

Quantum Physics 101

Quantum mechanics was developed in the beginning of the last century as a means to explain certain mystical new phenomena that had been observed in experiments involving atoms, electrons and light. The development of quantum mechanics during the first thirty years of the last century led to a revolution in physics and, more broadly, in how we look upon the nature of reality. THIS NEEDS WORK!

Nowadays, even though quantum physics still might sound mysterious and abstract, it is very much a vital part of our daily lives through its many applications in modern technologies.

Classical physics¹ is completely deterministic. It is in theory possible to know everything about a classical system, and furthermore, once we know enough about the system, we can determine everything about its future through the basic laws of classical physics such as Newtonian mechanics and the theory of relativity.

One of the mysterious, or some would even say disturbing, facts about quantum mechanics is that this is no longer true. Quantum mechanics is inherently a non-deterministic, or probabilistic, theory.

In this Chapter we will give a lightning introduction to the wonderful world of quantum mechanics, with of course a special eye towards the applications in computer science. The mathematical language of quantum mechanics is mainly that of linear algebra, and much of the material will therefore hopefully be familiar, but perhaps presented in a way that is different from how you learned it in preschool.

We will also discuss the probabilistic nature of quantum mechanics and how this affects results of measurements; how quantum systems evolve with time; the quantum harmonic oscillator; and finally, we will discuss the quantum analogue of the classical bit of computer science, the so called qubit.

1. Quantum states

1.1. States, probability and measurements in a classical world. Let us start with a simple thought experiment. Imagine throwing an ordinary die, or flipping a coin. The resulting outcomes will be either $\{1, 2, 3, 4, 5, 6\}$ or $\{\text{Heads}, \text{Tails}\}$, respectively. We refer to this as saying that the *state* of the die or coin is in the value of the outcome, say 5 or Heads. Obviously, it does not make sense to say that for example the coin is in a mixture of heads and tails. It simply is in either the state heads or the state tails. We can summarize this by saying that, *in classical physics, a state takes values in a set.*

Furthermore, it is obvious to us that making a measurement, i.e., looking at the die or coin after it has landed, will not affect the system. If we throw the die and immediately cover it with our hand before seeing the outcome, it will still be in the state it lands on, say 5, before we remove the hand, and continue to be in the state 5 if we cover it again. We could even imagine doing something more complicated, for example, we could first look only at the number on top of the die (5) then cover it, and instead look only at the number on the side facing us, say 4, then cover it again. If we now look at the number on the top we of course still assume, and correctly so, that this will still be 5. This can be phrased as saying that *in classical physics, measurements does not affect the system.*

Later on, we will discuss the probabilistic nature of quantum mechanics, but the notion of probability is of course something we occasionally use when describing systems in the classical world as well. After all, playing board games would perhaps be a bit less fun if we always knew exactly how the dice would land. However, this notion of probability is simply a measure of how little information we have about the system. If we had some super computer that could completely characterize the initial state of the dice in

¹In this course, when we talk about classical physics we simply mean *not* quantum physics.

the thrower's hand, the force and angles of the hand that throw the dice, the atmospheric pressure and wind speed in the room when the dice are thrown, and so on, it could determine exactly how the dice would land. In classical physics, knowing everything about a system really means knowing everything. Using the laws of classical physics (and given a powerful enough computer) we can completely determine the future of any system once we know enough data. Or in other words, *classical physics is deterministic*.

Let us summarize what we have learned about classical physics so far:

- Classical states are elements of a set.
- Measurements does not affect the classical system.
- Classical physics is deterministic.

All of this hopefully seems rather obvious and intuitive to you and you might wonder why we are discussing such basic facts. Well, as we will see, when we step in to the quantum world, these basic things will no longer hold true and our daily life intuition about the world around us can more or less be thrown out the window.

1.2. Quantum states. One of the main differences between classical and quantum physics is the fact that quantum states are not just elements of a set, they are vectors in a complex-valued vector space. The strange thing is that we can give some meaning to the statement that a quantum state is in a mixture of states. If we had a quantum coin it could of course be either in the states heads or tails, but it could also be in a mixture of the two. This is called *superposition* and is one of the most fundamental concepts in quantum mechanics.

To see how this works, we first introduce some notation. We imagine that we have a system that is in some state, which we simply label by the letter ψ . This could in principle be anything we want, it is just a label for us to distinguish the state from another. For example, it could be a number corresponding to one of the classical states $\{1, 2, 3, 4, 5, 6\}$ of a die, but it could also be something else, such as \uparrow or \downarrow . The quantum state is then represented by a vector, which we denote by

$$|\psi\rangle.$$

This is called a *ket vector*, or simply a *ket*.² The ψ is just a label that we pick for our state while the encasing $|\cdot\rangle$ is there to remind us that this is a vector. Now, superposition tells us that it could happen that the physical system is in a combination of two (or more) states, e.g., we could have something like

$$|\psi\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle,$$

for some states $|\psi_1\rangle, |\psi_2\rangle$, and some (complex) numbers α and β . The numbers α and β are usually called the probability amplitude of the states $|\psi_1\rangle$ and $|\psi_2\rangle$, respectively.³ The notion of superposition is one of the key tools in quantum computing, and it is perhaps easy to see that this will grant us many more possibilities compared to the classical system.

The ket vectors satisfy the ordinary axioms of a vector space. There are two operations, vector addition and scalar multiplication. Under vector addition, the vector space is closed, associative and commutative. This means that for three vectors in the space $|a\rangle, |b\rangle, |c\rangle$, we have

$$\begin{aligned} |a\rangle + |b\rangle &= |c\rangle, & (\text{closed}), \\ (|a\rangle + |b\rangle) + |c\rangle &= |a\rangle + (|b\rangle + |c\rangle), & (\text{associative}), \\ |a\rangle + |b\rangle &= |b\rangle + |a\rangle, & (\text{commutative}). \end{aligned}$$

There is a unique identity element of vector addition, which we denote simply by 0 , such that

$$|\psi\rangle + 0 = |\psi\rangle.$$

²The notation here (together with the bra vector that we will introduce shortly, is usually called either the *bra-ket* notation or the Dirac notation, after the physicist Paul Dirac who invented it.

³This will be discussed in more detail later on, but it is important to note that the probability amplitude is not the same as a probability. For one thing, it is a complex number.

The reason why we do not use $|0\rangle$ here is because we want to reserve that notation for something completely different, as we will see later on. There is also a unique vector $(-|\psi\rangle)$ such that

$$|\psi\rangle + (-|\psi\rangle) = 0.$$

The vector space is linear and distributive under scalar multiplication. This means that for some complex numbers $z, z_1, z_2 \in \mathbb{C}$,

$$|(z_1 + z_2)\psi\rangle = z_1|\psi\rangle + z_2|\psi\rangle, \quad z(|\psi\rangle + |\varphi\rangle) = z|\psi\rangle + z|\varphi\rangle.$$

Finally, there also exists an identity element with respect to scalar multiplication, i.e., we can multiply with the number 1 and get back the same state, $1|\psi\rangle = |\psi\rangle$.

A basis for a vector space, $\{|a_1\rangle, \dots, |a_d\rangle\}$, is a minimal set of vectors that spans the space, the number of basis vectors needed, here d , gives the dimension of the vector space. A generic state $|\psi\rangle$ in this vector space can then be expressed as a superposition of such basis vectors,

$$|\psi\rangle = \sum_{j=1}^d \psi_j |a_j\rangle.$$

1.3. The dual space and inner product. There is also a corresponding dual vector space. The elements of this space are denoted

$$\langle\varphi|,$$

and are called *bra vectors*. The notation and their names becomes slightly more sensical when we introduce the inner product between the bra and the ket, or a *bra(c)ket*⁴

$$\langle\varphi|\psi\rangle.$$

This is simply a complex number. When we have a finite-dimensional vector space together with an inner product this defines what is called a *Hilbert space*⁵. Two vectors are said to be orthogonal if their inner product is zero. Furthermore, it is customary to normalize quantum states such that the inner product with itself is equal to one, such vectors are called unit vectors. We will do this automatically, or in other words, we will always set

$$\langle\psi|\psi\rangle = 1.$$

Vectors that are both normalized and orthogonal are then called *orthonormal*. This is, for example, a very good property to demand of a set of basis vectors. The normalization of quantum states will also play a vital role when we later discuss probabilities in quantum mechanics.

It is often useful to represent the kets as column vectors and the bras as row vectors. We then have the relation

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_d \end{pmatrix} \longleftrightarrow \langle\psi| = (\psi_1^*, \dots, \psi_d^*),$$

and the inner-product (or the bracket) then simply becomes the ordinary multiplication of vectors. We further see that the elements of the corresponding vectors are related by complex conjugation and we have

$$\langle\psi|\psi\rangle = |\psi_1|^2 + \dots + |\psi_d|^2.$$

Since the inner product between two states is just a complex number, we can ask what its complex conjugate is. This is given by

$$(\langle\varphi|\psi\rangle)^* = \langle\psi|\varphi\rangle,$$

and thus

$$|\langle\varphi|\psi\rangle|^2 = \langle\varphi|\psi\rangle\langle\psi|\varphi\rangle.$$

⁴Remember that quantum physics was invented long before the invention of the meme, so this was perhaps at the time considered funny. Dirac was also a famously strange man, [The strangest man](#)

⁵When the vector space is infinite-dimensional, some extra subtleties arise, but we will mostly be dealing with finite-dimensional vector spaces in this course, and we therefore ignore these subtleties for now.

1.4. Composite systems. If we imagine that we have several quantum systems, each in some state represented by some state vector, we can combine the separate system into a larger system using the tensor product of vector spaces, \otimes . If we imagine that we have one system where the state is given by $|\psi\rangle$ and another where the state is given by $|\varphi\rangle$, the state of the composite system is given by

$$|\psi\rangle \otimes |\varphi\rangle.$$

States that can be written in this simple way are called *product states*. We will discuss this name in more detail later on when we introduce the concept of entanglement. This way we can build complicated systems by combining several smaller systems. We will see this in action when we discuss quantum circuits. Note that the tensor product does not commute in general.

Sometimes, to save space, we denote a tensor product of states simply by writing

$$|\psi\rangle|\varphi\rangle := |\psi\rangle \otimes |\varphi\rangle.$$

EXERCISE 1.1. Consider an orthonormal set of basis vectors, $\{|u\rangle, |d\rangle\}$, for \mathbb{C}^2 .

a) Normalize the states:

$$\begin{aligned} |\psi_1\rangle &= (1 - i)|u\rangle + 2i|d\rangle, \\ |\psi_2\rangle &= |u\rangle \otimes |d\rangle - |d\rangle \otimes |u\rangle, \\ |\psi_3\rangle &= |u\rangle \otimes |u\rangle \otimes |u\rangle + |d\rangle \otimes |d\rangle \otimes |d\rangle. \end{aligned}$$

b) Represent the basis states as $|u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|d\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ and calculate the above (normalized) states in this representation.

Summary quantum states

- Quantum states are vectors in a complex vector space.
- A state is represented by the ket $|\psi\rangle$.
- The elements of the dual space are called bras and denoted $\langle\varphi|$.
- The inner product, or bracket, $\langle\varphi|\psi\rangle$, is a complex number, and its complex conjugate is given by $(\langle\varphi|\psi\rangle)^* = \langle\psi|\varphi\rangle$.
- We normalize the states such that $\langle\psi|\psi\rangle = 1$.
- Quantum states can be in a superposition of states, $|\psi\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle$, for some complex numbers α, β .
- More generally, we can express any quantum state in a vector space as a superposition of the basis vectors of that vector space, $|\psi\rangle = \sum_{j=1}^d \psi_j |a_j\rangle$, for some complex numbers ψ_j and basis vectors $|a_j\rangle$.

2. Measurements and probability

2.1. Observables. We have discussed how a quantum state is described by a state vector in a vector space. The quantum state is however not something that we can measure directly. In fact, it only tells us something about the *probability* of finding some result upon performing a measurement. Note that this is in stark contrast to the classical case where the state and the outcome of a measurement is for all intents and purposes equal to each other.

We refer to the properties of a state that we can measure as *observables*. If we consider a system representing a particle in some particular state, the observables would correspond to specific properties of this particle, such as its position, its velocity or its angular momentum. Observables are described in quantum mechanics by linear operators acting on the vector space of states. We thus say that a linear operator A acts on the state $|\psi\rangle$, and denote it by

$$A|\psi\rangle.$$

The corresponding action on the bra is given by the *Hermitian conjugate* (sometimes called the adjoint) of A , which we denote by a small dagger

$$A|\psi\rangle \longleftrightarrow \langle\psi|A^\dagger.$$

Note that the operator acts on the bra from the right and on the ket from the left.

When we represent the bras and kets as vectors the operators are naturally represented by matrices. The action of the dagger is then given by complex conjugation of the elements together with transposition of the matrix. For example,

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^\dagger = \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix}.$$

We can construct linear operators through the *outer product*

$$A = |\varphi_1\rangle\langle\varphi_2|.$$

Acting with such an operator on a state $|\psi\rangle$ gives

$$A|\psi\rangle = (|\varphi_1\rangle\langle\varphi_2|)|\psi\rangle = \langle\varphi_2|\psi\rangle|\varphi_1\rangle.$$

In words, we say that A transforms $|\psi\rangle$ into the state $|\varphi_1\rangle$ multiplied by the complex number $\langle\varphi_2|\psi\rangle$.

A very important and useful identity can be derived by considering a complete orthonormal basis $\{|v_j\rangle\}$ and expressing $|\psi\rangle = \sum_j \psi_j |v_j\rangle$, then introduce the operator $A = \sum_j |v_j\rangle\langle v_j|$. Here both sums are over the complete set of basis states. We notice that

$$A|\psi\rangle = \left(\sum_j |v_j\rangle\langle v_j| \right) |\psi\rangle = \sum_j |v_j\rangle\langle v_j|\psi\rangle = \sum_j \sum_k \psi_k |v_j\rangle\langle v_j|v_k\rangle = \sum_j \psi_j |v_j\rangle = |\psi\rangle,$$

which implies that $\sum_j |v_j\rangle\langle v_j| = \mathbb{1}$, the identity operator on the vector space. This relation is called a *completeness relation*, or sometimes a resolution of identity, and can be a very useful trick in many computations and proofs in quantum mechanics.

For any observable, say A , there exists a particular set of vectors called the *eigenvectors*, $|a_j\rangle$. They are defined through the relation

$$A|a_j\rangle = a_j|a_j\rangle,$$

where a_j is a complex number called the *eigenvalue* corresponding to the eigenvector $|a_j\rangle$ of A . We will typically use the above notation where the eigenvalues and eigenvectors have the same symbol, i.e., the eigenvalue of the eigenvector $|a_j\rangle$ is given by a_j . This is standard, and hopefully does not introduce too much confusion.

An especially important class of operators is the class of *Hermitian* operators. They are defined by having the property $A^\dagger = A$. From this definition, one can easily prove the important property that the eigenvalues of Hermitian operators are always real numbers. For this reason, physical observables in quantum mechanics are always given by Hermitian operators. The reason, as we will see later, is that the result of a measurement in quantum mechanics is given by the eigenvalues of the observable we are measuring, and the results of any physical measurement should of course be a real number. Another important property of Hermitian operators is that their eigenvectors form a complete set, i.e., any state can be expressed in the eigenvectors. Note however, that if the eigenvalues are the same the eigenvectors need not be orthogonal.

An operator A is called *normal* if it satisfies $A^\dagger A = A A^\dagger$. Such operators satisfy an important theorem called the spectral decomposition theorem. It states that an operator is normal if and only if it is diagonalizable with respect to some basis. This means that we can always express a normal operator, A , as $A = \sum_j a_j |j\rangle\langle j|$, where a_j are the eigenvalues of A and $|j\rangle$ an orthonormal basis where each vector is also an eigenvector of A (with eigenvalue a_j). Obviously, Hermitian operators are always normal.

A third class of operators that will play a very important role in this course is the class of *unitary* operators. They are defined by the property $A^{-1} = A^\dagger$, or in words, that the Hermitian conjugate is equal to the inverse operator. This means that $A^\dagger A = \mathbb{1}$.

Suppose now that we have two different observables A and B and we want to know if we can express them both in terms of the same basis. Or in other words, if we can write $A = \sum_j a_j |j\rangle\langle j|$ and $B = \sum_j b_j |j\rangle\langle j|$.

If this is possible we say that A and B are *simultaneously diagonalizable*. It turns out that this can only be done if A and B commute with each other, that is, if and only if

$$[A, B] := AB - BA = 0.$$

The notation $[A, B]$ is called the *commutator* of A and B and is a very frequently used operation in quantum mechanics.

We can again use the tensor product to build larger systems. If we have a system that is a composite system of say two different vector spaces

$$|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle,$$

we can build composite operators acting on this tensor product as

$$A = A_1 \otimes A_2, \quad A|\psi\rangle = A_1|\psi_1\rangle \otimes A_2|\psi_2\rangle.$$

2.2. The wave function. Consider now a complete set of commuting observables, A, B, C, \dots together with an orthonormal basis $|a, b, c, \dots\rangle$, where a, b, c, \dots are the corresponding eigenvalues of the observables. An arbitrary state $|\psi\rangle$ can then be expanded in this basis as

$$|\psi\rangle = \sum_{a, b, c, \dots} \psi(a, b, c, \dots) |a, b, c, \dots\rangle.$$

The set of coefficients,

$$\{\psi(a, b, c, \dots) = \langle a, b, c, \dots | \psi \rangle\},$$

is called the *wave function* of the system in the a, b, c, \dots basis. As we have mentioned before, the individual coefficients $\psi(a, b, c, \dots)$ are also called the *probability amplitude* for finding the system in the state $|a, b, c, \dots\rangle$. It is important to note that this is not the same as the probability for finding the system in this state, as we will see next. For one thing, the probability amplitude is in general a complex number. The actual probability of finding the eigenvalues corresponding to $|a, b, c, \dots\rangle$, is instead given by the absolute value squared of $\psi(a, b, c, \dots)$.

2.3. Measurements. The idea of a measurement in quantum mechanics is that we measure some observable A and the outcome will be an eigenvalue of A , where the corresponding probability of getting this result is captured by the coefficient of the state when expanded in the eigenvectors of the measured observable.

In other words, we start with an observable A that we want to measure for some system $|\psi\rangle$. We express it in its complete basis of eigenvectors $A = \sum_j a_j |a_j\rangle$. We further expand our system in this basis as $|\psi\rangle = \sum_j \psi_j |a_j\rangle$. The measurement will then return an eigenvalue of A , let us say a_j , and the probability of finding this specific result is given by $|\psi_j|^2$. Remember that we always normalize the states such that

$$1 = \langle \psi | \psi \rangle = \sum_j |\psi_j|^2,$$

so this interpretation as a probability makes sense.

After the measurement, the system has “collapsed” to the state $|a_j\rangle$ and we can measure A again to find the same result, a_j .⁶

At this point you might be wondering what all the fuss is about. We said in the beginning of this chapter that quantum mechanics is supposed to undermine our classical intuition that measurements does not affect the system. But, now we are saying that if we measure an observable A and find that the system is in, say, the state $|a_1\rangle$, then making another measurement asking if the system is in state $|a_1\rangle$ will give a positive answer with probability one. Is this not exactly what we said about the experiment with throwing a die and covering it? Can we not just say that the system was in state $|a_1\rangle$ all along?

⁶The word “collapsed” here is a standard one used in a majority of the literature, but is definitely the subject of much debate. What exactly happens in the moment of measurement is at the core of the debate among various interpretations of quantum mechanics that have appeared over the years. We will give a very brief account of various such interpretation later in this Chapter.

Well, the tricky thing with quantum mechanics is that if we now measure another observable that is not commuting with A , say B , and find the result $|b_1\rangle$, and then afterwards return to measure A again, it is no longer true that we are certain to find the result a_1 . We are basically back at square one and the only thing we can say is that there is a probability $|\langle b_1|a_1\rangle|^2$ to find the result a_1 . This would be like throwing the die, looking at the number on top, then looking at one of the numbers on the side and then finally looking at the number on top again to find that it is no longer the same.

With the above interpretations we can define the expectation value of an observable A in the state $|\psi\rangle$ in the ordinary way. This is denoted $\langle A \rangle_\psi$ and defined by

$$\langle A \rangle_\psi := \langle \psi | A | \psi \rangle = \sum_j a_j |\langle \psi | a_j \rangle|^2,$$

where $|a_j\rangle$ is the complete set of eigenvectors of A .

Let us consider a simple example, namely that of a two-level system. This means that we have a two-dimensional vector space.⁷ We introduce an orthonormal basis

$$\{|u\rangle, |d\rangle\},$$

such that we can express any state as

$$|\psi\rangle = \alpha|u\rangle + \beta|d\rangle, \quad |\alpha|^2 + |\beta|^2 = 1.$$

Next, we introduce an observable σ_z defined by

$$\sigma_z|u\rangle = |u\rangle, \quad \sigma_z|d\rangle = -|d\rangle.$$

I.e., the basis vectors are eigenvectors of σ_z with eigenvalues ± 1 , respectively.

We now measure σ_z and get some result. Let us assume that this is $+1$, and the state collapses to $|u\rangle$. As said before, we can now measure σ_z again and again and every time we will get the result $+1$.

But, there is of course nothing special with the basis defined by $|u\rangle$ and $|d\rangle$, we could as easily pick another basis. For example,

$$|l\rangle := \frac{1}{\sqrt{2}}(|u\rangle + |d\rangle), \quad |r\rangle := \frac{1}{\sqrt{2}}(|u\rangle - |d\rangle).$$

Related to this basis we can introduce a new observable, σ_x , that has these vectors as eigenvectors,

$$\sigma_x|l\rangle = |l\rangle, \quad \sigma_x|r\rangle = -|r\rangle,$$

and which does not commute with σ_z .⁸ If we now measure σ_x in our system, which has collapsed to $|u\rangle$ after the first measurement, we will get the results ± 1 with probabilities

$$\begin{aligned} |\langle u|l\rangle|^2 &= \frac{1}{2} |\langle u|(|u\rangle + |d\rangle)|^2 = \frac{1}{2}, \\ |\langle u|r\rangle|^2 &= \frac{1}{2} |\langle u|(|u\rangle - |d\rangle)|^2 = \frac{1}{2}. \end{aligned}$$

Let us again assume that the result is $+1$ such that the state collapses to $|l\rangle$. Now you might start to see the problem. If we return to measure σ_z , we will no longer find $+1$ with probability one but instead we have

$$\begin{aligned} |\langle l|u\rangle|^2 &= \frac{1}{2}, \\ |\langle l|d\rangle|^2 &= \frac{1}{2}. \end{aligned}$$

The two outcomes are now equally probable. This is part of the mysterious and indeterministic nature of quantum mechanics. It is, perhaps, easy to see that, if the observables do commute we can measure them simultaneously. Since we can then diagonalize them in the same basis.

The uncertainty in measuring non-commuting observables is captured by the famous *Heisenberg's uncertainty principle*. This principle is one of the fundamental results of quantum mechanics and has so

⁷This kind of system will of course be the main protagonist of this course, since the qubit is a two-level system. But for now we simply think of it in slightly more abstract terms.

⁸This follows from the definitions.

many big implications for the physical world. It therefore makes sense to take a few moments to derive it.

When we talk about uncertainty in this setting we typically mean with respect to the standard deviation, ΔA , for some observable A . This is defined by the following equation,

$$(\Delta A)_\psi^2 := \sum (a_j - \langle A \rangle_\psi)^2 |\langle \psi | a_j \rangle|^2.$$

We may simplify things and assume that the expectation value of A is zero, which implies that we have the simpler form

$$(\Delta A)_\psi^2 = \langle \psi | A^2 | \psi \rangle.$$

Let us now consider two observables A and B . The Cauchy-Schwartz inequality,

$$2|X||Y| \geq |\langle X|Y \rangle + \langle Y|X \rangle|,$$

applied to the combinations $|X\rangle = A|\psi\rangle$ and $|Y\rangle = iB|\psi\rangle$ gives us⁹

$$\Delta A \Delta B \geq \frac{1}{2} |\langle \psi | [A, B] | \psi \rangle|.$$

This is the uncertainty principle in its general form. In words it simply says that the product of the uncertainties in the two observables A and B , can not be smaller than the expectation value of the commutator of A and B . This is exactly what we mentioned earlier, namely that if two observables does not commute, then we can not measure them with certainty at the same time.

This is an enormously important consequence of the laws of quantum mechanics, and it has many important consequences of its own. It is for example believed to be the reason why there are galaxies and planets in the universe as well as part of the leading explanation to why the universe is expanding with an accelerating speed.

Let us finally note two important facts about quantum states. Firstly, if we have two states that only differ by an overall phase, say, $|\psi\rangle$ and $|\varphi\rangle = e^{i\gamma}|\psi\rangle$, then the statistical properties of these states are the same. This is easily seen from the fact that we have

$$|\varphi\rangle = e^{i\gamma}|\psi\rangle \implies \langle \varphi | = \langle \psi | e^{-i\gamma},$$

and we thus have

$$\langle \varphi | \varphi \rangle = \langle \psi | e^{-i\gamma} e^{i\gamma} | \psi \rangle = \langle \psi | \psi \rangle = \sum_j |\psi_j|^2.$$

For this reason, in quantum mechanics, we do not distinguish between states that differ only by an overall phase.

Secondly, we can notice that it is only possible to distinguish two quantum states with complete certainty if they are orthogonal. Otherwise they will have some component along the same direction and the result of the measurement has some probability of being the same for the two states.

EXERCISE 1.2. Consider the matrices

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

- Show that these matrices are Hermitian and unitary.
- Calculate all commutators between them.
- Calculate their eigenvectors and eigenvalues.

EXERCISE 1.3. Show that the eigenvalues of a Hermitian matrix are all real.

EXERCISE 1.4. For the (normalized) state $|\psi_1\rangle$ in Exercise 1.1, calculate the probabilities of getting the results ± 1 when measuring the observable given by the matrix Z defined in the previous exercise.

EXERCISE 1.5. Calculate the expectation value of the observable $Z \otimes Z$ in the (normalized) state $|\psi_2\rangle$ defined in Exercise 1.1.

⁹here we are assuming that the expectation values of both A and B are zero,

EXERCISE 1.6. Show that the set of vectors $\{|l\rangle, |r\rangle\}$, as defined above, gives an orthonormal set of basis vectors for \mathcal{C}^2 .

EXERCISE 1.7. Fill in the missing steps of the derivation of the uncertainty principle.

Summary observables and measurements

- Observables in quantum mechanics are represented as linear operators acting on the state space. They act on a ket from the left, $A|\psi\rangle$, and on a bra from the right $\langle\psi|A^\dagger$, where † denotes the Hermitian conjugate.
- Normal operators are defined by having $A^\dagger A = AA^\dagger$, and such operators satisfy the spectral decomposition theorem.
- Unitary operators are defined by having $A^\dagger = A^{-1}$.
- Hermitian operators are defined by having $A^\dagger = A$. They are normal operators and their eigenvalues are all real.
- Physical observables are described by Hermitian operators.
- The commutator between two operators A and B is denoted $[A, B] = AB - BA$. Two observables can only be simultaneously diagonalizable if they commute, i.e. if $[A, B] = 0$.
- Measurements “collapses” the quantum state into an eigenstate of the measured observable.
- Heisenberg’s uncertainty principle states that we can not know two properties of a quantum system simultaneously, unless their respective operators commute.

3. Evolution

3.1. Unitary operators. An interesting question to ask at this point might be how a quantum system evolves in time? To answer this, we first consider a system that at some time t is in the state $|\psi(t)\rangle$. We then ask how this is related to the state at some other time, say $t = 0$? We encode this change in an operator that we call $U(t)$ such that we have

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle.$$

Now, to be able to say something more about this mysterious operator $U(t)$ we want to introduce some restrictions. First of all, we want to demand that it is linear. This is natural from what we have discussed before. Quantum operators are typically linear. Less trivial is the statement that we want to enforce the operator to preserve distinguishability. This means that, if we have two orthogonal states, such that they are distinguishable by a measurement, we want them to still be orthogonal after the time evolution. Furthermore, we want the probabilities to be preserved, i.e., the normalization should remain intact.

Let us see what consequences this has. If we pick two elements $|a_j\rangle$ and $|a_k\rangle$ of an orthonormal basis to represent the states at $t = 0$, we have the condition

$$\langle a_j | a_k \rangle = \delta_{jk},$$

where δ_{jk} is the Kronecker symbol.¹⁰ But if we now let them evolve in time using $U(t)$ we want to have

$$\langle a_j | U^\dagger(t)U(t) | a_k \rangle = \delta_{jk},$$

and we see that $U^\dagger(t)U(t)$ acts as the unit operator. From this you can prove that the same is true for the action on any states. We thus need the time evolution operator to satisfy $U^\dagger(t)U(t) = \mathbb{1}$. This is exactly what we mentioned earlier as the definition of a unitary operator. So, time evolution in quantum mechanics is described by a unitary operator.

3.2. The Schrödinger equation. A slightly different view of the evolution of a system is due to thinking about a very important operator in quantum mechanics, namely the *Hamilton operator*, or sometimes just the *Hamiltonian*. This is the observable corresponding to the energy of the system.¹¹

¹⁰ $\delta_{jk} = 1$ if $j = k$ and 0 if $j \neq k$.

¹¹The Hamiltonian, named after William Rowan Hamilton, as a quantity describing the energy of a system is of course also important in classical physics. In classical mechanics it is however not an operator but an ordinary function.

The Hamiltonian determines the evolution of the system through the Schrödinger equation¹²

$$i\hbar \frac{d|\psi\rangle}{dt} = H|\psi\rangle. \quad (1.1)$$

More specifically, this is called the time-dependent Schrödinger equation. Here, \hbar (pronounced *h-bar*) is the famous Planck's constant, $\hbar \sim 1.0546 \times 10^{-34} \text{kg m}^2/\text{s}$ ¹³. As you see it is a very small constant when measured in units of our ordinary life, and this is basically the reason why our daily life does not prepare us with a good intuition for quantum physics.

The Hamiltonian is Hermitian and we can expand it in its complete set of eigenvectors,

$$H = \sum_j E_j |E_j\rangle\langle E_j|.$$

These eigenstates are called the energy eigenstates and the corresponding eigenvalues are the results of a measurement of the energy of the system. Since the $|E_j\rangle$ are eigenstates of the Hamiltonian we have

$$H|E_j\rangle = E_j|E_j\rangle,$$

which is sometimes called the time-independent Schrödinger equation.

By solving Schrödinger's equation, we find the connection to the operator $U(t)$ discussed earlier. Namely,

$$U(t) = e^{-\frac{i}{\hbar}Ht}. \quad (1.2)$$

We thus see that we can consider two different pictures, one where the state itself changes with time. The change is governed by the Schrödinger equation (1.1) and the corresponding picture is aptly called the *Schrödinger picture*. In the other picture we can instead think of the states as being constant while the time dependence is all due to the operators, as in Eq. (1.2). This picture is called the *Heisenberg picture*.

3.3. A note on (in)determinism. As we have mentioned already in the introduction, and seen in the discussion of measurements, quantum mechanics is inherently non-deterministic. But the discussion of time evolution of the quantum state looks very deterministic, right? This is true. The time evolution of the quantum state is a deterministic process, but this does not necessarily mean that quantum mechanics is deterministic.

In classical physics, making measurements does not affect the system and the result of a measurement is equivalent to the state of the system, both before and after the measurement. This is the basis of the determinism in classical physics. By knowing the state and knowing the equations of motion, we can determine where the state came from and where it is going. As we have seen, this is no longer true in quantum physics. Time evolution of the quantum state is deterministic, but knowing the state does not tell you with certainty the result of a general measurement.

¹²Named after its inventor, the cat-friendly Austrian Erwin Schrödinger.

¹³The German physicist Max Planck was the person who, sort of by mistake, started the whole field of quantum physics. He introduced a constant which he called h , which was later divided by 2π to give the constant $\hbar := \frac{h}{2\pi}$, which we now call Planck's constant.

Summary: Quantum postulates

Let us summarize what we have learned so far into four postulates of quantum mechanics.

- (1) States are described by unit vectors in a complex vector space (in fact a Hilbert space), and observables are described by linear Hermitian operators.
- (2) The possible outcomes of a measurement are given by the eigenvalues of the operator corresponding to the observable being measured.
- (3) If the system is in a state $|\psi\rangle$, and we measure an observable A with eigenvectors $|a_j\rangle$ and eigenvalues a_j , the probability of measuring eigenvalue a_j is given by

$$P(a_j) = |\langle a_j | \psi \rangle|^2 = \langle \psi | a_j \rangle \langle a_j | \psi \rangle.$$

- (4) The evolution of a quantum system is described by unitary operators.

4. What actually is the quantum state?

TO BE REWRITTEN

At this point, you might be asking yourself what the meaning of the quantum state is. After all, measurements tells us that eventually the state will not be in a superposition, the thing we observe is a definitive classical state, so how do we know that the state was ever in a superposition of other states? Well, such questions have given rise to a large number of debates on the interpretation of quantum mechanics. ¹⁴

Many early interpretations of quantum mechanics involved hidden variables, i.e., that there are some hidden variables that we do not know about which determines the measurements in a deterministic fashion. These have been essentially refuted by a number of results, such as Gleason's theorem and variations thereof. These type of results typically go under the name of Bell's theorem, and in principle they rule out almost all hidden variables theories. The experimental verification of these results was the subject of the Nobel prize in physics 2022. ¹⁵

In contrast, the widely considered Copenhagen interpretation of quantum mechanics (with variations) is essentially Bayesian. In this interpretation, the nature of quantum mechanics is essentially non-deterministic, and we should not require one to consider the "exponential" dimension of the quantum state prior to measurement any more so than we require a person throwing a die to consider the probability distribution over the outcomes. Measurements give rise to a (practically) irreversible process in which the state is affected.

Another famous interpretation is the many-worlds interpretation due to Hugh Everett. Here, time is considered as a tree, having many branches and each branch corresponds to a possible result of a measurement. This gives rise to an uncountable number of worlds or universes. The many-worlds interpretation is thus inherently deterministic, as the universal wave function never collapses to one particular state.

Finally, let us mention the de Broglie-Bohm interpretation. This is a kind of hidden variables theory where the problems of Bell's theorem are circumvented by embracing non-locality. Locality is basically the concept that only things near to each other can affect each other. This is one of the main building blocks of Einstein's theory of special relativity. The de Broglie-Bohm interpretation is thus a deterministic theory and particles have a definite configuration at all times, even when not observed. This has gained some interest in recent years and researcher are currently working on how to align it with the ideas of special relativity.

¹⁴See for example [Wikipedia](#)

¹⁵Awarded to the three experimentalists Alain Aspect, John Clauser and Anton Zeilinger.

5. The qubit

Let us now introduce the main protagonist of the course, the qubit. In a classical computer we use classical bits that are systems whose states takes values in the set $\{0, 1\}$. The corresponding quantum system is called a *qubit* (sometimes QBit, q-bit or quantum bit). This system is described by a two-dimensional complex vector space. To make the connection to classical bits even stronger we denote a set of basis vectors in this state space as

$$\{|0\rangle, |1\rangle\}.$$

Note that, as was mentioned before, we use the notation $|0\rangle$ to denote a basis vector, not the zero vector. This basis is typically referred to as the *computational basis*. Another frequently appearing basis is given by the states

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle).$$

You may recognize these bases as the u, d and l, r basis we studied earlier. The $|\pm\rangle$ basis is sometimes called the Hadamard basis. Any qubit can be expanded in either of these bases,

$$|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle = \alpha_+|+\rangle + \alpha_-|-\rangle,$$

for some numbers α_j , with the extra conditions $|\alpha_0|^2 + |\alpha_1|^2 = |\alpha_+|^2 + |\alpha_-|^2 = 1$.

We will often represent the computational basis by the vectors

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Linear operators acting on a qubit will now be described by 2×2 complex matrices. Of special importance are the so called *Pauli operators*.¹⁶ These are a set of three matrices that together with the identity matrix spans the vector space of 2×2 Hermitian matrices. In the computational basis, they read

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

As an easy, but informative and extremely useful, exercise, we can study how the Pauli operators act on our basis states. The Pauli matrices are some of the most used operation in quantum circuits, and these kinds of actions on the basis states will be used many many times throughout the course. We find¹⁷

$$\sigma_x \begin{Bmatrix} |0\rangle \\ |1\rangle \\ |+\rangle \\ |-\rangle \end{Bmatrix} = \begin{Bmatrix} |1\rangle \\ |0\rangle \\ |+\rangle \\ -|-\rangle \end{Bmatrix}, \quad \sigma_y \begin{Bmatrix} |0\rangle \\ |1\rangle \\ |+\rangle \\ |-\rangle \end{Bmatrix} = \begin{Bmatrix} i|1\rangle \\ -i|0\rangle \\ -i|-\rangle \\ i|+\rangle \end{Bmatrix}, \quad \sigma_z \begin{Bmatrix} |0\rangle \\ |1\rangle \\ |+\rangle \\ |-\rangle \end{Bmatrix} = \begin{Bmatrix} |0\rangle \\ -|1\rangle \\ |-\rangle \\ |+\rangle \end{Bmatrix}.$$

When discussing quantum gates, the σ_x operator is sometimes referred to as the NOT gate, since it interchanges the states $|0\rangle$ and $|1\rangle$, similar to the NOT gate of ordinary computers.

5.1. The Bloch sphere. We know that we can express any qubit as a superposition of the two basis vectors $|0\rangle, |1\rangle$, and that the corresponding coefficients must satisfy $|\alpha_0|^2 + |\alpha_1|^2 = 1$. We can then use a little trigonometry to express any qubit as

$$|\psi\rangle = e^{i\gamma} \left(\cos \frac{\theta}{2} |0\rangle + e^{i\phi} \sin \frac{\theta}{2} |1\rangle \right).$$

Where γ, ϕ and θ are some real numbers. However, we also saw earlier that we can not distinguish states that only differ by an overall phase, so we can disregard the overall phase factor $e^{i\gamma}$. We can thus describe any qubit in terms of two real numbers ϕ and θ through the identification

$$|\psi\rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\phi} \sin \frac{\theta}{2} |1\rangle.$$

This is simply the spherical coordinates of the unit sphere, and we have thus found that any qubit can be represented by a point on the unit sphere. This representation of the state space of a qubit as a sphere goes under the name of the *Bloch sphere*. See Figure 1.1 for an example of how we can visualize

¹⁶Named after the Austrian physicist Wolfgang Pauli, who is counted as one of the main inventors of quantum mechanics.

¹⁷perhaps you recognize some of these properties from when we studied the up/down/left/right system earlier,

the state $|+\rangle$ on the Bloch sphere. Here we clearly see the difference between a classical bit and a qubit. A classical bit can only take the values 1 or 2 while the qubit can in principle be in any state that correspond to a point on the Bloch sphere, i.e., we have a continuum of possible states.

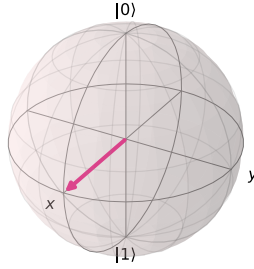


FIGURE 1.1. The Bloch sphere. The vector denotes the qubit state $|\psi\rangle = |+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. The labels x and y represent the Euclidean x and y directions.

It can be easily seen from the previous calculations that the Pauli matrices act as rotations along the different axes of the Bloch sphere. For example, acting with σ_x on $|0\rangle$ rotates the state 180° , or π radians, around the x -axis to give the state $|1\rangle$, and so on. All the standard one qubit gates can be visualized in a similar manner as their action on the Bloch sphere.

5.2. Several qubits. Just as before, we can combine simple systems into larger ones by using the tensor product of vector spaces. This will be vital when constructing quantum circuits, since, obviously, having just one qubit would perhaps not be all that exciting.

So, using the tensor product we can build larger systems of several qubits, for example

$$|0\rangle \otimes |0\rangle \otimes |+\rangle \otimes |1\rangle \otimes \dots \otimes |1\rangle.$$

We will often be lazy and use the notation

$$|\psi_{n-1} \dots \psi_0\rangle := |\psi_{n-1}\rangle \otimes |\psi_{n-2}\rangle \otimes \dots \otimes |\psi_0\rangle.$$

For example, for the two-qubit system, given by a four-dimensional vector space, we then have the basis vectors

$$|00\rangle = |0\rangle \otimes |0\rangle, \quad |01\rangle = |0\rangle \otimes |1\rangle, \quad |10\rangle = |1\rangle \otimes |0\rangle, \quad |11\rangle = |1\rangle \otimes |1\rangle.$$

It is easy to show that these span the vector space of states. Sometimes a further simplification of notation is used for these types of combined systems where we imagine the product to indicate a binary representation of an integer, so that we write for example $|01\rangle = |1\rangle_2$ and $|11\rangle = |3\rangle_2$ and so on, where the subscript indicates how many qubits there are in the system. The subscript is of course needed because 001 and 1 are both binary representations of the number 1, while here the former would be a three qubit system and the latter a one qubit system.

5.3. Physical implementations. There are several physical implementations of a qubit, including:

- **Superconducting qubits:** These qubits are made from tiny loops of superconducting wire, which can carry electrical current without resistance. The state of a superconducting qubit can be controlled by applying electromagnetic pulses to the loop.
- **Trapped-ion qubits:** These qubits are made by trapping a single ion (an electrically charged atom) in a magnetic or electric field. The state of a trapped-ion qubit can be controlled by shining laser light on the ion.
- **Topological qubits:** These qubits are based on the properties of certain materials, such as topological insulators, that can carry electrical current on their surface while insulating inside.
- **Quantum dots:** These qubits are made by confining a single electron or hole (an absence of an electron) in a tiny semiconductor structure called a quantum dot.

- Nuclear Magnetic Resonance (NMR) qubits: These qubits are based on the spin of the nuclei of certain atoms.
- Photonic qubits: These qubits are based on the properties of individual photons (particles of light). For example, the polarization state of a photon can be used as a qubit, with the two possible states being horizontal and vertical polarization.
- Single-molecule spin qubits: These qubits are based on the spin of individual electrons or nuclei in a single molecule. The state of the qubit can be controlled by applying magnetic fields to the molecule. These qubits are still in the research stage and not yet commercialized.

EXERCISE 1.8. Consider the computational basis representation

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

- a) Calculate the vectors

$$|00\rangle, |01\rangle, |10\rangle, |11\rangle,$$

in this basis.

- b) Calculate $\sigma_x \otimes \sigma_z$ and $\sigma_z \otimes \sigma_x$. Are these matrices Hermitian? Unitary? What is the commutator?

EXERCISE 1.9. The Hadamard transform is a 1-qubit operation, typically denoted H , and acts on the computational basis in the following way:

$$|0\rangle \rightarrow |+\rangle, \quad |1\rangle \rightarrow |-\rangle.$$

- a) Find the unitary operator U_H which implements H with respect to the basis $\{|0\rangle, |1\rangle\}$.
 b) Find the inverse of this operator.
 c) Find its matrix representation in the computational basis:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

and in the Hadamard basis

$$|0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

6. The harmonic oscillator

Models of most physical implementations of qubits rely on various variations of the quantum harmonic oscillator. To give some intuition behind the physical qubits, as well as to illustrate the many concepts we have introduced so far, we will show how to extend the classical harmonic oscillator to the quantum harmonic oscillator, highlighting the differences.¹⁸

6.1. The classical harmonic oscillator. Classical systems follow Newton's three laws of mechanics. In particular, the second law states that the force is equal to the mass times the acceleration,

$$F = ma.$$

A harmonic oscillator is a particle that undergoes harmonic motion around an equilibrium point. Think for example of a spring with a mass attached to its end such that it bounces back and forth around an equilibrium.

Let us focus on the one-dimensional case and set the equilibrium point to be $x = 0$. The system is described by a mass m and a restoring force that pushes the mass towards the equilibrium point,

$$F = -m\omega^2 x,$$

¹⁸The harmonic oscillator could very well be the single most important system in all of physics, so a basic knowledge of this system is probably a good thing to have in life.

where ω is called the angular frequency. The minus sign tells us that the force is driving the spring back towards its equilibrium point. Combining this with Newton's second law we get

$$ma = m\ddot{x} = -m\omega^2x.$$

The solution of this second order differential equation is

$$x(t) = A \cos(\omega t + \phi),$$

where A is the amplitude of the oscillations (giving the turning points of the motion) and ϕ the initial phase.

SOME PICTURES COULD DEFINITELY BE ADDED IN THE ABOVE!

The potential energy of the system is given by

$$V = \frac{1}{2}m\omega^2x^2.$$

This gives a parabola as shown in Figure 1.2. The reason why the harmonic oscillator is so important as a physical system is that almost any smooth function can be approximated by a parabola near its minimum points.

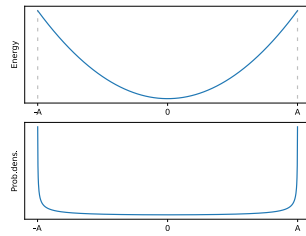


FIGURE 1.2. The potential energy (top) and probability density (bottom) of the classical harmonic oscillator, with amplitude A .

Remember that the total energy of the system is given by the sum of the potential energy, V , and the kinetic energy $\frac{1}{2}mv^2$. At the turning points $x = \pm A$, the velocity, and therefore the kinetic energy, is zero, and the potential energy reaches its maximum. The total energy of the system thus simply says something about how far away from the equilibrium it can move. For example, the zero-energy harmonic oscillator simply sits still at its equilibrium. At the equilibrium point, on the other hand, the kinetic energy reaches its maximum and the potential energy is zero, this means that the particle attains the greatest velocity here. This further implies that for a classical harmonic oscillator, the probability is highest to find it close to the turning points $x = \pm A$, since this is where it moves at its slowest, and thus spends the most time. This is shown in the bottom picture of Fig. 1.2

6.2. The quantum harmonic oscillator. The quantum harmonic oscillator is, as the name suggests, the quantum analogue of the classical system. As we discussed earlier, in quantum mechanics (and also in classical mechanics) an important role is played by the Hamiltonian of the system. This is simply constructed as the sum of the kinetic and potential energy. So to construct the Hamiltonian we simply take the expression for the classical kinetic and potential energy and sum them,

$$H = \frac{1}{2}mv^2 + \frac{1}{2}m\omega^2x^2.$$

But in quantum mechanics, as we have seen, observables should be operators, so we also promote the position and momentum ($p = mv$) variables to operators.¹⁹ This results in the expression

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2,$$

¹⁹There are many reasons why we use momentum instead of velocity as the go-to operator in quantum mechanics, the most important one being that momentum is a conserved quantity, while velocity is not.

where we, in this section only, adopted the very common practice of putting hats on quantum operators, to distinguish them from their classical variable analogues. Note that, in contrast to most of the rest of this course, we are here considering an infinite-dimensional Hilbert space of states, since both \hat{x} and \hat{p} take continuous values. This does introduce some extra subtleties that we however simply gloss over at the moment.

In quantum mechanics, the energy of the system is described by the time-independent Schrödinger equation

$$\hat{H}|\psi_E\rangle = E|\psi_E\rangle,$$

where the subscript E on ψ_E is there to remind us that these are the eigenvectors of \hat{H} corresponding to the energy eigenvalues E . To solve this, we express the wave function $\psi_E(x) = \langle x|\psi_E\rangle$ in the coordinate basis. In this basis we can represent the momentum operator \hat{p} as a derivative $\hat{p} = -i\hbar\frac{\partial}{\partial x}$, and the equation takes the form

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi_E(x)}{\partial x^2} + \frac{1}{2}m\omega^2x^2\psi_E(x) = E\psi_E(x).$$

This does not look like something we want to explicitly solve in this course, we leave that for a full course on quantum mechanics or perhaps a course on differential equations.^[20] Instead, we simply state that under the assumptions that the wave function is normalizable and symmetric around the equilibrium $x = 0$, we have an infinite family of solutions labeled by a level (or *quantum number*) n

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right), \quad n = 0, 1, 2, \dots$$

Here, $H_n(y)$ are the so called (physicist's) Hermite polynomials, with the first few being

$$\begin{aligned} H_0(y) &= 1, \\ H_1(y) &= 2y, \\ H_2(y) &= 4y^2 - 2, \\ H_3(y) &= 8y^3 - 12y, \\ &\vdots \end{aligned}$$

The corresponding energy eigenvalues are

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right).$$

These are the values that would be returned upon a measurement of the Hamiltonian of the quantum harmonic oscillator. Two important things to note are, first that the energies are quantized, i.e., they come in discrete steps; and secondly the lowest value is not equal to zero, but rather $E_0 = \frac{\hbar\omega}{2}$. This second point is a consequence of the uncertainty principle.

To connect with the classical system we can calculate the amplitudes, A_n , of a classical harmonic oscillator with the corresponding energies of the quantum one. We find

$$E_n = \frac{1}{2}m\omega^2 A_n^2 \implies A_n = \sqrt{(2n+1)\frac{\hbar}{m\omega}}.$$

Note that these increase with the quantum number n .

Figure 1.3 shows the probability amplitudes, $\psi_n(x)$, and probability densities, $|\psi_n(x)|^2$ of finding the system at the location x , for the first few energy levels in the positional basis. We note two big differences with the classical oscillator. First, there is a non-zero probability of finding the particle outside the values $x = \pm A_n$, this is not possible in the classical system. This is due to something called *quantum tunneling*. Secondly, the probability density distribution for the lowest-energy state $\psi_0(x)$, is highest at the origin $x = 0$, while for the higher values of n we see that the system starts looking more like the classical one, i.e., that it is most likely to find the system near the turning points. This is an illustration of something called the Bohr correspondence principle. Namely that quantum physics should become classical physics in the limit of large quantum numbers (or when \hbar becomes small in comparison to the energy).

²⁰Of course you are welcome to solve it yourselves. A nice trick one can use is to first guess or argue for the expression of the lowest energy state, and then use the fact that $[\hat{x}, \hat{p}] = i\hbar$ together with the algebra given by introducing the *creation* and *annihilation* operators $a^\pm \propto \hat{p} \pm i\omega\hat{x}$ to construct the higher energy states.

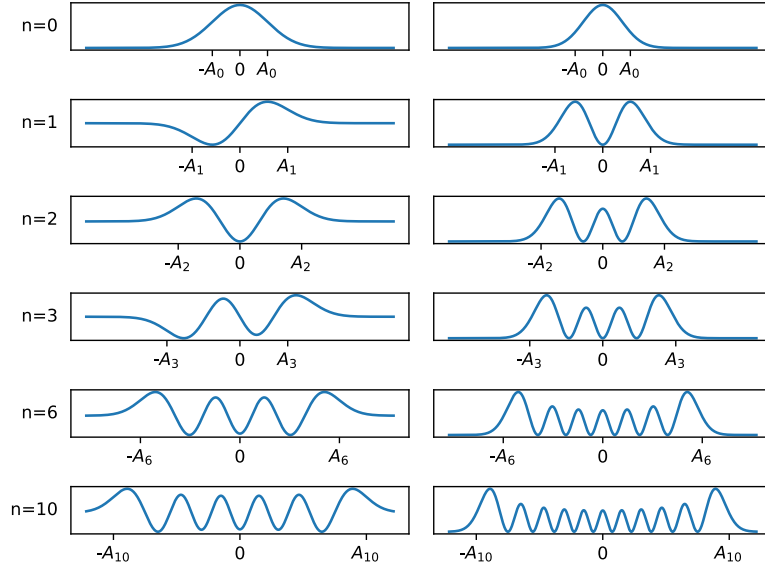


FIGURE 1.3. The probability amplitudes (left) and probability densities (right) for some levels of the quantum harmonic oscillator. The classical amplitudes A_n are indicated.

2D HARMONIC OSCILLATOR??

6.3. The transmon qubit. TBC

7. Entanglement

Let us end this chapter by discussing one of the most mysterious concepts in quantum mechanics, namely that of *entanglement*. We will also elaborate on some of its important consequences for quantum computers.

7.1. Product states. We have seen that if we have two physical systems $|\psi_A\rangle$ and $|\psi_B\rangle$, we can combine them into a composite system

$$|\psi_{AB}\rangle = |\psi_A\rangle \otimes |\psi_B\rangle.$$

Let us study this concept in more detail. For simplicity, let us consider a two-qubit system. We then have that both systems $|\psi_A\rangle$ and $|\psi_B\rangle$ can be expressed as a linear combination of the basis states $|0\rangle$ and $|1\rangle$,

$$|\psi_A\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle, \quad |\psi_B\rangle = \beta_0|0\rangle + \beta_1|1\rangle,$$

with the ordinary normalization conditions $|\alpha_0|^2 + |\alpha_1|^2 = |\beta_0|^2 + |\beta_1|^2 = 1$. The combined system looks like

$$|\psi_{AB}\rangle = (\alpha_0|0\rangle + \alpha_1|1\rangle) \otimes (\beta_0|0\rangle + \beta_1|1\rangle) = \alpha_0\beta_0|00\rangle + \alpha_0\beta_1|01\rangle + \alpha_1\beta_0|10\rangle + \alpha_1\beta_1|11\rangle. \quad (1.3)$$

Furthermore, we have seen that we do not need to consider overall phases for the two individual systems. All in all this means that we have four real degrees of freedom in the combined system. Two coming from each qubit. But, let us now instead consider the most general two-qubit system

$$\gamma_{00}|00\rangle + \gamma_{01}|01\rangle + \gamma_{10}|10\rangle + \gamma_{11}|11\rangle,$$

with the normalization condition now being

$$|\gamma_{00}|^2 + |\gamma_{01}|^2 + |\gamma_{10}|^2 + |\gamma_{11}|^2 = 1.$$

Here, we only have one overall phase to disregard. The generic two-qubit system thus have six real degrees of freedom. Which of course is larger than the four we had before. It is easy to see that the first

case is a special case of the more general second case. The extra degrees of freedom between the two cases are exactly what give rise to the mysterious concept of *entanglement*.

A state that can be written on the form (1.3), or more generally as a product

$$|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle \otimes \dots,$$

is, somewhat naturally, called a *product state*, while those that can not be written on this form are called entangled. A simple example would be the state

$$|\psi^-\rangle := \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle).$$

This is called a *maximally entangled state* for reasons that will become clear later.

7.2. Non-locality. In 1935, Einstein, Podolsky and Rosen (EPR) published a paper called “Can quantum-mechanical description of physical reality be considered complete?” [Einstein et al. 1935]. In this paper, they considered a simple thought experiment that pinpointed some of the mysteries of entanglement. EPR were interested in the question of *completeness* of a physical theory. They defined a complete theory as one where each element of *physical reality*²¹ must have a counterpart in the physical theory. They proposed one simple requirement for an element of physical reality such that “if, without in any way disturbing a system, we can predict with certainty (i.e., a probability equal to unity) the value of a physical quantity, then there exists an element of physical reality corresponding to this physical quantity.” [Einstein et al. 1935]. They would thus say that two physical quantities corresponding to two non-commuting observables could not have a simultaneous reality, since they can not be measured simultaneously.

We will now give a simple example highlighting how quantum mechanics, or more specifically entanglement, challenges this simple idea.

Let us start with stating a simple fact. A quick calculation shows that for a generic qubit state, $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, we have the result

$$\langle\sigma_x\rangle_\psi^2 + \langle\sigma_y\rangle_\psi^2 + \langle\sigma_z\rangle_\psi^2 = 1.$$

This can be interpreted as saying that there is always some direction that has eigenvalue +1 for the qubit. It is furthermore easy to check that this continues to hold for the product states (1.3). Let us now look at the entangled state $|\psi^-\rangle$ which we defined above. To this end, we calculate the expectation values of the operators $\sigma_{x,y,z} \otimes \mathbb{1}$ and $\mathbb{1} \otimes \sigma_{x,y,z}$ ²². The result turns out to be zero for all choices. Having a zero expectation value of course simply means that both outcomes are equally likely. We thus see that, even though we know the exact state the system is in, namely $|\psi^-\rangle$, we can not say anything about the individual pieces, i.e., the states of the two individual qubits.

Next, we can note that an operator such as $\sigma_z \otimes \sigma_z$ will have $|\psi^-\rangle$ as an eigenstate, more specifically, we have

$$(\sigma_z \otimes \sigma_z)|\psi^-\rangle = -|\psi^-\rangle.$$

Which of course tells us that $\langle\sigma_z \otimes \sigma_z\rangle_{\psi^-} = -1$ ²³. This is peculiar for the following reason: We can imagine having the two-qubit system $|\psi^-\rangle$ and distributing each qubit to two people, say Alice and Bob. We then imagine that Alice flies off to Mars with her qubit and Bob stays behind here on Earth. If at Mars, Alice suddenly (and randomly) decides to measure the spin along the z -axis of her qubit (i.e. measure σ_z), she will find one of the results ± 1 , but since the combined eigenvalue of hers and Bob’s measurement of σ_z must be equal to -1 , she will immediately know what the result of Bob’s measurement would be. For example, if Alice finds the result $+1$ she immediately knows that Bob must find -1 and vice versa. Similarly, if she instead measures σ_x or σ_y . This is what Einstein famously called *spooky action at a distance*. According to the EPR paper, this would mean that Bob’s system should have definitive and simultaneous values for the measurements σ_z and σ_x , but quantum mechanics does not agree with this.

²¹whatever that is,

²²By the notation $\sigma_{x,y,z}$ we simply mean that we can take any of the three indices.

²³Note that the same result holds for $\sigma_x \otimes \sigma_x$ and $\sigma_y \otimes \sigma_y$.

7.3. Bell inequalities and CHSH. The EPR paper did not receive a lot of attention after its publication. By many it was mostly considered to be a philosophical detail that one need not care about when doing physics. But, in 1964, almost 30 years after the original paper, John Bell published an idea for an experiment that could make use of the entanglement introduced by EPR to make predictions about the nature of quantum mechanics [Bell 1964]. Since then, this has been verified in real experiments, and today entanglement plays an essential role in quantum information theory and quantum computing.

We will discuss a variant of Bell's proposed experiment due to Clauser, Horne, Shimony and Holt (CHSH) [Clauser et al. 1969].

We consider the following game. We have two players, Alice (A) and Bob (B) and one game host, Charlie (C). Charlie chooses two questions $xy \in \{00, 01, 10, 11\}$ uniformly. He then asks x to Alice and y to Bob, who will answer with a single bit a and b , respectively. Alice and Bob will win if $a \oplus b = x \wedge y$.^[24] In other words, we need

$$\begin{aligned} a(0) \oplus b(0) &= 0, \\ a(0) \oplus b(1) &= 0, \\ a(1) \oplus b(0) &= 0, \\ a(1) \oplus b(1) &= 1. \end{aligned} \tag{1.4}$$

If we consider classical (and deterministic) strategies, we can easily see that there are 16 possible ones. For example, one strategy would be for both Alice and Bob to always answer every question with zero. By comparing the different strategies with the winning ones of (1.4) we can see that there is no classical strategy that can win every time. The best we can do is to choose a strategy that wins 3/4 of the times. One such example is the strategy of always answering zero to every question.^[25]

The big question is now if we can do better by considering quantum strategies. For simplicity we consider the answers to be either ± 1 instead of 0 and 1. This of course makes no real difference, we can for example consider the map $a \mapsto (-1)^a$ to take us from one convention to the other.

In the quantum version we consider Alice and Bob to share an entangled state, say

$$|\varphi^+\rangle := \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle),$$

such that they have one qubit each of this state. Before answering the question they both make a measurement on their corresponding qubit, such that $a(0)$ corresponds to the measurement of σ_z , $a(1)$ of σ_x , $b(0)$ of $H = \frac{1}{\sqrt{2}}(\sigma_z + \sigma_x)$ and $b(1)$ of $\frac{1}{\sqrt{2}}(\sigma_z - \sigma_x)$. We thus have the expectation values

$$\langle a(0) \otimes b(0) \rangle_{\varphi^+} = \langle a(0) \otimes b(1) \rangle_{\varphi^+} = \langle a(1) \otimes b(0) \rangle_{\varphi^+} = \frac{1}{\sqrt{2}}, \quad \langle a(1) \otimes b(1) \rangle_{\varphi^+} = -\frac{1}{\sqrt{2}}.$$

These expectation values measures the expectation that Alice and Bob win minus the expectation that they loose on each of the questions $\{00, 01, 10\}$ and minus this on the question $xy = 11$. Therefore, we find that the total probability of winning minus the probability of loosing is

$$\frac{1}{4} \langle \varphi^+ | a(0) \oplus b(0) + a(0) \otimes b(1) + a(1) \otimes b(0) - a(1) \otimes b(1) | \varphi^+ \rangle = \frac{1}{\sqrt{2}},$$

and the probability of winning is therefore

$$\frac{1}{2} \left(1 + \frac{1}{\sqrt{2}} \right) \sim 0.85.$$

This is of course better than the 3/4 probability in the classical setting.

In physics literature, this is more often stated as the fact that the inequality, known as a Bell inequality,^[26]

$$a(0)b(0) + a(0)b(1) + a(1)b(0) - a(1)b(1) \leq 2,$$

²⁴Here, \oplus means addition modulo 2.

²⁵As an exercise you can assure yourself that we can not do better by considering probabilistic strategies.

²⁶more specifically here the CHSH inequality,

which clearly holds for classical variables $a, b \in [-1, 1]$, can be violated by considering the above quantum situation, which gives

$$\langle a(0) \otimes b(0) \rangle_{\varphi^+} + \langle a(0) \otimes b(1) \rangle_{\varphi^+} + \langle a(1) \otimes b(0) \rangle_{\varphi^+} - \langle a(1) \otimes b(1) \rangle_{\varphi^+} = 2\sqrt{2}.$$

7.4. The GHZ paradox. Greenberger, Horn and Zeilinger (GHZ) [Greenberger et al. \[1989\]](#) came up with a stronger version of the Bell inequality game with a perhaps even more striking result. Namely, it gives a problem where the quantum strategy can win with certainty every time, while the classical can not.

For the GHZ setup, we consider a three-party game where Alice, Bob and Charlie each are asked one out of two questions (0 or 1), chosen uniformly from $xyz = \{000, 011, 101, 110\}$ with possible answers again given by a bit, a , b and c . They now win if $a \oplus b \oplus c = x \vee y \vee z$. The winning strategies should thus satisfy

$$\begin{aligned} a(0) \oplus b(0) \oplus c(0) &= 0, \\ a(0) \oplus b(1) \oplus c(1) &= 1, \\ a(1) \oplus b(0) \oplus c(1) &= 1, \\ a(1) \oplus b(1) \oplus c(0) &= 1. \end{aligned}$$

It is straightforward to once again assure us that no classical strategy can do better than win 75% of the time.

For the quantum strategy, we consider the case that Alice, Bob and Charlie are each given one qubit from the entangled state

$$|GHZ\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle).$$

The measurements can then correspond to σ_x and σ_y , since we can easily check that

$$\begin{aligned} \sigma_x \otimes \sigma_x \otimes \sigma_x |GHZ\rangle &= +|GHZ\rangle, \\ \sigma_x \otimes \sigma_y \otimes \sigma_y |GHZ\rangle &= -|GHZ\rangle, \\ \sigma_y \otimes \sigma_x \otimes \sigma_y |GHZ\rangle &= -|GHZ\rangle, \\ \sigma_y \otimes \sigma_y \otimes \sigma_x |GHZ\rangle &= -|GHZ\rangle. \end{aligned}$$

Where we again considered the answers ± 1 instead of 0 and 1. By the same argument as in the CHSH game of before we can now see that the GHZ game has a strategy that wins every time.

7.5. Bell basis and measurements. We have seen two examples of maximally entangled two-qubit states, $|\psi^-\rangle$ and $|\varphi^+\rangle$. They are in fact two out of four basis states of maximally entangled states. This basis is called the Bell basis,

$$\begin{aligned} |\varphi^\pm\rangle &:= \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle), \\ |\psi^\pm\rangle &:= \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle). \end{aligned}$$

As we have seen, and will continue to see, they play an important role in various thought experiments involving quantum entanglement.

Due to their importance in quantum theory, it is worthwhile to consider how we can construct the Bell states out of two generic qubits. If we start from a state in the computational basis we can create a Bell state by acting with an operator called the Hadamard gate, $H = \frac{1}{\sqrt{2}}(\sigma_x + \sigma_z)$ on the first qubit and then the so called controlled NOT, or CNOT, gate, with the newly transformed first qubit as the control. The CNOT gate acts by first controlling the state of the control qubit. If this is 0 it does nothing to the other qubit, while if it is 1 it acts with σ_x on the other qubit, flipping it between 0 and 1.²⁷ For example, if we start from the state $|00\rangle$, we find first that

$$H \otimes \mathbb{1}|00\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)|0\rangle,$$

²⁷These gates will be more properly introduced later as they are, of course, very important for the course.

and the CNOT thus transforms this into

$$\frac{1}{\sqrt{2}}\text{CNOT}(|0\rangle + |1\rangle)|0\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) = |\varphi^+\rangle.$$

Similarly, we find that the same circuit transforms $|11\rangle$ into $|\varphi^-\rangle$, $|01\rangle$ into $|\psi^+\rangle$ and $|10\rangle$ into $|\psi^-\rangle$.

Equally important is the Bell measurement. Given two maximally entangled qubits we can perform a Bell measurement to determine which of the Bell states the entangled qubits are in, and thus entangle the information. Algorithmically, this measurement is simply the Bell creation circuit, just presented, run in the opposite order. We start by acting with the CNOT gate, followed by the Hadamard on the control qubit. This is a key ingredient in the quantum teleportation protocol, which we discuss next.

7.6. Teleportation. The notion of entanglement is a very powerful one. To show some of its consequences, we will now discuss how quantum mechanics allows a form of teleportation of information.

We return again to our dear friends Alice and Bob. Alice was recently given a qubit

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle,$$

that she wants to send to Bob. However, they are very far away from each other and only have access to a measuring device and a telephone. So this seems hard. But perhaps there is a way? In other words, Alice needs to share some classical information over the phone such that Bob can recreate her state $|\psi\rangle$. There is a deep result in quantum mechanics called the *no-cloning theorem* that states that Bob can not simply copy Alice's state exactly.²⁸ Instead what we will see is that Alice will make a certain measurement changing her state but allowing her to retrieve some information that she can send to Bob such that he can rebuild the original state $|\psi\rangle$. This procedure is then what is called *quantum teleportation*.

First of all, let us note that we have seen that quantum mechanics does not allow for any direct measurement of Alice to simply get the numbers α and β such that she can communicate them to Bob. Since the measurement would change the state and she would not get the complete information of the original state. Instead we will come up with another prescription.

For this to work we imagine that besides the original qubit $|\psi\rangle$, Alice and Bob both have one qubit each from an entangled Bell pair $|\varphi_{AB}\rangle$. The procedure is simple, and given by four short steps:

- (1) Alice makes a Bell measurement of her combined system of two qubits $|\psi\rangle$ and $|\varphi_A\rangle$;
- (2) Alice makes a measurement to decide which states $|00\rangle$, $|01\rangle$, $|10\rangle$ or $|11\rangle$ her combined system is in;
- (3) depending on the outcome she gives an instruction to Bob, as follows:
 - if $|00\rangle$ do nothing;
 - if $|01\rangle$ apply σ_x ;
 - if $|10\rangle$, apply σ_z ;
 - if $|11\rangle$, apply $\sigma_z\sigma_x$.
- (4) if Bob chooses to follow Alice's instructions, he will now have the state $|\psi\rangle$.

So why does this work? Let us do the maths. For the Bell pair we take $|\varphi_{AB}\rangle = |\varphi^+\rangle$. The original system is then

$$|\psi\rangle \otimes |\varphi_{AB}\rangle = \frac{1}{\sqrt{2}}(\alpha|0\rangle + \beta|1\rangle) \otimes (|00\rangle + |11\rangle) = \frac{1}{\sqrt{2}}(\alpha|000\rangle + \alpha|011\rangle + \beta|100\rangle + \beta|111\rangle).$$

Alice then makes a Bell measurement on the first two qubits of this system. Remember that this means CNOT followed by Hadamard on the first qubit:

$$\begin{aligned} (H \otimes \mathbb{1} \otimes \mathbb{1})(\text{CNOT} \otimes \mathbb{1})(|\psi\rangle \otimes |\varphi_{AB}\rangle) &= (H \otimes \mathbb{1} \otimes \mathbb{1}) \frac{1}{\sqrt{2}}(\alpha|000\rangle + \alpha|011\rangle + \beta|110\rangle + \beta|101\rangle) \\ &= \frac{1}{2}(\alpha(|000\rangle + |011\rangle + |100\rangle + |111\rangle) + \beta(|010\rangle - |110\rangle + |001\rangle - |101\rangle)). \end{aligned}$$

²⁸You could try and derive this theorem, everything you need has been discussed in the course already.

This can be rearranged into

$$\frac{1}{2} (|00\rangle(\alpha|0\rangle + \beta|1\rangle) + |01\rangle(\alpha|1\rangle + \beta|0\rangle) + |10\rangle(\alpha|0\rangle - \beta|1\rangle) + |11\rangle(\alpha|1\rangle - \beta|0\rangle)).$$

Next, Alice measures her two qubits. This will give one of the results $|00\rangle$, $|01\rangle$, $|10\rangle$ or $|11\rangle$, with equal probability, projecting Bob's state to the corresponding parenthesis in the above expression. We thus see that if Alice obtains the result corresponding to $|00\rangle$ Bob's state will be $|\psi\rangle$, which is what we wanted, so no further action is needed. If Alice finds $|01\rangle$, Bob's state is $\alpha|1\rangle + \beta|0\rangle$, and acting on this with σ_x gives $|\psi\rangle$. Similarly, if Alice finds $|10\rangle$ Bob should act with σ_z and $|11\rangle$ means that he should act with $\sigma_z\sigma_x$ to get $|\psi\rangle$.

As we stated in the beginning, we also see that Alice's qubit is of course no longer in the state $|\psi\rangle$, it has collapsed to an eigenstate of her measurement. We thus say that she has teleported her state to Bob.

8. Further reading

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