_z (see Section 4.2.1).

Exercise 4.20.

A. Calculate the tensor product operator

$$A \equiv S_x \otimes S_z, \tag{4.67}$$

[33] Here, $\simeq$ means "isomorphic to".

where S_x and S_z were defined in (4.31).

B. Calculate the tensor product state

$$|\Psi\rangle \equiv |+\rangle \otimes |1\rangle\,, \tag{4.68}$$

where $|+\rangle$ and $|1\rangle$ were defined in Section 4.2.1.

C. Calculate the expectation value $\langle A\rangle_\Psi$.

4.3.3 Quantum Entanglement

Consider a composite system of two qubits. In the computational (standard) basis, each of the qubits is a superposition of the two basis eigenstates $|0\rangle$ and $|1\rangle$. Let us name the first qubit A and the second qubit B. In the composite Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, the computational basis has four eigenstates:

$$|0\rangle \otimes |0\rangle\,, \qquad |0\rangle \otimes |1\rangle\,, \qquad |1\rangle \otimes |0\rangle\,, \qquad |1\rangle \otimes |1\rangle\,, \tag{4.69}$$

where in each of these, the first state is the state of qubit A and the second is the state of qubit B. Thus $|0\rangle \otimes |0\rangle$ corresponds to $|0\rangle$ for both qubits, $|0\rangle \otimes |1\rangle$ corresponds to $|0\rangle$ for qubit A and $|1\rangle$ for qubit B, $|1\rangle \otimes |0\rangle$ corresponds to $|1\rangle$ for qubit A and $|0\rangle$ for qubit B, and $|1\rangle \otimes |1\rangle$ corresponds to $|1\rangle$ for both qubits.

These four eigenstates have the following representations in terms of vectors in $\mathbb{C}^4$:

$$|0\rangle \otimes |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad |0\rangle \otimes |1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \tag{4.70}$$

$$|1\rangle \otimes |0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \qquad |1\rangle \otimes |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \tag{4.71}$$

So we see that they are, in fact, just the standard basis of $\mathbb{C}^4$.

The most general state of both qubits is described as a superposition of all possible combinations:

$$|\Psi\rangle = \alpha_{00}\,|0\rangle \otimes |0\rangle + \alpha_{01}\,|0\rangle \otimes |1\rangle + \alpha_{10}\,|1\rangle \otimes |0\rangle + \alpha_{11}\,|1\rangle \otimes |1\rangle = \begin{pmatrix} \alpha_{00} \\ \alpha_{01} \\ \alpha_{10} \\ \alpha_{11} \end{pmatrix}, \tag{4.72}$$

where $\alpha_{00}, \alpha_{01}, \alpha_{10}, \alpha_{11} \in \mathbb{C}$ and, of course, the coefficients should be chosen such that the state

is normalized to 1:

$$|\alpha_{00}|^2 + |\alpha_{01}|^2 + |\alpha_{10}|^2 + |\alpha_{11}|^2 = 1. \tag{4.73}$$

We would now like to ask: when do the two qubits depend on each other? More precisely, under what conditions can qubit A be $|0\rangle$ or $|1\rangle$ **independently** of the state of qubit B, and vice versa? As we will now see, this depends on the coefficients α_{ij}.

A *separable state* is a state which can be written as just **one** tensor product instead of a **sum** of tensor products, that is, a state of the form

$$|\Psi\rangle = |\Psi_A\rangle \otimes |\Psi_B\rangle\,, \tag{4.74}$$

where $|\Psi_A\rangle$ is the state of qubit A and $|\Psi_B\rangle$ is the state of qubit B. If we can write the state in this way, then we have **separated** the states from one another, in the sense that whatever value $|\Psi_A\rangle$ has is completely independent of the value of $|\Psi_B\rangle$ (and vice versa). In other words, the overall state of the composite system is just the tensor product of the independent states of the individual systems.

A simple example of a separable state would be:

$$|\Psi\rangle = |0\rangle \otimes |0\rangle\,. \tag{4.75}$$

This just means that both qubits are, with 100% probability, in the state $|0\rangle$:

$$|\Psi_A\rangle = |0\rangle\,, \qquad |\Psi_B\rangle = |0\rangle\,. \tag{4.76}$$

A more interesting separable state is:

$$|\Psi\rangle = \frac{1}{2}\left(|0\rangle \otimes |0\rangle + |0\rangle \otimes |1\rangle + |1\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle\right). \tag{4.77}$$

To see that it is separable, we simplify it using the distributive property, and get:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right). \tag{4.78}$$

In other words, both qubits are in a state where either 0 or 1 is possible with 50% probability, that is:

$$|\Psi_A\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right), \qquad |\Psi_B\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right). \tag{4.79}$$

A state which is **not** separable is called an *entangled state*. Here is an example of an entangled state:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle \otimes |1\rangle + |1\rangle \otimes |0\rangle\right). \tag{4.80}$$

No matter how much we try, we can never write it as just one tensor product; it is always going to be the sum of two tensor products! This means that the state of each qubit is no longer independent of the state of the other qubit. Indeed, if qubit A is in the state $|0\rangle$ then

qubit B must be in the state $|1\rangle$ (due to the first term), and if qubit A is in the state $|1\rangle$ then qubit B must be in the state $|0\rangle$ (due to the second term). This is precisely what it means for two systems to be entangled.

More generally, consider again a composite system in the state

$$|\Psi\rangle = \alpha_{00}\,|0\rangle \otimes |0\rangle + \alpha_{01}\,|0\rangle \otimes |1\rangle + \alpha_{10}\,|1\rangle \otimes |0\rangle + \alpha_{11}\,|1\rangle \otimes |1\rangle = \begin{pmatrix} \alpha_{00} \\ \alpha_{01} \\ \alpha_{10} \\ \alpha_{11} \end{pmatrix}, \tag{4.81}$$

where $\alpha_{00}, \alpha_{01}, \alpha_{10}, \alpha_{11} \in \mathbb{C}$. If it is separable, then we should be able to write it in the form

$$|\Psi\rangle = (\beta_0\,|0\rangle + \beta_1\,|1\rangle) \otimes (\gamma_0\,|0\rangle + \gamma_1\,|1\rangle)\,, \tag{4.82}$$

where $\beta_0, \beta_1, \gamma_0, \gamma_1 \in \mathbb{C}$. Expanding the last equation, we get

$$|\Psi\rangle = \beta_0\gamma_0\,|0\rangle \otimes |0\rangle + \beta_0\gamma_1\,|0\rangle \otimes |1\rangle + \beta_1\gamma_0\,|1\rangle \otimes |0\rangle + \beta_1\gamma_1\,|1\rangle \otimes |1\rangle\,. \tag{4.83}$$

So we should have:

$$\alpha_{ij} = \beta_i\gamma_j, \qquad i, j \in \{0, 1\}\,, \tag{4.84}$$

or explicitly:

$$\alpha_{00} = \beta_0\gamma_0, \qquad \alpha_{01} = \beta_0\gamma_1, \qquad \alpha_{10} = \beta_1\gamma_0, \qquad \alpha_{11} = \beta_1\gamma_1. \tag{4.85}$$

If this is true, then in particular

$$\begin{aligned} \alpha_{00}\alpha_{11} - \alpha_{01}\alpha_{10} &= (\beta_0\gamma_0)\,(\beta_1\gamma_1) - (\beta_0\gamma_1)\,(\beta_1\gamma_0) \\ &= \beta_0\beta_1\gamma_0\gamma_1 - \beta_0\beta_1\gamma_0\gamma_1 \\ &= 0. \end{aligned}$$

Now, if α_{ij} are the components of a matrix[34],

$$\alpha = \begin{pmatrix} \alpha_{00} & \alpha_{01} \\ \alpha_{10} & \alpha_{11} \end{pmatrix}, \tag{4.88}$$

then the quantity $\alpha_{00}\alpha_{11} - \alpha_{01}\alpha_{10}$ is called the *determinant* of the matrix, denoted $\det \alpha$:

$$\det \alpha \equiv \alpha_{00}\alpha_{11} - \alpha_{01}\alpha_{10}. \tag{4.89}$$

We have proven that, **if** the composite state is separable (not entangled), **then** the matrix of the coefficients has vanishing determinant. Below you will prove that this also works in the opposite direction; thus, a composite state of two qubits is separable **if and only if** $\det \alpha = 0$. Let us check this. The state in (4.75) is separable, since it has

$$\det \alpha = 1 \cdot 0 - 0 \cdot 0 = 0. \tag{4.90}$$

The state in (4.77) is also separable, since it has

$$\det \alpha = \frac{1}{2} \cdot \frac{1}{2} - \frac{1}{2} \cdot \frac{1}{2} = 0. \tag{4.91}$$

However, the state in (4.80) is entangled, since it has

$$\det \alpha = 0 \cdot 0 - \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}} = -\frac{1}{2} \neq 0. \tag{4.92}$$

Unfortunately, this simple rule only works for a composite system of 2 qubits. The problem of finding whether a given state of a composite system is separable or entangled is called the *separability problem*, and it is, for general states, a difficult problem to solve!

Problem 4.21. Prove that, for a composite state of two qubits given by

$$|\Psi\rangle = \alpha_{00} |0\rangle \otimes |0\rangle + \alpha_{01} |0\rangle \otimes |1\rangle + \alpha_{10} |1\rangle \otimes |0\rangle + \alpha_{11} |1\rangle \otimes |1\rangle , \tag{4.93}$$

[34]This is actually the matrix that would be obtained if, instead of writing the composite state of two qubits as a vector in $\mathbb{C}^4$, we wrote it as the outer products of the qubits, which would be a 2×2 matrix. Explicitly, you can check that:

$$|0\rangle \langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad |0\rangle \langle 1| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad |1\rangle \langle 0| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \qquad |1\rangle \langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{4.86}$$

so in this representation, we would get

$$|\Psi\rangle = \alpha_{00} |0\rangle \langle 0| + \alpha_{01} |0\rangle \langle 1| + \alpha_{10} |1\rangle \langle 0| + \alpha_{11} |1\rangle \langle 1| = \begin{pmatrix} \alpha_{00} & \alpha_{01} \\ \alpha_{10} & \alpha_{11} \end{pmatrix}. \tag{4.87}$$

The reason we do not use the outer product representation for two-qubit states is that writing them as vectors in $\mathbb{C}^4$ allows us to act on them with operators given by 4×4 matrices, just as we would act on single qubit with operators given by 2×2 matrices.

the state is separable if

$$\det \begin{pmatrix} \alpha_{00} & \alpha_{01} \\ \alpha_{10} & \alpha_{11} \end{pmatrix} = \alpha_{00}\alpha_{11} - \alpha_{01}\alpha_{10} = 0. \tag{4.94}$$

This is the opposite direction to what we proved above, which is that **if** the determinant is zero, **then** the state is separable.

Problem 4.22. Find two separable states and two entangled states of **three** qubits, and prove that they are separable/entangled.

4.3.4 The Bell States

Let us define the Bell states, also known as[35] *EPR states*:

$$\left|\beta_{xy}\right\rangle \equiv \frac{1}{\sqrt{2}} \left(|0\rangle \otimes |y\rangle + (-1)^x |1\rangle \otimes |1-y\rangle\right), \qquad x, y \in \{0,1\}. \tag{4.95}$$

Explicitly, the four choices for x and y give:

$$|\beta_{00}\rangle \equiv \frac{1}{\sqrt{2}} \left(|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle\right), \tag{4.96}$$

$$|\beta_{01}\rangle \equiv \frac{1}{\sqrt{2}} \left(|0\rangle \otimes |1\rangle + |1\rangle \otimes |0\rangle\right), \tag{4.97}$$

$$|\beta_{10}\rangle \equiv \frac{1}{\sqrt{2}} \left(|0\rangle \otimes |0\rangle - |1\rangle \otimes |1\rangle\right), \tag{4.98}$$

$$|\beta_{11}\rangle \equiv \frac{1}{\sqrt{2}} \left(|0\rangle \otimes |1\rangle - |1\rangle \otimes |0\rangle\right). \tag{4.99}$$

It is useful to adopt a shorthand notation where we write

$$|xy\rangle \equiv |x\rangle \otimes |y\rangle, \tag{4.100}$$

so

$$|00\rangle \equiv |0\rangle \otimes |0\rangle, \qquad |01\rangle \equiv |0\rangle \otimes |1\rangle, \qquad |10\rangle \equiv |1\rangle \otimes |0\rangle, \qquad |11\rangle \equiv |1\rangle \otimes |1\rangle. \tag{4.101}$$

In this notation, the Bell states are

$$|\beta_{00}\rangle \equiv \frac{1}{\sqrt{2}} \left(|00\rangle + |11\rangle\right), \tag{4.102}$$

$$|\beta_{01}\rangle \equiv \frac{1}{\sqrt{2}} \left(|01\rangle + |10\rangle\right), \tag{4.103}$$

[35] EPR stands for Einstein, Podolsky, and Rosen.

$$|\beta_{10}\rangle \equiv \frac{1}{\sqrt{2}}\left(|00\rangle - |11\rangle\right), \tag{4.104}$$

$$|\beta_{11}\rangle \equiv \frac{1}{\sqrt{2}}\left(|01\rangle - |10\rangle\right). \tag{4.105}$$

The Bell states have important applications in quantum information and computation, as we will see below.

Exercise 4.23. Write down the representations of the four Bell states as 4-vectors in $\mathbb{C}^2 \otimes \mathbb{C}^2 \simeq \mathbb{C}^4$.

Problem 4.24. Prove that the four Bell states form an orthonormal basis for the composite Hilbert space of two qubits, by showing that they span that space, are linearly independent, are orthogonal, and are normalized to 1.

Problem 4.25. Prove that each of the four Bell states is entangled.

Exercise 4.26. Write down the four Bell states in terms of $|+\rangle$ and $|-\rangle$, the eigenstates of σ_x. You may wish to use the shorthand notation $|\pm\pm\rangle \equiv |\pm\rangle \otimes |\pm\rangle$.

4.3.5 Entanglement Does Not Transmit Information

Now that we have rigorously defined quantum entanglement, let us debunk the most common misconception associated with it: that quantum entanglement allows us to transmit information, and in particular, that it allows us to do so faster than the speed of light (or even instantaneously), in violation of relativity. This is, in fact, not true.

To illustrate this, imagine the following scenario. Alice and Bob create an entangled pair of qubits, for example in the Bell state

$$|\beta_{01}\rangle \equiv \frac{1}{\sqrt{2}}\left(|01\rangle + |10\rangle\right). \tag{4.106}$$

Alice takes the first qubit in the pair, and Bob takes the second qubit. Alice then stays on Earth, while Bob embarks on a long journey to Alpha Centauri, about 4.4 light years away. When Bob gets there, he measures his qubit. He has a 50% chance to observe 0 and a 50% chance to observe 1. However, if he observes 0 he knows that Alice will surely observe 1 whenever she measures her qubit, and if he observes 1 he knows that Alice will surely observe 0, since the qubits must have opposite values.

So it seems that Bob now knows something about Alice's qubit that he did not know before. Furthermore, he knows that **instantly** – even though Alice is 4.4 light years away, and thus according to relativity, that information should have taken at least 4.4 years to travel between them. But has any information actually been transferred between them?

The answer is no! All Bob did was observe a **random** event. Bob cannot **control** which value he observes when he measures the qubit, 0 or 1; he can only observe it, and randomly get

whatever he gets. He gains information about Alice's qubit, which is completely random, but he does not receive any specific message from Alice, nor can he transmit any specific information to Alice by observing his qubit.

In fact, there is a theorem called the *no-communication theorem* which rigorously proves that no information can be transmitted using quantum entanglement, whether faster than light or otherwise. Whatever you measure, it must be completely random. (Unfortunately, the proof of this theorem uses some advanced tools that we will not learn in this course, so we will not present it here.)

The fact that a measurement of one qubit determines the measurement of another qubit might seem like it indicates that some information must be transmitted between the qubits themselves, so that they "know" about each other's states. However, there isn't any actual need to transmit information between the two entangled qubits in order for them to match their measurements! After all, the entangled state does **not** depend on the distance between the qubits, whether in time or in space; it is simply the combined state of the two qubits, wherever or whenever they might be.

Consider now the following completely classical scenario. Let's say I write 0 on one piece of paper and 1 on another piece of paper. I then put each piece of paper in a separate sealed envelope, and randomly give one envelope to Alice and the other to Bob. When Bob gets to Alpha Centauri, he opens his envelope. If he sees 0 he knows that Alice's envelope says 1, and if he sees 1 he knows that Alice's envelope says 0.

Obviously, this does not allow any information to be transmitted between Alice and Bob, nor does each envelope need to "know" what's inside the other envelope in order for the measurements to match. If Bob sees 0, then the piece of paper saying 0 was inside the envelope **all along**, and the piece of paper saying 1 was inside Alice's envelope all along – and vice versa. The envelopes are **classically correlated**, and nothing weird is going on. What, then, is the difference between this classical correlation and quantum entanglement? The answer to this question can be made precise using *Bell's theorem*, which we will now formulate.

4.3.6 Bell's Theorem and Bell's Inequality

Bell's theorem proves that the predictions of quantum theory cannot be explained by theories of *local hidden variables*, which we first mentioned in Section 4.2.4. These are *deterministic* theories, where measurements of quantum systems such as qubits have **pre-existing** values. For example, if we measured 0, then the qubit always had the value 0; we could have, in fact, predicted the exact value 0, and not just the probability to measure it (which is what quantum theory can predict), if we knew the value of a "hidden variable" that quantum theory does not take into account.

Local hidden variable theories are essentially no different than the envelope scenario described above; the envelope always had the number 0 inside it, and if we were able to look inside the envelope (at the "hidden variable") without opening it, we would have been able to make a deterministic prediction. In this sense, local hidden variable theories have classical correlation,

and Bell's theorem proves that quantum entanglement is different, and in a precise sense we will discuss below, **stronger** than classical correlation.

Consider the following experiment. I prepare two qubits, and give one to Alice and another to Bob. Alice can measure one of two different physical observables[36] of her qubit, Q or R, both having two possible outcomes, $+1$ or -1. Similarly, Bob can measure one of two different physical observables of his qubit, S or T, both having two possible outcomes, $+1$ or -1.

We now make two crucial assumptions:

1. *Locality*: Both Alice and Bob measure their qubits at the same time in different places, so that their measurements cannot possibly disturb or influence each other without sending information faster than light. This ensures that the predicted probabilities for Alice's and Bob's measurements are completely independent of each other. This condition puts the "local" in "local hidden variable theory".

2. *Realism*: The values of the physical observables Q, R, S, T exist independently of observation, that is, they have certain definite values q, r, s, t which are already determined before any measurements took place, as in the envelope scenario. This condition puts the "hidden variable" in "local hidden variable theory".

Together, these two assumptions form the principle of *local realism*. Classical relativity definitely satisfies this principle; there are no faster-than-light interactions, and everything is deterministic. Local hidden variable theories also satisfy this principle. Non-local hidden variable theories satisfy realism, but not locality.

Now, whatever the values of q, r, s, t are, we must always have

$$rs + qs + rt - qt = (r + q)\, s + (r - q)\, t = \pm 2. \tag{4.107}$$

To see that, note that since $r = \pm 1$ and $q = \pm 1$, we must either have $r + q = 0$ if they have opposite signs, or $r - q = 0$ if they have the same sign. So one of the terms must always vanish. In the first case we have $(r - q)\, t = \pm 2$ because $t = \pm 1$ and in the second case we have $(r + q)\, s = \pm 2$ because $s = \pm 1$.

Using this information, we can calculate the expectation value of this expression. To do that, we assign a probability $p\,(q, r, s, t)$ to each outcome of q, r, s, t. For example, we could simply assign a uniform probability distribution, where all probabilities are equal:

$$p\,(q, r, s, t) = \frac{1}{16}, \tag{4.108}$$

for any values of q, r, s, t. However, the probability distribution can be arbitrary. Even though we don't know the probabilities in advance, we we can nonetheless still calculate an **upper**

[36] Alice could take, for example, $Q = \sigma_z$ and $R = \sigma_x$ – which is indeed what we will take below. However, for our purposes, it doesn't matter what the physical observables being measured actually are. For that matter, the physical systems don't need to be qubits, either; it's just easier to talk about qubits since they are the simplest non-trivial quantum systems. This scenario is very general, and does not depend on any specific systems or observables, which is good since we are trying to capture a **general** property of quantum theory.

bound on the expectation value:

$$\begin{aligned}\langle RS + QS + RT - QT\rangle &= \sum_{q,r,s,t\in\{-1,+1\}} p\left(q,r,s,t\right)\left(rs + qs + rt - qt\right)\\ &\leq 2 \sum_{q,r,s,t\in\{-1,+1\}} p\left(q,r,s,t\right)\\ &= 2.\end{aligned}$$

To go to the second line we used the fact that $rs + qs + rt - qt = \pm 2$, as we proved in (4.107), and thus it is always less than or equal to 2 for any values of q, r, s, t. To go to the third line we used the fact that the sum of all possible probabilities must be 1. Also, since the expectation value function is linear, we have

$$\langle RS + QS + RT - QT\rangle = \langle RS\rangle + \langle QS\rangle + \langle RT\rangle - \langle QT\rangle\,. \tag{4.109}$$

We thus obtain the *Bell inequality*[37]:

$$\langle RS\rangle + \langle QS\rangle + \langle RT\rangle - \langle QT\rangle \leq 2. \tag{4.110}$$

To summarize, we have proven that in any locally realistic theory, the expectation value considered here must be less than or equal to 2.

Now, let us assume that I prepared the two qubits in the following Bell state:

$$|\beta_{11}\rangle = \frac{1}{\sqrt{2}}\left(|01\rangle - |10\rangle\right). \tag{4.111}$$

Alice gets the first qubit, and Bob gets the second qubit. We define the observables Q, R, S, T in terms of the Pauli matrices. Alice measures the observables

$$Q = \sigma_z, \qquad R = \sigma_x, \tag{4.112}$$

while Bob measures the observables

$$S = -\frac{1}{\sqrt{2}}\left(\sigma_x + \sigma_z\right), \qquad T = -\frac{1}{\sqrt{2}}\left(\sigma_x - \sigma_z\right). \tag{4.113}$$

In Exercise 4.27 you will prove that

$$\langle RS\rangle = \langle QS\rangle = \langle RT\rangle = \frac{1}{\sqrt{2}}, \qquad \langle QT\rangle = -\frac{1}{\sqrt{2}}, \tag{4.114}$$

where we used the shorthand notation $RS \equiv R \otimes S$ and so on, and the expectations values

[37] More precisely, there are many different Bell inequalities, and this specific one is called the *CHSH (Clauser-Horne-Shimony-Holt) inequality*.

are calculated with respect to the state $|\beta_{11}\rangle$. We thus get:

$$\langle RS\rangle + \langle QS\rangle + \langle RT\rangle - \langle QT\rangle = 2\sqrt{2} \approx 2.8, \tag{4.115}$$

which violates the Bell inequality (4.110)!

Importantly, this is not just a theoretical result; many different experiments have verified that the Bell inequality is indeed violated in nature. This means that our assumptions, either locality or realism (or both), must be incorrect. In particular, it also means that quantum entanglement is stronger than classical correlation, which is locally realistic – since with classical correlation, the best you can do for the expectation value considered here is 2, but quantum entanglement allows you to get a larger expectation value of $2\sqrt{2}$.

This pretty much rules out any local hidden variable theory. Instead, we should consider the following options:

1. Locality is an incorrect assumption[38], but realism is correct. This is the essence of non-local hidden variable theories, such as *de Broglie–Bohm theory*, which we briefly discussed in Section 4.2.4 – where the state of each particle depends on the states of every other particle in the universe! However, most physicists don't like these theories, since they are complicated and contrived, and lack the simplicity, elegance, and universality of quantum theory.

2. Realism is an incorrect assumption, but locality is correct. This is the option that most physicists prefer, even though it is less intuitive and contradicts our experience with the classical world. Surely, if you open the fridge to get an apple, the apple has always been there, even before you observed it; but the same does not have to be true for observing a qubit.

Another important lesson of Bell's theorem is that there is something fundamentally profound and powerful about quantum entanglement, which classical correlation does not have. This property of quantum entanglement is exactly what makes quantum computers more powerful than classical computers, as we will see below. It also has some other interesting applications, such as quantum teleportation (which we will discuss in Section 5.1.2) and quantum cryptography.

Exercise 4.27. Prove (4.114) by explicitly calculating the expectation values of the given operators with respect to the state $|\beta_{11}\rangle$.

[38] That would be the "spooky action at a distance" you hear about all the time. However, note that even if locality is violated, this still does not necessarily mean faster-than-light communication is possible. As we discussed in the previous section, communication between two people requires a form of non-locality that is **controllable**, so that Bob can **choose** which state he measures, and by doing that, send a message to Alice, which she will discover when she measures her qubit. Thus a theory can be non-local while still violating neither the no-communication theorem nor relativity.

Problem 4.28. Consider two qubits in the composite state

$$|\beta_{11}\rangle = \frac{1}{\sqrt{2}}\left(|01\rangle - |10\rangle\right). \tag{4.116}$$

Since $|0\rangle$ and $|1\rangle$ are the eigenstates of the observable S_z corresponding to positive and negative spin respectively along the z direction (recall Section 4.2.2), it is easy to see that a measurement of spin along the z direction will always yield opposite spins for the qubits: if one qubit has positive spin in the z direction (i.e. $|0\rangle$), then the other qubit must have negative spin in the z direction (i.e. $|1\rangle$). This state is historically known as a *spin singlet*.

Now, let $\mathbf{v}\in\mathbb{R}^3$ be a unit vector pointing in some direction in space (the real space, not the Hilbert space!). Then the observable $S_{\mathbf{v}}$ defined in (4.33) corresponds to a measurement of spin along the direction of $\mathbf{v}$. Prove that if the system is in the state $|\beta_{11}\rangle$, then the measurement of spin along **any** direction $\mathbf{v}$ will **always** yield opposite spins for the qubits: if one qubit has positive spin along the direction $\mathbf{v}$, then the other must have negative spin along the same direction $\mathbf{v}$.

This is remarkable, since it means if Alice measures her qubit on Earth and Bob measures his qubit on Alpha Centauri at the same time, and both of them measure spin along the same direction, then somehow both qubits must "know" to have opposite spins along this direction, no matter which direction Alice and Bob choose!

4.4 Non-Commuting Observables and the Uncertainty Principle

4.4.1 Commuting and Non-Commuting Observables

In Problem 4.13 we defined the *commutator* of two operators:

$$[A, B] \equiv AB - BA. \tag{4.117}$$

If the operators commute, then $AB = BA$ and thus the commutator vanishes: $[A, B] = 0$. Otherwise, $AB \neq BA$ and the commutator is non-zero: $[A, B] \neq 0$. The commutator thus tells us if the operators commute or not. Note that any operator commutes with itself: $[A, A] = 0$ for any A.

Problem 4.29. Prove that the commutator is anti-symmetric:

$$[B, A] = -\left[A, B\right]. \tag{4.118}$$

Problem 4.30. Prove that the commutator is linear:

$$[A + B, C] = [A, C] + [B, C], \tag{4.119}$$

$$[A, B + C] = [A, B] + [A, C]. \tag{4.120}$$

Problem 4.31. Prove that

$$[A, B]^\dagger = [B^\dagger, A^\dagger]. \tag{4.121}$$

Problem 4.32. Prove the useful identities

$$[AB, C] = A\,[B, C] + [A, C]\,B, \tag{4.122}$$

$$[A, BC] = B\,[A, C] + [A, B]\,C. \tag{4.123}$$

Problem 4.33. Prove the *Jacobi identity*:

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0. \tag{4.124}$$

4.4.2 The Uncertainty Principle

When two quantum observables do not commute, we get an *uncertainty relation*. *Uncertainty* is just another name for *standard deviation*, which we defined in Section 3.3.4. The most well-known such relation is the *position-momentum uncertainty relation*[39]:

$$\Delta x \Delta p \geq \frac{1}{2}. \tag{4.125}$$

Here, x and p are two Hermitian operators, corresponding to the observables position and momentum respectively. This inequality means that the product of uncertainty in position Δx and the uncertainty in momentum Δp cannot go below $1/2$; it follows that Δx and Δp cannot both be zero at the same time, so we can never know both the position and momentum with arbitrarily high certainty.

Let us prove this relation for the general case of any two observables represented by Hermitian operators, A and B, which do not commute:

$$[A, B] \neq 0. \tag{4.126}$$

Recall that the (square of the) standard deviation ΔA of A is given by

$$(\Delta A)^2 = \left\langle (A - \langle A \rangle)^2 \right\rangle. \tag{4.127}$$

We have seen that expectation values in quantum theory are calculated using the inner product "sandwich"

$$\langle A \rangle = \langle \Psi | A | \Psi \rangle, \tag{4.128}$$

where $|\Psi\rangle$ is the state with respect to which the expectation value is calculated. The (square

[39] Recall that we are using units where $\hbar = 1$!

of the) standard deviation is thus

$$\begin{aligned}(\Delta A)^2 &= \langle\Psi|\left(A-\langle A\rangle\right)^2|\Psi\rangle \\ &= \langle\Psi|\left(A-\langle A\rangle\right)\left(A-\langle A\rangle\right)|\Psi\rangle.\end{aligned}$$

Let us now define a new vector:

$$|a\rangle = \left(A-\langle A\rangle\right)|\Psi\rangle. \tag{4.129}$$

Then we simply have[40]

$$(\Delta A)^2 = \langle a|a\rangle = \|a\|^2. \tag{4.130}$$

Similarly, for B we define

$$|b\rangle = \left(B-\langle B\rangle\right)|\Psi\rangle, \tag{4.131}$$

and get

$$(\Delta B)^2 = \langle b|b\rangle = \|b\|^2. \tag{4.132}$$

The product of the (squares of the) standard deviations in A and B is thus

$$(\Delta A)^2(\Delta B)^2 = \|a\|^2\|b\|^2. \tag{4.133}$$

Using the Cauchy-Schwarz inequality (3.153), we have

$$\begin{aligned}(\Delta A)^2(\Delta B)^2 &= \|a\|^2\|b\|^2 \\ &\geq |\langle a|b\rangle|^2 \\ (*) &= \left(\mathrm{Re}\langle a|b\rangle\right)^2+\left(\mathrm{Im}\langle a|b\rangle\right)^2 \\ (**) &\geq \left(\mathrm{Im}\langle a|b\rangle\right)^2 \\ (***) &= \left(\frac{\langle a|b\rangle-\langle b|a\rangle}{2i}\right)^2,\end{aligned}$$

where in $(*)$ we used (3.17), in $(**)$ we used the fact that $\left(\mathrm{Im}\langle a|b\rangle\right)^2 \geq 0$ since it's the square of a real number, and in $(***)$ we used (3.14) and the fact that $\langle b|a\rangle = \langle a|b\rangle^*$.

[40] $A-\langle A\rangle$ is the **operator** A minus the **real number** $\langle A\rangle$ times the identity operator 1 (the identity operator is implied). Thus $A-\langle A\rangle$ is Hermitian, and the bra of $\left(A-\langle A\rangle\right)|\Psi\rangle$ is $\langle\Psi|\left(A-\langle A\rangle\right)$.

Next, we note that

$$\begin{aligned}\langle a|b\rangle &= \langle\Psi|\left(A-\langle A\rangle\right)\left(B-\langle B\rangle\right)|\Psi\rangle\\ &= \langle\left(A-\langle A\rangle\right)\left(B-\langle B\rangle\right)\rangle\\ &= \langle AB - A\langle B\rangle - \langle A\rangle B + \langle A\rangle\langle B\rangle\rangle\\ &= \langle AB\rangle - \langle A\langle B\rangle\rangle - \langle\langle A\rangle B\rangle + \langle\langle A\rangle\langle B\rangle\rangle\\ &= \langle AB\rangle - \langle A\rangle\langle B\rangle - \langle A\rangle\langle B\rangle + \langle A\rangle\langle B\rangle\\ &= \langle AB\rangle - \langle A\rangle\langle B\rangle,\end{aligned}$$

where we used the linearity of the expected value, (3.177). Similarly,

$$\langle b|a\rangle = \langle BA\rangle - \langle A\rangle\langle B\rangle. \tag{4.134}$$

Thus

$$\begin{aligned}\langle a|b\rangle - \langle b|a\rangle &= \left(\langle AB\rangle - \langle A\rangle\langle B\rangle\right) - \left(\langle BA\rangle - \langle A\rangle\langle B\rangle\right)\\ &= \langle AB\rangle - \langle BA\rangle\\ &= \langle[A,B]\rangle,\end{aligned}$$

and so we get

$$\left(\Delta A\right)^2\left(\Delta B\right)^2 \geq \left\langle\frac{1}{2\,\mathrm{i}}\left[A,B\right]\right\rangle^2. \tag{4.135}$$

Now, by definition, ΔA and ΔB are real and non-negative. If $\left\langle\frac{1}{2\mathrm{i}}\left[A,B\right]\right\rangle$ is also real, we could take the square root (but we have to add an absolute value because it could actually be negative):

$$\Delta A\Delta B \geq \frac{1}{2}\left|\langle[A,B]\rangle\right|. \tag{4.136}$$

You will show in Problem 4.34 that it is indeed always real. Note that the uncertainty relation we found still depends on the choice of state $|\Psi\rangle$ with which to calculate the expected values and standard deviations, but sometimes, as in the position-momentum uncertainty relation, the same relation applies to all states.

As we will explain in more details later, when we discuss continuous systems, the operators x and p have the commutator

$$[x,p] = \mathrm{i}\,. \tag{4.137}$$

By plugging this commutator into the uncertainty relation (4.136), we indeed get the familiar result

$$\Delta x\Delta p \geq \frac{1}{2}. \tag{4.138}$$

Problem 4.34. Inequalities are only defined for real numbers, not complex numbers. Let us prove that if A and B are Hermitian, then $\langle[A,B]\rangle$ must always be an imaginary number, and thus $\left\langle\frac{1}{2\mathrm{i}}\left[A,B\right]\right\rangle$ is always real, so the inequality we found is well-defined.

An *anti-Hermitian operator* O is an operator which satisfies

$$O^\dagger = -O. \tag{4.139}$$

Just as a Hermitian operator is the matrix analogue of a real number, an anti-Hermitian operator is the matrix analogue of an imaginary number.

A. Prove that the eigenvalues of an anti-Hermitian operator are all purely imaginary, as defined in Problem 3.2.

B. Prove that an anti-Hermitian operator is normal, and thus it has an orthonormal eigenbasis (see Section 3.2.14).

C. Prove that if A and B are Hermitian, then $[A, B]$ must be anti-Hermitian.

D. Prove that if $[A, B]$ is anti-Hermitian, then the expectation value $\langle [A, B] \rangle_\Psi$ is imaginary for any state $|\Psi\rangle$.

Exercise 4.35. Calculate the uncertainty relation for σ_x and σ_y given an arbitrary qubit:

$$|\Psi\rangle = a\,|0\rangle + b\,|1\rangle\,, \qquad |a|^2 + |b|^2 = 1. \tag{4.140}$$

That is, find the right-hand side of

$$\Delta\sigma_x \Delta\sigma_y \geq (?)\,. \tag{4.141}$$

Comment on the consequences of the relation you found for choices of different states, that is, different values of a and b.

4.4.3 Simultaneous Diagonalization

Why is there uncertainty when two observers don't commute? Some insight may be gained from the fact that two Hermitian operators may be *simultaneously diagonalizable* if and only if they commute[41].

Recall that in Section 3.2.16 we proved that for any Hermitian matrix[42] A there exists a unitary matrix P such that

$$P^\dagger A P = D, \tag{4.142}$$

where D is a diagonal matrix. Furthermore, the elements on the diagonal are none other than the eigenvalues of A. This is called *diagonalizing* the matrix A.

Now, let A_1 and A_2 be two Hermitian matrices. We say that A_1 and A_2 are *simultaneously*

[41] This is a special case of a more general theorem: a set of diagonalizable matrices commute if and only if they are simultaneously diagonalizable. Of course, here we are dealing specifically with Hermitian matrices, and such matrices are always diagonalizable; furthermore, for our purposes it is enough to talk about two matrices rather than a larger set.

[42] Or more generally for any normal matrix, which satisfies $A^\dagger A = A A^\dagger$. As we mentioned before, both Hermitian and unitary matrices are special cases of normal matrices.

diagonalizable if both matrices are diagonalizable using the **same** unitary matrix P:

$$P^\dagger A_1 P = D_1, \qquad P^\dagger A_2 P = D_2, \tag{4.143}$$

where D_1 and D_2 are two diagonal matrices.

If A_1 and A_2 are simultaneously diagonalizable, we can invert (4.143) (by multiplying both sides by P from the left and $P^\dagger$ from the right) to find:

$$A_1 = PD_1P^\dagger, \qquad A_2 = PD_2P^\dagger. \tag{4.144}$$

Then the commutator of the two matrices is

$$\begin{aligned}
[A_1, A_2] &\equiv A_1A_2 - A_2A_1 \\
&= \left(PD_1P^\dagger\right)\left(PD_2P^\dagger\right) - \left(PD_2P^\dagger\right)\left(PD_1P^\dagger\right) \\
&= PD_1\left(P^\dagger P\right)D_2P^\dagger - PD_2\left(P^\dagger P\right)D_1P^\dagger \\
&= PD_1D_2P^\dagger - PD_2D_1P^\dagger \\
&= P\left(D_1D_2 - D_2D_1\right)P^\dagger \\
&= P\left[D_1, D_2\right]P^\dagger.
\end{aligned}$$

However, any two diagonal matrices commute with each other. Indeed, if

$$D_1 \equiv \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_n \end{pmatrix}, \qquad D_2 \equiv \begin{pmatrix} \mu_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \mu_n \end{pmatrix}, \tag{4.145}$$

then it is easy to see that

$$D_1D_2 = D_1D_2 = \begin{pmatrix} \lambda_1\mu_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_n\mu_n \end{pmatrix}. \tag{4.146}$$

Therefore $[D_1, D_2] = 0$, and we conclude that A_1 and A_2 commute:

$$[A_1, A_2] = 0. \tag{4.147}$$

It is possible to prove the opposite direction as well: **if** A_1 and A_2 commute, **then** they are simultaneously diagonalizable. However, we won't do this here.

So what does this mean? Let A_1 and A_2 be two commuting observables, represented by Hermitian operators. Then they are simultaneously diagonalizable. Now, remember that in Section 3.2.16 we said that the unitary matrix P, which in this case diagonalizes both matrices,

has for its columns an orthonormal eigenbasis $|B_i\rangle$:

$$P = \begin{pmatrix} |B_1\rangle & \cdots & |B_n\rangle \end{pmatrix}. \tag{4.148}$$

By inspecting (4.143) and (4.145), we see that the basis states $|B_i\rangle$ are eigenstates of **both** A_1 and A_2, with the eigenvalues:

$$A_1 |B_i\rangle = \lambda_i |B_i\rangle, \qquad A_2 |B_i\rangle = \mu_i |B_i\rangle. \tag{4.149}$$

This means that the eigenstates $|B_i\rangle$ are states where the system **simultaneously** has the exact value λ_i for the observable A_1 and the exact value μ_i for the observable A_2.

Conversely, since this is an if-and-only-if relationship, if A_1 and A_2 **don't** commute, then one **cannot** find a basis of eigenstates of both observables simultaneously (since if we found such a basis, then they would be simultaneously diagonalizable, in contradiction). This is essentially where the uncertainty principle comes from: if A_1 and A_2 don't commute and the system is in an eigenstate of A_1, then in general it can't also be in an eigenstate of A_2. This means it must instead be in a **superposition** of eigenstates of A_2, so there are many different possible values for the measurement of A_2 with different probabilities. So being certain of the value of A_1 means being necessarily uncertain of the exact value of A_2.

Exercise 4.36.

A. Show that the following Hermitian operator commutes with the Pauli operator σ_x:

$$A \equiv \begin{pmatrix} 1 & -3 \\ -3 & 1 \end{pmatrix}, \qquad \sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{4.150}$$

Therefore, they are simultaneously diagonalizable.

B. Show that the eigenstates of σ_x (see Section 4.2.1) are also eigenstates of A, and find their eigenvalues.

C. Find a unitary matrix P which diagonalizes both A and σ_x, and find the resulting diagonal matrices.

4.5 Dynamics, Transformations, and Measurements

4.5.1 Unitary Transformations and Evolution

We have covered almost all of the basic properties of quantum theory. However, notice that so far we only talked about quantum systems that are in one given state, and never change. In real life, physical systems change all the time, whether it's because some transformation was explicitly done to the system, or simply because time has passed. To account for that in the mathematical framework of quantum theory, let us introduce a new axiom:

The Evolution Axiom: If the system is in the state $|\Psi_1\rangle$ at some point in time, and in another state $|\Psi_2\rangle$ at another point in time, then the two states must be related by the action of some unitary operator U:

$$|\Psi_2\rangle = U|\Psi_1\rangle. \tag{4.151}$$

This is called *unitary evolution* or *unitary transformation*.

The exact form of U is determined by the specific quantum system in question and the specific transformation performed, for example rotating the system, moving it in space, or letting it "move itself" in time (i.e. just waiting for time to pass). All the Evolution Axiom tells us is that U must be a unitary operator – just like the Observable Axiom tells us that an observable must be represented by a Hermitian operator, but the exact form of the Hermitian operator depends on the specific system and the specific observable.

Now, in Section 3.2.13 we proved that unitary operators preserve the inner product between two states. This means that if we two states $|\Psi_1\rangle$ and $|\Phi_1\rangle$ at one time, and they evolve to $|\Psi_2\rangle = U|\Psi_1\rangle$ and $|\Phi_2\rangle = U|\Phi_1\rangle$ at another time, then the inner product of the new states $\langle\Psi_2|\Phi_2\rangle$ is equal to the inner product of the old states $\langle\Psi_1|\Phi_1\rangle$, because $U^\dagger U = 1$:

$$\langle\Psi_2|\Phi_2\rangle = \left(\langle\Psi_1|U^\dagger\right)(U|\Phi_1\rangle) = \langle\Psi_1|U^\dagger U|\Phi_1\rangle = \langle\Psi_1|\Phi_1\rangle. \tag{4.152}$$

Therefore, probability amplitudes are preserved by unitary evolution.

As a corollary, unitary evolution also preserves the norm of a vector – that is, $|\Psi\rangle$ and $U|\Psi\rangle$ have the same norm:

$$\|U\Psi\| = \sqrt{\langle\Psi|U^\dagger U|\Psi\rangle} = \sqrt{\langle\Psi|\Psi\rangle} = \|\Psi\|. \tag{4.153}$$

This has to be the case, since quantum states must have norm 1! So if we start with a properly normalized quantum state, we end up with another properly normalized quantum state.

Furthermore, recall that probabilities must sum to one. This means that, for an orthonormal eigenbasis $|B_i\rangle$, we must have

$$\sum_{i=1}^{n} |\langle B_i|\Psi\rangle|^2 = 1, \tag{4.154}$$

as we indeed proved in Section 4.1.4. Again, since each of the probability amplitudes $\langle B_i|\Psi\rangle$ is preserved by unitary evolution, we are guaranteed that the probabilities still sum to 1 after the states have evolved.

Lastly, observe that since any unitary operator is invertible (with the inverse of U being $U^{-1} = U^\dagger$), any unitary transformation has an inverse transformation. This means that unitary evolution is always reversible, and therefore quantum mechanics has *time-reversal symmetry*: it works exactly the same forwards in time and backwards in time.

If at time t_1 the system is in the state $|\Psi_1\rangle$ and at time $t_2 > t_1$ the system is in the state $|\Psi_2\rangle$, then they are either related by $|\Psi_2\rangle = U|\Psi_1\rangle$, evolving **forward** in time, or $|\Psi_1\rangle = U^\dagger|\Psi_2\rangle$ for the same U, evolving **backwards** in time. As far as quantum mechanics is concerned,

there is no distinction between the future and the past, and everything works the same if we take $t \mapsto -t$ so that $t_2 < t_1$, as long as we also replace every unitary evolution operator by its adjoint.

Exercise 4.37. The system was previously in the state

$$|\Psi_1\rangle = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2\,\mathrm{i} \end{pmatrix}. \tag{4.155}$$

Now, it is in the state

$$|\Psi_2\rangle = \frac{1}{\sqrt{5}} \begin{pmatrix} 2\,\mathrm{i} \\ -1 \end{pmatrix}. \tag{4.156}$$

Which unitary operator U was responsible for this evolution (such that $|\Psi_2\rangle = U\,|\Psi_1\rangle$)? What will be the state of the system after the same amount of time has passed again (i.e. after another evolution with U)?

4.5.2 Quantum Logic Gates

In a classical computer, bits are manipulated using *logic gates*. In logic terms, these gates treat 0 as "false" and 1 as "true". Let us list some examples of logic gates.

NOT gets a single bit as input, and outputs 1 minus that bit. In logic terms, it outputs "true" if it gets "false" and vice versa, so the output is the negation of the input:

Input	NOT
0	1
1	0

AND gets two bits as input, and outputs 1 if both bits are 1, otherwise it outputs 0. In logic terms, it outputs "true" only if both bit A **and** bit B are "true":

Input A	Input B	AND
0	0	0
0	1	0
1	0	0
1	1	1

OR gets two bits as input, and outputs 1 if at least one of the bits is 1, otherwise it outputs 0. In logic terms, it outputs "true" if either bit A **or** bit B **or both** are "true":

Input A	Input B	OR
0	0	0
0	1	1
1	0	1
1	1	1

XOR (*eXclusive OR*, pronounced "ex or") gets two bits as input, and outputs 1 if exactly one of the bits is 1, otherwise it outputs 0. In logic terms, it outputs "true" if either bit A **or** bit B, but **not both**, are "true":

Input A	Input B	XOR
0	0	0
0	1	1
1	0	1
1	1	0

In quantum computers we have qubits instead of classical bits, and thus we must use *quantum logic gates*, or *quantum gates* for short. Since they transform qubits from one state to the other, quantum gates must take the form of unitary operators, by the Evolution Axiom.

As a simple example, let us define the *quantum NOT gate*, which flips $|0\rangle \leftrightarrow |1\rangle$, just like a classical NOT gate flips $0 \leftrightarrow 1$. This gate is none other than the Pauli matrix σ_x, which is of course unitary:

$$\text{NOT} \equiv X \equiv \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{4.157}$$

(The notation X for the NOT gate is common in quantum computing.) Indeed, we have

$$\text{NOT}\,|0\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle\,, \tag{4.158}$$

$$\text{NOT}\,|1\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle\,. \tag{4.159}$$

Since unitary transformations are linear, this means that for a general qubit state we have

$$\text{NOT}\,(a\,|0\rangle + b\,|1\rangle) = a\,|1\rangle + b\,|0\rangle\,, \tag{4.160}$$

where of course $|a|^2 + |b|^2 = 1$.

In classical computers there is only one non-trivial single-bit gate, the NOT gate; the two other options would be the gate $0 \mapsto 0$, $1 \mapsto 0$ and the gate $0 \mapsto 1$, $1 \mapsto 1$, which are trivial gates since their output is fixed and does not depend on the input. However, in quantum computers, since qubits are in a superposition of $|0\rangle$ and $|1\rangle$, we have more options; in fact, we have an **infinite** number of possible single-qubit gates, since any unitary operator can be a single-qubit gate.

One example of a useful quantum gate is the *Z gate*, which is just the Pauli matrix σ_z:

$$Z \equiv \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{4.161}$$

and has the action

$$Z|0\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle\,, \tag{4.162}$$

$$Z|1\rangle = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix} = -|1\rangle\,, \tag{4.163}$$

so it leaves $|0\rangle$ unchanged but flips the phase of $|1\rangle$.

Another example is the *Hadamard gate*:

$$H \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{4.164}$$

which turns $|0\rangle$ and $|1\rangle$ (the eigenstates of σ_z) into $|+\rangle$ and $|-\rangle$ respectively (the eigenstates of σ_x):

$$H|0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) = |+\rangle\,, \tag{4.165}$$

$$H|1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) = |-\rangle\,. \tag{4.166}$$

What about two-qubit gates? Notice that classical two-bit gates such as AND, OR, and XOR are **irreversible**, since if we are given the single output bit of any of these gates, we cannot in general reconstruct the two input bits. For example, if AND outputs 0, then the inputs could have been any of 00, 01, or 10. In contrast, quantum gates must be represented by unitary operators, and as we saw in Section 4.5.1, unitary transformations are **reversible**. Thus we cannot use AND, OR, XOR, and other irreversible logic gates in quantum computing.

We can, however, define other two-qubit quantum gates. A very useful example is the *controlled-NOT* or CNOT gate. Here, the first qubit controls whether the second qubit gets flipped or not. If the first qubit is $|0\rangle$, then the second qubit is unchanged; if the first qubit is $|1\rangle$, then the second qubit is flipped $|0\rangle \leftrightarrow |1\rangle$. So, given an input state of two qubits, we have:

$$\text{CNOT}\,|0\rangle \otimes |0\rangle = |0\rangle \otimes |0\rangle\,, \tag{4.167}$$

$$\text{CNOT}\,|0\rangle \otimes |1\rangle = |0\rangle \otimes |1\rangle\,, \tag{4.168}$$

$$\text{CNOT}\,|1\rangle \otimes |0\rangle = |1\rangle \otimes |1\rangle\,, \tag{4.169}$$

$$\text{CNOT}\,|1\rangle \otimes |1\rangle = |1\rangle \otimes |0\rangle\,. \tag{4.170}$$

As you will verify in Exercise 4.38, the CNOT gate can be represented by the unitary matrix

$$\text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{4.171}$$

Alternatively, as you will verify in Exercise 4.39, the CNOT gate can be represented by a tensor product of outer products:

$$\text{CNOT} = |0\rangle\langle 0| \otimes \Big(|0\rangle\langle 0| + |1\rangle\langle 1| \Big) + |1\rangle\langle 1| \otimes \Big(|0\rangle\langle 1| + |1\rangle\langle 0| \Big). \tag{4.172}$$

Exercise 4.38. Verify that the matrix definition of the CNOT operator given in (4.171) indeed has the action described in equations (4.167), (4.168), (4.169), and (4.170).

Exercise 4.39. Verify that the CNOT operator has the outer product representation

$$\text{CNOT} = |0\rangle\langle 0| \otimes \Big(|0\rangle\langle 0| + |1\rangle\langle 1| \Big) + |1\rangle\langle 1| \otimes \Big(|0\rangle\langle 1| + |1\rangle\langle 0| \Big). \tag{4.173}$$

You can either do so by explicitly calculating the matrix representations of the outer products and tensor products and adding them up to get the matrix in (4.171), or by showing that this operator has the required action on the two-qubit basis states.

Exercise 4.40. Show that the Hadamard gate turns $|+\rangle$ back into $|0\rangle$ and $|-\rangle$ back into $|1\rangle$. Note: You don't actually have to do an explicit calculation, you can simply use a certain property of the matrix H itself.

Problem 4.41. Find an outer product representation for the Hadamard operator (4.164).

Problem 4.42. Show how you can generate each of the four entangled Bell states by acting on the separable state $|0\rangle \otimes |0\rangle$ with various quantum gates. This means that quantum gates can be used to generate entanglement if it's not already there.

4.5.3 The Measurement Axiom (Projective)

In Section 4.1.4, we formulated the Probability Axiom: if the system is in the state $|\Psi\rangle$, then the probability to measure the eigenvalue λ_i corresponding to the eigenstate $|B_i\rangle$ of an observable is given by $|\langle B_i|\Psi\rangle|^2$. This axiom was good enough at the time, but after all that we have learned in the previous sections, we can now see that this axiom is missing two important things:

1. It doesn't tell us what happens if we measure just one part of a composite system,
2. It doesn't tell us about dynamics: what happens to the system after we perform the measurement.

To correct that, we now replace the Probability Axiom with a new and improved axiom, which we call the Measurement Axiom. In order to formulate it, let us recall that in Problem 3.55 you proved that if A is normal (so in particular, if it is Hermitian and thus an observable), then it has the outer product representation

$$A = \sum_{i=1}^{n} \lambda_i |B_i\rangle \langle B_i| , \tag{4.174}$$

where $|B_i\rangle$ is an orthonormal eigenbasis and λ_i are the eigenvalues of the eigenstates $|B_i\rangle$. More generally, for any observable we can write

$$A = \sum_{i=1}^{n} \lambda_i P_i, \tag{4.175}$$

where P_i is the *projector* onto the vector space of the eigenvectors corresponding to the eigenvalue λ_i, called the *eigenspace* of λ_i (see Problem 4.43). Using projectors allows us to:

1. Deal with the case of *degenerate eigenvectors*, where two eigenvectors have the same eigenvalue; so far we have always implicitly assumed that observables do not have any degenerate eigenvectors. A trivial example of an operator with degenerate eigenvalues is the identity matrix 1, which has only one eigenvalue – namely, 1 – for which **every** vector in the space is an eigenvector.

2. Measure only part of a composite Hilbert space, for example one qubit in a composite system of two qubits, as we will see below.

In the simple case where there is no degeneracy of eigenvectors and the measurement is performed on the entire Hilbert space, the projector can take the simple form

$$P_i \equiv |B_i\rangle \langle B_i| , \tag{4.176}$$

and we recover (4.174). Using projectors, we can now define a very general Measurement Axiom, which employs so-called *projective measurements*.

The Measurement Axiom (Projective): Consider an observable A of the form

$$A = \sum_{i=1}^{n} \lambda_i P_i. \tag{4.177}$$

If the system is in the state $|\Psi\rangle$, then the probability to measure the eigenvalue λ_i is given by

$$\langle \Psi | P_i | \Psi \rangle. \tag{4.178}$$

The measurement yields exactly one of the eigenvalues λ_i, and after the measurement, the

system *collapses* to the state[43]

$$|\Psi\rangle \mapsto \frac{P_i |\Psi\rangle}{\sqrt{\langle\Psi|P_i|\Psi\rangle}}, \tag{4.179}$$

where P_i is the projector corresponding to the specific eigenvalue λ_i that was measured.

Problem 4.43. Let A be a normal operator with eigenvalues λ_i. Each eigenvalue has a corresponding eigenspace, which is the set of all vectors which have the eigenvalue λ_i. Prove that each eigenspace is a vector space by showing that it satisfies the properties of a vector space as defined in Section 3.2.1.

Exercise 4.44. Find the eigenvalues of the CNOT operator (4.171) and their corresponding eigenvectors and eigenspaces.

4.5.4 Applications of the Measurement Axiom

Let us now see some examples of the Measurement Axiom in action. First of all, consider a qubit in the general state

$$|\Psi\rangle = a|0\rangle + b|1\rangle, \qquad |a|^2 + |b|^2 = 1. \tag{4.180}$$

The observable corresponding to the eigenbasis $|0\rangle, |1\rangle$ is the Pauli matrix σ_z, which has the outer product representation

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = |0\rangle\langle 0| - |1\rangle\langle 1|. \tag{4.181}$$

This means that we have[44]

$$\lambda_0 = +1, \qquad P_0 = |0\rangle\langle 0|, \tag{4.182}$$

$$\lambda_1 = -1, \qquad P_1 = |1\rangle\langle 1|. \tag{4.183}$$

The probability to measure the eigenvalue $+1$ (corresponding to a value of 0 for the qubit) is thus

$$\langle\Psi|P_0|\Psi\rangle = \langle\Psi|\Big(|0\rangle\langle 0|\Big)|\Psi\rangle = \langle\Psi|0\rangle\langle 0|\Psi\rangle = |\langle 0|\Psi\rangle|^2 = |a|^2, \tag{4.184}$$

and the probability to measure the eigenvalue -1 (corresponding to a value of 1 for the qubit) is

$$\langle\Psi|P_1|\Psi\rangle = \langle\Psi|\Big(|1\rangle\langle 1|\Big)|\Psi\rangle = \langle\Psi|1\rangle\langle 1|\Psi\rangle = |\langle 1|\Psi\rangle|^2 = |b|^2. \tag{4.185}$$

[43] Notice that the square root of the probability is not necessarily the probability amplitude. For example, if the amplitude is $\mathrm{i}/2$ then the probability is $1/4$, but the square root of that is $1/2$, which is not the amplitude we started with! However, recall that the two vectors $|\Psi\rangle$ and $\mathrm{e}^{\mathrm{i}\phi}|\Psi\rangle$, which differ by an overall complex phase $\mathrm{e}^{\mathrm{i}\phi}$, represent the same state. Since the square root of the probability is the same as the amplitude up to a complex phase, dividing by $\mathrm{i}/2$ or $1/2$ both result in the **same** state.

[44] Note that I decided to start counting i from 0 to 1 instead of from 1 to 2, so that the subscript of λ_i will correspond to the value of the qubit. Also, recall that the eigenvalue of $|0\rangle$ is **not** 0, it's -1, and the eigenvalue of $|1\rangle$ is **not** 1, it's $+1$; this is confusing, but unfortunately it's standard notation, since qubits are analogous to classical bits which have the values 0 and 1.

This indeed matches the old Probability Axiom. The new part is that after the measurement, if we measured 0, then the system will collapse to the state

$$|\Psi\rangle \mapsto \frac{P_0\,|\Psi\rangle}{\sqrt{\langle\Psi|P_0|\Psi\rangle}} = \frac{|0\rangle\langle 0|\Psi\rangle}{|a|} = \frac{a}{|a|}|0\rangle \simeq |0\rangle\,, \tag{4.186}$$

where by $\simeq$ we mean that $\frac{a}{|a|}|0\rangle$ and $|0\rangle$ are the same state, since they only differ by a complex phase (see Footnote 43; in polar coordinates we have $a = |a|\,\mathrm{e}^{\mathrm{i}\,\phi}$ where $\mathrm{e}^{\mathrm{i}\,\phi}$ is the phase of a, so if we divide a by $|a|$ we are left with just the phase). Similarly, if we measured 1 then the system will collapse to the state

$$|\Psi\rangle \mapsto \frac{P_1\,|\Psi\rangle}{\sqrt{\langle\Psi|P_1|\Psi\rangle}} = \frac{|1\rangle\langle 1|\Psi\rangle}{|b|} = \frac{b}{|b|}|1\rangle \simeq |1\rangle\,. \tag{4.187}$$

Consider now the general composite state of two qubits given in (4.72):

$$|\Psi\rangle = \alpha_{00}\,|0\rangle\otimes|0\rangle + \alpha_{01}\,|0\rangle\otimes|1\rangle + \alpha_{10}\,|1\rangle\otimes|0\rangle + \alpha_{11}\,|1\rangle\otimes|1\rangle\,, \tag{4.188}$$

which is of course normalized such that

$$\|\Psi\|^2 = |\alpha_{00}|^2 + |\alpha_{01}|^2 + |\alpha_{10}|^2 + |\alpha_{11}|^2 = 1. \tag{4.189}$$

We can define an observable corresponding to a measurement of only the **first** qubit as follows:

$$\sigma_z \otimes 1 = \Big(\,|0\rangle\,\langle 0| - |1\rangle\,\langle 1|\Big)\otimes 1, \tag{4.190}$$

where 1 is the identity operator. So we have

$$P_0 = |0\rangle\,\langle 0|\otimes 1, \qquad P_1 = |1\rangle\,\langle 1|\otimes 1. \tag{4.191}$$

Then the probability to measure 0 for the first qubit is

$$\langle\Psi|P_0|\Psi\rangle = \langle\Psi|\,\Big(|0\rangle\langle 0|\otimes 1\Big)\,|\Psi\rangle. \tag{4.192}$$

Let us first calculate[45] the action of the operator $P_0 = |0\rangle\langle 0| \otimes 1$ on the ket $|\Psi\rangle$:

$$\begin{aligned} P_0 |\Psi\rangle &= \Big(|0\rangle\langle 0| \otimes 1\Big) |\Psi\rangle \\ &= \Big(|0\rangle\langle 0| \otimes 1\Big) \Big(\alpha_{00} |0\rangle \otimes |0\rangle + \alpha_{01} |0\rangle \otimes |1\rangle + \alpha_{10} |1\rangle \otimes |0\rangle + \alpha_{11} |1\rangle \otimes |1\rangle\Big) \\ &= |0\rangle \otimes \Big(\alpha_{00}\langle 0|0\rangle |0\rangle + \alpha_{01}\langle 0|0\rangle |1\rangle + \alpha_{10}\langle 0|1\rangle |0\rangle + \alpha_{11}\langle 0|1\rangle |1\rangle\Big) \\ &= |0\rangle \otimes \Big(\alpha_{00} |0\rangle + \alpha_{01} |1\rangle\Big), \end{aligned}$$

since $|0\rangle$ and $|1\rangle$ form an orthonormal basis, so $\langle 0|0\rangle = \langle 1|1\rangle = 1$ and $\langle 0|1\rangle = \langle 1|0\rangle = 0$. Then we act with the bra $\langle\Psi|$ from the left:

$$\begin{aligned} \langle\Psi|P_0|\Psi\rangle &= \langle\Psi| \Big(|0\rangle\langle 0| \otimes 1\Big) |\Psi\rangle \\ &= \langle\Psi| \Big(|0\rangle \otimes (\alpha_{00} |0\rangle + \alpha_{01} |1\rangle)\Big) \\ &= \Big(\alpha_{00}^* \langle 0| \otimes \langle 0| + \alpha_{01}^* \langle 0| \otimes \langle 1| + \alpha_{10}^* \langle 1| \otimes \langle 0| + \alpha_{11}^* \langle 1| \otimes \langle 1|\Big) \Big(|0\rangle \otimes \Big(\alpha_{00} |0\rangle + \alpha_{01} |1\rangle\Big)\Big) \\ &= \alpha_{00}^* \langle 0| \Big(\alpha_{00} |0\rangle + \alpha_{01} |1\rangle\Big) + \alpha_{01}^* \langle 1| \Big(\alpha_{00} |0\rangle + \alpha_{01} |1\rangle\Big) \\ &= |\alpha_{00}|^2 + |\alpha_{01}|^2 . \end{aligned}$$

Similarly, we also find that the probability to measure 1 for the first qubit is

$$\langle\Psi|P_1|\Psi\rangle = \langle\Psi| \Big(|1\rangle\langle 1| \otimes 1\Big) |\Psi\rangle = |\alpha_{10}|^2 + |\alpha_{11}|^2 . \tag{4.193}$$

These very complicated calculations tell us what we could have just guessed from common sense: the total probability to measure $|0\rangle$ is the sum of the probabilities to measure all the composite states which have $|0\rangle$ as the state of the first qubit, and similarly for $|1\rangle$.

What about collapse? If we measured 0, then the system will collapse to the state

$$\frac{P_0 |\Psi\rangle}{\sqrt{\langle\Psi|P_0|\Psi\rangle}} = \frac{\alpha_{00}|0\rangle \otimes |0\rangle + \alpha_{01}|0\rangle \otimes |1\rangle}{\sqrt{|\alpha_{00}|^2 + |\alpha_{01}|^2}}, \tag{4.194}$$

and if we measured 1, it will collapse to the state

$$\frac{P_1 |\Psi\rangle}{\sqrt{\langle\Psi|P_1|\Psi\rangle}} = \frac{\alpha_{10}|1\rangle \otimes |0\rangle + \alpha_{11}|1\rangle \otimes |1\rangle}{\sqrt{|\alpha_{10}|^2 + |\alpha_{11}|^2}}. \tag{4.195}$$

Again, we could have just guessed the result: the qubit that we measured collapses into either $|0\rangle$ or $|1\rangle$, while the other qubit stays in a superposition. The denominator is there simply to normalize the vector so it has norm 1, and can thus represent a state.

[45] To understand this calculation, you might want to review how tensor products work, which we discussed in Section 4.3.1.

Problem 4.45. Consider a composite system of three qubits. Which projectors will you use to measure only the state of the middle qubit in the $|+\rangle, |-\rangle$ eigenbasis? Which projectors will you use to measure only the state of the first two qubits in the $|0\rangle, |1\rangle$ eigenbasis?

4.5.5 The Measurement Axiom (Simplified)

Now that we understand how projective measurements works, we can formulate a simpler version of the Measurement Axiom, which does not require projective measurements, and will be sufficient for our purposes in the rest of this course.

The Measurement Axiom (Simplified):

- Consider an observable with an eigenbasis of non-degenerate eigenstates $|B_i\rangle$ corresponding to eigenvalues λ_i. If the system is in the state $|\Psi\rangle$, then the probability to measure the eigenvalue λ_i corresponding to the eigenstate $|B_i\rangle$ is given by

$$|\langle B_i|\Psi\rangle|^2 . \tag{4.196}$$

  After the measurement, if the eigenvalue λ_i was measured, then the system will collapse to the eigenstate $|B_i\rangle$:

$$|\Psi\rangle \mapsto |B_i\rangle . \tag{4.197}$$

  This works the same whether the system in question is composite or not, provided that the measurement is performed on the entire system at once.

- Now consider a composite system and an observable defined only on part of that system, with non-degenerate eigenstates $|B_i\rangle$ corresponding to eigenvalues λ_i. The total probability to measure the eigenvalue λ_i is the sum of the probabilities for all the possible ways in which this eigenvalue can be measured – that is, the sum of the magnitude-squared of the probability amplitudes of all the composite states where the part being measured is in the eigenstate $|B_i\rangle$. After the measurement, if the eigenvalue λ_i was measured, then only the system we measured will collapse to the eigenstate $|B_i\rangle$, while the other systems will stay in a superposition.

The process described by the Measurement Axiom, where the state of the system changes after a measurement, is what people mean when they talk about *wavefunction collapse*. However, we haven't yet defined what a "wavefunction" is. This is because in the modern abstract formulation of quantum mechanics, which is what we have been studying so far, **states** are the fundamental entities, not wavefunctions. We will explain this in more detail when we define wavefunctions in Section 6.5.

Problem 4.46. A composite system of two qubits is in the state

$$|\Psi\rangle = \frac{1}{\sqrt{14}} \left(2|00\rangle - \mathrm{i}|10\rangle + 3|11\rangle\right) . \tag{4.198}$$

A measurement is performed on only the first qubit, in the $|+\rangle, |-\rangle$ eigenbasis. For each of the two possible outcomes, what is the probability to measure that outcome and what will be the state of the system after the measurement?

Problem 4.47. A composite system of three qubits is in the state

$$|\Psi\rangle = \frac{1}{\sqrt{35}} \left(|000\rangle + 2\,|010\rangle - 3\,\mathrm{i}\,|011\rangle - 4\,|101\rangle + \mathrm{i}\,|110\rangle + 2\,\mathrm{i}\,|111\rangle \right), \tag{4.199}$$

where $|000\rangle \equiv |0\rangle \otimes |0\rangle \otimes |0\rangle$ and so on. A measurement is performed on only the **first two** qubits in the $|0\rangle, |1\rangle$ basis. For each of the **four** possible outcomes, what is the probability to measure that outcome and what will be the state of the system after the measurement? You can either solve this problem by inspection using the simplified axiom, or by explicit calculation using the projectors you found in Problem 4.45.

4.5.6 Interpretations of Quantum Mechanics and the Measurement Problem

If you consider the collapse process carefully, you will realize that it is actually incompatible with the Evolution Axiom. This is because the collapse is a type of time evolution: the system was in the state $|\Psi\rangle$ before the measurement, and will be in one of the eigenstates $|B_i\rangle$ after the measurement. However, this evolution is not unitary, because it is not invertible.

Given the probabilistic nature of the measurement, the information that the system is currently in the eigenstate $|B_i\rangle$ is not enough to reconstruct the state $|\Psi\rangle$ of the system before the measurement, which was a superposition of all the eigenstates $|B_1\rangle, |B_2\rangle, \ldots, |B_n\rangle$. The information about the coefficients of each eigenstate in the superposition is lost forever.

This incompatibility, and more generally our failure to understand the exact nature of measurement and collapse in quantum mechanics, is called the *measurement problem*. Many physicists believe that quantum theory will remain fundamentally incomplete until we manage to solve the measurement problem, and this is an area of active research. The current approaches towards solving this problem largely fall into several distinct groups, which more or less coincide with specific *interpretations of quantum mechanics*. Let us list some of them.

"Shut up and calculate": This approach simply ignores the measurement problem. It is not necessarily associated with any particular interpretation, since it doesn't care about trying to interpret the theory in the first place. However, one could associate it with the *Copenhagen interpretation*, the earliest interpretation of quantum mechanics, which essentially just accepts the Measurement Axiom at face value, without attempting to explain why there is a collapse. This interpretation regards quantum states as merely a tool to calculate probabilities, and ignores questions like "what was the spin of the particle before I measured it".

This approach is, by far, the most popular one among physicists, with a recent survey indicating that around a third of physicists subscribe to the Copenhagen interpretation and another third don't have any preferred interpretation. However, this definitely doesn't mean it is the "best" approach. It is popular simply because in practice, as long as quantum mechan-

ics enables us to make accurate predictions, it doesn't matter how (or even if) the collapse happens.

The applications of quantum mechanics to theoretical, experimental, and applied physics, as well as to other fields of science and technology, do not require us to solve the measurement problem. However, as practical as this approach is, adopting it means ignoring deep and fundamental questions about the nature of reality which, if answered, could have far-reaching consequences.

There is no collapse: This approach claims that collapse does not actually happen. The most well-known example of this approach is the *Everett or "many-worlds" interpretation*, which gets rid of the collapse by considering the state of every system to be part of a huge composite state which describes the entire universe. Measurements then simply correspond to entangling two parts of that composite state – the system being measured, and the observer. Instead of a collapse, the observer is now in a superposition of having measured each eigenvalue. For example, if I measured a qubit, I will then be in a superposition of "I measured 0" and "I measured 1". This process is completely unitary (and invertible), thus there is no collapse and no incompatibility with the Evolution Axiom.

It is a common misconception that the name "many worlds" means measurements somehow "create" new "parallel universes", one for each measurement outcome. What really happens is that there is just one universe, but that universe is in a superposition of many different possibilities – the sum total of every single superposition of every individual system since the Big Bang. For example, a toy universe made of n qubits will be in a superposition of 2^n different possibilities or "parallel universes". However, it's important to stress that the defining property of this interpretation is **not** the "many worlds" part – it is the "no collapse" part!

Let's see how exactly this works. Say Alice is measuring a qubit. The individual states of the qubit and Alice before the measurement are

$$|\text{qubit}\rangle = a\,|0\rangle + b\,|1\rangle\,, \qquad |\text{Alice}\rangle = |\text{Alice hasn't measured yet}\rangle\,. \tag{4.200}$$

The composite state of both of them together before the measurement is thus

$$|\Psi_1\rangle \equiv |\text{qubit}\rangle \otimes |\text{Alice}\rangle = (a\,|0\rangle + b\,|1\rangle) \otimes |\text{Alice hasn't measured yet}\rangle\,. \tag{4.201}$$

Notice that $|\Psi_1\rangle$ is **separable** – it is just a tensor product of the state of the qubit with the state of Alice, and those states are independent of each other.

After the qubit is measured, the system undergoes evolution with a unitary operator U into:

$$|\Psi_2\rangle \equiv U\,|\Psi_1\rangle\,, \tag{4.202}$$

$$|\Psi_2\rangle = a\,|0\rangle \otimes |\text{Alice measured 0}\rangle + b\,|1\rangle \otimes |\text{Alice measured 1}\rangle\,. \tag{4.203}$$

Intuitively, we can see that this evolution is unitary because it works similarly to a CNOT

gate; U essentially checks the state of the qubit, and changes Alice's state accordingly. In Problem 4.49 you will find the exact form of this unitary operator. We can see that the new state $|\Psi_2\rangle$ is **entangled** – the states of the qubit and Alice are now correlated.

We can think of each term in the superposition as a different "parallel universe" or "world", but this isn't quite the same as the typical (incorrect) science-fiction treatment of the many-worlds interpretation, since the two versions of Alice, the Alice who measured 0 and the Alice who measured 1, can never communicate with each other, and there is no sense in which you can "travel" from one "parallel universe" to another – since you can't change which term in the superposition you are in!

Crucially, notice that in the calculation we did above, there is no collapse. It **looks like** there is a collapse from the point of view of each of the Alices, since the Alice who measured 0 can only access the qubit in the state $|0\rangle$ (with which she is entangled) and the Alice who measured 1 can only access the qubit in the state $|1\rangle$. However, the overall state of the qubit and Alice (and more broadly, of the entire universe) in fact evolves in a way that is perfectly compatible with the Evolution Axiom, and at no point does it reduce to a single eigenstate.

This interpretation is probably the most popular among the approaches which are not Copenhagen or "shut up and calculate". This is perhaps due to its simplicity – it does not introduce any new assumptions, as most other interpretations do, and in fact it even gets rid of an assumption, namely the collapse part of the Measurement Axiom, so it arguably makes quantum theory even simpler.

However, it has several unresolved issues. One of its main problems is that it is unclear where exactly probabilities come from. If I split into several observers after the measurement, and the different versions of me collectively measured every single possible outcome of the measurement, then why is the probability for me to find myself as one observer different from the probability to find myself as another observer? And what does this probability have to do with the coefficients of the superposition?

Hidden variables: This approach is associated with interpretations such as *De Broglie–Bohm theory*, which we already mentioned in Sections 4.2.4 and 4.3.6 in the context of non-locality.

To remind you, theories of hidden variables involve adding supplemental variables which make the theory deterministic "behind the scenes", but we can't actually know the values of these variables and use them to make deterministic predictions, since they're "hidden". As the system is deterministic, there is no collapse.

One serious problem with this approach is, as we discussed earlier, that theories of hidden variables tend to be complicated, and many physicists find them contrived and ad-hoc. Therefore, if we subscribe to the principle of *Occam's razor*, which states that theories with less assumptions should be preferred, we should discard hidden variables in favor of simpler interpretations.

Collapse models: This approach modifies quantum mechanics by adding an actual physical mechanism for collapse. This can be done by assuming that there is a more general type of evolution, which is compatible with both unitary evolution and collapse. Collapse models

have the same problem as hidden variable theories; they require additional assumptions and more complicated equations, which are not necessarily justified except in that they give the desired results.

For example, one collapse model, the *GRW model*, assumes that quantum systems collapse spontaneously – at random, without any relation to measurements. This happens very rarely, but when you have a big enough composite system with a very large number of subsystems, it happens frequently enough to explain collapse.

Problem 4.48. There are many other interpretations of quantum mechanics, each attempting to solve the measurement problem in a different way. We will not discuss them here, but you are encouraged to look them up and discuss them with your classmates. Which interpretation is your favorite?

Problem 4.49. Find the unitary operator U in (4.202). Treat Alice as a 3-state system with an orthonormal basis

$$|A_0\rangle \equiv |\text{Alice measured } 0\rangle\,, \tag{4.204}$$

$$|A_1\rangle \equiv |\text{Alice measured } 1\rangle\,, \tag{4.205}$$

$$|A\rangle \equiv |\text{Alice hasn't measured yet}\rangle\,. \tag{4.206}$$

You can either write U as an outer product representation, or as a matrix represented in the basis constructed from tensor products of the bases of each system, namely $|0\rangle\,, |1\rangle$ and $|A\rangle\,, |A_0\rangle\,, |A_1\rangle$. Hint: $|A\rangle\,, |A_0\rangle\,, |A_1\rangle$, represented in their own basis, are just the standard basis vectors of $\mathbb{C}^3$. You may have to do some guesswork regarding the precise form of U. Prove that the operator U that you found is unitary and that it transforms $|\Psi_1\rangle$ into $|\Psi_2\rangle$.

4.5.7 Superposition Once Again: Schrödinger's Cat

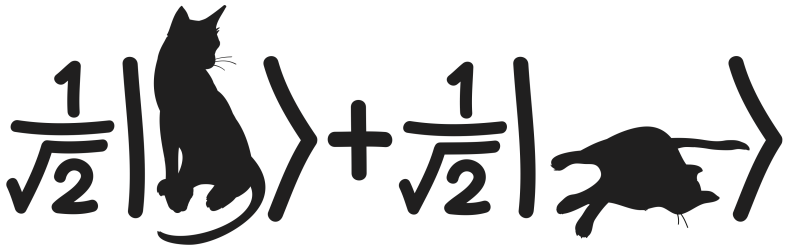

Figure 4.2: Schrödinger's Cat. *Source: Found via Google Image Search, original source unknown.*

Suppose that, inside a box, there is a cat and a qubit in the state $|+\rangle$:

$$|+\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right). \tag{4.207}$$

A measurement apparatus measures the qubit. If it measures 0 (with 50% probability), the cat dies[46]. If it measures 1 (with 50% probability), the cat stays alive. Therefore, the state of the cat is now a superposition of dead and alive (see Figure 4.2):

$$|\text{cat}\rangle = \frac{1}{\sqrt{2}} \left(|\text{dead}\rangle + |\text{alive}\rangle \right). \tag{4.208}$$

Before we open the box and measure the state of the cat, is it "actually" dead, or alive? A qubit being in a superposition of 0 and 1, compared to a classical bit which can only be either 0 or 1, might not be intuitive, but it is nevertheless an experimental fact. The thought of an animal being in a superposition of dead and alive, on the other hand, seems absurd.

This thought experiment was suggested by Schrödinger in the early days of quantum mechanics to illustrate this discrepancy between the quantum world (of elementary particles, atoms, qubits, and so on) and the classical world (of cats and everything else we know from our daily life).

So what exactly is the difference between a qubit and a cat? Well, the qubit has an infinite number of eigenbases, corresponding to measurements of spin up or down along every possible direction – as we saw in Section 4.2.2. All of these eigenbases are completely equivalent; there is no preferred basis. So being in an eigenstate of σ_z ($|0\rangle$ or $|1\rangle$) isn't any more "natural" for the qubit than being in an eigenstate of σ_x ($|+\rangle$ or $|-\rangle$, which can both be written as a superposition of $|0\rangle$ and $|1\rangle$).

However, the cat definitely has a preferred eigenbasis: the one composed of eigenstates of the "is the cat alive" operator, namely $|\text{dead}\rangle$ and $|\text{alive}\rangle$. There is no operator that has $\left(|\text{dead}\rangle + |\text{alive}\rangle \right) / \sqrt{2}$ as one of its eigenstates (like σ_x is to σ_z). This is because the cat is **not** a two-state system; it is composed of a huge number of entangled quantum particles that interact with each other in complicated ways, and the Hilbert space required to describe the states of the system has many orders of magnitude more than two dimensions.

Now, even a qubit, which is described by a 2-dimensional Hilbert space, is already extremely fragile. As soon as it interacts with the environment, it gets entangled with it, and loses its superposition and other quantum properties in a process called *quantum decoherence*. This is one of the reasons it is so hard to build quantum computers: qubits will inevitably interact with the environment, since they cannot be completely isolated. There is a certain time, called the *decoherence time*, after which different physical realizations of qubits undergo decoherence; the time it takes the quantum gate to operate must be shorter than the decoherence time.

It should therefore not be a surprise that the cat, which is incredibly more complicated, is also incredibly harder to keep in a superposition. The cat is still a quantum system, just like anything else in the universe, but it is so complicated, that it can't be in arbitrary states. Instead, with almost certain probability, it will be in one of the states $|\text{dead}\rangle$ or $|\text{alive}\rangle$.

Finally, let us address two common misconceptions about Schrödinger's cat. The first one

[46] For example, poison is released into the box. This is just a thought experiment, please do not attempt it at home!

(which is also a misconception about quantum mechanics in general) is that a conscious observer is needed to collapse the cat into being alive or dead. In fact, consciousness plays no role whatsoever in quantum mechanics! There is nothing special about conscious observers that unconscious measurement devices do not have. In both cases, the interaction of the quantum system with a larger system – whether it's a human or a particle detector – causes it to undergo decoherence and appear classical.

The second misconception occurs when Schrödinger's cat is invoked in any situation where the state of something is unknown until it is measured. Usually this takes the form of "Schrödinger's X" for some X. For example, I heard the term "Schrödinger's millionaire" being used to describe someone who has a lottery ticket which they have not yet checked to see if it's the winning ticket; therefore, that person is "both a millionaire and not a millionaire until the ticket is checked". However, the fact that you don't know the state of something until you measure it is completely trivial, and has nothing to do with Schrödinger's cat, or even with quantum mechanics in general. The purpose of the Schrödinger's cat thought experiment is to illustrate the difference between the classical and quantum worlds.

4.6 The Foundations of Quantum Theory: Summary

Quantum theory is a fundamental mathematical framework for describing physical systems in our universe. For discrete systems, which have finite-dimensional Hilbert spaces, we defined this framework using a set of seven axioms:

1. **The System Axiom:** Discrete physical systems are represented by complex n-dimensional Hilbert spaces $\mathbb{C}^n$, where n depends on the specific system.

2. **The State Axiom:** The states of the system are represented by unit n-vectors in the system's Hilbert space, up to a complex phase.

3. **The Operator Axiom:** The operators on the system, which act on states to produce other states, are represented by $n \times n$ matrices in the system's Hilbert space.

4. **The Observable Axiom:** Physical observables in the system are represented by Hermitian operators on the system's Hilbert space. The eigenvalues of the observable (which are always real, since it's Hermitian) represent its possible measured values. The eigenstates of the observable can be used to form an orthonormal eigenbasis of the Hilbert space.

    - **Superposition:** Any state $|\Psi\rangle$ can be written as a linear combination of the eigenstates $|B_i\rangle$ of an observable:

$$|\Psi\rangle = \sum_{i=1}^{n} |B_i\rangle\langle B_i|\Psi\rangle. \tag{4.209}$$

5. **The Composite System Axiom:** The Hilbert space of a composite system is represented by the tensor product of the individual systems.

- **Entanglement:** A state of a composite system that cannot be written as a single tensor product of states of the individual systems is entangled. Quantum entanglement is a form of correlation between systems, and by Bell's theorem, it is stronger than classical correlation.

6. **The Evolution Axiom:** If the system is in the state $|\Psi_1\rangle$ at some point in time, and in another state $|\Psi_2\rangle$ at another point in time, then the two states must be related by the action of some unitary operator U:

$$|\Psi_2\rangle = U|\Psi_1\rangle. \tag{4.210}$$

7. **The Measurement Axiom:** Consider an observable A of the form

$$A = \sum_{i=1}^{n} \lambda_i P_i. \tag{4.211}$$

If the system is in the state $|\Psi\rangle$, then the probability to measure the eigenvalue λ_i is given by

$$\langle\Psi|P_i|\Psi\rangle. \tag{4.212}$$

After the measurement, if the eigenvalue λ_i was measured, then the system will collapse to the state

$$|\Psi\rangle \mapsto \frac{P_i|\Psi\rangle}{\sqrt{\langle\Psi|P_i|\Psi\rangle}}. \tag{4.213}$$

- **The Simplified Measurement Axiom:** Consider an observable with an eigenbasis of non-degenerate eigenstates $|B_i\rangle$ corresponding to eigenvalues λ_i. If the system is in the state $|\Psi\rangle$, then the probability to measure the eigenvalue λ_i corresponding to the eigenstate $|B_i\rangle$ is given by

$$|\langle B_i|\Psi\rangle|^2. \tag{4.214}$$

After the measurement, if the eigenvalue λ_i was measured, then the system will collapse to the eigenstate $|B_i\rangle$:

$$|\Psi\rangle \mapsto |B_i\rangle. \tag{4.215}$$

If a measurement is performed only on part of a composite system, the total probability to measure the eigenvalue λ_i is the sum of the probabilities for all the possible ways in which this eigenvalue can be measured. After the measurement, if the eigenvalue λ_i was measured, then only the system we measured will collapse to the eigenstate $|B_i\rangle$, while the other systems will stay in a superposition.

- **Expectation Value:** If the system is in the state $|\Psi\rangle$, the expectation value for the measurement of the observable A is given by $\langle\Psi|A|\Psi\rangle$.
- **Uncertainty Principle:** If two observables A and B don't commute, the standard

deviations of their measurements satisfy the uncertainty relation

$$\Delta A \Delta B \geq \frac{1}{2} \left| \langle [A, B] \rangle \right| . \tag{4.216}$$

The mathematical framework we have defined here is not enough on its own; one must use the framework to define different *model*s, which map the framework to specific physical systems. A model is a specific choice of the following ingredients:

- A Hilbert space describing a specific physical system,
- Hermitian operators corresponding to specific physical observables that may be measured for the system,
- Unitary operators corresponding to the time evolution and other possible transformations of the system,
- The states on which these operators act, which correspond to different configurations of the system.

In the simple case of a qubit, we saw that the Hilbert space is $\mathbb{C}^2$, the Hermitian operators corresponding to observables are linear combinations of the Pauli matrices, the unitary operators corresponding to transformations are the quantum gates, and the states are the two possible values of the qubits, 0 and 1 (and superpositions thereof).

Of course, not every possible model we can make will actually correspond to a physical system that we can find in nature. However, amazingly, the opposite statement does seem to be true: every physical system that we find in nature[47] can be precisely described by a model built using the ingredients of quantum theory.

We can think of quantum theory as a sort of **language**. Just like English is a language with rules such as grammar and spelling, so is quantum theory a language with its own rules: observables must be Hermitian operators, possible measurement results are given by the eigenvalues of these operators, and so on. And just like we can use English to make any sentence we want, both true and false, we can use quantum theory to make any model we want, both models that correspond to real physical systems and those that do not.

5 Quantum Information and Computation

Now that we have successfully formulated the mathematical basis of quantum theory, I would like to discuss two of its modern applications: *quantum information* and *quantum computation*. We will only present a few basic concepts and examples from these cutting-edge areas of research, but I encourage you to look them up and read more about them.

[47] Except perhaps general relativity, but we are pretty sure that there is a quantum theory of general relativity, we just don't have a consistent formulation of it yet. If time permits, we will discuss this theory – quantum gravity – at the end of this course.

5.1 The No-Cloning Theorem and Quantum Teleportation

5.1.1 The No-Cloning Theorem

The *no-cloning theorem* states that it is impossible to make a copy of an unknown quantum state. Note that it is possible, in principle, to generate a **known** quantum state as many times as we want; all we need to do is repeat whatever process is known to generate that state. However, if someone gives you an **unknown** quantum state $|\Psi\rangle$ and doesn't tell you anything about it, the no-cloning theorem states that you will never be able to make another copy of $|\Psi\rangle$.

To prove the theorem, let us assume that we have a "copying operator" U which gets a tensor product of two states as input, and copies the state from the first slot into the second slot:

$$U\Big(|\Psi\rangle \otimes |?\rangle\Big) = |\Psi\rangle \otimes |\Psi\rangle\,. \tag{5.1}$$

The second state $|?\rangle$ in the input can be anything – it doesn't matter what it was originally, since it will be overwritten with the state $|\Psi\rangle$ that we are copying.

We are looking for a **universal** copying operator, which can copy **any** state $|\Psi\rangle$, even if we don't know in advance what the state is. If this operator only works for a **specific** state $|\Psi\rangle$, that means we must know what $|\Psi\rangle$ is in advance, in order to choose the specific U that copies it. Let us use U to copy two states, $|\Psi_1\rangle$ and $|\Psi_2\rangle$:

$$U\Big(|\Psi_1\rangle \otimes |?\rangle\Big) = |\Psi_1\rangle \otimes |\Psi_1\rangle\,, \tag{5.2}$$

$$U\Big(|\Psi_2\rangle \otimes |?\rangle\Big) = |\Psi_2\rangle \otimes |\Psi_2\rangle\,. \tag{5.3}$$

We can take the inner product of the last two equations by turning the second equation into a bra:

$$\Big(\langle\Psi_2| \otimes \langle ?|\Big)\, U^\dagger U\, \Big(|\Psi_1\rangle \otimes |?\rangle\Big) = \Big(\langle\Psi_2| \otimes \langle\Psi_2|\Big)\, \Big(|\Psi_1\rangle \otimes |\Psi_1\rangle\Big)\,. \tag{5.4}$$

By the Evolution Axiom, U must be a unitary operator, so we have $U^\dagger U = 1$:

$$\Big(\langle\Psi_2| \otimes \langle ?|\Big)\, \Big(|\Psi_1\rangle \otimes |?\rangle\Big) = \Big(\langle\Psi_2| \otimes \langle\Psi_2|\Big)\, \Big(|\Psi_1\rangle \otimes |\Psi_1\rangle\Big)\,. \tag{5.5}$$

The inner product can be calculated using (4.55):

$$\langle\Psi_2|\Psi_1\rangle\langle ?|?\rangle = \langle\Psi_2|\Psi_1\rangle\langle\Psi_2|\Psi_1\rangle. \tag{5.6}$$

On the right-hand side, we have $\langle\Psi_2|\Psi_1\rangle\langle\Psi_2|\Psi_1\rangle = \langle\Psi_2|\Psi_1\rangle^2$:

$$\langle\Psi_2|\Psi_1\rangle\langle ?|?\rangle = \langle\Psi_2|\Psi_1\rangle^2. \tag{5.7}$$

Finally, even though we haven't specified the state $|?\rangle$ (since we don't care what it is), we still

know it must be normalized such that $\langle ?|?\rangle = 1$, since otherwise it won't be a proper state. Therefore, we obtain:

$$\langle \Psi_2|\Psi_1\rangle = \langle \Psi_2|\Psi_1\rangle^2. \tag{5.8}$$

This is a quadratic equation, so it has two solutions:

- The first solution is $\langle \Psi_2|\Psi_1\rangle = 1$, in which case the states must be the same state: $|\Psi_1\rangle = |\Psi_2\rangle$. So U is a copying operator that can only copy one specific state, in contradiction with our requirement above that U is universal.
- The second solution is $\langle \Psi_2|\Psi_1\rangle = 0$, in which case $|\Psi_1\rangle$ and $|\Psi_2\rangle$ must be orthogonal. Again, this means that U cannot be universal, since it can only copy states that are orthogonal to a specific state, and thus we cannot clone an unknown quantum state.

In conclusion, we have proven that it is impossible to find a unitary operator U that can clone any arbitrary state $|\Psi\rangle$.

By the way, this is one of the reasons quantum computers are so hard to build. In a classical computer, we can just make several copies of each bit, and use that for error correction in case the bit gets corrupted. In a quantum computer, we cannot do that, since we cannot make copies of a qubit, due to the no-cloning theorem. Still, quantum error correction is possible – but it is much more complicated.

Problem 5.1. The opposite of the no-cloning theorem is the *no-deleting theorem*, which states that given two identical copies[48] of the same **unknown** quantum state, one can never delete one of them and end up with just one copy. Prove the no-deleting theorem.

Problem 5.2. Remarkably, if cloning a quantum state **was** possible, it would have allowed faster-than-light communication! Assuming Alice and Bob each have one qubit of an entangled Bell state, and Bob can make as many copies of his qubit as he wants, show that it is possible for Alice to send Bob a message instantaneously, regardless of the distance between them.

This result is especially noteworthy due to the fact that we can freely copy classical bits, and yet classical correlation definitely does not allow instantaneous communication. This demonstrates something very special about quantum entanglement, which does not apply to classical correlation.

5.1.2 Quantum Teleportation

We discovered that it is impossible to copy a quantum state, which is quite surprising. *Quantum teleportation* is another surprising discovery, which also serves to illustrate the powerful consequences of entanglement. We begin with the Bell state (4.102):

$$|\beta_{00}\rangle \equiv \frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle\right), \tag{5.9}$$

[48] Of course, deleting just one copy of a quantum state is trivial – all you need to do is measure it!

where we again used the shorthand notation $|xy\rangle \equiv |x\rangle \otimes |y\rangle$. Alice takes the first qubit, Bob takes the second, and they go their separate ways. In this entangled state, if Alice measures 0, Bob will also measure 0, and if Alice measures 1, Bob will also measure 1.

Later, Alice receives an arbitrary qubit

$$|\Psi\rangle = a\,|0\rangle + b\,|1\rangle\,, \qquad |a|^2 + |b|^2 = 1, \tag{5.10}$$

but she does **not** know the state of the qubit, that is, the coefficients a and b. Alice needs to transfer this unknown qubit in its entirety to Bob using only two **classical** bits. This seems impossible, for two different reasons:

1. The exact state of the qubit is determined by the two arbitrary complex numbers a and b. Even if Alice did know the values of these numbers, transferring that information requires much more than two classical bits – in fact, to transmit the **precise** value of an arbitrary complex (or even real) number, an **infinite** number of bits are required.

2. Even if Alice was somehow able to magically transmit two complex numbers using only two classical bits, there is no way she could determine the values of a and b in the first place. Any measurement that Alice makes on her qubit will simply result in either 0 or 1; it does not tell Alice anything about the probabilities, not to mention the probability amplitudes. To get information about the probabilities, Alice must make a large number of measurements (in fact, an infinite number of them, if she wants to know the precise values of the probabilities). However, this is impossible due to the no-cloning theorem; Alice can only measure the qubit once, and that's it.

To make the impossible possible, Alice can use the fact that her half of the Bell state is entangled with Bob's half. All three qubits can be represented together by the composite state

$$\begin{aligned} |\gamma\rangle &\equiv |\Psi\rangle \otimes |\beta_{00}\rangle \\ &= \frac{1}{\sqrt{2}}\left(a\,|0\rangle + b\,|1\rangle\right) \otimes \left(|00\rangle + |11\rangle\right) \\ &= \frac{1}{\sqrt{2}}\Big(a\left(|000\rangle + |011\rangle\right) + b\left(|100\rangle + |111\rangle\right)\Big)\,, \end{aligned}$$

where we used the shorthand notation

$$|xyz\rangle \equiv |x\rangle \otimes |y\rangle \otimes |z\rangle\,. \tag{5.11}$$

Here the first qubit is the one that is to be teleported from Alice to Bob, the second is Alice's half of the Bell state, and the third is Bob's half.

First, Alice sends the first qubit (the unknown qubit $|\Psi\rangle$) and the second qubit (her half of the Bell state) through a CNOT gate, which as you recall, flips the second qubit only if the first

qubit is $|1\rangle$:

$$\begin{aligned}\mathrm{CNOT}_{1,2}\,|\gamma\rangle &= \frac{1}{\sqrt{2}}\Big(a\,(|000\rangle + |011\rangle) + b\,(|110\rangle + |101\rangle)\Big)\\ &= \frac{1}{\sqrt{2}}\Big(a\,|0\rangle \otimes (|00\rangle + |11\rangle) + b\,|1\rangle \otimes (|10\rangle + |01\rangle)\Big)\,.\end{aligned}$$

Here we used the notation $\mathrm{CNOT}_{1,2}$ to indicate that the gate only acts on qubits 1 and 2 out of the three qubits. Explicitly, this would be the tensor product of the CNOT gate on the left with the 2×2 identity matrix on the right:

$$\mathrm{CNOT}_{1,2} \equiv \mathrm{CNOT} \otimes 1 = \begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0\\ 0 & 1 \end{pmatrix}. \tag{5.12}$$

Next, she sends the first qubit through the Hadamard gate, which as you recall, takes $|0\rangle$ to $|+\rangle \equiv (|0\rangle + |1\rangle)/\sqrt{2}$ and $|1\rangle$ to $|-\rangle \equiv (|0\rangle - |1\rangle)/\sqrt{2}$:

$$\begin{aligned}H_1 \cdot \mathrm{CNOT}_{1,2}\,|\gamma\rangle &= \frac{1}{\sqrt{2}}\Big(a\,|+\rangle \otimes (|00\rangle + |11\rangle) + b\,|-\rangle \otimes (|10\rangle + |01\rangle)\Big)\\ &= \frac{1}{2}\Big(a\,(|0\rangle + |1\rangle) \otimes (|00\rangle + |11\rangle) + b\,(|0\rangle - |1\rangle) \otimes (|10\rangle + |01\rangle)\Big)\\ &= \frac{1}{2}\Big(a\,((|000\rangle + |011\rangle) + |100\rangle + |111\rangle) + b\,(|010\rangle + |001\rangle - |110\rangle - |101\rangle)\Big)\\ &= \frac{1}{2}a\,(|00\rangle \otimes |0\rangle + |01\rangle \otimes |1\rangle + |10\rangle \otimes |0\rangle + |11\rangle \otimes |1\rangle) +\\ &\quad + \frac{1}{2}b\,(|01\rangle \otimes |0\rangle + |00\rangle \otimes |1\rangle - |11\rangle \otimes |0\rangle - |10\rangle \otimes |1\rangle)\,.\end{aligned}$$

Again, the notation H_1 means we act with the Hadamard gate only on the first qubit:

$$H_1 \equiv H \otimes 1 \otimes 1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1\\ 1 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0\\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0\\ 0 & 1 \end{pmatrix}. \tag{5.13}$$

We can rearrange the transformed state as follows:

$$\begin{aligned}H_1 \cdot \mathrm{CNOT}_{1,2}\,|\gamma\rangle = \frac{1}{2}\,|00\rangle \otimes (a\,|0\rangle + b\,|1\rangle) +\\ + \frac{1}{2}\,|01\rangle \otimes (a\,|1\rangle + b\,|0\rangle) +\\ + \frac{1}{2}\,|10\rangle \otimes (a\,|0\rangle - b\,|1\rangle) +\\ + \frac{1}{2}\,|11\rangle \otimes (a\,|1\rangle - b\,|0\rangle)\,.\end{aligned}$$

Finally, Alice performs a measurement on the first two qubits (the one to be teleported, and her half of the Bell state), and obtains one of four results: 00, 01, 10, or 11. These are **two classical bits**, which she can then send to Bob. With this information, Bob can read from the last equation exactly which operations he has to perform on his qubit (which you will determine in Problem 5.4) in order to obtain the original qubit $|\Psi\rangle = a|0\rangle + b|1\rangle$. The qubit has been successfully teleported from Alice to Bob!

Note that since Alice measured the original qubit, it collapsed and its quantum state has been destroyed. Therefore, quantum teleportation does not violate the no-cloning theorem; the state of the qubit was not cloned or copied, it was just moved from one qubit to another. Also, since Alice had to send two classical bits to Bob – for example through a cable or radio waves – the speed of teleportation is limited by the speed of light, and there is no violation of relativity.

Finally, since quantum teleportation requires Alice and Bob to already have one half of an entangled pair each, and the entanglement is destroyed in the process due to Alice's measurement, the number of qubits they can teleport is limited by the number of entangled pairs they have. Once they run out of entangled pairs, they can no longer teleport any qubits until they physically exchange more entangled pairs. This means that you can't just establish two teleportation stations on, say, two planets, and teleport qubits between them forever; you will have to actually send a spaceship from one planet to the other with a fresh supply of entangled particles every once in a while.

Problem 5.3. Quantum teleportation has been demonstrated experimentally in many different experiments, over distances of up to 1400 km, and not just with qubits but even with more complicated systems. Whenever a new quantum teleportation experiment happens, articles appear in the media with sensationalist headlines such as "scientists demonstrate teleportation is possible!" or "is teleportation closer than we think?", where by "teleportation" they actually mean the **science-fiction** concept of "teleportation", where a macroscopic object is sent from one place to another without going through the space in between. Is the word "teleportation" in "quantum teleportation" indeed justified? In what ways is quantum teleportation the same as science-fiction teleportation, and in what ways is it different?

Problem 5.4. For each of the four results of Alice's measurement, 00, 01, 10, and 11, determine which unitary transformations Bob must perform on his qubit in order to obtain the original $|\Psi\rangle = a|0\rangle + b|1\rangle$.

Problem 5.5. Write a computer program[49] that gets an arbitrary composite state of n qubits as input and allows the user to perform the following actions:

- Analyze whether or not any two of the qubits are entangled.
- Act on one or more of the qubits with a quantum gate; for example, act with Hadamard on one qubit or with CNOT on two qubits.

[49] As in Problem 3.65, I recommend either Mathematica or Python, but feel free to use whatever language you like.

- Simulate a measurement of one or more of the qubits as dictated by the Projective Measurement Axiom, with the result determined randomly according to the appropriate probability distribution, and the state collapsing after the measurement according to the value that was measured.

Use your program to simulate quantum teleportation, and show that it indeed works.

5.2 Quantum Algorithms

5.2.1 Quantum Parallelism

It's a common misconception that quantum computers work by using superposition to "calculate the answer for every possible combination of qubits in parallel". As the claim goes, if you have a quantum computer with n qubits, then because each qubit can be "0 and 1 at the same time", then you can operate on all 2^n possible combinations at once.

You've probably already heard this incorrect claim before – perhaps even from someone with a PhD in physics! This misconception stems from the more general misconception about the meaning of superposition which we discussed in Section 4.2.4. Sure, it would have been great if this kind of parallelism was actually possible... but unfortunately, it's not.

So how do quantum computers actually work? Generally, they make clever use of properties of quantum states, such as superposition, entanglement, and interference, to solve certain problems. Just as classical computers operate by sending one or more classical bits through classical logic gates, quantum computers operate by sending one or more qubits through quantum logic gates (recall Section 4.5.2). The arrangement of gates is called a *quantum circuit*, and algorithms which make use of qubits and quantum gates are called *quantum algorithms*.

Even though quantum computers don't really "calculate everything in parallel", there is still a concept called *quantum parallelism* which is used in most quantum algorithms. Let us demonstrate it with a simple example. Consider a function $f(x) : \{0,1\} \to \{0,1\}$ which takes one bit as input and gives one bit as output. There are, in fact, exactly 4 such functions, because each of the input bits 0 or 1 can be sent to either 0 or 1 as output:

$$f(x) = 0, \qquad f(x) = 1, \qquad f(x) = x, \qquad f(x) = 1 - x. \tag{5.14}$$

Say have a quantum computer which can manipulate two qubits. Let U_f be a unitary operator which transforms any composite 2-qubit state $|x, y\rangle$, where $x, y \in \{0,1\}$, as follows:

$$U_f |x, y\rangle = |x, y \oplus f(x)\rangle, \tag{5.15}$$

where $\oplus$ means addition modulo 2, that is,

$$0 \oplus 0 = 0, \qquad 0 \oplus 1 = 1, \qquad 1 \oplus 0 = 1, \qquad 1 \oplus 1 = 0. \tag{5.16}$$

The form of U_f depends on the choice of $f(x)$. For example, if $f(x) = 0$, then U_f is simply

the identity operator. In Problem 5.6 you will find the exact form of U_f for each choice of $f(x)$ and see that it is indeed unitary.

We assume that initially, the state of the two qubits in our quantum computer is

$$|\Psi\rangle = |0\rangle \otimes |0\rangle \equiv |00\rangle . \tag{5.17}$$

The first qubit, which will store the input, is called the *data register*, and the second qubit, which will store the output, is called the *target register*. We now build a quantum circuit as follows. First, recall the Hadamard gate (4.164):

$$H \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{5.18}$$

which acts as follows:

$$H|0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) , \tag{5.19}$$

$$H|1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) . \tag{5.20}$$

Let us apply it to the first qubit of $|\Psi\rangle$:

$$\begin{aligned} H_1 |\Psi\rangle &= \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \otimes |0\rangle \\ &= \frac{1}{\sqrt{2}} (|00\rangle + |10\rangle) . \end{aligned}$$

We now apply U_f to this state. Since U_f is a linear operator, it acts on both terms in the superposition independently:

$$U_f H_1 |\Psi\rangle = \frac{1}{\sqrt{2}} (|0, f(0)\rangle + |1, f(1)\rangle) . \tag{5.21}$$

Even though we applied U_f only once, the state now contains information about the value of $f(x)$ for both 0 and 1! This is an example of quantum parallelism. Does this actually mean we "calculated all the possibilities in parallel", as the common misconception says? Not exactly. The state is still in a superposition; there is no way to tell the values of $f(x)$ from the state, since **we don't know the state**; we can only **measure** the state, and the result of the measurement will be either $|0, f(0)\rangle$ or $|1, f(1)\rangle$ with probability $1/2$. Thus we can only know **one** of the values of $f(x)$, chosen at random.

Problem 5.6. Find the form of the operator U_f described above for each possible choice of $f(x)$ and prove that it is indeed unitary for each choice.

Exercise 5.7. For each of the functions $f(x) = x$ and $f(x) = 1 - x$, find the matrix representation of $U_f H_1$ and show that it takes the vector $|\Psi\rangle = |00\rangle$ to the Bell states $|\beta_{00}\rangle$ and $|\beta_{01}\rangle$ respectively, as given in (4.102) and (4.103).

5.2.2 Deutsch's algorithm

If we can only know one of the values of $f(x)$, and not all of them, then what's the point of quantum parallelism? Well, the point isn't to know all the values at once; it's to take advantage of the parallelism to find **relations** between the different values. Consider, for example, the problem of determining whether $f(x)$ is **constant** or not.

Classically, it is clear that we must evaluate both $f(0)$ and $f(1)$. The function is constant if $f(0) = f(1)$ or not constant if $f(0) \neq f(1)$, but we must know **both** values to find the answer. However, with a quantum computer, that is not the case. We can determine if the function is constant **without** knowing both of its values, and in fact, without knowing **any** of its values!

This can be done using *Deutsch's algorithm*. In this algorithm, we start with the state

$$|\Psi\rangle = |0\rangle \otimes |1\rangle \equiv |01\rangle\,, \tag{5.22}$$

and then act on **both** qubits with a Hadamard gate:

$$H_{12}\,|\Psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right). \tag{5.23}$$

Next, we notice that

$$U_f\left(|x\rangle \otimes \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right)\right) = |x\rangle \otimes \frac{1}{\sqrt{2}}\left(|f(x)\rangle - |1 + f(x)\rangle\right). \tag{5.24}$$

On the right-hand side, we have

$$\begin{aligned}\frac{1}{\sqrt{2}}\left(|f(x)\rangle - |1 + f(x)\rangle\right) &= \begin{cases} \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right) & f(x) = 0, \\ \frac{1}{\sqrt{2}}\left(|1\rangle - |0\rangle\right) & f(x) = 1, \end{cases} \\ &= (-1)^{f(x)}\,\frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right),\end{aligned}$$

which means that

$$U_f\left(|x\rangle \otimes \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right)\right) = (-1)^{f(x)}\,|x\rangle \otimes \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right). \tag{5.25}$$

Using this information, we can act with U_f on the full state:

$$U_f H_{12}\,|\Psi\rangle = \frac{1}{\sqrt{2}}\left((-1)^{f(0)}\,|0\rangle + (-1)^{f(1)}\,|1\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle - |1\rangle\right). \tag{5.26}$$

If $f(x)$ is constant, then $f(0) = f(1)$, and both terms in the first qubit have the same sign, either both $+$ or both $-$. However, if $f(x)$ is not constant, then the terms will have opposite

signs, one $+$ and one $-$. In other words:

$$U_f H_{12} |\Psi\rangle = \begin{cases} \pm \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) & f(0) = f(1), \\ \pm \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) & f(0) \neq f(1). \end{cases} \tag{5.27}$$

Next, we pass the first qubit through a Hadamard gate again:

$$H_1 U_f H_{12} |\Psi\rangle = \begin{cases} \pm |0\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) & f(0) = f(1), \\ \pm |1\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) & f(0) \neq f(1), \end{cases} \tag{5.28}$$

where we used the fact that the Hadamard gate is its own inverse:

$$H \left(\frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \right) = \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) + \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \right) = |0\rangle, \tag{5.29}$$

$$H \left(\frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \right) = \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) - \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \right) = |1\rangle. \tag{5.30}$$

Finally, we note that

$$f(0) \oplus f(1) = \begin{cases} 0 & f(0) = f(1), \\ 1 & f(0) \neq f(1), \end{cases} \tag{5.31}$$

so we can write concisely

$$H_1 U_f H_{12} |\Psi\rangle = \pm |f(0) \oplus f(1)\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle). \tag{5.32}$$

To determine if $f(x)$ is constant or not, all we need to do is simply to measure the first qubit. If it's 0, then we know $f(x)$ is constant, and if it's 1, then we know $f(x)$ is not constant!

Exercise 5.8. For each of the functions $f(x) = 0$ (constant) and $f(x) = x$ (not constant), find the matrix representation of $H_1 U_f H_{12}$ and demonstrate by explicit matrix multiplication that it takes the vector $|\Psi\rangle = |01\rangle$ to a state of the form (5.32).

5.2.3 The Deutsch-Jozsa Algorithm

You may be asking yourself: okay, we can determine if the function is constant, but so what? We could also just calculate both its values. Well, imagine now that $f(x)$ is much more complicated. Instead of getting just one bit as input, it gets n bits. This means that the input can be any integer between 0 and $2^n - 1$, as can be seen from the following table:

Binary (n bits)	Decimal
$000\ldots000$	0
$000\ldots001$	1
$000\ldots010$	2
$000\ldots011$	3
$\vdots$	$\vdots$
$111\ldots100$	2^n-4
$111\ldots101$	2^n-3
$111\ldots110$	2^n-2
$111\ldots111$	2^n-1

For example, for the case of $n = 3$ we have:

Binary (3 bits)	Decimal
000	0
001	1
010	2
011	3
100	4
101	5
110	6
111	7

In this case $2^n = 8$, so $2^n - 1 = 7$. For a large number of bits, the number of possible input values increases **exponentially**. For example, if we have $n = 64$ bits, then the maximum input value is $2^{64} - 1 \approx 1.8 \times 10^{19}$.

Assume that we are given the information that $f(x)$ is one of two kinds of functions:

1. A **constant** function, that is, $f(x)$ **always** gives the same value regardless of the input; either $f(x) = 0$ for all x or $f(x) = 1$ for all x.
2. A **balanced** function, that is, $f(x) = 0$ for **exactly half** of all of possible values of x and $f(x) = 1$ for the other half.

$f(x)$ can never be anything in between, e.g. equal to 0 for all values of x except one; it must be one of these two options. The problem is now to determine whether $f(x)$ is constant or balanced.

With a classical computer, in the best case scenario, we only need to calculate $f(x)$ for two different values of x. For example, if $f(0) = 0$ and $f(1) = 1$, then we immediately know that $f(x)$ cannot be constant, and thus it must be balanced. However, in the worst case scenario we will have to calculate $f(x)$ for $2^{n-1} + 1$ different values of x.

The worst case scenario occurs when the first 2^{n-1} values (i.e. half of all the possible values) all turn out the be the same. That is still not enough to know if the function is constant or

balanced; it could still be either of the two. We must calculate one more value, and if that is **also** the same, then we know the function must be constant, otherwise it must be balanced. Hence the total number of calculations required is $2^{n-1}+1$.

This means that we may need to calculate $f(x)$ for a very large number of values. For example, if $n = 64$, then we may need to make up to $2^{63}+1 \approx 9.2 \times 10^{18}$ calculations. Even if each calculation only takes the classical computer one microsecond (a millionth of a second), it would still take around **300,000 years** to finish all the required calculations in the worst-case scenario!

Things become much easier if we happen to have a quantum computer with $n+1$ qubits. The algorithm is a straightforward generalization of Deutsch's algorithm, replacing the single input qubit with n input qubits. We start in the initial state

$$|\Psi\rangle = |0\rangle^{\otimes n} \otimes |1\rangle\,, \tag{5.33}$$

where the notation $|0\rangle^{\otimes n}$, the order-n *tensor power* of $|0\rangle$, means "the tensor product of $|0\rangle$ with itself n times", that is,

$$|0\rangle^{\otimes n} \equiv \underbrace{|0\rangle \otimes \cdots \otimes |0\rangle}_{n \text{ copies}}\,. \tag{5.34}$$

Let us send each of the first n qubits through a Hadamard gate. This is called a *Hadamard transform*. We get:

$$H_{1,\ldots,n}\,|0\rangle^{\otimes n} = \underbrace{\frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \otimes \cdots \otimes \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)}_{n \text{ copies}}\,. \tag{5.35}$$

Consider, for clarity, the case of $n = 3$. Then we have:

$$\begin{aligned} H_{123}\,|0\rangle^{\otimes 3} &= \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \\ &= \frac{1}{\sqrt{2^3}}\left(|000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle + |111\rangle\right), \end{aligned}$$

or in other words, $H_{123}\,|0\rangle^{\otimes 3}$ is a superposition of all the possible combinations of 3 qubits, with equal probabilities. We can write this in a compact notation as follows:

$$H_{123}\,|0\rangle^{\otimes 3} = \frac{1}{\sqrt{2^3}} \sum_{x \in \{0,1\}^3} |x\rangle\,, \tag{5.36}$$

where the notation $\{0,1\}^3$ means "all the possible combinations of 3 bits", and as we have seen in the table above, is equivalent to a sum over the integers from 0 to $2^3 - 1 = 7$. Generalizing to n bits, we see that:

$$H_{1,\ldots,n}\,|0\rangle^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle\,, \tag{5.37}$$

where now the sum on x is over all n-bit integers, so from 0 to $2^n - 1$. The Hadamard transform thus takes n qubits in the state $|0\rangle$ and transforms them into a superposition of every possible combination of n qubits with equal probabilities. In conclusion, applying this to the first n qubits of the full state $|\Psi\rangle = |0\rangle^{\otimes n} \otimes |1\rangle$, we get:

$$H_{1,\dots,n} |\Psi\rangle = \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle \otimes |1\rangle . \tag{5.38}$$

Let us also send the target qubit, number $n+1$, which started in the state $|1\rangle$, through the Hadamard gate:

$$H_{n+1} H_{1,\dots,n} |\Psi\rangle = \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) . \tag{5.39}$$

We now use the same U_f from (5.15). In our discussion of Deutsch's algorithm, we found in (5.25) that

$$U_f \left(|x\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \right) = (-1)^{f(x)} |x\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) . \tag{5.40}$$

Therefore

$$U_f H_{n+1} H_{1,\dots,n} |\Psi\rangle = \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} (-1)^{f(x)} |x\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) . \tag{5.41}$$

Notice that we now automatically get the results of calculating $f(x)$, all 2^n of them, in the **amplitudes** of each state in the superposition, even though we never actually calculated the function for each input individually!

However, as I stressed before, this information cannot actually be obtained, since we need to perform a **measurement**, and we will get only one value of x chosen at random; and even then, we won't actually know the value of $f(x)$ for that x, since it's hidden in the amplitude. The amplitude determines the probability, but we cannot measure it directly, and even the probability is actually determined by the **magnitude-squared** of the amplitude, which means we lose the phase $(-1)^{f(x)}$ in any case.

Nonetheless, there is still a clever way to extract the information we want – whether $f(x)$ is constant or balanced – by taking advantage of **quantum interference**. That it, we make all the different amplitudes interfere with each other constructively or destructively in a specific way. Let us see how this works.

The action of the Hadamard gate on one qubit can be written succinctly as follows:

$$H |x\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle + (-1)^x |1\rangle \right) , \qquad x \in \{0,1\} . \tag{5.42}$$

You can check that this works for each of the options $x = 0$ and $x = 1$. We can write it even

more compactly as follows:

$$H|x\rangle = \frac{1}{\sqrt{2}} \sum_{z\in\{0,1\}} (-1)^{xz} |z\rangle , \qquad x, z \in \{0,1\} . \tag{5.43}$$

Let us consider how the Hadamard transform acts on an n-qubit state $|x\rangle$ for some $x \in \{0,1\}^n$. Explicitly, the state is

$$|x\rangle \equiv |x_1, \ldots, x_n\rangle \equiv |x_1\rangle \otimes \cdots \otimes |x_n\rangle , \qquad x_i \in \{0,1\} \text{ for all } i \in \{0, \ldots, n\} . \tag{5.44}$$

Thus:

$$\begin{aligned} H_{1,\ldots,n}|x\rangle &= \frac{1}{\sqrt{2}} \sum_{z_1\in\{0,1\}} (-1)^{x_1 z_1} |z_1\rangle \otimes \cdots \otimes \frac{1}{\sqrt{2}} \sum_{z_n\in\{0,1\}} (-1)^{x_n z_n} |z_n\rangle \\ &= \frac{1}{\sqrt{2^n}} \sum_{z_1,\ldots,z_n\in\{0,1\}} (-1)^{x_1 z_1 + \ldots + x_n z_n} |z_1\rangle \otimes \cdots \otimes |z_n\rangle , \end{aligned}$$

where we simply combined all the phases $(-1)^{x_i z_i}$ into one.

Just as we treat $x_1, \ldots, x_n$ as the bits of an integer x between 0 and $2^n - 1$, we can also treat $z_1, \ldots, z_n$ as the bits of an integer z. We can then define a *bitwise inner product*:

$$x \odot z \equiv x_1 z_1 + \ldots + x_n z_n . \tag{5.45}$$

This allows us to write the result of the Hadamard transform simply as:

$$H_{1,\ldots,n}|x\rangle = \frac{1}{\sqrt{2^n}} \sum_{z\in\{0,1\}^n} (-1)^{x\odot z} |z\rangle . \tag{5.46}$$

Using this equation, we can now calculate the Hadamard transform of the first n qubits of (5.41):

$$\begin{aligned} H_{1,\ldots,n} U_f H_{n+1} H_{1,\ldots,n} |\Psi\rangle &= \frac{1}{\sqrt{2^n}} \sum_{x\in\{0,1\}^n} (-1)^{f(x)} \left(H_{1,\ldots,n}|x\rangle \right) \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \\ &= \frac{1}{\sqrt{2^n}} \sum_{x\in\{0,1\}^n} (-1)^{f(x)} \left(\frac{1}{\sqrt{2^n}} \sum_{z\in\{0,1\}^n} (-1)^{x\odot z} |z\rangle \right) \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \\ &= \frac{1}{2^n} \sum_{x,z\in\{0,1\}^n} (-1)^{x\odot z + f(x)} |z\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) . \end{aligned}$$

We can write this in a more suggestive way as follows:

$$H_{1,\ldots,n} U_f H_{n+1} H_{1,\ldots,n} |\Psi\rangle = \sum_{z\in\{0,1\}^n} \left(\frac{1}{2^n} \sum_{x\in\{0,1\}^n} (-1)^{x\odot z + f(x)} \right) |z\rangle \otimes \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) . \tag{5.47}$$

This means that, when we measure the first n qubits, the amplitude to measure the integer z is given by the **sum**:

$$A(z) \equiv \frac{1}{2^n} \sum_{x \in \{0,1\}^n} (-1)^{x \odot z + f(x)}. \tag{5.48}$$

Consider specifically the amplitude to measure $z = 0$, that is, the term in the superposition where all n qubits $z_1, \ldots, z_n$ are zero. In that case $x \odot z = 0$, so the amplitude will simply be:

$$A(0) = \frac{1}{2^n} \sum_{x \in \{0,1\}^n} (-1)^{f(x)}. \tag{5.49}$$

The sum will depend on which of the two possible kinds of $f(x)$ we have:

- If $f(x)$ is **constant**, then we have

$$A(0) = \begin{cases} \frac{1}{2^n} \sum_{x \in \{0,1\}^n} (+1) = +1 & f(x) = 0, \\ \frac{1}{2^n} \sum_{x \in \{0,1\}^n} (-1) = -1 & f(x) = 1. \end{cases} \tag{5.50}$$

  In each case, we are summing over 2^n terms which are all the same (either $+1$ or -1), and then dividing by 2^n, so the result is just $+1$ or -1 depending on the constant value of $f(x)$. But this means that the amplitude has magnitude 1, so the probability to measure $z = 0$ is $|A(0)|^2 = 1$. In other words, if $f(x)$ is **constant**, then we will **always** measure $z = 0$, with 100% probability, and we can never measure any other values for z, since they must have a 0% probability. Notice that in this case we got **constructive interference** between the amplitudes.

- If $f(x)$ is **balanced**, then it is equal to 0 for exactly half the values of x and to 1 for the other half. Therefore, in the sum $\sum_{x \in \{0,1\}^n} (-1)^{f(x)}$, half the terms will be $+1$ and half will be -1. The terms will exactly cancel each other, and the amplitude will be zero, so the probability to measure $z = 0$ is $|A(0)|^2 = 0$. In other words, if $f(x)$ is **balanced**, then we will **never** measure $z = 0$, since that outcome has 0% probability. Notice that in this case we got **destructive interference** between the amplitudes.

In conclusion, if we measure $z = 0$ (all qubits are 0) then we know for sure that $f(x)$ is constant, and if we measure $z \neq 0$ (at least one qubit is 1) then we know for sure that $f(x)$ is balanced. We found this just by passing the qubits through a few gates, without having to actually calculate $2^{n-1} + 1$ values of $f(x)$ as in the classical case. Going back to our example of $n = 64$, a classical computer could take it up to 300,000 years to find the answer, while a quantum computer can find it in the time it takes to pass the qubits through the gates, which shouldn't be more than a few seconds!

This result is very impressive, but we should also mention that an algorithm for determining whether a function is constant or balanced is not something you would ever realistically need. This problem was specifically designed to show the potential benefits of quantum computers, but it has no known applications.

A more useful quantum algorithm, that you may have heard of, is *Shor's algorithm*, which is used to factorize integers, and can do so much faster than any known classical algorithm. Factorizing integers is a very common problem, especially in cryptography. This algorithm is a bit more complicated, so we will not discuss it here, but you should look up this and other quantum algorithms if you're interested.

Problem 5.9. You meet a layperson with no knowledge of the math of quantum mechanics. They tell you about an amazing YouTube video with 100 million likes, where a famous YouTuber with 10 million subscribers talked about quantum computers. According to the famous YouTuber, who has a master's degree in physics, quantum computers are so immensely powerful because they can apply any calculation to all the possible inputs in parallel, while a classical computer can only calculate them one at a time. Explain to the layperson, in simple terms and without using any math, what the YouTuber got wrong. Identify the concepts on which the YouTuber's misconception is most likely based, and explain how the YouTuber applied these concepts incorrectly. Then clarify how quantum computers really work.

Problem 5.10.

A. In Problem 5.5 you wrote a computer program which allows the user to pass qubits through quantum gates and perform measurements. Your program should therefore be able to do anything a quantum computer can. Use it to perform the Deutsch-Jozsa algorithms.

B. You program is running on a classical computer, so obviously, it shouldn't be able to reproduce the speedup of a quantum computer. How can you reconcile this with the fact that the program is able to perform the Deutsch-Jozsa algorithm? You should be able to answer this part of the question even if you didn't do Problem 5.5 or part A, but writing the program should give you some insight into the answer.

6 Continuous Quantum Systems

Quantum mechanics is a confusing and unintuitive theory, and requires the introduction of many new concepts. One of the main goals of this course is to introduce quantum mechanics to students in a way that is mathematically as simple as possible, so that they won't have to struggle with complicated math on top of trying to understand new physical concepts.

It is quite remarkable that we have managed to describe all of the axioms of quantum theory, and almost all of its important aspects such as superposition, entanglement, and the uncertainty principle, using only linear algebra – without any calculus. Moreover, by focusing on discrete two-state systems, or qubits, we actually managed to do everything almost exclusively in $\mathbb{C}^2$, the simplest non-trivial complex vector space.

Unfortunately, in real life not all systems are discrete, and the time has finally come to start introducing some calculus and talking about continuous quantum systems, which are described by infinite-dimensional Hilbert spaces. However, the student may take comfort in the fact that this is going to be merely a straightforward generalization of what we've already

learned. The only real difference is that now states are going to be functions instead of vectors, and operators are going to be derivatives instead of matrices.

6.1 Mathematical Preliminaries

6.1.1 Exponentials and Logarithms

The *exponential function* is defined on arbitrary complex numbers $z \in \mathbb{C}$ using a *power series* as follows:

$$\mathrm{e}^z \equiv \sum_{n=0}^{\infty} \frac{z^n}{n!} = 1 + z + \frac{1}{2}z^2 + \frac{1}{3!}z^3 + \cdots . \tag{6.1}$$

The complex number z is called the *exponent*. If the exponent is zero, then all the terms in the series vanish except the first one, and we get $\mathrm{e}^0 = 1$. If the exponent is a natural number $n \in \mathbb{N}$, then (6.1) turns out to be the same as taking the real number[50] $\mathrm{e} \approx 2.718$ to the power of n, that is, multiplying it by itself n times. This can then be expanded to negative integers using the formula

$$\mathrm{e}^{-n} \equiv \frac{1}{\mathrm{e}^n}, \tag{6.2}$$

and to rational numbers using

$$\frac{a}{b} \in \mathbb{Q} \quad \Longrightarrow \quad \mathrm{e}^{a/b} \equiv \sqrt[b]{\mathrm{e}^a}. \tag{6.3}$$

However, for arbitrary real or complex numbers, we generally use the power series definition (6.1) directly, or an equivalent definition such as the ones you will prove in problems 6.2 and 6.3 below.

By taking the complex conjugate of the series (6.1), we get:

$$\left(\mathrm{e}^z\right)^* = \mathrm{e}^{z^*}, \tag{6.4}$$

so the conjugate operation commutes with taking the exponential. In particular, given a complex number in the polar representation (see Section 3.1.4), we have

$$z = r\,\mathrm{e}^{\mathrm{i}\phi} \quad \Longrightarrow \quad z^* = r\,\mathrm{e}^{-\mathrm{i}\phi}, \qquad r, \phi \in \mathbb{R}. \tag{6.5}$$

This indeed makes sense, as taking the complex conjugate mean reflecting z across the real line, and thus turns the angle ϕ, which is the angle with respect to the real line, into its negative – see Figure 3.1.

One can also prove from the definition (6.1) that $\mathrm{e}^{z+w} = \mathrm{e}^z\,\mathrm{e}^w$, so

$$e^{\mathrm{i}\phi} e^{-\mathrm{i}\phi} = e^{\mathrm{i}\phi - \mathrm{i}\phi} = \mathrm{e}^0 = 1. \tag{6.6}$$

[50] But of course, in order to know the value of the number e in the first place, we need to calculate the power series (6.1) for $z = 1$!

Therefore the magnitude of z is

$$|z| = \sqrt{zz^*} = \sqrt{re^{\mathrm{i}\,\phi} \cdot re^{-\mathrm{i}\,\phi}} = \sqrt{r^2} = r, \tag{6.7}$$

as expected.

The exponential function is its own derivative:

$$\frac{\mathrm{d}}{\mathrm{d}z}\,\mathrm{e}^z = \mathrm{e}^z\,. \tag{6.8}$$

In fact, it can be **defined** using this property, as you will prove in Problem 6.1. Using the chain rule, we get the more general result

$$\frac{\mathrm{d}}{\mathrm{d}z}\,\mathrm{e}^{\lambda z} = \frac{\mathrm{d}}{\mathrm{d}z}\,(\lambda z)\,\mathrm{e}^{\lambda z} = \lambda\,\mathrm{e}^{\lambda z}, \tag{6.9}$$

where λ is any **constant** complex number (i.e. independent of z).

The inverse function of the exponential is the *logarithm*:

$$w = \mathrm{e}^z \quad \Longleftrightarrow \quad z = \log w, \qquad \mathrm{e}^{\log z} = \log \mathrm{e}^z = z. \tag{6.10}$$

This is also called the *natural logarithm*, since it is taken with respect to the "natural" *base* $\mathrm{e} \approx 2.718$. More generally, a logarithm with respect to the base b satisfies

$$w = b^z \quad \Longleftrightarrow \quad z = \log_b w, \qquad b^{\log_b z} = \log_b b^z = z. \tag{6.11}$$

For a general base b we have

$$\frac{\mathrm{d}}{\mathrm{d}z} b^z = b^z \log_{\mathrm{e}} b, \tag{6.12}$$

and the extra term vanishes when $b = \mathrm{e}$, since $\log_{\mathrm{e}} \mathrm{e} = 1$. This explains why the base $\mathrm{e} \approx 2.718$ is "natural"; it is the unique base for which the function b^z is its own derivative, without the extra term. Sometimes the notation ln is also used for the natural logarithm: $\ln \equiv \log_e$. Since $b = \mathrm{e}^{\ln b}$, the power series definition (6.1) can be used to define the exponential of any base b with respect to arbitrary complex numbers z using the formula

$$b^z = \left(\mathrm{e}^{\ln b}\right)^z = \mathrm{e}^{z \ln b}\,. \tag{6.13}$$

Problem 6.1. By assuming a generic power series expansion

$$f\,(z) = \sum_{n=0}^{\infty} a_n z^n, \tag{6.14}$$

prove that if $f\,(z)$ is its own derivative, then it must be the exponential function, i.e. $a_n = 1/n!$.

Problem 6.2. The power series expansions of the trigonometric functions $\cos x$ and $\sin x$ are

$$\cos x \equiv \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} x^{2n} = 1 - \frac{1}{2}x^2 + \frac{1}{4!}x^4 + \cdots, \tag{6.15}$$

$$\sin x \equiv \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} x^{2n+1} = x - \frac{1}{3!}x^3 + \frac{1}{5!}x^5 + \cdots. \tag{6.16}$$

Use them to prove *Euler's formula*

$$\mathrm{e}^{\mathrm{i}\,x} = \cos x + \mathrm{i} \sin x. \tag{6.17}$$

As a corollary, show that

$$\cos x = \mathrm{Re}\left(\mathrm{e}^{\mathrm{i}\,x}\right) = \frac{\mathrm{e}^{\mathrm{i}\,x} + \mathrm{e}^{-\mathrm{i}\,x}}{2}, \tag{6.18}$$

$$\sin x = \mathrm{Im}\left(\mathrm{e}^{\mathrm{i}\,x}\right) = \frac{\mathrm{e}^{\mathrm{i}\,x} - \mathrm{e}^{-\mathrm{i}\,x}}{2\,\mathrm{i}}. \tag{6.19}$$

Problem 6.3. The *binomial theorem* states that for $x, y \in \mathbb{C}$ and $n \in \mathbb{N}$:

$$(x+y)^n = \sum_{k=0}^{n} \binom{n}{k} x^{n-k} y^k, \tag{6.20}$$

where the *binomial coefficients* are defined as

$$\binom{n}{k} \equiv \frac{n!}{k!\,(n-k)!}. \tag{6.21}$$

So, explicitly, we have

$$(x+y)^n = x^n + n x^{n-1} y + \frac{1}{2} n\,(n-1)\, x^{n-2} y^2 + \cdots. \tag{6.22}$$

Using the binomial theorem and the power series definition of the exponential (6.1), prove the equivalent definition

$$\mathrm{e}^z = \lim_{n \to \infty} \left(1 + \frac{z}{n}\right)^n. \tag{6.23}$$

6.1.2 Matrix and Operator Exponentials

To generalize the exponential to complex matrices A, we define the *matrix exponential*:

$$\mathrm{e}^A \equiv \sum_{n=0}^{\infty} \frac{A^n}{n!} = 1 + A + \frac{1}{2}A^2 + \frac{1}{3!}A^3 + \cdots, \tag{6.24}$$

where 1 is now the identity matrix, and A^n means the product of the matrix A with itself n times. Note that it satisfies

$$\mathrm{e}^0 = 1, \tag{6.25}$$

that is, the exponential of the zero matrix is the identity matrix, in analogy with the fact that the exponential of zero is one. It also satisfies, as you will prove in Problem 6.4,

$$\left(\mathrm{e}^{A}\right)^{\dagger} = \mathrm{e}^{A^{\dagger}}, \tag{6.26}$$

in analogy with (6.4).

Things start to become more complicated when we consider the product of two exponentials, $\mathrm{e}^{A}\,\mathrm{e}^{B}$. For numbers (which can be considered 1×1 matrices) we have $\mathrm{e}^{z}\,\mathrm{e}^{w} = \mathrm{e}^{z+w}$, but to prove that, we used the fact that numbers commute. For arbitrary $n \times n$ matrices A and B, it is in general not true that $\mathrm{e}^{A}\,\mathrm{e}^{B} = \mathrm{e}^{A+B}$. However, in Problem 6.5 you will prove that this identity is true if $[A, B] = 0$, that is, if A and B commute.

The *matrix logarithm* is the inverse function of the matrix exponential:

$$B = \mathrm{e}^{A} \quad \Longleftrightarrow \quad A = \log B, \qquad \mathrm{e}^{\log A} = \log \mathrm{e}^{A} = A. \tag{6.27}$$

This is analogous to (6.10). However, although every complex number has a logarithm[51], a matrix has a logarithm if and only if it is invertible. One of the directions of this proof is easy: if a matrix B has a logarithm $A = \log B$, then we can write $B = \mathrm{e}^{A}$, and then the inverse will be $B^{-1} = \mathrm{e}^{-A}$. We won't prove the other direction here.

Recall that we said that Hermitian matrices are analogous to real numbers, and unitary matrices are analogous to complex numbers with unit norm. Since for real ϕ we have $\left|\mathrm{e}^{\mathrm{i}\,\phi}\right| = 1$, we should expect that the exponential of i times a Hermitian matrix will be a unitary matrix. Let H be a Hermitian matrix and let $t \in \mathbb{R}$ be a real number, and let us define[52]

$$U \equiv \mathrm{e}^{-\mathrm{i}\,Ht}. \tag{6.29}$$

To prove that U is unitary, let us take its adjoint:

$$U^{\dagger} = \left(\mathrm{e}^{-\mathrm{i}\,Ht}\right)^{\dagger} = \mathrm{e}^{-\mathrm{i}^{*}\,H^{\dagger}t^{*}} = \mathrm{e}^{\mathrm{i}\,Ht}, \tag{6.30}$$

since $H^{\dagger} = H$ due to H being Hermitian, $t^{*} = t$ due to t being real, and $\mathrm{i}^{*} = -\,\mathrm{i}$. Thus:

$$UU^{\dagger} = \mathrm{e}^{-\mathrm{i}\,Ht}\,\mathrm{e}^{\mathrm{i}\,Ht} = \mathrm{e}^{0} = 1, \tag{6.31}$$

so $\mathrm{e}^{-\mathrm{i}\,Ht}$ is indeed unitary. Note that here we used the fact that H commutes with itself, and

[51] In fact, every complex number has an **infinite** number of logarithms. The arbitrary complex number $z = r\,\mathrm{e}^{\mathrm{i}\,\phi}$ can also be written as $z = r\,\mathrm{e}^{\mathrm{i}(\phi+2\pi n)}$ for all integer n, since adding a multiple of 2π to the angle ϕ results in the same angle. Thus we have

$$\log z = \log\left(r\,\mathrm{e}^{\mathrm{i}(\phi+2\pi n)}\right) = \log r + \log \mathrm{e}^{\mathrm{i}(\phi+2\pi n)} = \log r + \mathrm{i}\,(\phi + 2\pi n)\,, \tag{6.28}$$

where n can be any integer. Here we used the identity $\log(ab) = \log a + \log b$, which follows from the identity $\mathrm{e}^{z}\,\mathrm{e}^{w} = \mathrm{e}^{z+w}$.

[52] The minus sign here is a convention; the inverse matrix, $\mathrm{e}^{\mathrm{i}\,Ht}$, is of course unitary as well.

therefore the product of the exponentials is the exponential of the sum, as we discussed above. In fact, since all unitary matrices are invertible, and all invertible matrices have a logarithm, **any** unitary matrix U can be written as $\mathrm{e}^{-\mathrm{i}H}$ for some Hermitian matrix H, where

$$H = \mathrm{i}\log U \quad \Longrightarrow \quad U = \mathrm{e}^{-\mathrm{i}H}. \tag{6.32}$$

Finally, (6.9) generalizes to matrices as well:

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{At} = A\,\mathrm{e}^{At}, \tag{6.33}$$

where A is any **constant** complex matrix (i.e. independent of t).

Everything we described here was defined for matrices; however, it actually also applies to general operators on any Hilbert space – and in the infinite-dimensional case it is less convenient to think about operators as matrices, since those matrices would be infinite-dimensional as well. The *operator exponential* is defined is exactly the same way as the matrix exponential, with the identity matrix replaced by the identity operator (which does not change the state it acts on), the power A^n means the operator A is applied n times, and so on.

Problem 6.4. Prove that $\left(\mathrm{e}^{A}\right)^{\dagger} = \mathrm{e}^{A^{\dagger}}$.

Problem 6.5. Prove that if two matrices A and B commute, that is, $[A, B] = 0$, then

$$\mathrm{e}^{A}\,\mathrm{e}^{B} = \mathrm{e}^{A+B}. \tag{6.34}$$

One way to do this is using the power series definition (6.24).

Problem 6.6.

A. Prove that the exponential of a diagonal matrix with diagonal elements λ_i is a diagonal matrix with diagonal elements e^{λ_i}:

$$\exp\begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & \\ 0 & 0 & \lambda_n \end{pmatrix} = \begin{pmatrix} \mathrm{e}^{\lambda_1} & 0 & 0 \\ 0 & \ddots & \\ 0 & 0 & \mathrm{e}^{\lambda_n} \end{pmatrix}. \tag{6.35}$$

B. Prove that if B is an invertible matrix, then for any matrix A :

$$\mathrm{e}^{BAB^{-1}} = B\,\mathrm{e}^{A}\,B^{-1}. \tag{6.36}$$

C. Using (A) and (B), prove that if A is diagonalizable, that is, $A = PDP^{-1}$ for some matrix P and a diagonal matrix D (recall Section 3.2.16), then

$$\mathrm{e}^{A} = P\,\mathrm{e}^{D}\,P^{-1}. \tag{6.37}$$

This gives us a straightforward way to calculate the exponential of any diagonalizable matrix (and in particular every normal matrix, since they are always diagonalizable).

Problem 6.7. Find the matrix exponential $e^{-i\theta\sigma_y}$ where σ_y is the Pauli matrix

$$\sigma_y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{6.38}$$

Does the result look familiar?

6.2 Continuous Time Evolution, Hamiltonians, and the Schrödinger Equation

When we described the Evolution Axiom, we only talked about evolution from one discrete point in time to another. As a first step towards quantum mechanics of continuous systems, let us discuss time evolution with a continuous time variable.

6.2.1 The Schrödinger Equation and Hamiltonians: Preface

Usually, in introductory quantum mechanics courses, the *Schrödinger equation* is introduced at the very beginning – as a fundamental postulate, without any explanation or motivation. The student is simply told that this is the equation they are going to be working with, and typically, much of the rest of the course consists of solving the Schrödinger equation for different systems.

In this course, I chose to do the exact opposite, and introduce the Schrödinger equation only at the very end of the course. The reason is that the Schrödinger equation is actually **not** a fundamental component of the modern 21st-century formulation of quantum theory[53]. What is truly fundamental about quantum theory is what we spent the majority of this course studying: the abstract formulation of the theory in terms of Hilbert spaces, states, and operators, using the axioms we have presented above. The Schrödinger equation turns out to be merely a **special case** of the Evolution Axiom – which, as you recall, simply says that quantum states evolve by the action of unitary operators.

The Evolution Axiom applies to **any** kind of evolution, whether in time or due to some transformation performed on the system; and with regards to evolution in time, the time variable can be either discrete or continuous. Quantum gates, which are the main type of evolution we have seen so far, correspond to discrete time evolution – the qubit is in some state now, and will be in another state after it passes through the gate, but these are two **discrete** points in time, and nothing of interest is happening in the gap between them.

In the specific case when the evolution is the system's natural evolution in time (so not a result of some explicit transformation, like a rotation) and with respect to a **continuous** time variable, it is useful in practice to replace the Evolution Axiom, which is very abstract, with the Schrödinger equation, which is a concrete differential equation that can be solved, either exactly or approximately, for a variety of different systems. The focus then shifts from

[53] In fact, entire books have been written about fields such as quantum computation and quantum gravity without mentioning the Schrödinger equation even once!

the unitary evolution operator of the Evolution Axiom to a Hermitian operator called the *Hamiltonian*. We will see below precisely how these two operators are related to each other.

To further illustrate the fact that the Evolution Axiom is more fundamental than the Schrödinger equation, consider the fact that the Evolution Axiom is an almost **inevitable** result of the mathematical framework of quantum theory – indeed, if quantum states evolved with non-unitary operators, then probabilities would no longer sum to 1, and the theory wouldn't make any sense. While the Schrödinger equation also preserves probabilities (as it must), this fact is not immediately obvious from the form of the equation.

6.2.2 Derivation of the Schrödinger Equation

Let us recall the Evolution Axiom from Section 4.5.1, with slightly different notation. If the system is in the state $|\Psi(t_1)\rangle$ at time t_1, and in another state $|\Psi(t_2)\rangle$ at time t_2, then the two states must be related by the action of some unitary operator $U(t_2 \leftarrow t_1)$:

$$|\Psi(t_2)\rangle = U(t_2 \leftarrow t_1)\,|\Psi(t_1)\rangle\,. \tag{6.39}$$

The main difference between this formulation and the one we had for discrete systems is that now we are letting U be a **continuous function** of t_1 and t_2, so that we can encode the unitary evolution of the system from any point in time to any other point in time. This is very different than what we discussed in the discrete case, where for example, a quantum gate is not a function of time – it is the same quantum gate at all times.

However, this is still just a special case of the Evolution Axiom; the axiom simply states that evolution between any two points in time must be encoded in some unitary operator, but it will in general be a different operator for different start and end times, so here we have explicitly encoding the different operators as one universal function $U(t_2 \leftarrow t_1)$.

In (6.39), if we assume that $t_2 = t_1$ (that is, no time has passed) then we get

$$|\Psi(t_1)\rangle = U(t_1 \leftarrow t_1)\,|\Psi(t_1)\rangle\,. \tag{6.40}$$

Since this must be true for **every** state $|\Psi(t_1)\rangle$ and for **every** time t_1, we see[54] that if no time has passed, $U(t_1 \leftarrow t_1)$ must be the identity operator:

$$U(t_1 \leftarrow t_1) = 1, \qquad \forall t_1 \in \mathbb{R}. \tag{6.41}$$

Let us now assume that the system is in the state $|\Psi(t_3)\rangle$ at time t_3. Then from (6.39) we must have on the one hand

$$|\Psi(t_3)\rangle = U(t_3 \leftarrow t_1)\,|\Psi(t_1)\rangle\,, \tag{6.42}$$

but on the other hand

$$|\Psi(t_3)\rangle = U(t_3 \leftarrow t_2)\,|\Psi(t_2)\rangle = U(t_3 \leftarrow t_2)\,U(t_2 \leftarrow t_1)\,|\Psi(t_1)\rangle\,. \tag{6.43}$$

[54] Recall Problem 3.29!

Therefore, U must satisfy the *composition property*[55]:

$$U\left(t_3 \leftarrow t_1\right) = U\left(t_3 \leftarrow t_2\right) U\left(t_2 \leftarrow t_1\right), \qquad \forall t_1, t_2, t_3 \in \mathbb{R}. \tag{6.44}$$

In particular, if $t_3 = t_1$ we get

$$1 = U\left(t_1 \leftarrow t_1\right) = U\left(t_1 \leftarrow t_2\right) U\left(t_2 \leftarrow t_1\right). \tag{6.45}$$

Therefore we must have

$$U\left(t_1 \leftarrow t_2\right) = U^{-1}\left(t_2 \leftarrow t_1\right) = U^{\dagger}\left(t_2 \leftarrow t_1\right), \qquad \forall t_1, t_2 \in \mathbb{R}, \tag{6.46}$$

or in other words, evolution to the past is given by the adjoint (or inverse) of the evolution to the future, as we discussed in Section 4.5.1.

We now change notation slightly by taking $t_1 \mapsto t_0$ and $t_2 \mapsto t$ in (6.39):

$$\left|\Psi\left(t\right)\right\rangle = U\left(t \leftarrow t_0\right)\left|\Psi\left(t_0\right)\right\rangle. \tag{6.47}$$

For any **arbitrary** time t, the evolution of the system from a **fixed** time t_0 is given by this equation. Let us take the time derivative of the equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left|\Psi\left(t\right)\right\rangle = \frac{\mathrm{d}U\left(t \leftarrow t_0\right)}{\mathrm{d}t}\left|\Psi\left(t_0\right)\right\rangle, \tag{6.48}$$

where we consider $\left|\Psi\left(t_0\right)\right\rangle$ to be independent of t since t_0 is a fixed time. From (6.47) we find, by multiplying both sides by $U^{\dagger}\left(t \leftarrow t_0\right)$ from the left, that

$$\left|\Psi\left(t_0\right)\right\rangle = U^{\dagger}\left(t \leftarrow t_0\right)\left|\Psi\left(t\right)\right\rangle. \tag{6.49}$$

We plug that into (6.48) and find

$$\frac{\mathrm{d}}{\mathrm{d}t}\left|\Psi\left(t\right)\right\rangle = \frac{\mathrm{d}U\left(t \leftarrow t_0\right)}{\mathrm{d}t} U^{\dagger}\left(t \leftarrow t_0\right)\left|\Psi\left(t\right)\right\rangle, \tag{6.50}$$

where the time derivative only acts on U and not on $U^{\dagger}$. Now, let us define a new operator H called the *Hamiltonian* as follows:

$$H\left(t\right) \equiv \mathrm{i}\,\frac{\mathrm{d}U\left(t \leftarrow t_0\right)}{\mathrm{d}t} U^{\dagger}\left(t \leftarrow t_0\right). \tag{6.51}$$

Note that H can in general be a function of t, but it is **independent** of t_0, which is why we

[55] This property is the reason we used the notation $U\left(t_2 \leftarrow t_1\right)$: we wanted the t_2 in $U\left(t_2 \leftarrow t_1\right)$ and the t_2 in $U\left(t_3 \leftarrow t_2\right)$ to be adjacent. If the times were arranged from left to right, we would have had $U\left(t_2 \rightarrow t_3\right) U\left(t_1 \rightarrow t_2\right)$ which does not make it clear that the operator on the left starts when the operator on the right ends. Note that when applying operators to a ket, the operators always act from right to left. So in $U\left(t_3 \leftarrow t_2\right) U\left(t_2 \leftarrow t_1\right)\left|\Psi\left(t_1\right)\right\rangle$ the operator $U\left(t_2 \leftarrow t_1\right)$ acts on the state first, to take it to t_2, and then $U\left(t_3 \leftarrow t_2\right)$ acts on the result, to take it to t_3.

called it $H(t)$ and not $H(t, t_0)$ or $H(t \leftarrow t_0)$. Also, the Hamiltonian is Hermitian. You will prove both of these facts in Problem 6.8.

In terms of the Hamiltonian, (6.50) becomes

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle. \tag{6.52}$$

This equation is called the *Schrödinger equation*[56][57].

Problem 6.8.

A. Prove that $H(t)$ as defined in (6.51) is independent of t_0, thus justifying the notation $H(t)$, as well as its use in the Schrödinger equation (6.52), where t is the only variable.

B. Prove that $H(t)$ is a Hermitian operator.

6.2.3 Time-Independent Hamiltonians

Let us now assume that the Hamiltonian is constant, that is, *time-independent*. Although in some quantum systems the Hamiltonian does depend on time, this is not very common; most quantum systems have time-independent Hamiltonians.

We can rewrite (6.51) as follows:

$$\frac{\mathrm{d}U(t \leftarrow t_0)}{\mathrm{d}t} = -\mathrm{i}HU(t \leftarrow t_0). \tag{6.54}$$

Compare this with (6.33):

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{At} = A\,\mathrm{e}^{At}, \tag{6.55}$$

which we derived assuming that A is constant. If the Hamiltonian H is constant, then $A \equiv -\mathrm{i}H$ is also constant. In addition, we can replace t with $t - t_0$ in the exponent, since that

[56] In non-natural units, this equation features the reduced Planck constant $\hbar$:

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle. \tag{6.53}$$

Of course, as we discussed in Section 4.1.1, $\hbar$ is dimensionful and therefore its numerical value doesn't matter, so we can just choose units such as the Planck units, where it simply has the value $\hbar \equiv 1$.

[57] In the Schrödinger equation, a time derivative $\mathrm{d}/\mathrm{d}t$ is acting on the state $|\Psi(t)\rangle$. Therefore, one might wonder whether $\mathrm{d}/\mathrm{d}t$ is an operator on the Hilbert space. However, the answer is no. This is because here we are dealing with non-relativistic quantum mechanics, and non-relativistic theories – both classical and quantum – treat space and time differently: while x is an operator (as we will see below), t is just a **label**. See also Footnote 66.

In this section we defined a function $|\Psi(t)\rangle$, which takes some real number t as input, and returns some state in the Hilbert space as output. The derivative $\mathrm{d}/\mathrm{d}t$ doesn't act on the vectors in the Hilbert space, which is what operators do; instead, it acts on this function. Therefore, $\mathrm{d}/\mathrm{d}t$ is not an operator on the Hilbert space.

To illustrate this further, consider a system with a finite Hilbert space, such as a qubit. We can define a function $|\Psi(t)\rangle$ which returns a particular state of the qubit given a particular point t in time. Then $\mathrm{d}/\mathrm{d}t$ would be the derivative of that function with respect to time. But as we have seen, operators on finite Hilbert spaces take the form of matrices acting on vectors in the space. $\mathrm{d}/\mathrm{d}t$ is not a matrix, so it is not an operator on the Hilbert space – it's just a derivative with respect to a label.

does not change the derivative (because t_0 is constant). Hence, we see that the solution[58] to the differential equation (6.54) is

$$U(t \leftarrow t_0) \equiv \mathrm{e}^{-\mathrm{i}H(t-t_0)}. \tag{6.56}$$

In other words, if we take $U(t \leftarrow t_0) \equiv \mathrm{e}^{-\mathrm{i}H(t-t_0)}$, then its time derivative will be $-\mathrm{i}HU(t \leftarrow t_0)$, and thus it will satisfy (6.54). Don't get confused by the notation: $H(t-t_0)$ in the exponent is the **constant** H **times** the **number** $t-t_0$, not the function H evaluated at $t-t_0$!

The reason we wrote $t-t_0$ instead of t in the exponential is that from (6.41) we have the initial condition

$$U(t_0 \leftarrow t_0) = 1. \tag{6.57}$$

This condition is indeed satisfied for U as defined in (6.56), since

$$U(t_0 \leftarrow t_0) = \mathrm{e}^{-\mathrm{i}H(t_0-t_0)} = \mathrm{e}^0 = 1, \tag{6.58}$$

by (6.25). However, it would **not** be satisfied if we just wrote $\mathrm{e}^{-\mathrm{i}Ht}$, since then we would have $U(t_0 \leftarrow t_0) = \mathrm{e}^{-\mathrm{i}Ht_0} \neq 1$. In general, when solving differential equations, the solution always depends on the initial (or boundary) conditions.

We can rewrite (6.56) to match the notation in the beginning of Section 6.2.2 as follows:

$$U(t_2 \leftarrow t_1) \equiv \mathrm{e}^{-\mathrm{i}H(t_2-t_1)}. \tag{6.59}$$

The evolution operator between any two arbitrary points in time, t_1 and t_2, is given by (6.59).

It is interesting that, since H is constant, the unitary evolution operator is not a function of both t_1 and t_2, but only the **difference** between them, t_2-t_1. So for example, the evolution from time $t_1=3$ to time $t_2=4$ and from time $t_1=4$ to time $t_2=5$ will be given by the **same** unitary operator, $\mathrm{e}^{-\mathrm{i}H}$, since in both cases the time difference is $t_2-t_1=1$.

Problem 6.9. For the unitary operator defined in (6.59):

A. Verify that it satisfies the composition property (6.44).

B. Verify that it is invariant under the *time shift* transformation

$$t_1 \mapsto t_1+t, \qquad t_2 \mapsto t_2+t, \tag{6.60}$$

where $t \in \mathbb{R}$.

C. Verify that under a *time-reversal* transformation

$$t_1 \mapsto -t_1, \qquad t_2 \mapsto -t_2, \tag{6.61}$$

the evolution operator is replaced with its adjoint (or inverse). Thus the evolution equation

[58] Even if the Hamiltonian is time-dependent, it is still possible to solve the differential equation (6.54); however, the solution is then much more complicated and involves *time-ordered exponentials*, which we will not cover in this course.

(6.39) is invariant under time reversal if we also replace U by its adjoint. This is an explicit example of the *time-reversal symmetry* of quantum mechanics, which we discussed in Section 4.5.1.

Problem 6.10. In Section 4.5.2 we discussed several unitary operators which act on qubits. For example, the quantum Z gate is given by the Pauli matrix σ_z

$$Z \equiv \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{6.62}$$

and its action is to leave $|0\rangle$ unchanged but flip the phase of $|1\rangle$. Find the Hamiltonian corresponding to this unitary evolution operator. Since this is a discrete evolution, the time coordinate is discrete and not continuous, and we can take the time interval to be 1. In other words, you need to find the H in the equation $Z = \mathrm{e}^{-\mathrm{i}H}$.

6.2.4 Hamiltonians and Energy

In Problem 6.8, you proved that the Hamiltonian is a Hermitian operator. Therefore, it should correspond to an **observable**. Indeed, it does; this observable is the *energy* of the system. Its (real) eigenvalues E_i correspond to *energy eigenstates* $|E_i\rangle$ which, as usual, make up an orthonormal basis[59]:

$$H\,|E_i\rangle = E_i\,|E_i\rangle\,. \tag{6.63}$$

This is often referred to as the *time-independent Schrödinger equation*, but it's really just an eigenvalue equation!

The basis eigenstate $|E_i\rangle$ corresponds to a measurement of E_i for the energy. There will always be a state of **lowest** energy, that is, a state $|E_0\rangle$ for which the eigenvalue E_0 is the lowest among all the eigenvalues:

$$E_0 < E_i, \qquad \forall i > 0. \tag{6.64}$$

Such a state is called the *ground state*.

As we have seen, the Hamiltonian is used to evolve continuous systems in time. What does energy have to do with time, you ask? Well, from relativity we know that momentum in spacetime is described by a 4-vector called the *4-momentum*, which is defined as follows:

$$\mathbf{p}\,(t,x,y,z) \equiv \begin{pmatrix} E \\ p_x \\ p_y \\ p_z \end{pmatrix}. \tag{6.65}$$

Here, p_x, p_y, and p_z are the momenta in the x, y, and z directions respectively. In the first component, which is the one in the time direction, we have the energy E. Thus energy is

[59] Here we used slightly different notation than usual, with the basis eigenstates being $|E_i\rangle$ instead of $|B_i\rangle$ and the eigenvalues being E_i instead of λ_i – compare (3.143).

actually "momentum in the time direction"! Indeed, in relativity we will often write p_0 for the energy. Just like momentum moves you in space, so does energy move you in time. This is exactly why the Hamiltonian is responsible for evolution in time. It is also why Hamiltonians are usually time-independent – if they are not, then energy is not conserved!

6.3 Hamiltonian Mechanics and Canonical Quantization

We have seen that in order to create a model for a specific physical system in quantum theory, we must choose a specific Hilbert space with specific states and specific operators. But how do we know which Hilbert space, states, and operators to use for a given physical system? This is often a hard question to answer. For example, we currently do not have a consistent and experimentally verified quantum model for general relativity; the problem of finding such a model is known as *quantum gravity*, and it is one of the hardest problems in physics.

Luckily, it turns out that there is a certain prescription that allows us to take a classical theory and turn it into a quantum theory in a straightforward way. The properties of the classical theory will dictate the type of Hilbert space, states, and operators we should use in the corresponding quantum theory. This process is known as *quantization*. It doesn't work for every classical theory; for example, it doesn't work for general relativity, which is why quantizing gravity is so hard. However, it does work, in an experimentally verifiable way, for most classical theories of interest.

6.3.1 A Quick Review of Classical Hamiltonian Mechanics

Classical mechanics can be reformulated using a quantity called the *(classical) Hamiltonian*. This is basically the total energy of the system, usually written as *kinetic energy* plus *potential energy* and in terms of the *canonical coordinates* q and p. Here we will consider the case where q and p represent position and momentum respectively, and therefore we will label them x and p instead.

The *phase space* of the system consists of all the possible values of the canonical coordinates; for a particle, the phase space includes both "actual" space (all the values of x) and *momentum space* (all the values of p).

Since we have limited time, and we are interested in quantum mechanics and not classical mechanics, we will not go over the Hamiltonian formulation in detail. Instead, we will just review certain important definitions and results.

The Hamiltonian is generally of the form

$$H = K(p) + V(x), \tag{6.66}$$

where K is the kinetic energy, which depends only on the momentum p, and V is the potential energy, which depends only on the position x.

Let us consider the specific case of a single particle of mass m. In Newtonian mechanics, the particle's momentum is defined as

$$p \equiv mv, \qquad \text{where } v \equiv \dot{x} \equiv \frac{\mathrm{d}x}{\mathrm{d}t}. \tag{6.67}$$

The kinetic energy is defined as $\frac{1}{2}mv^2$, and we can write it in terms of the momentum as follows:

$$K = \frac{1}{2}mv^2 = \frac{1}{2m}(mv)^2 = \frac{p^2}{2m}. \tag{6.68}$$

We conclude that for a particle of mass m, the Hamiltonian will generally be of the form

$$H = \frac{p^2}{2m} + V(x). \tag{6.69}$$

The kinetic energy of a particle will always be $p^2/2m$, but the potential energy $V(x)$ depends on the forces acting on the particle, such as gravity or electromagnetism.

Now, let us define the *Poisson brackets* of two functions f, g of position x and momentum p as follows:

$$\{f, g\} \equiv \frac{\partial f}{\partial x}\frac{\partial g}{\partial p} - \frac{\partial g}{\partial x}\frac{\partial f}{\partial p}. \tag{6.70}$$

In Problem 6.11 you will prove some properties of these brackets; in particular they are anti-symmetric, $\{g, f\} = -\{f, g\}$ which means that $\{f, f\} = 0$ for any f. For x and p themselves we have

$$\{x, x\} = \{p, p\} = 0, \tag{6.71}$$

and

$$\{x, p\} = \frac{\partial x}{\partial x}\frac{\partial p}{\partial p} - \frac{\partial p}{\partial x}\frac{\partial x}{\partial p} = 1, \tag{6.72}$$

since x and p are assumed to be **independent** variables, so their derivatives with respect to each other vanish. Even though in Newtonian mechanics we **define** the momentum to be $p \equiv m\dot{x}$, in Hamiltonian mechanics we "forget" about this relation and just assume that x and p are two completely independent degrees of freedom of the system, thus generalizing the concept of momentum to any kind of system.

The dynamics of the system in Hamiltonian mechanics are determined as follows. If A is any function of x and p, then its time derivative is given by[60]

$$\dot{A} \equiv \frac{\mathrm{d}A}{\mathrm{d}t} = \{A, H\}. \tag{6.74}$$

[60] Here we are assuming that A does not depend on t **explicitly**, but only **implicitly** via its dependence on x and p. If A does have explicit dependence on t, then this equation becomes

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \{A, H\} + \frac{\partial A}{\partial t}. \tag{6.73}$$

For x and p themselves, we get

$$\dot{x} \equiv \frac{\mathrm{d}x}{\mathrm{d}t} = \{x, H\} = \frac{\partial x}{\partial x}\frac{\partial H}{\partial p} - \frac{\partial H}{\partial x}\frac{\partial x}{\partial p} = \frac{\partial H}{\partial p}, \tag{6.75}$$

$$\dot{p} \equiv \frac{\mathrm{d}p}{\mathrm{d}t} = \{p, H\} = \frac{\partial p}{\partial x}\frac{\partial H}{\partial p} - \frac{\partial H}{\partial x}\frac{\partial p}{\partial p} = -\frac{\partial H}{\partial x}. \tag{6.76}$$

In other words, the evolution of each parameter depends on the derivative of the Hamiltonian with respect to the other parameter. Equations (6.75) and (6.76) are called *Hamilton's equations*.

For a point particle with Hamiltonian (6.69), we get

$$\dot{x} \equiv \frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\partial}{\partial p}\left(\frac{p^2}{2m} + V(x)\right) = \frac{p}{m}, \tag{6.77}$$

$$\dot{p} \equiv \frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial}{\partial x}\left(\frac{p^2}{2m} + V(x)\right) = -V'(x). \tag{6.78}$$

The first equation relates the two independent variables x and p to each other: $p = m\dot{x}$. Of course, this is just the definition of the momentum of a particle in Newtonian mechanics, but Hamiltonian mechanics allows us to consider more general systems and define a *generalized momentum* for any kind of system. For example, in a rotating system p will be the angular momentum, and so on.

The second equation is *Newton's second law*: the time derivative of momentum is the force, and the force is given by minus the derivative of the potential[61]. We can take the derivative of (6.77) and plug (6.78) into it to get

$$\ddot{x} \equiv \frac{\mathrm{d}^2x}{\mathrm{d}t^2} = \frac{\mathrm{d}\dot{x}}{\mathrm{d}t} = \frac{1}{m}\frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{1}{m}V'(x). \tag{6.80}$$

Multiplying by m, we get the familiar form of Newton's law:

$$F = ma = m\ddot{x} \equiv m\frac{\mathrm{d}^2x}{\mathrm{d}t^2} = -V'(x), \tag{6.81}$$

where a is the acceleration.

Problem 6.11. Prove the following properties of the Poisson brackets:

- **Anti-symmetry:** For all functions f, g

$$\{f, g\} = -\{g, f\}. \tag{6.82}$$

[61] Here we are working in one spatial dimension, for simplicity. In the 3-dimensional case, the force is minus the gradient of the potential:

$$\mathbf{F} = -\boldsymbol{\nabla} V = -\left(\frac{\partial V}{\partial x}, \frac{\partial V}{\partial y}, \frac{\partial V}{\partial z}\right). \tag{6.79}$$

- **Linearity:** For all functions f, g, h and numbers α, b

$$\{\alpha f + \beta g, h\} = \alpha \{f, h\} + \beta \{g, h\}. \tag{6.83}$$

- **Leibniz rule:** For all functions f, g, h

$$\{fg, h\} = f \{g, h\} + \{f, h\} g. \tag{6.84}$$

- **Jacobi identity:**

$$\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0. \tag{6.85}$$

6.3.2 Canonical Quantization

Recall the definition of the expectation value for the measurement of an observable A when the system is in the state $|\Psi\rangle$:

$$\langle A \rangle \equiv \langle \Psi | A | \Psi \rangle. \tag{6.86}$$

Let us take the time derivative of this, assuming that the state $|\Psi\rangle$ depends on time but the observable A doesn't (which is usually the case):

$$\frac{\mathrm{d} \langle A \rangle}{\mathrm{d}t} = \left(\frac{\mathrm{d}}{\mathrm{d}t} \langle \Psi | \right) A | \Psi \rangle + \langle \Psi | A \left(\frac{\mathrm{d}}{\mathrm{d}t} | \Psi \rangle \right). \tag{6.87}$$

By the Schrödinger equation (6.52), we have

$$\frac{\mathrm{d}}{\mathrm{d}t} |\Psi\rangle = -\mathrm{i} H |\Psi\rangle. \tag{6.88}$$

We can take the adjoint of this equation to get (remember that H is Hermitian so $H = H^\dagger$)

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle \Psi | = \mathrm{i} \langle \Psi | H. \tag{6.89}$$

Plugging into (6.87), we get

$$\begin{aligned} \frac{\mathrm{d} \langle A \rangle}{\mathrm{d}t} &= \mathrm{i} \langle \Psi | HA | \Psi \rangle - \mathrm{i} \langle \Psi | AH | \Psi \rangle \\ &= -\mathrm{i} \langle \Psi | (AH - HA) | \Psi \rangle \\ &= -\mathrm{i} \langle \Psi | [A, H] | \Psi \rangle \\ &= -\mathrm{i} \langle [A, H] \rangle, \end{aligned}$$

so in conclusion,

$$\frac{\mathrm{d} \langle A \rangle}{\mathrm{d}t} = -\mathrm{i} \langle [A, H] \rangle. \tag{6.90}$$

Comparing this with (6.74),

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \{A, H\}\,, \tag{6.91}$$

we find a very interesting result: the **quantum** expectation value of the observable A evolves in time just as **classical** Hamiltonian mechanics predicts, provided we relate the Poisson brackets of functions and the commutator of operators as follows:

$$[A, H] \equiv \mathrm{i}\,\{A, H\}\,, \tag{6.92}$$

or more generally for any two observables A and B,

$$[A, B] \equiv \mathrm{i}\,\{A, B\}\,. \tag{6.93}$$

This is called the *canonical commutation relation*.

Equation (6.93) makes sense, because in Problem 6.11 you proved some properties of Poisson brackets, and these properties also happen to be satisfied by the commutator, as you proved in problems 4.29, 4.30, 4.32, and 4.33!

In particular, for x and p themselves, according to (6.72) we have $\{x, p\} = 1$, so in the quantum theory we will have[62]

$$[x, p] = \mathrm{i}\,. \tag{6.94}$$

What we have derived (or at least, motivated) here is called *canonical quantization*. Given a classical system described by a Hamiltonian, we can turn it into a quantum system – *quantize* it – by *"promoting"* classical functions on the phase space, including the variables x and p themselves, to Hermitian operators. We are not provided with any specific information about these operators, except that they are Hermitian (which they must be, since in classical physics all variables are real!) and that the quantum commutators should be related to the classical Poisson brackets according to the prescription (6.93).

These Hermitian operators now represent observables in the quantum theory; they have eigenstates and eigenvalues which represent possible measurement outcomes. This means that the values of x and p are no longer uniquely determined from some initial conditions, as in the classical theory; they become **probabilistic**. In addition, the time evolution of the system is no longer described by Hamilton's equations, but rather, by the Schrödinger equation.

Note that what we did here does not constitute a proof that **all** classical theories are related to quantum theories in this way. Canonical quantization merely ensures that expectation values of the observables in the quantum theory evolve in time in the same way as the observables in the classical theory, which is something that we expect to be true, but it is not by itself a sufficient condition for creating a sensible quantum theory. Indeed, there are known cases where canonical quantization doesn't quite work, or is at least ambiguous, because two Poisson brackets which in the classical theory are equal to each other will have different values in the quantum theory, generating an inconsistency.

[62] With $\hbar$, this equation will take the form $[x, p] = \mathrm{i}\,\hbar$.

Nevertheless, canonical quantization works incredibly well in the vast majority of cases – and indeed, most classical theories, from a single point particle to very complicated systems with many different particles and forces, can be quantized in this way, and the results have been verified experimentally to high precision!

Just as in the case of the Schrödinger equation, in introductory quantum mechanics courses canonical quantization is usually just presented as an arbitrary axiom. I hope I managed to motivate it and give you some intuition as to why classical and quantum theories are related in this way.

6.4 The Harmonic Oscillator

6.4.1 The Classical Harmonic Oscillator

The *quantum harmonic oscillator* is the quantization of the *classical harmonic oscillator*, and just like the qubit, it is a reasonably simple quantum system which turns out to describe many different realistic physical systems, either exactly or approximately. This makes sense, because the classical harmonic oscillator itself describes or approximates many different classical systems!

In particular, quantum harmonic oscillators form the basis of *quantum field theory*, which is the theory describing all of the known elementary particles, including matter particles (such as electrons and *quarks*), particles which mediate fundamental interactions (such as photons, which mediate the electromagnetic force, and *gluons*, which mediate the *strong nuclear force*), and others (such as the *Higgs boson*).

The (simple) classical harmonic oscillator has the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2. \tag{6.95}$$

We have the standard kinetic energy term $K(p) = p^2/2m$, where m is the mass of the particle, and the potential energy

$$V(x) \equiv \frac{1}{2}m\omega^2 x^2, \tag{6.96}$$

where ω is a numerical constant called the *frequency* or *angular frequency*, because it represents the frequency in which the oscillator oscillates.

It is easy to find the *equations of motion* using Hamilton's equations (6.75) and (6.76). Alternatively, since this is a particle with a Hamiltonian of the standard form (6.69), we can just use Newton's second law (6.81) directly:

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -\frac{1}{m}\frac{\partial}{\partial x}V(x) = -\frac{1}{m}\frac{\partial}{\partial x}\left(\frac{1}{2}m\omega^2 x^2\right) = -\omega^2 x. \tag{6.97}$$

To solve this differential equation, we can use the fact that

$$\frac{\mathrm{d}}{\mathrm{d}t}\cos t = -\sin t, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\sin t = \cos t, \tag{6.98}$$

which means that

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\cos t = -\frac{\mathrm{d}}{\mathrm{d}t}\sin t = -\cos t. \tag{6.99}$$

If we replace t by $\omega t + \phi$, where both ω and ϕ are constant (independent of t), then since

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\omega t + \phi\right) = \omega, \tag{6.100}$$

we get, by the chain rule, that each derivative generates a factor of ω, so

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}\cos\left(\omega t + \phi\right) = -\omega\frac{\mathrm{d}}{\mathrm{d}t}\Big(\sin\left(\omega t + \phi\right)\Big) = -\omega^2\cos\left(\omega t + \phi\right). \tag{6.101}$$

Therefore, this differential equation has the solution:

$$x\left(t\right) = A\cos\left(\omega t + \phi\right), \tag{6.102}$$

where the *integration constants* A and ϕ are real numbers determined by the initial conditions. Now we see why this is called a harmonic oscillator: the position of the particle oscillates repeatedly between $+A$ and $-A$ over time.

Problem 6.12. Prove that the most general solution for the classical harmonic oscillator can also be written as

$$x\left(t\right) = B\cos\left(\omega t\right) + C\sin\left(\omega t\right), \tag{6.103}$$

where B and C are integration constants, or as

$$x\left(t\right) = D\,\mathrm{e}^{\mathrm{i}\,\omega t} + E\,\mathrm{e}^{-\mathrm{i}\,\omega t}, \tag{6.104}$$

where D and E are integration constants. All of these solutions are equivalent; find the relationships between the integration constants $\{A, \phi\}$, $\{B, C\}$, and $\{D, E\}$ – that is, write each pair in terms of another pair.

Problem 6.13. As an example of solving the equation of motion for specific initial conditions, if the particle starts at time $t = 0$ at position $x\left(0\right) = 1$ with velocity $\dot{x}\left(0\right) = 0$, then we have

$$\dot{x}\left(0\right) = -\omega A\sin\phi = 0 \quad \Longrightarrow \quad \phi = 0, \tag{6.105}$$

$$x\left(0\right) = A = 1 \quad \Longrightarrow \quad A = 0, \tag{6.106}$$

and thus the solution is

$$x\left(t\right) = \cos\left(\omega t\right). \tag{6.107}$$

Similarly, find a solution for the classical harmonic oscillator with the initial conditions

$x(0) = 0$ and $\dot{x}(0) = \omega$.

Problem 6.14. By plugging the general solution (6.102) into the Hamiltonian (6.95), show that the total energy of the system is

$$H = \frac{1}{2} m\omega^2 A^2. \tag{6.108}$$

Thus the Hamiltonian is time-independent, and energy is conserved.

6.4.2 Quantizing the Harmonic Oscillator

Let us now quantize the simple harmonic oscillator by promoting x and p to operators. We are interested in finding the energy eigenstates of this quantum system. Instead of finding them by solving a differential equation, we will use an easier and more intuitive method. We define the *ladder operators*:

$$a = \sqrt{\frac{m\omega}{2}} \left(x + \frac{\mathrm{i}}{m\omega} p \right), \qquad a^\dagger = \sqrt{\frac{m\omega}{2}} \left(x - \frac{\mathrm{i}}{m\omega} p \right), \tag{6.109}$$

where $a^\dagger$ is called the *creation operator* and a is called the *annihilation operator*. Notice that $a^\dagger$ is indeed the adjoint of a, since the numbers m, ω are real and the operators x, p are Hermitian. These definitions may be inverted to get the position and momentum operators in terms of the ladder operators:

$$x = \sqrt{\frac{1}{2m\omega}} \left(a^\dagger + a \right), \qquad p = \mathrm{i} \sqrt{\frac{m\omega}{2}} \left(a^\dagger - a \right). \tag{6.110}$$

Now, notice that

$$\begin{aligned}
\omega a^\dagger a &= \omega \sqrt{\frac{m\omega}{2}} \left(x - \frac{\mathrm{i}}{m\omega} p \right) \cdot \sqrt{\frac{m\omega}{2}} \left(x + \frac{\mathrm{i}}{m\omega} p \right) \\
&= \frac{1}{2} m\omega^2 \left(x - \frac{\mathrm{i}}{m\omega} p \right) \left(x + \frac{\mathrm{i}}{m\omega} p \right) \\
&= \frac{1}{2} m\omega^2 \left(x^2 + \frac{\mathrm{i}}{m\omega} xp - \frac{\mathrm{i}}{m\omega} px - \left(\frac{\mathrm{i}}{m\omega} p \right)^2 \right) \\
&= \frac{1}{2} m\omega^2 \left(\frac{p^2}{m^2\omega^2} + x^2 + \frac{\mathrm{i}}{m\omega} [x, p] \right) \\
&= \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 + \frac{1}{2} \mathrm{i}\, \omega\, [x, p].
\end{aligned}$$

Recall that in the classical theory we have $\{x, p\} = 1$, so in the quantum theory we have $[x, p] = \mathrm{i}$. Therefore:

$$\omega a^\dagger a = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 - \frac{1}{2} \omega. \tag{6.111}$$

Comparing this to the Hamiltonian operator (6.95):

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \tag{6.112}$$

we see that we can write

$$H = \omega\left(a^\dagger a + \frac{1}{2}\right). \tag{6.113}$$

Finally, we define a new operator called the *number operator*:

$$N \equiv a^\dagger a. \tag{6.114}$$

Now the Hamiltonian may be written as

$$H = \omega\left(N + \frac{1}{2}\right). \tag{6.115}$$

The Hamiltonian has been simplified considerably! Since both ω and $1/2$ are just numbers, the problem of finding the eigenvalues and eigenstates of H now reduces to finding the eigenvalues and eigenstates of N.

Problem 6.15.

A. Show that N is Hermitian.

B. Show that if $|n\rangle$ is an eigenstate of N with the eigenvalue n, that is,

$$N|n\rangle = n|n\rangle, \tag{6.116}$$

then $|n\rangle$ is also an eigenstate of H with the eigenvalue $\omega\left(n + \frac{1}{2}\right)$.

C. Calculate, using the canonical commutation relation $[x, p] = \mathrm{i}$, the following commutators:

$$[a, a^\dagger] = 1, \qquad [N, a^\dagger] = a^\dagger, \qquad [N, a] = -a. \tag{6.117}$$

6.4.3 The Energy Eigenstates of the Harmonic Oscillator

Let $|n\rangle$ be an eigenstate of N with eigenvalue n:

$$N|n\rangle = n|n\rangle. \tag{6.118}$$

Since N is Hermitian, we know that n must be a real number. Let us calculate the expectation value of the observable N with respect to the eigenstate $|n\rangle$:

$$\langle N\rangle_n = \langle n|N|n\rangle = \langle n|a^\dagger a|n\rangle = \|an\|^2, \tag{6.119}$$

where we used the fact that $\langle n|\, a^\dagger$ is the bra of $a|n\rangle$. On the other hand, we have

$$\langle N\rangle_n = \langle n|N|n\rangle = n\langle n|n\rangle = n, \tag{6.120}$$

where we used (6.118) and the fact that the state $|n\rangle$ is normalized to 1. By comparing the two equations, we see that

$$n = \|an\|^2 \geq 0, \tag{6.121}$$

that is, n is not only real but also non-negative.

Next, we act with Na and $Na^\dagger$ on $|n\rangle$. In Problem 6.15 you showed that

$$Na - aN = [N, a] = -a, \tag{6.122}$$

$$Na^\dagger - a^\dagger N = [N, a^\dagger] = a^\dagger, \tag{6.123}$$

so we have

$$Na = aN - a = a\,(N-1)\,, \qquad Na^\dagger = a^\dagger N + a^\dagger = a^\dagger\,(N+1)\,, \tag{6.124}$$

and thus

$$Na\,|n\rangle = a\,(N-1)\,|n\rangle = (n-1)\,a\,|n\rangle\,, \tag{6.125}$$

$$Na^\dagger\,|n\rangle = a^\dagger\,(N+1)\,|n\rangle = (n+1)\,a^\dagger\,|n\rangle\,, \tag{6.126}$$

where we used (6.118) and the fact that since $n \pm 1$ is a number, it commutes with operators and can be moved to the left. Writing this result in a different way, we see that

$$N\left(a\,|n\rangle\right) = (n-1)\left(a\,|n\rangle\right), \tag{6.127}$$

$$N\left(a^\dagger\,|n\rangle\right) = (n+1)\left(a^\dagger\,|n\rangle\right), \tag{6.128}$$

or in other words, $a\,|n\rangle$ is an eigenstate of N with eigenvalue $n-1$, and $a^\dagger\,|n\rangle$ is an eigenstate of N with eigenvalue $n+1$. However, by definition, the normalized eigenstates of N with eigenvalues $n-1$ and $n+1$ are $|n-1\rangle$ and $|n+1\rangle$ respectively. Thus, we conclude that $a\,|n\rangle$ is proportional to $|n-1\rangle$ and $a^\dagger\,|n\rangle$ is proportional to $|n+1\rangle$. The proportionality factors must be chosen so that the states are normalized. Let us therefore calculate the norms. The norm $\|an\|^2$ was already calculated above:

$$\|an\|^2 = \langle n|a^\dagger a|n\rangle = \langle n|N|n\rangle = n. \tag{6.129}$$

To calculate $\|a^\dagger n\|^2$, we recall from Problem 6.15 that

$$aa^\dagger - a^\dagger a = [a, a^\dagger] = 1, \tag{6.130}$$

and thus

$$aa^\dagger = a^\dagger a + 1 = N + 1. \tag{6.131}$$

We therefore get

$$\|a^\dagger n\|^2 = \langle n|aa^\dagger|n\rangle = \langle n|\,(N+1)\,|n\rangle = \langle n|N|n\rangle + \langle n|n\rangle = n + 1. \tag{6.132}$$

To summarize, the norms are

$$\|an\| = \sqrt{n}, \qquad \|a^\dagger n\| = \sqrt{n+1}. \tag{6.133}$$

The normalized eigenstates are now obtained, as usual, by dividing by the norm:

$$|n-1\rangle = \frac{1}{\sqrt{n}} a\,|n\rangle\,, \qquad |n+1\rangle = \frac{1}{\sqrt{n+1}} a^\dagger\,|n\rangle\,. \tag{6.134}$$

Another way to write this, from a different point of view, is as the action of the operators a and $a^\dagger$ on the state $|n\rangle$:

$$a\,|n\rangle = \sqrt{n}\,|n-1\rangle\,, \qquad a^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle\,. \tag{6.135}$$

We see that a **reduces** the energy eigenvalue by 1, while $a^\dagger$ **increases** the energy eigenvalue by 1. In other words, $a^\dagger$ gets us to the state of next higher energy (it "creates one quantum of energy") while a gets us to the state of next lower energy (it "annihilates one quantum of energy"). This is the reason we called $a^\dagger$ the *creation operator* and a the *annihilation operator*. We call them the *ladder operators* because they let us "climb the ladder" of energy eigenstates. Going back to the definition of the Hamiltonian in terms of the number operator, we see that

$$H\,|n\rangle = \omega\left(n + \frac{1}{2}\right)|n\rangle\,, \tag{6.136}$$

and thus, as you proved in Problem 6.15, $|n\rangle$ is an energy eigenstate with eigenvalue

$$E_n \equiv \omega\left(n + \frac{1}{2}\right). \tag{6.137}$$

In particular, since we showed above that n must be non-negative, and since we now also see that it has to be an integer (as it can only be increased or decreased by 1!), the possible eigenstates are found to be

$$|0\rangle\,, |1\rangle\,, |2\rangle\,, |3\rangle\,, \ldots. \tag{6.138}$$

We found that the energy of the quantum harmonic oscillator is discrete, or *quantized*, and the system can only have energy which differs from $\omega/2$ by equal steps of ω. The state of lowest energy, also called the *ground state*, is $|0\rangle$. It has the energy eigenvalue

$$E_0 = \frac{1}{2}\omega. \tag{6.139}$$

If we act on the ground state with the annihilation operator, we get

$$a\,|0\rangle = 0, \tag{6.140}$$

which is **not** a state, because it has norm 0 and cannot be normalized. This means that we

cannot generate states with energy lower than that of the ground state. If we act on $|0\rangle$ with the creation operator, we get

$$a^\dagger |0\rangle = |1\rangle . \tag{6.141}$$

We say that $a^\dagger$, which takes us from $|0\rangle$ to $|1\rangle$, *excites* the harmonic oscillator from the ground state to the *first excited state*, which has exactly one *"quantum"* of energy. The state $|n\rangle$ has exactly n quanta, while the ground state $|0\rangle$ has no quanta.

As we mentioned above, the quantum harmonic oscillator may be used to describe many different physical systems. In quantum field theory, the operator N corresponds to the number of particles excited from the field. So $|0\rangle$ is the *vacuum state*, or a state with no particles[63]; $|1\rangle$ is a state where one particle has been excited from the field (e.g. one photon has been excited from the electromagnetic field); $|2\rangle$ is a state with two particles; and so on.

Problem 6.16. Prove that

$$|n\rangle = \frac{\left(a^\dagger\right)^n}{\sqrt{n!}} |0\rangle . \tag{6.142}$$

This means that, once we know the ground state, we can create any energy eigenstate by simply applying n times the operator $a^\dagger$ and normalizing.

Problem 6.17.

A. Find $\langle V \rangle$ for the harmonic oscillator given that the system is in the energy eigenstate $|n\rangle$.

B. How is the expectation value of the potential energy related to the total energy?

C. What is the expectation value of the kinetic energy?

6.5 Wavefunctions, Position, and Momentum

6.5.1 The Position Operator

When canonically quantizing a particle, the position function x is promoted to a Hermitian *position operator*. We usually denote this operator with a *hat*, $\hat{x}$, to distinguish it from its eigenvalues, which are confusingly also written as x. Even more confusingly, we denote the *position eigenstate* corresponding to a measurement of position x as $|x\rangle$:

$$\hat{x} |x\rangle = x |x\rangle , \qquad x \in \mathbb{R}. \tag{6.143}$$

As usual, since $\hat{x}$ is a Hermitian operator, its eigenstates $|x\rangle$ form an orthonormal basis[64]. Recall that for an orthonormal basis $|B_i\rangle$, $i \in \{1, \ldots, n\}$ in a finite-dimensional Hilbert space,

[63] Notice that the vacuum state, despite having no particles, still has non-zero energy $\omega/2$! This is called *zero-point energy*, and it is simply the energy of the field itself.

[64] Our Hilbert space is now infinite-dimensional, and a rigorous discussion of such a space requires dealing with many mathematical subtleties, but we will mostly ignore them in this course due to lack of time.

the orthonormality condition is given by (3.53):

$$\langle B_i | B_j \rangle = \delta_{ij} = \begin{cases} 0 & \text{if } i \neq j, \\ 1 & \text{if } i = j. \end{cases} \tag{6.144}$$

The *Kronecker delta* δ_{ij} has the property that, when evaluated inside a sum over an index i, it "chooses" the term in the sum with index j:

$$\sum_{i=1}^{n} f_i \delta_{ij} = f_j, \tag{6.145}$$

where f_i represents the terms to be summed upon. You don't actually need to evaluate the sum, since all of the terms with $i \neq j$ vanish, and you are left with just one term, the one with $i = j$.

The infinite-dimensional version of this is that for two basis states $|x\rangle$ and $|x'\rangle$, where $x, x' \in \mathbb{R}$, we have

$$\langle x | x' \rangle = \delta\left(x - x'\right), \tag{6.146}$$

where $\delta\left(x - x'\right)$ is the *Dirac delta function*. This function is zero everywhere except when $x = x'$, in which case it is divergent. More precisely, the Dirac delta isn't actually a function, it is a *distribution*, which basically means it is only well-defined when used inside an integral. For any function f, the Dirac delta satisfies the condition

$$\int_{-\infty}^{+\infty} f(x)\, \delta\left(x - x'\right) \mathrm{d}x = f\left(x'\right). \tag{6.147}$$

In other words, when evaluated inside an integral over a variable x, the delta function $\delta\left(x - x'\right)$ simply "chooses" the value of the integrand for which $x = x'$. This is simply a generalization the property of the Kronecker delta in (6.145). You don't need to evaluate the integral, since all of the terms with $x \neq x'$ vanish, and you are left with just one term, the one with $x = x'$.

Problem 6.18. Prove the following properties of the Dirac delta function:

A.

$$\int_{-\infty}^{+\infty} f(x)\, \delta(x) \mathrm{d}x = f(0). \tag{6.148}$$

B.

$$\int_{-\infty}^{+\infty} \delta(x) \mathrm{d}x = 1. \tag{6.149}$$

C.

$$\delta(x) = \delta(-x). \tag{6.150}$$

D.

$$\delta(\lambda x) = \frac{1}{|\lambda|} \delta(x), \qquad \lambda \in \mathbb{R}. \tag{6.151}$$

Problem 6.19. Let us define the *Heaviside step function*:

$$\Theta(x) \equiv \begin{cases} 0 & x < 0, \\ \frac{1}{2} & x = 0, \\ 1 & x > 0. \end{cases} \tag{6.152}$$

Prove that

$$\frac{\mathrm{d}}{\mathrm{d}x}\Theta(x) = \delta(x), \tag{6.153}$$

where $\delta(x)$ is the Dirac delta function.

6.5.2 Wavefunctions in the Position Basis

Since $|x\rangle$ is an orthonormal eigenbasis, we should be able to write down any state $|\Psi\rangle$ as a linear combination – or superposition – of the basis eigenstates. Let us recall that in the finite-dimensional case, with a finite basis $|B_i\rangle$, we have

$$|\Psi\rangle = \sum_{i=1}^{n} |B_i\rangle\langle B_i|\Psi\rangle. \tag{6.154}$$

In Section 3.2.7 we said that $\langle B_i|\Psi\rangle$ – the probability amplitudes – are the coordinates of the representation of the vector $|\Psi\rangle$ with respect to the basis $|B_i\rangle$, and they can be collected into an n-dimensional vector:

$$|\Psi\rangle\Big|_B \equiv \begin{pmatrix} \langle B_1|\Psi\rangle \\ \vdots \\ \langle B_n|\Psi\rangle \end{pmatrix}. \tag{6.155}$$

In the infinite-dimensional case, we simply replace the sum with an integral (and optionally add time dependence, since we now have a continuous time coordinate):

$$|\Psi(t)\rangle = \int_{-\infty}^{+\infty} |x\rangle \langle x \,|\, \Psi(t)\rangle \,\mathrm{d}x. \tag{6.156}$$

In this case, $\langle x|\Psi(t)\rangle$ are the *coordinates* of the *representation* of the vector $|\Psi(t)\rangle$ with respect to the basis $|x\rangle$. Since there is one coordinate for each real number x, we cannot collect them into a vector; instead, we define a function:

$$\psi(t,x) \equiv \langle x \,|\, \Psi(t)\rangle. \tag{6.157}$$

The complex-valued function $\psi(t,x)$, which returns the probability amplitude to measure the particle at position x at time t, is called the *wavefunction*.

Given a wavefunction $\psi(t,x)$, the *probability density* to find the particle at position x at time t

is given by the magnitude squared of the probability amplitude:

$$|\psi(t,x)|^2 = |\langle x \,|\, \Psi(t)\rangle|^2 . \tag{6.158}$$

The reason this is a probability **density**, and not a probability, is that continuous probability distributions behave a bit differently than discrete ones. The probability to find the particle somewhere in the *real interval* $[a,b] \subset \mathbb{R}$ at time t is given by the integral

$$\int_a^b |\psi(t,x)|^2 \,\mathrm{d}x. \tag{6.159}$$

If $a = b$, then the integral evaluates to zero. This means that the probability to find a particle at any one specific point x is actually **zero**! A set containing just one point, or even a countable number of discrete points, is a set of *Lebesgue measure zero*, which means it has no length. It only makes sense to talk about finding a particle inside an interval such as $[a,b]$ with $a \neq b$, which has non-zero Lebesgue measure and thus non-zero length.

Also, instead of the probabilities summing to 1, we must demand that the integral of the probability densities over the entire real line evaluates to 1:

$$\int_{-\infty}^{+\infty} |\psi(t,x)|^2 \,\mathrm{d}x = 1. \tag{6.160}$$

This makes sense, because there is 100% probability to find the particle **somewhere** on the real line, that is, inside the interval $(-\infty, +\infty)$.

Using the wavefunction $\psi(t,x) = \langle x \,|\, \Psi(t)\rangle$, we can rewrite (6.156) as follows:

$$|\Psi(t)\rangle = \int_{-\infty}^{+\infty} \psi(t,x)\,|x\rangle \,\mathrm{d}x. \tag{6.161}$$

If we are given a state $|\Psi(t)\rangle$, we can use (6.157) to convert it to a wavefunction, and conversely, if we are given a wavefunction $\psi(t,x)$, we can use (6.161) to convert it to a state. This is, of course, a consequence of the wavefunction being a representation of the state in a specific basis. For this reason, you will sometimes hear the term "wavefunction" used as a synonym for "state"; for systems where a wavefunction description exists, such as a quantized particle, these two descriptions are equivalent.

However, it should be noted that wavefunctions are **not** fundamental entities in modern quantum theory. The fundamental entities are the states, since any quantum system has states, but only some systems have wavefunctions. For example, there is no wavefunction for a qubit, since there are no continuous variables with respect to which the wavefunction can be defined[65]. Even for systems that do have wavefunctions, the description using states is more general, since a state is independent of a basis, while a wavefunction is only defined in a particular basis.

[65] This is why, in the discussion of the Measurement Axiom, I used the term "collapse" rather than the more popular "wavefunction collapse". Qubits also collapse, but they do not have wavefunctions!

Next, recall the completeness relation (3.81):

$$\sum_{i=1}^{n} |B_i\rangle\langle B_i| = 1. \tag{6.162}$$

We can use (6.156) to derive an infinite-dimensional analogue. We simply note that $|\Psi(t)\rangle$ does not explicitly depend on the variable x, so it can actually be taken out of the integral, and we get:

$$|\Psi(t)\rangle = \left(\int_{-\infty}^{+\infty} |x\rangle\langle x| \, \mathrm{d}x\right) |\Psi(t)\rangle, \tag{6.163}$$

from which we get the *infinite-dimensional completeness relation*

$$\int_{-\infty}^{+\infty} |x\rangle\langle x| \, \mathrm{d}x = 1. \tag{6.164}$$

This relation allows us to define an explicit *inner product* between states on our infinite-dimensional Hilbert space as follows:

$$\begin{aligned}\langle\Psi(t)|\Phi(t')\rangle &= \langle\Psi(t)| \left(\int_{-\infty}^{+\infty} |x\rangle\langle x| \, \mathrm{d}x\right) |\Phi(t')\rangle \\ &= \int_{-\infty}^{+\infty} \langle\Psi(t)|x\rangle\langle x|\Phi(t')\rangle \mathrm{d}x \\ &= \int_{-\infty}^{+\infty} \psi^*(t,x)\,\phi(t',x)\,\mathrm{d}x,\end{aligned}$$

where $\psi^*(t,x) \equiv \langle\Psi(t)|x\rangle$ is the complex conjugate of the wavefunction for $|\Psi(t)\rangle$ defined in (6.157) (since as usual, switching the order of states in the inner product turns it into its complex conjugate), and $\phi(t',x) \equiv \langle x|\Phi(t')\rangle$ is the wavefunction for the state $|\Phi(t')\rangle$.

This is really nothing more than the familiar inner product we defined all the way back in Section 3.2.2, except instead of summing on the components of a vector, we are integrating on the values of a function! The vector in the discrete case was the representation of the state in a particular basis (such as the standard basis), while the function in the continuous case is also the representation of the state in a particular basis, in this case the position basis.

Now we can see that the normalization condition in (6.160) simply says that the *norm* of a state has to be 1, as usual:

$$\|\Psi(t)\| \equiv \sqrt{\langle\Psi(t)|\Psi(t)\rangle} = \sqrt{\int_{-\infty}^{+\infty} |\psi(t,x)|^2 \, \mathrm{d}x} = 1. \tag{6.165}$$

Problem 6.20. The expectation value of the position, given that the state of the system is $|\Psi(t)\rangle$, is defined as usual by

$$\langle x\rangle \equiv \langle\Psi(t)|\hat{x}|\Psi(t)\rangle. \tag{6.166}$$

By inserting the completeness relation (6.164), show that, in terms of the wavefunction $\psi(t,x)$,

the expectation value of x is

$$\langle x \rangle = \int_{-\infty}^{+\infty} x \, |\psi(t,x)|^2 \, \mathrm{d}x. \tag{6.167}$$

Problem 6.21. Let $V(x)$ be an arbitrary smooth function of x. When we promote x into an operator, $V(x)$ becomes the operator $V(\hat{x})$. (For example, if $V(x) = x^2$, then $V(\hat{x})$ is the operator $\hat{x}^2$.) By expanding $V(\hat{x})$ in a Taylor series, show that $|x\rangle$ is an eigenstate of $V(\hat{x})$ with eigenvalue $V(x)$:

$$V(\hat{x}) \, |x\rangle = V(x) \, |x\rangle . \tag{6.168}$$

As a corollary, show that

$$\langle x | \, V(\hat{x}) \, |\Psi(t)\rangle = V(x) \, \psi(t,x) . \tag{6.169}$$

Exercise 6.22. A wavefunction is given by

$$\psi(t,x) = A \, \mathrm{e}^{-x^2}, \qquad A \in \mathbb{C}. \tag{6.170}$$

Find a value of A for which the wavefunction is properly normalized, that is, (6.160) is satisfied. Then, calculate the expectation value $\langle x \rangle$ for this wavefunction.

6.5.3 The Momentum Operator

When we canonically quantize a particle, in addition to the position operator, we also promote the momentum function to a Hermitian *momentum operator* $\hat{p}$. This operator has *momentum eigenstates* $|p\rangle$, which correspond to measurements of momentum p:

$$\hat{p} \, |p\rangle = p \, |p\rangle . \tag{6.171}$$

Everything that we discussed in the previous two sections also applies to the momentum operator and its eigenstates – simply replace x with p. This also includes the wavefunction, which can be represented in the momentum basis as

$$\psi(t,p) \equiv \langle p \, | \, \Psi(t) \rangle . \tag{6.172}$$

Now, let us recall that in Section 6.2 we found out that the unitary operator responsible for shifts in time can be written as the exponential of the Hamiltonian. This can be written in slightly different notation

$$\mathrm{e}^{-\mathrm{i}Ht_0} \, |\Psi(t)\rangle = |\Psi(t+t_0)\rangle . \tag{6.173}$$

From this relation, we derived the Schrödinger equation (6.52), which tells us that the Hamiltonian – the Hermitian operator corresponding to energy – acts on states as a time derivative:

$$H \, |\Psi(t)\rangle = \mathrm{i} \frac{\mathrm{d}}{\mathrm{d}t} |\Psi(t)\rangle . \tag{6.174}$$

Since the energy is just the momentum in the time direction, we expect, in analogy, that the momentum operator will act on states as a derivative with respect to **position**, and that its

exponential will translate states in **space**. However, here we encounter a complication: in non-relativistic quantum mechanics, time is considered to be just a **label** on the states $|\Psi(t)\rangle$, while position is the **eigenvalue** of the position operator[66]. Due to this complication, we won't give the derivation here, but simply state the result:

$$\langle x|\hat{p}|\Psi(t)\rangle = -\mathrm{i}\frac{\partial}{\partial x}\langle x\,|\,\Psi(t)\rangle = -\mathrm{i}\frac{\partial}{\partial x}\psi(t,x)\,. \tag{6.175}$$

This means that the **representation** of the momentum operator in the position basis is given by the derivative with respect to position (times $-\mathrm{i}$, which is a convention). This result will be very useful in Section 6.6, when we discuss solution to the Schrödinger equation. Equation (6.175) is often written simply as

$$\hat{p} = -\mathrm{i}\frac{\partial}{\partial x}, \tag{6.176}$$

but this actually incorrect (or at the very least, serious abuse of notation), since the momentum operator is an abstract operator, and only becomes a derivative when represented in the position basis!

By exponentiating the momentum operator, we get the *translation operator* $\mathrm{e}^{-\mathrm{i}\hat{p}a}$, a unitary operator (as it has to be, since it must preserve norms) which translates position eigenstates a distance a in space:

$$\mathrm{e}^{-\mathrm{i}\hat{p}a}\,|x\rangle = |x+a\rangle\,. \tag{6.177}$$

By taking the adjoint of this expression and acting on a state $|\Psi(t)\rangle$, we get

$$\langle x|\,\mathrm{e}^{\mathrm{i}\hat{p}a}\,|\Psi(t)\rangle = \langle x+a|\Psi(t)\rangle = \psi(t,x+a)\,. \tag{6.178}$$

Therefore, the translation operator translates not only position eigenstates but also wavefunctions.

Problem 6.23. Calculate the expectation value of the momentum, $\langle p\rangle$, given that the state of the system is $|\Psi(t)\rangle$, in terms of the wavefunction $\psi(t,x)$.

6.5.4 Quantum Interference

Let us consider the *double-slit experiment*, which we discussed all the way back in Section 2.1.3. Schematically, the particle's state can be described as a superposition of passing through slit A and passing through slit B:

$$|\Psi\rangle = a\,|\Psi_A\rangle + b\,|\Psi_B\rangle\,, \qquad |a|^2 + |b|^2 = 1. \tag{6.179}$$

[66]This is, in fact, a big problem when trying to combine quantum mechanics with special relativity, since relativity merges space and time into a 4-dimensional spacetime, and this means space and time must be treated on equal footing. However, we won't go into that here. See also Footnote 57.

We suppress the time dependence here, for brevity. The probability amplitude to measure the particle at the position x is given by

$$\psi(x) \equiv \langle x|\Psi\rangle = a\langle x|\Psi_A\rangle + b\langle x|\Psi_B\rangle \equiv a\psi_A(x) + b\psi_B(x). \tag{6.180}$$

The probability density is then, as usual, the magnitude squared of the amplitude:

$$\begin{aligned}
|\psi(x)|^2 &= |a\psi_A(x) + b\psi_B(x)|^2 \\
&= \left(a^*\psi_A^*(x) + b^*\psi_B^*(x)\right)\left(a\psi_A(x) + b\psi_B(x)\right) \\
&= a^*a\psi_A^*(x)\,\psi_A(x) + b^*b\psi_B^*(x)\,\psi_B(x) + a^*b\psi_A^*(x)\,\psi_B(x) + b^*a\psi_B^*(x)\,\psi_A(x) \\
&= |a|^2|\psi_A(x)|^2 + |b|^2|\psi_B(x)|^2 + 2\,\mathrm{Re}\left(a^*b\psi_A^*(x)\,\psi_B(x)\right).
\end{aligned}$$

The terms $|a|^2|\psi_A(x)|^2$ and $|b|^2|\psi_B(x)|^2$ are always positive, for any x. However, the third term $2\,\mathrm{Re}\left(a^*b\psi_A^*(x)\,\psi_B(x)\right)$, called the *interference term* or sometimes the *cross term* (because it "crosses" ψ_A and ψ_B), is a real number which can be either positive or negative, depending on the specific values of a and b, as well as the specific position x in which $\psi_A^*(x)$ and $\psi_B(x)$ are calculated.

The interference term will either increase or decrease the probability to find the particle at x. If it increases the probability, this is *constructive interference*, and it if decreases the probability, this is *destructive interference*. This is precisely what is responsible for the interference pattern in the double-slit experiment, illustrated in Figure 2.5; for different values of x, there will be different amounts of constructive and destructive interference.

6.6 Solutions of the Schrödinger Equation

6.6.1 The Schrödinger Equation for a Particle

Recall the Schrödinger equation (6.52):

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}|\Psi(t)\rangle = H|\Psi(t)\rangle. \tag{6.181}$$

For a particle, we have the Hamiltonian (6.69):

$$H = \frac{p^2}{2m} + V(x). \tag{6.182}$$

Therefore, the Schrödinger equation becomes

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}|\Psi(t)\rangle = \left(\frac{\hat{p}^2}{2m} + V(\hat{x})\right)|\Psi(t)\rangle, \tag{6.183}$$

where we promoted the position and momentum to operators. To find the representation of this equation in the position basis, we multiply by $\langle x|$ from the left:

$$\langle x| \, \mathrm{i} \frac{\mathrm{d}}{\mathrm{d}t} |\Psi(t)\rangle = \langle x| \left(\frac{\hat{p}^2}{2m} + V(\hat{x}) \right) |\Psi(t)\rangle . \tag{6.184}$$

On the left-hand side, since the position eigenstate $|x\rangle$ is independent of time, we can move the time derivative out of the inner product:

$$\langle x| \, \mathrm{i} \frac{\mathrm{d}}{\mathrm{d}t} |\Psi(t)\rangle = \mathrm{i} \frac{\mathrm{d}}{\mathrm{d}t} \langle x \,|\, \Psi(t)\rangle = \mathrm{i} \frac{\mathrm{d}}{\mathrm{d}t} \psi(t,x) . \tag{6.185}$$

On the right-hand side, since in the position representation we have

$$\hat{p} = -\mathrm{i} \frac{\partial}{\partial x}, \tag{6.186}$$

the first term will be

$$\begin{aligned} \langle x| \frac{\hat{p}^2}{2m} |\Psi(t)\rangle &= \frac{1}{2m} \left(-\mathrm{i} \frac{\partial}{\partial x} \right)^2 \psi(t,x) \\ &= \frac{1}{2m} \left(-\mathrm{i} \frac{\partial}{\partial x} \right) \left(-\mathrm{i} \frac{\partial}{\partial x} \right) \psi(t,x) \\ &= -\frac{1}{2m} \frac{\partial^2}{\partial x^2} \psi(t,x) . \end{aligned}$$

As for the second term, in Problem 6.21 you showed that

$$\langle x| \, V(\hat{x}) \, |\Psi(t)\rangle = V(x) \, \psi(t,x) . \tag{6.187}$$

In total, we get:

$$\mathrm{i} \frac{\mathrm{d}}{\mathrm{d}t} \psi(t,x) = \left(-\frac{1}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi(t,x) . \tag{6.188}$$

This is the Schrödinger equation in the position basis. It is a concrete differential equation that one can solve for a variety of different potentials $V(x)$.

Problem 6.24. In this problem you will prove *Ehrenfest's theorem*, which states that:

$$\langle p \rangle = m \frac{\mathrm{d} \langle x \rangle}{\mathrm{d}t}, \tag{6.189}$$

$$\frac{\mathrm{d} \langle p \rangle}{\mathrm{d}t} = -\left\langle V'(x) \right\rangle . \tag{6.190}$$

(6.189) shows that the expectation values of the position and momentum in the quantum theory satisfy the same relation as the position and momentum in the classical theory. (6.190) is Newton's second law (6.78) in terms of the expectation values of the momentum and the force $F \equiv -V'(x)$.

A. Using the identities you proved in Section 4.4.1, calculate the commutator

$$[x^n, p]\,, \tag{6.191}$$

where n is a positive integer. (**Hint:** Make an educated guess and prove it by induction.**)**

B. Using the result of (A), calculate the commutator

$$[f\,(x)\,, p]\,, \tag{6.192}$$

where $f\,(x)$ is an analytic function.

C. Recall (6.90):

$$\frac{\mathrm{d}\,\langle A\rangle}{\mathrm{d}t} = -\,\mathrm{i}\,\langle [A, H]\rangle\,. \tag{6.193}$$

Use this equation, and the result of (B), to prove equations (6.189) and (6.190).

D. In Problem 6.20, you showed that

$$\langle x\rangle = \int_{-\infty}^{+\infty} x\,|\psi\,(t,x)|^2\,\mathrm{d}x, \tag{6.194}$$

and in Problem 6.23, you calculated $\langle p\rangle$. Prove equations (6.189) and (6.190) using these results and the Schrödinger equation in the position basis, (6.188).

Hint: You will have to use integration by parts, and assume[67] that $\psi\,(t,x) \to 0$ as $x \to \pm\infty$.

E. Does (6.190) imply that the expectation values of x and p obey Newton's laws? If so, prove this for a general $V\,(x)$. If not, find some $V\,(x)$ which provides a counterexample.

Problem 6.25. Recall the time-independent Schrödinger equation (6.63), which is just the eigenvalue equation for the Hamiltonian:

$$H\,|E_i\rangle = E_i\,|E_i\rangle\,. \tag{6.195}$$

Let us denote the wavefunctions corresponding to the energy eigenstates as follows:

$$\psi_i\,(x) \equiv \langle x|E_i\rangle. \tag{6.196}$$

They don't depend on t, since we are assuming the Hamiltonian doesn't depend on t either, and energy is constant. Show that (for a point particle with mass m) these wavefunctions satisfy the equation

$$\left(-\frac{1}{2m}\frac{\partial^2}{\partial x^2} + V\,(x)\right)\psi_i\,(x) = E_i\psi_i\,(x)\,. \tag{6.197}$$

[67] This is pretty much always assumed to be true about wavefunctions in quantum mechanics. It can be justified in two ways. First, according to (6.160), $|\psi\,(t,x)|^2$ has to integrate to 1 so that the state is normalized. Therefore, it makes sense that $\psi\,(t,x)$ should vanish at infinity – although, if you look hard enough (you are encouraged to try!), you can find normalized wavefunctions which nonetheless do not vanish at infinity. Second, if we create a particle in the lab, we would expect the probability to find this particle a trillion light years away to be very close to zero...

6.6.2 Separation of Variables

Let us assume that the wavefunction can be separated into a part which depends only on x and a part which depends only on t:

$$\psi(t,x) = \psi_i(x)\,\psi_t(t). \tag{6.198}$$

By plugging this into the Schrödinger equation (6.188) and dividing by ψ, we obtain the equation

$$\frac{\mathrm{i}}{\psi_t}\frac{\mathrm{d}\psi_t}{\mathrm{d}t} = -\frac{1}{2m}\frac{1}{\psi_i}\frac{\partial^2\psi_i}{\partial x^2} + V(x). \tag{6.199}$$

Since the left-hand side only depends on t and the right-hand side only depends on x, we conclude that they must in fact both be **constant**, that is, independent of **both** t and x – otherwise, if for example the left-hand side was a function of t, then the right-hand side would have to be a function of t also, in contradiction with our assumption that it only depends on x. This is called *separation of variables*.

Let E_i be the constant that both sides are equal to. Then we get two equations. The first equation will just be the eigenvalue equation (6.197), which therefore implies that E_i is the energy (and thus must be real). The other equation will be

$$\frac{\mathrm{d}\psi_t}{\mathrm{d}t} = -\,\mathrm{i}\,E_i\psi_t. \tag{6.200}$$

Recalling (6.9), we see that the solution to (6.200) is simply

$$\psi_t = \mathrm{e}^{-\,\mathrm{i}\,E_i t}. \tag{6.201}$$

Therefore, any **separable** solution to the Schrödinger equation is given by a wavefunction of the form

$$\psi(t,x) = \psi_i(x)\,\mathrm{e}^{-\,\mathrm{i}\,E_i t}. \tag{6.202}$$

These are called *stationary states*. Since these states are energy eigenstates, they have a well-defined energy E_i.

As it turns out, since the Schrödinger equation is linear, the **most general solution** to the equation is a linear combination of stationary states:

$$\psi(t,x) = \sum_i \alpha_i\psi_i(x)\,\mathrm{e}^{-\,\mathrm{i}\,E_i t}, \tag{6.203}$$

where $\alpha_i \in \mathbb{C}$ are constant coefficients and E_i are all the possible energy eigenstates, of which there can be infinitely many. Of course, this is nothing other than a **superposition** of energy eigenstates, represented in the position basis, and therefore the coefficients α_i are none other than the **probability amplitudes** to measure each energy E_i given the state $|\Psi(t)\rangle$.

In other words, the general solution to the Schrödinger equation simply amounts to writing

the state of the system as a superposition with respect to the eigenbasis of a particular observable – the Hamiltonian. With the time dependence out of the way, all that remains is to solve the time-independent Schrödinger equation (6.197) for ψ_i, and find the coefficients α_i. The solution will depend on the explicit form of the potential $V(x)$. However, this is, of course, the hard part! Thousands upon thousands of pages have been written in the last 100 years or so about solutions (or even just approximations of solutions) to the Schrödinger equation for all kinds of different potentials.

Unfortunately, our course has come to an end, and we won't have time to work out any specific solutions. The focus of this course has been on developing deep intuition and conceptual understanding of quantum theory, as it is formulated in modern 21st-century theoretical physics. For this reason, we spent the vast majority of the course developing the entire mathematical framework of the theory from scratch, highlighting and debunking common misconceptions, focusing on concepts and their meaning rather than calculations, and giving examples from discrete systems, where the math is simple, so we could concentrate our efforts on understanding the physics without being bogged down by the math.

Still, solving the Schrödinger equation is something every physicist should know how to do, and in Problem 6.28 you will find the solutions corresponding to two simple potentials, related to scattering and tunneling of particles in one dimension.

Problem 6.26. Show that the probability density of a stationary state, as well as the expectation value of any observable A with respect to that state, are independent of t.

Exercise 6.27. A wavefunction is given at time $t = 0$ by

$$\psi(0, x) = \alpha_1 \psi_1(x) + \alpha_2 \psi_2(x). \tag{6.204}$$

What is the wavefunction $\psi(t, x)$ at some other time t, and what is the corresponding probability density?

Problem 6.28. Solve the Schrödinger equation for particular potentials. Solve it for the following two simple potentials:

- *Finite square well – scattering*:

$$V(x) = \begin{cases} 0 & x < -a, \\ -V_0 & -a < x < a, \\ 0 & x > a. \end{cases} \tag{6.205}$$

- *Finite square barrier – tunneling*:

$$V(x) = \begin{cases} 0 & x < -a, \\ +V_0 & -a < x < a, \\ 0 & x > a. \end{cases} \tag{6.206}$$

In both cases, a and V_0 are two positive numbers. Make nice plots of the potentials and the wavefunctions. The solutions are not trivial, and you are allowed – even encouraged – to make use of textbooks and online resources. However, you should write the solutions **in your own words** and summarize what you learned from the results.

6.7 Lagrangian Mechanics and the Path Integral Formulation

In this section, we will learn the basics of *path integral quantization*. This is a significantly different method of quantizing a classical system, and it is in fact the preferred method in much of 21st-century physics, including quantum field theory, quantum gravity, and other fundamental quantum theories.

6.7.1 A Quick Review of Classical Lagrangian Mechanics

Just as canonical quantization starts from a classical system formulated using *Hamiltonian mechanics*, path integral quantization starts from a classical system formulated using *Lagrangian mechanics*. In Hamiltonian mechanics, the degrees of freedom are position x and momentum p, or more generally a set of positions $\mathbf{x} = (x_1, \ldots, x_n)$ and momenta $\mathbf{p} = (p_1, \ldots, p_n)$, and they can be used to construct a *Hamiltonian* $H(x, p)$. In Lagrangian mechanics, the degrees of freedom are position x and velocity $\dot{x}$, or more generally a set of positions $\mathbf{x} = (x_1, \ldots, x_n)$ and velocities $\dot{\mathbf{x}} = (\dot{x}_1, \ldots, \dot{x}_n)$, and they can be used to construct a *Lagrangian* $L(x, \dot{x})$.

For example, the Lagrangian of a point particle is:

$$L(x, \dot{x}) = \frac{1}{2} m \dot{x}^2 - V(x). \tag{6.207}$$

Notice that the first term is just the usual Newtonian kinetic energy term $\frac{1}{2}mv^2$. Compare this to the Hamiltonian of a point particle (6.69):

$$H = \frac{p^2}{2m} + V(x). \tag{6.208}$$

The first term in both is the kinetic energy, except that in the Lagrangian we use the velocity $\dot{x}$ and in the Hamiltonian we use the momentum $p \equiv m\dot{x}$. The second term is the potential energy, but in the Hamiltonian we **add** the potential energy (so that the Hamiltonian is the **total** kinetic + potential energy) while in the Lagrangian we **subtract** the potential energy (so that the Lagrangian is the **difference** between kinetic and potential energy).

It is possible to do some classical mechanics using just the Lagrangian itself, but to understand its meaning from first principles, and to apply Lagrangian mechanics to more complicated systems, we must go one step further and define the *action*:

$$S[x] \equiv \int L(x, \dot{x}) \, \mathrm{d}t. \tag{6.209}$$

This is simply the integral of the Lagrangian over time. The action is an example of a *functional*, which is a map that takes a function and returns a real number[68]. Given a particular function $x(t)$, the action functional produces a real number by integrating the Lagrangian in terms of this function and its derivative.

However, the integration itself is almost never actually performed! Usually, we simply use the action functional as an abstract quantity in order to derive the equations of motion from it. This is done using the *principle of stationary action*: the equations of motion are given by *stationary points* of the action.

A stationary points is any point where the derivative is zero: either a minimum, maximum, or inflection point[69]. Sometimes you might hear the expression "principle of least action", but that is only a historical term and should **not** be used, because the equations of motion don't always correspond to a minimum of the action! As an example, in general relativity, the action for a point particle is the particle's proper time, and the equations of motion correspond to the **maximum** of proper time[70].

The principle of stationary action can be given in terms of the *functional differential* as follows:

$$\delta S[x] = 0. \tag{6.210}$$

You can think of the functional differential as the change in S due to an infinitesimal change in the function $x(t)$. This is similar to the usual notion of a differential $\mathrm{d}f$ of a function $f(x)$, which is the change in f due to an infinitesimal change in the argument x, which is a number. However, in the case of a functional differential, we change an entire **function**, not a number. Since $x(t)$ specifies the **path** (or trajectory) of the particle as a function of time, we can think of an infinitesimal change in $x(t)$ as a slight deformation of this path, which can be in different amounts at different points along the path.

This condition $\delta S[x] = 0$ is equivalent to the differential (or derivative) of a function vanishing, so it is a generalization of the concept of a stationary point, except that now instead of a **point** where the derivative vanishes, we have a **function** where the *functional derivative* vanishes.

Let us calculate this explicitly between two arbitrary points in time, t_1 and t_2:

$$\delta S = \int_{t_1}^{t_2} \delta L \, \mathrm{d}t = \int_{t_1}^{t_2} \left(\frac{\partial L}{\partial x} \delta x + \frac{\partial L}{\partial \dot{x}} \delta \dot{x} \right) \mathrm{d}t. \tag{6.211}$$

[68] More generally, a functional on any vector space is a map from vectors to scalars. So in $\mathbb{C}^n$, a bra $\langle \psi |$ is actually a functional, since it takes any vector $|\phi\rangle$ to a complex number. The space of continuous real functions is a vector space over the field of real numbers (prove this!), so f is a functional on this space.

[69] An **inflection point** is one where the function changes from being concave to convex. For example, the function x^3 at $x = 0$ has vanishing derivative at $x = 0$, but it's neither a minimum nor a maximum, it's an inflection point.

[70] You might claim that if the action was the **negative** of the proper time, then this would actually be the minimum. However, this is misleading because the proper time is the **square root** of a quantity (the spacetime interval), so we can actually take it to be either positive or negative in any case. No matter the sign, the equations of motion always correspond to the maximum of the **magnitude** of the action.

Here we used the chain rule[71]. The functional derivative commutes with the usual derivative, so we have

$$\delta\dot{x} = \delta\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right) = \frac{\mathrm{d}}{\mathrm{d}t}\left(\delta x\right). \tag{6.212}$$

Therefore we can integrate by parts. From the product rule we get

$$\frac{\partial L}{\partial \dot{x}}\delta\dot{x} = \frac{\partial L}{\partial \dot{x}}\frac{\mathrm{d}}{\mathrm{d}t}\left(\delta x\right) = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}}\delta x\right) - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}}\right)\delta x, \tag{6.213}$$

and so

$$\begin{aligned}
\delta S &= \int_{t_1}^{t_2}\left(\frac{\partial L}{\partial x}\delta x + \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}}\delta x\right) - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}}\right)\delta x\right)\mathrm{d}t \\
&= \int_{t_1}^{t_2}\left(\left(\frac{\partial L}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}}\right)\right)\delta x + \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}}\delta x\right)\right)\mathrm{d}t \\
&= \int_{t_1}^{t_2}\left[\left(\frac{\partial L}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}}\right)\right)\delta x\right]\mathrm{d}t + \left(\frac{\partial L}{\partial \dot{x}}\delta x\Big|_{t_1}^{t_2}\right).
\end{aligned}$$

The last term vanishes if we assume that the endpoints are fixed, that is, $\delta x\left(t_1\right) = \delta x\left(t_2\right) = 0$. This makes sense in the case of a particle, since we can assume that the particle must start and end at two specific points, and only the path connecting these two points can vary. We are thus left with

$$\delta S = \int_{t_1}^{t_2}\left[\left(\frac{\partial L}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}}\right)\right)\delta x\right]\mathrm{d}t. \tag{6.214}$$

To satisfy $\delta S = 0$, the integral must vanish for any choice of δx. Note that δx is a **function** of t, since it's a **functional** differential, and thus it is being integrated on – we can't take it out of the integral! The only way to guarantee that the integral vanishes for any $\delta x \neq 0$ is if the rest of the integrand always vanishes. Therefore, $\delta S = 0$ is equivalent to

$$\frac{\partial L}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}}\right) = 0. \tag{6.215}$$

This is called the *Euler-Lagrange equation*. Given a choice of Lagrangian L, we can use this equation to find the equation of motion for the system, which can then be solved to obtain $x\left(t\right)$.

As an example, consider the Lagrangian for a point particle (6.207):

$$L\left(x, \dot{x}\right) = \frac{1}{2}m\dot{x}^2 - V\left(x\right). \tag{6.216}$$

[71]The functional differential and functional derivative can be defined rigorously, and their properties, such as the chain rule, can be proven from this definition. Since this section is supposed to be just a quick review, and I'm only using these concepts in the derivation of the equations of motion, I will not attempt to give a rigorous definition or prove any properties here, but you are encouraged to look them up.

We have

$$\frac{\partial L}{\partial x} = \frac{\partial}{\partial x}\left(\frac{1}{2}m\dot{x}^2 - V(x)\right) = -V'(x) = F, \tag{6.217}$$

where F is the force due to the potential V, and

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}}\right) = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial}{\partial \dot{x}}\left(\frac{1}{2}m\dot{x}^2 - V(x)\right)\right) = \frac{\mathrm{d}}{\mathrm{d}t}(m\dot{x}) = m\ddot{x}, \tag{6.218}$$

where in both cases we assumed that x and $\dot{x}$ are **independent** variables. Therefore, the equation of motion is

$$F = m\ddot{x}, \tag{6.219}$$

which is just Newton's second law – the same equation we found from the Hamiltonian in (6.81).

In fact, the Lagrangian and Hamiltonian formulations are closely related. Given a Lagrangian L, we can find the momentum corresponding to x by

$$p \equiv \frac{\partial L}{\partial \dot{x}}. \tag{6.220}$$

This allows us to transform from $L(x, \dot{x})$, which uses the velocity $\dot{x}$, to $H(x, p)$, which uses the momentum p. This is known as a *Legendre transformation*. Aside from converting velocity to momentum, we also need to find the actual Hamiltonian. Intuitively, since $L = K(\dot{x}) - V(x)$ and $H = K(p) + V(x)$, this should involve writing the kinetic energy K in terms of p instead of $\dot{x}$ and then inverting the sign of V. In practice, it is not always clear which part of the Lagrangian is the kinetic energy and which part is the potential energy. However, there is a transformation that always works:

$$H = p\dot{x} - L\Big|_{\dot{x}\mapsto\dot{x}(p)}, \tag{6.221}$$

provided we can invert the relation (6.220) to find how to express $\dot{x}$ in terms of p. For example, in the case of a point particle we have

$$p = \frac{\partial L}{\partial \dot{x}} = \frac{\partial}{\partial \dot{x}}\left(\frac{1}{2}m\dot{x}^2 - V(x)\right) = m\dot{x}, \tag{6.222}$$

which is just the Newtonian momentum $p = mv$, and we can invert this to find $\dot{x} = p/m$. Thus we find that the Hamiltonian is

$$H = p\dot{x} - L\Big|_{\dot{x}\mapsto p/m} = p\left(\frac{p}{m}\right) - \left(\frac{1}{2}m\left(\frac{p}{m}\right)^2 - V(x)\right) = \frac{p^2}{2m} + V(x), \tag{6.223}$$

which indeed matches the Hamiltonian (6.69).

Problem 6.29. Any system can, in fact, be described by an infinite number of equivalent

Lagrangians. These Lagrangians are all related; find the most general relation between two arbitrary Lagrangians L and L' such that they produce the same equations of motion.

Problem 6.30. Prove that if instead of just one coordinate x we have a set of coordinates $\mathbf{x} = (x_1, \ldots, x_n)$, then the condition $\delta S = 0$ results in n Euler-Lagrange equations, one for each coordinate.

Problem 6.31. What form will the Euler-Lagrange equation take if instead of just the first derivative of x, the Lagrangian involved derivatives of x up to order N?

Problem 6.32. Show that Hamilton's equations (6.75) and (6.76) follow from the Euler-Lagrange equation (6.215) after performing a Legendre transformation. One way to do this is by calculating the differential of (6.221).

Problem 6.33. Consider an n-dimensional Lagrangian $L(\mathbf{x}, \dot{\mathbf{x}})$ where $\mathbf{x} = (x_1, \ldots, x_n)$. Assume that the Lagrangian is independent of x_i for some i; we then say that the coordinate x_i is a *cyclic coordinate*. Show that this implies there is a conserved quantity in the system, and find that quantity. This is a special simple case of *Noether's theorem*, which says that every continuous symmetry of the action has a corresponding conserved quantity. In this case, the symmetry is trivial since any change to x_i will not affect the action.

Exercise 6.34. Find the Lagrangian for the classical harmonic oscillator by applying a Legendre transformation to the Hamiltonian (6.95), and calculate the equations of motion using the Euler-Lagrange equation.

6.7.2 Motivation for Path Integral Quantization

Recall the definition of the unitary evolution operator (6.56):

$$U(t_F \leftarrow t_0) \equiv \mathrm{e}^{-\mathrm{i}H(t_F - t_0)}, \tag{6.224}$$

where H is the Hamiltonian, t_0 is the initial time, and t_F is the final time. Let $T \equiv t_F - t_0$ be the duration of evolution, then we can rewrite this operator as

$$U(T) \equiv \mathrm{e}^{-\mathrm{i}HT}. \tag{6.225}$$

Consider a particle at point x_0 at time t_0. What is the probability amplitude to find that particle at some other point x_F at time t_F?

We start with the eigenstate $|x_0\rangle$ at time t_0, then evolve it to the state $\mathrm{e}^{-\mathrm{i}HT}|x_0\rangle$ at time t_F, and finally perform a measurement of the position operator $\hat{x}$. As usual, the state can be expanded in a superposition in terms of the basis eigenstates of $\hat{x}$, and the amplitude to find the particle at point x_F will then be the coefficient of $|x_F\rangle$ in this superposition. The superposition is given by (6.156) with $|\Psi(t)\rangle = \mathrm{e}^{-\mathrm{i}HT}|x_0\rangle$:

$$\mathrm{e}^{-\mathrm{i}HT}|x_0\rangle = \int_{-\infty}^{+\infty} |x\rangle \langle x| \mathrm{e}^{-\mathrm{i}HT}|x_0\rangle \, \mathrm{d}x. \tag{6.226}$$

Then clearly the amplitude to find the particle at x_F is the inner product

$$A = \langle x_F | \, \mathrm{e}^{-\mathrm{i}HT} \, | x_0 \rangle \, . \tag{6.227}$$

Next, consider the *single-slit experiment*. A particle is emitted from x_0 at time t_0, passes through a slit on a barrier at x_1, and is detected at time t_F at some position x_F along the screen. What is the amplitude for this process?

Recall that the probability for two events to happen is the **product** of the probabilities of each event. For example, when rolling a 6-sided die, the probability to get a 1 is $1/6$. So when rolling two such dice, the probability to get 1 on both dice is $1/6 \cdot 1/6 = 1/36$. Since probability in quantum mechanics is the magnitude-squared of the amplitude, amplitudes must obey this rule as well. Therefore, assuming for simplicity that each half of the path takes an equal time $\Delta T \equiv T/2$, the amplitude for the path $x_0 \to x_1 \to x_F$ is:

$$A = \langle x_F | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_1 \rangle \, \langle x_1 | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_0 \rangle \, . \tag{6.228}$$

What if we have[72] two slits, $x_1^{(1)}$ and $x_1^{(2)}$, as in the *double-slit experiment* (Figure 2.3)? Now there are **two** paths that can result in the particle reaching x_F: one where it passes through $x_1^{(1)}$ and one where it passes through $x_1^{(2)}$.

Again, recall that the probability to get one of several specific outcomes for a measurement is the sum of the probabilities for each outcome. For example, the probability to get either 1 or 2 on a 6-sided die is $1/6 + 1/6 = 2/6$. Amplitudes also obey this rule, although in this case, adding the amplitudes might actually **lower** the probability due to destructive interference – indeed, that is exactly what makes quantum mechanics distinct from classical probabilistic theories!

Therefore, the total amplitude to find the particle at x_F must be the sum of the amplitudes **for each possible path** $x_0 \to x_1^{(1)} \to x_F$ and $x_0 \to x_1^{(2)} \to x_F$:

$$A = \langle x_F | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_1^{(1)} \rangle \langle x_1^{(1)} | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_0 \rangle + \langle x_F | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_1^{(2)} \rangle \langle x_1^{(2)} | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_0 \rangle . \tag{6.229}$$

Okay, so what if we have n slits $x_1^{(1)}, \ldots, x_1^{(n)}$? In this case, the amplitude will clearly be:

$$A = \sum_{i=1}^{n} \langle x_F | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_1^{(n)} \rangle \langle x_1^{(n)} | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_0 \rangle . \tag{6.230}$$

Now, imagine that there is **no barrier at all**; the particle doesn't pass through any slits, it just arrives directly at x_F. But if you think about it, this is actually equivalent to having the entire barrier "made of" an **infinite continuum of slits**! In this case, the sum over a finite number of discrete slits in the amplitude will become an integral over each possible value of the slit

[72] The reason for this weird notation is that in a bit I will introduce additional barriers. So the subscript is the number of the barrier, and the superscript is the number of the slit on that barrier.

location, which we label x_1:

$$A = \int \mathrm{d}x_1 \, \langle x_F | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_1 \rangle \, \langle x_1 | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_0 \rangle \, . \tag{6.231}$$

Notice that we can also write this as follows:

$$A = \langle x_F | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \left(\int | x_1 \rangle \, \langle x_1 | \, \mathrm{d}x_1 \right) \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_0 \rangle = \langle x_F | \, \mathrm{e}^{-\mathrm{i}HT} \, | x_0 \rangle \, , \tag{6.232}$$

where we used the fact that $T = \Delta T + \Delta T$ (the total time to get from x_0 to x_F is the sum of the time to go through each half of the path) and the completeness relation (6.164):

$$\int | x_1 \rangle \, \langle x_1 | \, \mathrm{d}x_1 = 1. \tag{6.233}$$

In other words, this result, which we arrived at by considering the different paths a particle could go through, is simply a trivial consequence of the completeness relation! Indeed, this provides a nice illustration of the physical meaning of the completeness relation.

But now, let us take this one step further. Imagine that there is another barrier at x_2, between x_1 and x_F. The amplitude to get from x_0 to x_F must now take into account going through different slits in **both** barriers, so it will be the product of **three** amplitudes: one for $x_0 \to x_1$, one for $x_1 \to x_2$, and one for $x_2 \to x_F$. Let us assume for simplicity that each of the 3 parts of the path $x_0 \to x_1 \to x_2 \to x_F$ takes equal time $\Delta T \equiv T/3$. If we treat x_2 in the same way as we did x_1, removing the barrier and considering the empty space to be composed of an infinite number of slits, then we get

$$A = \int \mathrm{d}x_1 \int \mathrm{d}x_2 \, \langle x_F | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_2 \rangle \, \langle x_2 | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_1 \rangle \, \langle x_1 | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_0 \rangle \, . \tag{6.234}$$

Note that, again, we could have also arrived at this by starting with $\langle x_F | \, \mathrm{e}^{-\mathrm{i}HT} \, | x_0 \rangle$, splitting the exponential into 3 equal parts, and inserting the completeness relation between each two exponentials.

This is the amplitude for 2 barriers. Let's increase this to N barriers at $x_1, \ldots, x_N$, and assume that each part of the path takes equal time $\Delta T \equiv T/\left(N+1\right)$. Then we should integrate over the infinite continuum of slits in each barrier:

$$A = \left(\prod_{j=1}^{N} \int \mathrm{d}x_j \right) \langle x_F | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_N \rangle \cdots \langle x_2 | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_1 \rangle \, \langle x_1 | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_0 \rangle \, . \tag{6.235}$$

A more concise way to write this is by taking $x_{N+1} \equiv x_F$, so that we have:

$$A = \left(\prod_{j=1}^{N} \int \mathrm{d}x_j \right) \left(\prod_{k=0}^{N} \langle x_{k+1} | \, \mathrm{e}^{-\mathrm{i}H\Delta T} \, | x_k \rangle \right) . \tag{6.236}$$

Note that j starts from 1 while k starts from 0, since we have N integrals but $N+1$ amplitudes,

with an integral inserted between each two adjacent amplitudes.

The way to generalize this even further should now be obvious: not only do we treat each barrier as an **infinite continuum of slits**, we also treat the entire space between x_0 and x_F as an **infinite continuum of barriers**. Schematically, this is achieved by taking $N \to \infty$. So in conclusion, we have:

$$\langle x_F | \, \mathrm{e}^{-\mathrm{i}\, HT} \, | x_0 \rangle = \lim_{N \to \infty} \left(\prod_{j=1}^{N} \int \mathrm{d}x_j \right) \left(\prod_{k=0}^{N} \langle x_{k+1} | \, \mathrm{e}^{-\mathrm{i}\, H \Delta T} \, | x_k \rangle \right), \tag{6.237}$$

where

$$x_{N+1} \equiv x_F, \qquad \Delta T \equiv \frac{T}{N+1}. \tag{6.238}$$

In other words, to calculate the amplitude for the particle to get from x_0 to x_F, we must take into account **every possible path** between these two points!

6.7.3 The Inner Product of Position and Momentum Eigenstates

What happens when we take the inner product of a momentum eigenstate with a position eigenstate? Recall equation (6.175):

$$\langle x | \hat{p} | \Psi(t) \rangle = -\mathrm{i} \frac{\partial}{\partial x} \langle x \,|\, \Psi(t) \rangle \,. \tag{6.239}$$

If we take $|\Psi(t)\rangle \mapsto |p\rangle$, that is, the state of the particle is a momentum eigenstate, we get:

$$\langle x | \hat{p} | p \rangle = -\mathrm{i} \frac{\partial}{\partial x} \langle x \,|\, p \rangle \,. \tag{6.240}$$

On the other hand, since $|p\rangle$ is an eigenstate of $\hat{p}$ with eigenvalue p, we have

$$\langle x | \hat{p} | p \rangle = p \langle x | p \rangle. \tag{6.241}$$

Comparing the two equations, we find a differential equation for $\langle x|p\rangle$:

$$\frac{\partial}{\partial x} \langle x | p \rangle = \mathrm{i}\, p \langle x | p \rangle. \tag{6.242}$$

In other words, the function $\langle x|p\rangle$ is its own derivative, with an additional factor of $\mathrm{i}\, p$. Recalling our discussion of the exponential function in Section 6.1.1, we immediately see that the solution to this equation is:

$$\langle x | p \rangle = A \, \mathrm{e}^{\mathrm{i}\, px}, \tag{6.243}$$

where A is an integration constant. To determine A, we start from the completeness relation in terms of the momentum eigenbasis:

$$\int |p\rangle \, \langle p| \, \mathrm{d}p = 1. \tag{6.244}$$

Multiplying by $|x\rangle$ on the right and $\langle x'|$ on the left, we get:

$$\int \langle x'|p\rangle\langle p|x\rangle \mathrm{d}p = \langle x'|x\rangle = \delta\left(x'-x\right). \tag{6.245}$$

On the other hand, plugging (6.243) into the integral, and inverting the inner product to get $\langle p|x\rangle = A^* \mathrm{e}^{-\mathrm{i}\,px}$, we get

$$\begin{aligned}\int \langle x'|p\rangle\langle p|x\rangle \mathrm{d}p &= \int \left(A\,\mathrm{e}^{\mathrm{i}\,px'}\right)\left(A^*\,\mathrm{e}^{-\mathrm{i}\,px}\right)\mathrm{d}p \\ &= |A|^2 \int \mathrm{e}^{\mathrm{i}\,p(x'-x)}\,\mathrm{d}p.\end{aligned}$$

Therefore, we have that

$$\delta\left(x'-x\right) = |A|^2 \int \mathrm{e}^{\mathrm{i}\,p(x'-x)}\,\mathrm{d}p. \tag{6.246}$$

However, a known representation for the Dirac delta distribution is

$$\delta\left(x'-x\right) = \frac{1}{2\pi}\int \mathrm{e}^{\mathrm{i}\,p(x'-x)}\,\mathrm{d}p. \tag{6.247}$$

This simply means that the *Fourier transform* of $\delta(x)$ is $\mathrm{e}^{\mathrm{i}\,px}$; you will prove it in Problem 6.35. Therefore, we conclude that (up to phase)

$$A = \frac{1}{\sqrt{2\pi}}, \tag{6.248}$$

and thus (6.243) becomes

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi}}\,\mathrm{e}^{\mathrm{i}\,px}. \tag{6.249}$$

Problem 6.35. Prove (6.247).

6.7.4 Deriving the Path Integral

Consider the simplest Hamiltonian, that of a *free particle*:

$$H = \frac{p^2}{2m}. \tag{6.250}$$

Let us find an expression for the amplitude $\langle x_{k+1}| \, \mathrm{e}^{-\,\mathrm{i}\,H\Delta T} \, |x_k\rangle$ for some k. We can insert the momentum completeness relation and use (6.249):

$$\begin{aligned}
\langle x_{k+1}| \, \mathrm{e}^{-\,\mathrm{i}\,\hat{p}^2\Delta T/m} \, |x_k\rangle &= \int \langle x_{k+1}| \, \mathrm{e}^{-\,\mathrm{i}\,\hat{p}^2\Delta T/2m} \, |p\rangle \langle p|x_k\rangle \mathrm{d}p \\
&= \int \mathrm{e}^{-\,\mathrm{i}\,p^2\Delta T/2m} \langle x_{k+1}|p\rangle \langle p|x_k\rangle \mathrm{d}p \\
&= \frac{1}{2\pi} \int \mathrm{e}^{-\,\mathrm{i}\,p^2\Delta T/2m} \, \mathrm{e}^{\mathrm{i}\,p(x_{k+1}-x_k)} \, \mathrm{d}p \\
&= \frac{1}{2\pi} \int \exp\left[\mathrm{i}\left(-\frac{\Delta T}{2m}p^2 + (x_{k+1}-x_k)\,p\right)\right] \mathrm{d}p,
\end{aligned}$$

where in line 2 we applied the **operator** $\mathrm{e}^{-\,\mathrm{i}\,\hat{p}^2\Delta T/m}$ to $|p\rangle$, which results in the **number** $\mathrm{e}^{-\,\mathrm{i}\,p^2\Delta T/m}$ (note that there is no hat on the p), and then moved this number to the left. This is a *Gaussian integral*, which may be calculated exactly, as you will prove in Problem 6.36. The result is:

$$\langle x_{k+1}| \, \mathrm{e}^{-\,\mathrm{i}\,\hat{p}^2\Delta T/m} \, |x_k\rangle = \sqrt{\frac{m}{2\pi\,\mathrm{i}\,\Delta T}} \exp\left(\mathrm{i}\,\frac{m}{2\Delta T}\,(x_{k+1}-x_k)^2\right), \tag{6.251}$$

which we rewrite as

$$\langle x_{k+1}| \, \mathrm{e}^{-\,\mathrm{i}\,\hat{p}^2\Delta T/m} \, |x_k\rangle = \sqrt{\frac{m}{2\pi\,\mathrm{i}\,\Delta T}} \exp\left(\mathrm{i}\,\frac{m}{2}\Delta T\left(\frac{x_{k+1}-x_k}{\Delta T}\right)^2\right). \tag{6.252}$$

This is the expression for one amplitude, so for the product (6.237) we find

$$\begin{aligned}
\langle x_F| \, \mathrm{e}^{-\,\mathrm{i}\,HT} \, |x_0\rangle &= \lim_{N\to\infty} \left(\prod_{j=1}^{N} \int \mathrm{d}x_j\right) \left(\prod_{k=0}^{N} \sqrt{\frac{m}{2\pi\,\mathrm{i}\,\Delta T}} \exp\left(\mathrm{i}\,\frac{m}{2}\Delta T\left(\frac{x_{k+1}-x_k}{\Delta T}\right)^2\right)\right) \\
&= \lim_{N\to\infty} \left(\frac{m}{2\pi\,\mathrm{i}\,\Delta T}\right)^{(N+1)/2} \left(\prod_{j=1}^{N} \int \mathrm{d}x_j\right) \left(\exp\left(\mathrm{i}\,\frac{m}{2}\Delta T \sum_{k=0}^{N}\left(\frac{x_{k+1}-x_k}{\Delta T}\right)^2\right)\right).
\end{aligned}$$

Instead of taking the limit $N \to \infty$, let us take the equivalent limit $\Delta T \equiv T/\,(N+1) \to 0$. Then we have from the definition of a derivative

$$\lim_{\Delta T\to 0} \frac{x_{k+1}-x_k}{\Delta T} = \dot{x}, \tag{6.253}$$

and we also know that the discrete sum becomes a continuous integral[73]:

$$\lim_{\Delta T\to 0} \left(\sum_{k=0}^{N} \Delta T\right) = \int_0^T \mathrm{d}t. \tag{6.254}$$

[73]Indeed, this is one way in which integrals can be rigorously defined. The sum is then called a *Riemann sum*, and if the limit exists, the function is called *Riemann integrable*.

Therefore

$$\lim_{\Delta T\to 0}\left(\frac{m}{2}\Delta T\sum_{k=0}^{N}\left(\frac{x_{k+1}-x_k}{\Delta T}\right)^2\right)=\int_0^T\frac{1}{2}m\dot{x}^2\mathrm{d}t. \tag{6.255}$$

We recognize here the Lagrangian of a free particle:

$$\int_0^T\frac{1}{2}m\dot{x}^2\mathrm{d}t=\int_0^T L\left(x,\dot{x}\right)\,\mathrm{d}t=S\left[x\right], \tag{6.256}$$

where we used the definition of the action, (6.209). Thus we get

$$\left\langle x_F\right|\mathrm{e}^{-\mathrm{i}HT}\left|x_0\right\rangle=\lim_{N\to\infty}\left(\frac{m}{2\pi\,\mathrm{i}\,\Delta T}\right)^{(N+1)/2}\left(\prod_{j=1}^{N}\int\mathrm{d}x_j\right)\mathrm{e}^{\mathrm{i}S[x]}. \tag{6.257}$$

We now define a *path integral* of a functional $F\left[x\right]$ as follows:

$$\int F\left[x\right]\mathcal{D}x\equiv\lim_{N\to\infty}\left(\frac{m}{2\pi\,\mathrm{i}\,\Delta T}\right)^{(N+1)/2}\left(\prod_{j=1}^{N}\int\mathrm{d}x_j\right)F\left[x\right]. \tag{6.258}$$

Here, $\mathcal{D}x$ means "integrate over all possible paths $x\left(t\right)$", so we are integrating not with respect to a numerical variable, but with respect to a **function**. In other words, this is a *functional integral*, and it is essentially the sum of the values of the functional for every possible path, times a suitable integration measure.

Unfortunately this definition **isn't quite rigorous**, and introduces a myriad of mathematical issues, the most important of which is whether this infinite product of integrals actually converges! Resolving these issues is very important, but much beyond the level of our course, so I will not discuss it here.

In conclusion, we find that the amplitude to get from x_0 to x_F is given by a path integral:

$$\left\langle x_F\right|\mathrm{e}^{-\mathrm{i}HT}\left|x_0\right\rangle=\int\mathrm{e}^{\mathrm{i}S[x]}\,\mathcal{D}x. \tag{6.259}$$

We did this calculation for a free particle, for simplicity, but it is in fact possible to do this for an **arbitrary** Hamiltonian, and the result will be the same: we will always get the integral of the corresponding Lagrangian, and hence the action, inside the exponential.

Problem 6.36.

A. Prove that

$$\int_{-\infty}^{+\infty}\mathrm{e}^{-x^2}\,\mathrm{d}x=\sqrt{\pi}. \tag{6.260}$$

B. Using the result of (A), prove the more general integral

$$\int_{-\infty}^{+\infty}\mathrm{e}^{-ax^2+bx+c}\,\mathrm{d}x=\sqrt{\frac{\pi}{a}}\exp\left(\frac{b^2}{4a}+c\right). \tag{6.261}$$

C. Using the result of (B), prove (6.251).

Problem 6.37. Here we derived the path integral representation for the amplitude to get from position x_0 to position x_F. This is an amplitude that involves only eigenstates of position. In the more general case, we want to know the amplitude to get from some initial state $|\Psi_0\rangle$ to some final state $|\Psi_F\rangle$, namely $\langle\Psi_F| e^{-iHT} |\Psi_0\rangle$. What will be the path integral for this amplitude?

6.7.5 Applications of Path Integrals

We found that to calculate the amplitude, we must integrate over all possible paths $x(t)$, with the integrand being none other than the exponential of the action times i. It is understood that the paths $x(t)$ we integrate over must start at x_0 and end at x_F, but other than that, the paths can be arbitrary.

In fact, some paths may be completely unrealistic, with the particle going to the Andromeda galaxy for a second and then coming back to Earth the following second! This, of course, violates relativity, but to properly impose the speed of light limit, we must use *quantum field theory*, a more fundamental theory which is consistent with both quantum mechanics (at the non-relativistic limit) and special[74] relativity (at the classical limit).

As you showed in Problem 6.37, the path integral allows us to calculate the amplitude to go from any state to any other state – using just the classical action, without the hassle of promoting functions to operators, imposing commutation relations, and acting with these operators on the states. It is possible to formulate all known quantum theories, including quantum field theory, in terms of path integrals, without doing any canonical quantization.

Another thing we can do with path integrals is to obtain the *classical limit* in an intuitive way. We can think of the classical limit as a composite system where numerous microscopic quantum particles make up a single macroscopic classical object. When we have many different quantum particles together in one system, the total action for the system is the sum of the individual actions for each particle. Therefore, it is sensible[75] to take the classical limit to be $S[x] \to \infty$, as we expect the total action to be very large in magnitude compared to the action of a single particle. In this limit, we can use the *stationary phase approximation* (as you will do in Problem 6.38) to obtain the approximation

$$\int e^{iS[x]} \mathcal{D}x \approx e^{iS[x_c]}, \tag{6.262}$$

where $x_c(t)$ is the *classical path*, that is, the path that solves the Euler-Lagrange equation (6.215) with the boundary conditions $x(t_0) = x_0$ and $x(t_F) = x_F$; in other words, $x_c(t)$ is a

[74] In fact, quantum field theory is also consistent with general relativity – as long as gravity remains classical, and only matter (as described by the fields) is quantum. It is currently unknown how to describe gravity itself, as described by general relativity, as a quantum theory; such a theory would be called *quantum gravity*.

[75] In most quantum mechanics textbooks, the integrand of the path integral is given by $e^{iS[x]/\hbar}$ where $\hbar$ is Planck's constant, and the classical limit is given by $\hbar \to 0$. However, this doesn't make much sense, as $\hbar$ is a dimensionful physical constant, so its numerical value has no physical meaning; all you're doing by taking $\hbar \to 0$ is redefining your units of measurement. Here I am keeping $\hbar \equiv 1$ fixed, and the classical limit is $S[x] \to \infty$, which is equivalent because $S[x]/\hbar \to \infty$ under both $\hbar \to 0$ and $S[x] \to \infty$.

stationary point of the action.

This happens because the exponential integrand is an oscillating function, and it can be shown that whenever S varies, the oscillations **cancel each other** by destructive interference. However, stationary points, where the action does not vary, do not get canceled. But as we have seen, stationary points are exactly those which correspond to classical paths. The classical path therefore has the highest probability, and this explains why we observe objects to follow classical trajectories even though each individual particle behaves according to the laws of quantum mechanics.

Unfortunately, as I mentioned earlier, it is hard to formulate a **rigorous** mathematical definition of the path integral. It can be defined rigorously for non-relativistic quantum mechanics using the dirty trick of taking time to be imaginary, $t \to \mathrm{i}\, t$, in which case the exponent becomes real and the integral becomes easier to define (this is called a *Wick rotation*). However, in quantum field theory, path integrals have not yet been defined rigorously except in some simple cases, such as for some fields in 2 spacetime dimensions. Physicists nevertheless use path integrals ubiquitously in quantum field theory, with great (and even experimentally verified) success, but the integrals themselves cannot be computed – instead, **perturbation theory** must be used to obtain approximate solutions.

In fact, as I mentioned in the beginning of this chapter, in 21st-century physics – and especially in quantum field theory, which is the fundamental framework used in most fields of modern theoretical physics – we usually prefer path integral quantization over canonical quantization. You can find more details in (recent) quantum field theory textbooks.

Problem 6.38. Prove (6.262) using the stationary phase approximation (if you are not already familiar with this approximation from other courses, look it up).

6.8 Epilogue

Unfortunately, our course has now come to an end. Even though this is a 4th-year undergraduate course, I taught you many advanced topics in quantum theory that most physicists only learn in graduate school – or not at all! I hope you had fun, and that this course helped you develop a deep intuition for quantum theory, understand its most important concepts and consequences, and demystify common misconceptions.

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