

Chapter 3

Quantum Mechanics

We now describe the full theory of quantum mechanics which emerged in the 1920s. There are four rules of quantum mechanics and they fully describe anything that we would like to calculate. These ideas will seem strange at first and it will probably take you a while to feel comfortable with them. Bohr himself said that “those who are not shocked when they first come across quantum mechanics cannot possibly have understood it”. It is, however, well worth the effort.

The rules are:

1. States of physical systems are represented by complex functions, called wave functions.
2. Observables of physical systems, things that we can measure, such as the position or momentum of a particle, are represented by Hermitian operators.
3. When we make a measurement of the system we probabilistically obtain the answer according to the modulus square of the wave function. This is the so-called Born measurement postulate.
4. The system, when not measured, evolves according to the Schrödinger equation.

The meaning of each of these statements will become clear as we start to develop quantum mechanics. Suffice it to say that the statements are neither intuitively clear nor physically motivated at this stage¹. The ultimate justification, as always for a physicist, is that these rules are in extremely good agreement with experimental results and tests. Quantum mechanics is our by far most accurate description of nature. With that in mind, let us proceed. First we will discuss the Schrödinger equation that appears in the fourth rule, which was in fact discovered well before the other postulates of quantum mechanics were phrased.

¹Some researchers believe that we need a better formulation, but there is no other formulation at present.

3.1. Schrödinger's Equation

If particles are waves then it would seem reasonable to expect to be able to write a wave equation for these quantum objects². So we need to understand how waves behave in the first place.

Waves were already well understood by physicists in the nineteenth century. A wave equation is usually an equation that involves a second derivative in space as well as in time. It reads something like

$$\frac{\partial^2 f(x, t)}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 f(x, t)}{\partial t^2} \quad (3.1)$$

Here v is the velocity at which the wave propagates. If the above is to describe light, then the velocity is simply the speed of light, if, on the other hand, we are describing sound, then v is the speed of sound and so on.

A solution to this equation is the so-called plane wave:

$$f(x, t) = Ae^{i(kx - \omega t)} \quad (3.2)$$

such that $\omega = vk$. Here, ω is the frequency of the wave oscillations and $k = 2\pi/\lambda$ is its wavenumber. A is known as the amplitude of the wave and for now we will treat it as an arbitrary constant. Its role will be discussed in more detail below. The number i is the imaginary number³ whose value is $\sqrt{-1}$.

The plane wave $f(x, t)$ is a complex function, i.e. a function involving complex numbers, which are combinations of real and imaginary numbers. In classical physics, however, waves are always real. Let us take the electromagnetic wave as an example. The electric field can be written in the following form (the same goes for the magnetic field):

$$E = E_0 \cos\left(\frac{2\pi}{\lambda}x - \omega t + \theta\right), \quad (3.3)$$

where all the symbols have their usual meaning and θ is the initial phase, which can take any value. In quantum mechanics, as we will now see, waves can have a genuinely complex nature and this is one of the key differences between quantum and classical physics.

²The story says that Schrödinger was giving a talk about de Broglie's ideas, when someone from the audience got up and said: "If matter is really made up of waves, then what is the wave equation describing its behaviour?" Schrödinger did not know the answer, but had to work it out over the following weekend. This resulted in his celebrated equation for which he was awarded the Nobel prize in 1933.

³The imaginary number was discovered when an Italian medieval mathematician encountered the equation $x^2 + 1 = 0$. He knew that the solution of $x^2 - 1 = 0$ was $x = \pm 1$, but the equation $x^2 + 1 = 0$ did not seem to him to have any real solution. So he introduced an imaginary unit i and the solution could then be written as $x = \pm i$. Imaginary numbers were attributed all sorts of mystical properties after that for a long time. In some parts of Europe they were even banned by the Inquisition and people who promoted them were persecuted. Anyway, as if to show that God had a sense of humour after all, these numbers ended up being indispensable in the most accurate description of the world we have – quantum mechanics.

Let us take an electron, for example, and try to derive a wave equation describing its behaviour. This is actually how Schrödinger arrived at it as well. The electron's kinetic energy is given by

$$E = \frac{p^2}{2M} = \frac{\hbar^2 k^2}{2M}, \quad (3.4)$$

but de Broglie also tells us that the energy should be like that of a wave, which means that we should be able to associate some natural frequency to this electron, i.e.

$$E = \hbar\omega. \quad (3.5)$$

By equating the two we see that

$$\omega = \frac{\hbar k^2}{2M}, \quad (3.6)$$

i.e. now the frequency of the electron is proportional to k^2 (and not to k as in our wave equation). If a wave is to be associated with an electron its plane wave form, i.e. its wave function, would be

$$\Psi = e^{i(kx - \hbar k^2 t / 2M)}. \quad (3.7)$$

Now, what differential wave equation in space and time would this be a solution to? We are in the funny position that we know the answer, but now we have to come up with an equation whose solution is the above wave. This was basically the task that Schrödinger had to undertake.

After staring at this for some time, it should become clear that we need a second derivative in space, as before in the wave equation, but, unlike in the wave equation, we need a first derivative in time. This is because we need the equation to hold true regardless of the value of k (or ω) and

$$\frac{\partial^2}{\partial x^2} \Psi = -k^2 e^{i(kx - \hbar k^2 t / 2M)} = -k^2 \Psi \quad (3.8)$$

while

$$\frac{\partial}{\partial t} \Psi = -i \frac{\hbar k^2}{2M} e^{i(kx - \hbar k^2 t / 2M)} = -i \frac{\hbar k^2}{2M} \Psi. \quad (3.9)$$

So if we equate the two derivatives above, the k^2 factors cancel and it is possible to write

$$\frac{-\hbar^2}{2M} \frac{\partial^2}{\partial x^2} \Psi = i\hbar \frac{\partial}{\partial t} \Psi. \quad (3.10)$$

This is the celebrated Schrödinger equation, albeit in a restricted form.

What if the particle is subject to an external force, whose potential is $V(x)$? Then the equation is modified in the following way

$$\left[\frac{-\hbar^2}{2M} \frac{\partial^2}{\partial x^2} + V(x) \right] \Psi = i\hbar \frac{\partial}{\partial t} \Psi \quad (3.11)$$

and this is the full Schrödinger equation in all its glory. We are only stating it in one dimension at the moment, but we will see shortly how it generalises to three-dimensional space. Later in the book we will also revisit this equation and discuss in more detail why it has the form that it does. We will see that it is nothing more than an expression of the conservation of energy written in a formal quantum mechanical way.

So, the most basic equation of motion in quantum mechanics is similar to a wave equation but, unlike the wave equation, space and time enter the Schrödinger equation in an asymmetric way. The Schrödinger equation is, therefore, more like a diffusion equation. This suggests that a wavepacket will spread out, or diffuse, with time. We can understand this better by briefly discussing the velocity of the propagation of waves.

There are two important velocities to mention: group and phase. They are defined as follows. The group velocity is

$$v_g = \frac{d\omega}{dk} \quad (3.12)$$

while the phase velocity is

$$v_p = \frac{\omega}{k}. \quad (3.13)$$

The actual physical velocity of wave propagation is always the group velocity. For the free particle we know that

$$\hbar\omega = \frac{\hbar^2 k^2}{2M} = \frac{Mv^2}{2} \quad (3.14)$$

and, therefore, $v_g = \hbar k/M$. The phase velocity, on the other hand, has half this value, $v_p = v_g/2$, for a free particle and is the speed of propagation of the points in phase. In some cases this can even exceed the speed of light.

The following example may help here. Suppose we add two sinusoidal waves whose frequencies and wavenumbers are very close to one another

$$\sin(kx - \omega t) + \sin[(k + dk)x - (\omega + d\omega)t] \approx 2 \sin(kx - \omega t) \cos\left(\frac{dkx - d\omega t}{2}\right).$$

We see that the overall wave is just like the original one, i.e. $\sin(kx - \omega t)$, but governed by an envelope, $\cos[(dkx - d\omega t)/2]$, which travels at the speed $d\omega/dk$, which is just the group velocity.

But why is the ψ wave function complex and not real? What does that mean? The imaginary number $i = \sqrt{-1}$ appears in Schrödinger's equation, but it never appears in any classical equations of Newton or Maxwell. This looks very unusual and it certainly puzzled Schrödinger and other people in the community at that time.

3.2. Born's Postulate

It seems that it is very difficult to attribute any reality to the wave function. It is a complex function and complex numbers never really appear in our measure-

ments. We always measure some physical observable, such as the position of a particle, and the outcome is always a real number. Interestingly enough, the meaning of the wave function was not clear to Schrödinger either, even though he had invented it in the first place⁴.

The German physicist Max Born resolved this issue in 1925 (for which he was awarded the Nobel prize in 1954), with what has become known as the Born interpretation⁵. He stated that the modulus squared of the wave function is the probability density for particle to be found at a position x ⁶. Therefore, the probability to find a particle located between x and $x + dx$ is given by

$$|\Psi(x)|^2 dx \quad (3.15)$$

The probability to find a particle in a finite interval between x_1 and x_2 is consequently

$$p = \int_{x_1}^{x_2} |\Psi(x)|^2 dx. \quad (3.16)$$

A direct consequence of this is that

$$\int_{-\infty}^{+\infty} |\Psi(x)|^2 dx = 1 \quad (3.17)$$

This means that the total probability for a particle to be somewhere must be one. This is often called the normalisation condition – it makes sure all the probabilities add up as they should.

3.3. Time-Independent Schrödinger Equation

We have seen that the full one-dimensional Schrödinger equation for a particle described by the wave function $\Psi(x, t)$ is,

$$-\frac{\hbar^2}{2M} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi = i\hbar \frac{\partial \Psi}{\partial t}. \quad (3.18)$$

Just like Newton's equations, Schrödinger's equation cannot be derived from any more fundamental principle – it is a *law* of quantum physics⁷. The reason we are happy to use it is simply that it works. No experiment has yet shown

⁴This is always the nature of doing something revolutionary – all the consequences are not immediately clear.

⁵Max Born's other claim to fame is as the grandfather of Olivia Newton-John.

⁶What he stated in the text of his paper in 1927 is that the wave function itself gives the probability density, but then he added a footnote in the revised version to say that “on closer inspection it is the square of the wave function that plays this role”.

⁷It is sometimes seen as a weakness of physics that it rests on unprovable laws. However, this view denies the scientific process, which is not about proving theories, but rather trying to disprove them. Schrödinger's equation is a scientific theory which has, so far, stood up against a century of rigorous testing, but that does not mean that someday it will not be superseded. The fact that science relies on unprovable laws also suggests that there are things that lie beyond the scope of science.

any deviation from its predictions. Importantly, Schrödinger's equation tells us how the wave function changes with time so, if we know the wave function at a particular time, we can use (3.18) to calculate the wave function at any other time. In order to calculate solutions to the Schrödinger equation, it is useful to first find its time-independent form.

To do this we look for solutions that have the separable form,

$$\Psi(x, t) = \psi(x)\eta(t), \quad (3.19)$$

where $\psi(x)$ is a function of x only and $\eta(t)$ is a function of t only. This method is known as the separation of variables technique (SVT) and is a useful tool for solving differential equations. You will meet it again later in the book when we come to solve the Schrödinger equation describing the electron in a Hydrogen atom. Substituting (3.19) into (3.18) and dividing both sides by Ψ gives,

$$-\frac{\hbar^2}{2M} \frac{1}{\psi(x)} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) = i\hbar \frac{1}{\eta(t)} \frac{\partial \eta(t)}{\partial t}. \quad (3.20)$$

Importantly, the left hand side of the equation depends only on x and the right hand side depends only on t , i.e. the variables have been separated. Since the x and t values are independent, i.e. if we change x or t on one side of the equation it cannot affect the other side, the two sides can only be equal if each is equal to the same constant. We will call this constant E since it turns out to be the total energy of the system.

Solving the equation for $\eta(t)$,⁸

$$i\hbar \frac{d\eta}{dt} = E\eta, \quad (3.21)$$

gives $\eta = \exp(-iEt/\hbar)$. The equation for $\psi(x)$ is,

$$-\frac{\hbar^2}{2M} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x). \quad (3.22)$$

This is called the time-independent Schrödinger equation. We note that the solution to the full time-dependent Schrödinger equation (3.18) is easily found from the solution, $\psi(x)$, to (3.22), i.e. $\Psi(x, t) = \psi(x) \exp(-iEt/\hbar)$. One important feature of solutions that take this form is,

$$|\Psi(x, t)|^2 = |\psi(x)|^2, \quad (3.23)$$

i.e. the probabilities do not change with time and so are called stationary states. For stationary states, we can use the time-independent form of the Schrödinger equation. This is the equation that we will be interested in for a large part of this book.

⁸ $i\hbar(\partial/\partial t)$ is called the energy operator. Operators are a very important part of quantum mechanics and we will discuss them in more detail later in the book.

3.4. Free Particle

We have already considered the simplest solution of the Schrödinger equation, i.e. a particle in free space where there is no potential present. This was the case that Schrödinger used to deduce the form of the wave equation for quantum particles. Let us now reconsider this system starting with the Schrödinger equation. Setting $V(x) = 0$, we can rewrite (3.22) as,

$$\frac{\partial^2 \psi(x)}{\partial x^2} = -k^2 \psi(x), \quad (3.24)$$

where $k = \sqrt{2ME}/\hbar$ is the wave number of the particle (since $E = \hbar^2 k^2 / 2M$). The solution to this is $\psi(x) = A \exp(\pm ikx)$, where A is the normalisation. The full time-dependent solution is, therefore,

$$\Psi(x, t) = A e^{i(\pm kx - Et/\hbar)} = A e^{i(\pm kx - \omega t)}, \quad (3.25)$$

where the last step follows because $E = \hbar\omega$ for a free particle. This is just a plane wave solution (travelling in either the $+x$ or $-x$ direction) and we note, in particular, that the probability of finding a particle anywhere does not depend on x , $|\Psi(x, t)|^2 = |A|^2$. In other words, the particle is equally likely to be found anywhere, as we might expect in free space.

In the next chapter, we will consider solving the Schrödinger equation in situations when the potential, $V(x)$ is not zero. This will lead to a number of interesting consequences and applications. Before we do that, we round off this chapter by introducing a few more key ideas in the theory of quantum mechanics.

3.5. Observables and Operators

Heisenberg understood that the main difference between classical and quantum mechanics is that observables in classical mechanics commute, while in quantum theory they do not. Classically, if we measure a position of a particle, and then its momentum, we would get the same numbers if we did it the other way round. This means that observables in classical physics can be represented simply by numbers (since 4 times 8 is the same as 8 times 4, i.e. numbers commute).

However, the same is not true in quantum mechanics and so observables in this case cannot just be numbers. Heisenberg used matrices for this purpose as he knew that they do not commute. In fact he developed a whole new formalism for quantum mechanics known as matrix mechanics (Hamilton had handily invented matrices some 60 years earlier). This is also the reason why a lot of quantum mechanics involves techniques from linear algebra and why a lot of the mathematics taught in an undergraduate physics degree involves manipulating matrices. But we will not use matrices just yet, we will meet them again later in the book. This is because here we are dealing with continuous systems and matrices could be awkward.

Let us first introduce the idea of operators. An operator is in general something that acts on one function to give us another one. Special kinds of operators (called Hermitian) represent observables. We will not spend too much time on this topic here as it will be covered in more detail later in the book, but it is useful to introduce the idea and see them in action. Here we will instead use differentials rather than matrices to represent operators. These are an equally good formalism to use since they also do not commute. We can see this in the following example. In one dimension, the position operator, \hat{x} , is simply x , when written in the position representation. In the same representation, the momentum operator, \hat{p} , representing the momentum observable, p , is given by

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}. \quad (3.26)$$

We did not just pull this one out of a hat. This really is the only reasonable choice for momentum. Von Neumann showed this a long time ago and we will show why this must be the case later in the book. In the meantime, however, you will just have to take it on faith. We now show that position and momentum do not commute. Namely $\hat{x}\hat{p} \neq \hat{p}\hat{x}$, which can be seen by its operation on some wave function, $\psi(x)$,

$$x \left(-i\hbar \frac{\partial}{\partial x} \right) \psi(x) \neq \left(-i\hbar \frac{\partial}{\partial x} \right) x\psi(x). \quad (3.27)$$

This is because the right hand side is

$$-i\hbar \frac{\partial}{\partial x} x\psi(x) = -i\hbar \left(\psi(x) + x \frac{\partial}{\partial x} \psi(x) \right) = -i\hbar \left(1 + x \frac{\partial}{\partial x} \right) \psi(x), \quad (3.28)$$

which is not the same as the left hand side.

Another important concept in quantum mechanics is the eigenvalue equation. It has the form

$$\hat{Q}u(x) = qu(x) \quad (3.29)$$

Where \hat{Q} is an operator, $u(x)$ is its eigenfunction and q is the corresponding eigenvalue. Let us consider the example of a free particle and the operator,

$$\hat{H} = -\frac{\hbar^2}{2M} \frac{d^2}{dx^2}. \quad (3.30)$$

From Eq. (3.22) with $V(x) = 0$, we see that we have

$$\hat{H}u(x) = Eu(x) \quad (3.31)$$

where E is the energy of the particle. This means that \hat{H} is the operator for the energy of the free particle. We have already seen another form of an operator for the total energy of a system, $i\hbar\partial/\partial t$, which means we can write,

$$\hat{H}u(x) = i\hbar \frac{\partial}{\partial t} u(x). \quad (3.32)$$

This is an alternative (shorthand) way of writing the Schrödinger equation. The meaning of the eigenvalue equation is the following. If the physical system is in an eigenfunction of an operator, then upon measurement of that operator, we will obtain the corresponding eigenvalue with certainty.

3.6. The Superposition Principle

The superposition principle is the cornerstone of quantum mechanics and its failure would signal the end of quantum theory. It really is the key feature that distinguishes quantum physics from classical theories⁹. It states that whenever we have two solutions of the Schrödinger equation, i.e. two possible physical states of a system, then any superposition of the two is also a solution. This is very easy to show from the form of the Schrödinger equation.

The implications of this can be very bizarre. If an atom can be located here, this is one possible state, and if it could be located on the Moon, that is a second possible state, then it can also be simultaneously here and on the Moon. Or, if a photon can be blue or yellow, then it can also be both blue and yellow at the same time.

When we have a superposition of two different energies, for example, then the resulting state does not have a well defined energy. Let us show that in a more formal way now. Suppose we have an operator, \hat{A} with two eigenstates ψ_1 and ψ_2 with corresponding eigenvalues a_1 and a_2 , i.e.

$$\hat{A}\psi_1 = a_1\psi_1 \quad (3.33)$$

$$\hat{A}\psi_2 = a_2\psi_2. \quad (3.34)$$

What happens when we superpose the eigenstates? We obtain

$$\hat{A}(\psi_1 + \psi_2) = \hat{A}\psi_1 + \hat{A}\psi_2 = a_1\psi_1 + a_2\psi_2 \neq a(\psi_1 + \psi_2) \quad (3.35)$$

for any a . Therefore, if ψ_1 and ψ_2 are both eigenstates of the operator A with different eigenvalues a_1 and a_2 , then their superposition is not. This fact is reflected in the statistical character of measurement outcomes in quantum mechanics.

Let us explain this a bit more. When the system is in a eigenstate of some observable, when we measure this observable, the outcome will (with 100% probability) be the eigenvalue corresponding to that eigenstate. Let us take position as an example. Say you prepare an electron at a specific place. If there are no forces disturbing the electron, next time you measure it you will find it in the same place. But what happens if you prepare an electron in two different places at the same time? Then, when you measure its position, it will sometimes be in one place and sometimes in the other one and you won't be able to predict which will happen at any given time. This randomness at the heart of nature is something that is very difficult to accept and has been the

⁹Richard Feynman famously said that "superposition is the only mystery in quantum mechanics". It is, however, a very big mystery!

source of much discussion and debate. The same goes for any quantum system, not just electrons, and for the measurement of any observable, not just position.

3.7. Expectation Values

In Section 3.2 we saw how the wave function can be used to determine the probability of finding a particle at a particular location. It can also be used to determine the expectation value of measuring some observable of the particle, e.g. position, momentum, or energy. It is straightforward to see how this works in the case of position. We know that the probability density for finding a particle at location x is $|\psi(x)|^2$, and so the expectation value for x is simply,

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx.$$

This is usually written in the equivalent form,

$$\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x) x \psi(x) dx.$$

More generally, the expectation value for some observable O is given by

$$\langle O \rangle = \int_{-\infty}^{\infty} \psi^*(x) \hat{O} \psi(x) dx,$$

where \hat{O} is the *operator* for the observable O . For position, the operator is simply x , for momentum it is $-i\hbar \frac{\partial}{\partial x}$, and for energy the operator is $i\hbar \frac{\partial}{\partial t}$, as we have seen. The expectation value for momentum, for example, is found by calculating,

$$\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \psi^*(x) \frac{\partial}{\partial x} \psi(x) dx.$$

One important property of the Schrödinger equation is that it is linear. This means that if we find two or more solutions, then any linear combination of those solutions will also be a solution. This introduces the idea of basis wave functions: the general solution to the Schrödinger equation can be written as a sum of components in different basis wave functions. This is similar to the idea that a general vector can be written as a sum of components in different basis directions, e.g. the x , y , and z directions in Cartesian coordinates. Often it is convenient to choose basis functions that are orthogonal, i.e. there is no overlap between them. The overlap between two wave functions $\psi(x)$ and $\phi(x)$ is,

$$\int_{-\infty}^{\infty} \phi^*(x) \psi(x) dx,$$

and the two states are orthogonal if this overlap is zero.

3.8. The Uncertainty Principle

Let us now exemplify the calculation of expectation values with the position and momentum observables. In the process we will demonstrate a very important result in quantum physics – Heisenberg’s uncertainty principle.

For the sake of simplicity, let us choose a Gaussian wave function for the particle

$$\Psi(x) = \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-x^2/4\sigma^2}, \quad (3.36)$$

where σ is a constant that represents the standard deviation of the Gaussian. The position variance of this state is $(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2$. The expectation value of x is zero, i.e. $\langle x \rangle = 0$, so

$$(\Delta x)^2 = \langle x^2 \rangle = \frac{1}{(2\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} x^2 e^{-x^2/2\sigma^2} dx = \sigma^2. \quad (3.37)$$

Similarly, the momentum variance is $(\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2$ and $\langle p \rangle = 0$, so

$$(\Delta p)^2 = \langle p^2 \rangle = \frac{1}{(2\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} -\hbar^2 e^{-x^2/2\sigma^2} \frac{d^2}{dx^2} e^{-x^2/2\sigma^2} dx = \frac{\hbar^2}{4\sigma^2}. \quad (3.38)$$

The product of the uncertainties is, therefore,

$$\Delta x \Delta p = \frac{\hbar}{2}. \quad (3.39)$$

This conforms to the uncertainty principle for position and momentum, which states,

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \quad (3.40)$$

In other words, the better we know x , i.e. the smaller Δx , the worse we know the momentum, i.e. the larger Δp . The two are exactly inversely proportional. We will revisit the uncertainty principle in a more formal (and more general) way later in the book.

3.9. Conceptual Foundations of Quantum Mechanics

Before we go on to describe how quantum mechanics can be applied to a range of different systems in the next chapter, it is worth pausing to think about what it all means. This question was asked right at the very beginning of quantum theory and it has driven a great deal of research in the past hundred years or so. Though we are still not quite sure what the answer is (despite the remarkable success of the theory), several distinct interpretations have emerged.

One of the ways you can start to ask questions about the meaning of quantum mechanics is to ask “what is it that waves in the wave function?”. Born’s answer

would, of course, be that it is the probability amplitude waves. If pushed to explain, then he would say that the modulus square of the wave function is the probability to find the system in a given location and this is what waves. But, is this probability a property of the system that we observe or is it all in our heads. In other words, is the system waving or is our knowledge about the system waving, or is it the relationship between the system and myself that is waving? No one really has any answer to this, but various attempts to answer it have led to a number of different ways of looking at quantum mechanics.

The fact that objects in quantum mechanics can exist in many different states at the same time is difficult to reconcile with our everyday (classical) intuition. Dealing with this notion has led to a number of different interpretations of the meaning of quantum mechanics. Here we will mention some of the most important ones. Although they are different, they are not necessarily unrelated to each other.

The earliest one is the Copenhagen interpretation and was mainly constructed by Bohr himself. His take on this was basically as follows. Quantum mechanics is weird and implies some fundamental complementarity between properties in the everyday world. Namely, either we can set up our apparatus to find out one property or we can find some other property with a different arrangement, but the two cannot be found at the same time. Bohr called this principle the principle of complementarity and he believed in its widespread validity. Therefore, the key issue for Bohr was that the experimental question – the measurement – defined what can be done. The measurement reveals physical properties and some experiments are simply mutually exclusive. Heisenberg, who was greatly influenced by Bohr, also subscribed to this view. Superpositions in this view are just our way of dealing with the weirdness of nature, but we don't really know and cannot know what the microscopic world is really like. In other words, we cannot ask questions about what is happening when we are not looking. Quantum physics is simply a tool for predicting measurement outcomes.

At the opposite extreme in some sense is the Many Worlds interpretation. This was actually first conceived by John von Neumann, but was fully developed into a framework by Hugh Everett in the 1950s. Everett did not like the fact that measurement plays such a central role, because its outcome is in general random. So Everett realised that the whole of quantum theory can be explained without the need for any measurements. The price to pay, however, is that we need to accept that we live in a multiverse and not in a universe. Everything that can happen does happen. Positions and momenta are known, but they exist in different universes and only one of these will be accessible to us. This view is appealing for many reasons, but it also leads to some bizarre consequences.

Finally, perhaps quantum mechanics simply fails at some level. Maybe some things just cannot be superposed. Different people have come up with variations of this interpretation and they all come under the collective term 'collapse of the wave function'. There are some big proponents of this idea with different ideas of how the collapse takes place. Unfortunately no experiment so far has ever indicated any failure of quantum mechanics. This is not to say, of course,

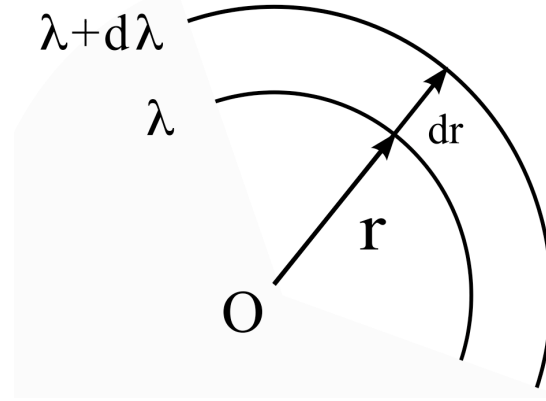


Fig. 3.1. How quantum mechanics reduces to classical. Consider an electron in a potential, V . At the radial distance r , from the origin, O , the electron has wavelength λ and at some infinitesimally larger distance $r + dr$, the wavelength is $\lambda + d\lambda$.

that future ones will not. As you learn more about quantum mechanics, you too will develop intuition as to which interpretation you are most inclined to accept. Until an experiment is able to distinguish these different interpretations you are, of course, free to choose any one you want. It is very much a question of taste.

Let us close this chapter by discussing one very important aspect of the consistency of quantum mechanics. We would like to show how it is possible to derive Newton's laws of motion from quantum mechanics. Rather than looking at the general case, which is a bit involved, though not too difficult, we will consider the specific case of an electron moving in an electromagnetic potential, V . What we would like to derive is that the radius of trajectory is governed by the balance between the centripetal force with the force derived from the electromagnetic potential.

At some radial distance r from the origin, the electron has wavelength λ and at some larger distance, $r + dr$, the wavelength is $\lambda + d\lambda$ (see Fig. 3.1). Now, we know that some integral number, n , of wavelengths must fit into the circumference, C . This gives

$$2\pi r = n\lambda \quad (3.41)$$

$$2\pi(r + dr) = n(\lambda + d\lambda). \quad (3.42)$$

Taking the ratio of these two equations, we get

$$\frac{r + dr}{r} = \frac{\lambda + d\lambda}{\lambda} \quad (3.43)$$

$$\implies \frac{dr}{r} = \frac{d\lambda}{\lambda}. \quad (3.44)$$

From this we can obtain

$$\frac{1}{r} = -\frac{1}{k} \frac{dk}{dr}, \quad (3.45)$$

where $k = 2\pi/\lambda$ is the wavenumber. Now, we know that k can be expressed as

$$k = \sqrt{2M(E - V(r))/\hbar} \quad (3.46)$$

since the kinetic energy is $\hbar^2 k^2/2M$. Plugging this into (3.45) we get

$$\frac{1}{r} = \frac{dV/dr}{2(E - V(r))}. \quad (3.47)$$

Noticing that $Mv^2 = 2(E - V(r))$, we finally reach the following expression

$$\frac{Mv^2}{r} = \frac{dV}{dr}, \quad (3.48)$$

which exactly encapsulates Newtonian dynamics. It states that the centripetal force, on the left hand side, matches the force due to the electromagnetic potential, on the right hand side. Therefore, Newtonian physics is just a special case of quantum mechanics.

3.10. Exercises

1. Suppose two travelling plane waves of momentum $\hbar k$, but travelling in opposite directions, are superposed.

Calculate the probability density of the resulting standing wave.

What are the nodes of this state?

Where is the probability maximal?

The quantum formula for probability current is given by

$$j = \frac{i\hbar}{2M} \left(\psi \frac{d}{dx} \psi^* - \psi^* \frac{d}{dx} \psi \right).$$

Calculate this for the above superposition of two travelling opposite waves. How would you interpret your result?

2. The state of a particle is represented by the wave function

$$\Psi(x) = A(a^2 - x^2) \quad -a \leq x \leq a$$

and is zero outside of this region.

Determine A from the normalisation condition.

Calculate the expectation values of x and x^2 .

Calculate the expectation values of p and p^2 .

Check that the uncertainty principle holds. What would happen to the momentum if the region halved in size, i.e. if a was reduced by a factor of 2?

3. Show that the probability density $|\Psi(x, t)|^2 dx$ for a free particle (plane wave) is conserved with time.

If, on the other hand, we have an unstable particle, with a lifetime τ (the mean disintegration time), the probability is no longer constant in time but behaves as

$$P(t) = \int_0^L |\Psi(x, t)|^2 dx = e^{-t/\tau},$$

where we assume that the particle exists on the interval $0 \leq x \leq L$.

Suppose that the particle is initially a free particle in the state

$$\Psi(x, 0) = A e^{i(kx - \omega t)}$$

where A is normalisation.

Derive the dependence of A on time if the probability is to behave as described.

What term V should be added in the Hamiltonian

$$H = \frac{-\hbar^2}{2M} \frac{d^2}{dx^2} + V$$

so that we recover the probability decrease above?

Now, suppose that the decay of the particle results in two photons, of identical frequency. Estimate their wavelengths as a function of τ if the whole process of decay is assumed to be energy conserving. You may fully neglect the kinetic part of the energy.

4. If $\psi_1(x, t)$ and $\psi_2(x, t)$ are both solutions to the 1-d time-dependent Schrödinger equation, show that the linear combination $\Psi = c_1\psi_1(x, t) + c_2\psi_2(x, t)$ is also a solution, where c_1 and c_2 are constants.