

1

Quantum mechanics

1.1 Introduction to quantum mechanics

Before attempting to investigate the workings of a tunnelling field-effect transistor, it is essential to be familiar with the concept of tunnelling. Tunnelling is a quantum phenomenon, with no counterpart in the everyday physics one encounters, or the physics that one applies while dealing with devices a few hundred nanometres in length. The initial two chapters will, therefore, help us develop an understanding of quantum phenomena. In this chapter, we will present an introduction to the field of quantum mechanics and the next chapter will discuss the phenomenon of tunnelling in detail.

The chapter begins with a description of a landmark experiment that conclusively proved the wave nature of particles, after which we will study the concept of wavefunctions and how to use Schrodinger's equation to obtain them. A few basic problems will be presented so that the readers may familiarise themselves with basic quantum concepts.

1.1.1 The double slit experiment

There are many experiments that led to the conception of quantum mechanics – blackbody radiation, the Stern Gerlach experiment, the photoelectric effect, the line spectrum, etc. However, for our purposes we will concentrate on one of the landmark experiments, that is the double slit experiment, which demonstrated the fundamental quantum nature (i.e. both wave and particle) of electrons.

Tunnel Field-Effect Transistors (TFET): Modelling and Simulation, First Edition. Jagadesh Kumar Mamidala, Rajat Vishnoi and Pratyush Pandey.

© 2017 John Wiley & Sons, Ltd. Published 2017 by John Wiley & Sons, Ltd.

2 TUNNEL FIELD-EFFECT TRANSISTORS (TFET)

You would have read that only waves can undergo superposition, and not particles. Superposition is the fundamental principle behind the occurrence of interference – therefore, if something exhibits interference, it must have a wave nature. The double slit experiment is famously associated with Thomas Young, who used it for the first time in the early nineteenth century to prove the wave nature of light. Before this experiment was performed, light had been associated with a particle nature (since the times of Newton), and the fact that it underwent interference was conclusive proof of its wave nature.

However, the behaviour of light that led Newton and others to believe that it had a particle nature could not be reconciled with this newly formed wave picture. It took another century of research and experiments to establish a rather astonishing result regarding the behaviour of light – that it displays both particle and wave natures. The particle nature leads to phenomena such as the photoelectric effect and rectilinear propagation of light in ray optics; the wave nature explained the interference and diffraction of light.

While this dual nature (that is both particle and wave natures) of light was being worked out, many people were, independently, studying the behaviour of subatomic particles. Phenomenon like the discrete line spectrum of hydrogen, the observed distribution of blackbody radiation, etc., could not be explained by any established theory. Theoretical physicists were in a quandary. At this point, de Broglie hypothesised that, just like light, particles possess a dual nature as well. When de Broglie made this hypothesis, there was little evidence to support his claim. A few years later, Davisson and Germer experimentally observed that electrons underwent diffraction just as light did. These were landmark moments in the history of physics – de Broglie received the Nobel Prize in physics (the second time it was awarded for a PhD thesis) and, later, so did Davisson and Germer. While the Davisson–Germer experiment was the first to establish the dual nature of matter, the double slit interference experiment is far easier to conceptually grasp and visualise, which is why we will use it to embark on our study of quantum phenomena.

The setup of an electron interferometer used in the double slit experiment is conceptually quite similar to that of a light interferometer (Figure 1.1). A parallel beam of electrons is incident on a screen with two slits. The electrons that pass through the slits impinge upon the optical screen, where their incidence is captured by a visible spot. First, let us think of these electrons as if they were the kind of particles we observe in our daily lives (classical particles) and see how they should behave. All the electrons in the initial beam have the same speed and direction of motion and they are heading towards the screen with two slits. All the electrons that hit this screen are blocked, except for the ones passing right through the slits. These electrons that passed through the slits should have no reason to change either their speed or the direction of their motion. They do not “know” that there

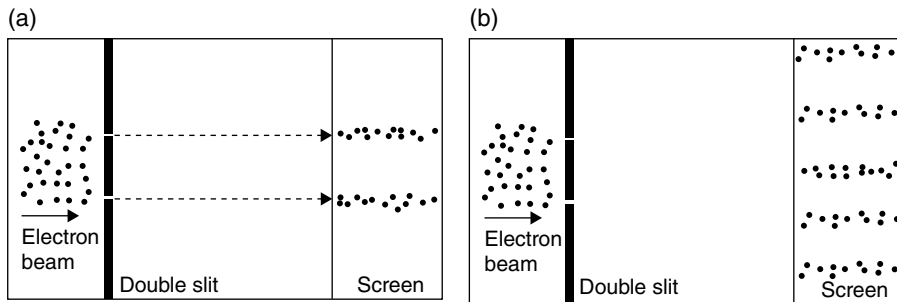


Figure 1.1 (a) Classically predicted electron pattern. It can be seen that interference fringes are experimentally observed, as opposed to the classically predicted pattern. This establishes the wave-like behaviour of electrons, (b) experimentally observed electron pattern.

was a screen in the first place – they pass through unaffected. They subsequently keep heading straight and hit the final screen as illustrated in Figure 1.1(a). Two narrow bands are formed on the screen, corresponding to the two thin beams of electrons that passed unaffected through the two small slits.

Now let us take a look at what was actually observed in the experiment. There was an interference pattern on the screen, as shown in Figure 1.1(b), a pattern uncannily similar to what is observed when we perform the same experiment with light instead of electrons. At this juncture, you might hypothesise this behaviour to result from some sort of statistical phenomenon due to the large number of electrons. However, the experiment is far from finished, and further strangeness lies ahead.

Let us now adjust the electron source so that instead of a beam of electrons it sends a single electron at a time. This time, we find something even more extraordinary – after a lot of electrons have hit the screen, the same interference pattern builds up as in the case of a beam of many electrons. There is no way this electron “knows” that it has been preceded by, or it will be followed by, another electron. What, then, could be happening? The answer is even more puzzling than the question, and will take you quite a while to come to terms with – *each and every electron is undergoing interference with itself*. This is what leads to the final conclusion that not just aggregates of particles but each and every particle exhibits a wave nature. To make this point clear, let us modify the experiment such that we are able to find out through which slit each electron passes. Independent of *how* we find out which slit each electron passes through, we get *exactly* the same result, that is the interference pattern vanishes and we get the pattern shown in Figure 1.1(a), as predicted by classical mechanics. Think about this very carefully, because this

point merits serious investigation. For a wave to show interference, there need to be two sources – the two slits in this case. Thus, for a single electron to show interference, *it must be passing through both slits*. However, this is not possible! At the very least, we cannot imagine such a situation. It is only reasonable to assume that the electron either goes through one slit or the other, but the moment we impose such a restriction on the electron, we are thinking of it as a classical particle. By just *knowing* which slit the electron is going through, and thereby imposing the condition that it will pass through either one slit or the other, we are restricting it to behave like a classical particle. While the mathematical foundations will be laid later in this chapter, for now the reader should try and grasp the underlying concept – the quantum electron passes through *both* the slits; it is a *superposition* of these two states (corresponding to passing through the upper or lower slit). You may think that the electron *actually* passes through either of the two slits and due to limitations of our experimental techniques, we do not know which slit it passes through. This is not the case – the electron is indeed passing through both the slits. This counterintuitive phenomenon is at the very root of quantum mechanics and it will take some time for us to be familiar with this kind of approach. You *cannot* ask of the *quantum* electron (or any general quantum particle), “Which slit does it pass through?” The question in itself is wrong. It passes through both. It should be noted that this wave nature of a particle becomes appreciable only at very small sizes, such as a few nanometres.

1.1.2 Basic concepts of quantum mechanics

1.1.2.1 Wavefunctions

The behaviour of classical particles can be fully explained by describing how their position changes with time. This information would be sufficient to give us the trajectory, the velocity, the momentum and the acceleration of the particle. However, what of the quantum particle? Surely, the electron that passed through both slits of the double slit experiment cannot be assigned a precise location. This leads us to the realisation that we need some new method to describe the quantum particle. The rest of this chapter is devoted to formulating a mathematical picture that is able to capture the unusual behaviour of quantum particles.

The search for this new method of description was helped by the knowledge that the quantum behaviour of particles closely resembled the behaviour displayed by waves. Waves of many kinds – electromagnetic waves, sound waves, etc. – had been extensively studied, and all these waves were described by wave equations. These equations described the behaviour of a wave at every point in space, and at all times. For example, in the case of sound waves, the wave equation described the displacement ($\Delta \vec{r}$) of each particle as a function of time:

$$\Delta \vec{r} = \vec{\psi}(x, y, z, t) \quad (1.1)$$

Similarly, for an electromagnetic wave, the wave equations described the electric (\vec{E}) or magnetic (\vec{B}) field at each and every point as a function of time:

$$\vec{E} = \vec{\psi}_E(x, y, z, t) \quad (1.2)$$

$$\vec{B} = \vec{\psi}_B(x, y, z, t) \quad (1.3)$$

Taking the cue from these equations, physicists assigned a similar wave equation to the quantum particle. This equation was called the wavefunction of the quantum particle and was usually denoted by the Greek symbol ψ (psi). Just like in the case of classical waves, this wavefunction contained all the information about the particle – its current state and the variation of its behaviour with time. It is important to note that while the previously described wave equations (1.1) to (1.3) were real functions, the wavefunction of a quantum particle is a complex function.

1.1.2.2 Born interpretation

While the wavefunction-based formulation of quantum mechanics was proposed by Erwin Schrodinger quite early, he was at a loss to ascribe any physical meaning to it. The theory he built up described what sort of mathematical operations one needed to perform on the wavefunction to get information relating to its various properties, such as its position, its momentum, its energy, etc. However, what this wavefunction *itself* meant was a mystery, especially because it was a complex function. Many interpretations were proposed as to the meaning of this wavefunction, but the one that is most widely accepted was proposed by Max Born. It is known as the “Born interpretation of quantum mechanics” and is one of the fundamental principles of quantum mechanics. According to this interpretation, the wavefunction ψ is the “probability amplitude” of the quantum particle, the square of whose magnitude gives us the probability density ρ of finding that particle at any point:

$$\rho = |\psi|^2 = \psi^* \psi \quad (1.4)$$

where ψ^* is the complex conjugate of ψ . Using this interpretation, the probability P of finding the particle in a volume V at any time t would be

$$P(V, t) = \iiint_V \rho \, dx \, dy \, dz \quad (1.5)$$

6 TUNNEL FIELD-EFFECT TRANSISTORS (TFET)

Since the probability of finding the particle in the entire space should always be unity, we can say that

$$\iiint_{-\infty}^{\infty} \psi^* \psi dx dy dz = 1 \quad (1.6)$$

A wavefunction that displays this property is called a “normalised” wavefunction.

It is very important to realise that the probabilistic behaviour that follows from the Born interpretation is different from the probabilistic behaviour encountered in statistical mechanics. For example, consider an ensemble of particles in a chamber each occupying a particular position. This allows us to calculate the probability of finding a particle at any position. If there were only a single classical particle in this chamber, we could always precisely identify its position. However, in quantum mechanics, every single particle is “spread out” in space, and its position is uncertain. Even if there is only a single electron, we cannot say, “The electron is at this particular point”. We can only talk about the probability of finding the electron at any given point once we measure its position. Thus, the Born interpretation provided a physical meaning to the wavefunction that was compatible with the fundamentally probabilistic behaviour of a quantum particle, and gave a mathematical approach to calculate the probability of finding a quantum particle at any region in space.

1.1.2.3 Measurement

Measurement is a fundamental process in our lives, yet it is so much a part of our instincts that we barely pay any attention to it. However, if you think carefully, most of the information you get is by the process of measurement. When you look at a tree, your eyes measure the frequency and amplitude of the incoming electromagnetic waves, giving you information regarding the colour and brightness of the tree. Subsequently, your eyes measure the angular difference between the signals received by the two eyes, and calculations by your brain tell you how far away this tree is. You may hear a bird chirping on this tree – once again, due to your ears measuring the frequency and location of the pressure waves (sound) impinging upon them. Similarly, any information we get about a quantum particle is by the process of measurement – measuring the position, energy, momentum, etc.

However, there is a very fundamental difference between measurement in classical physics and quantum physics. While the state of a classical particle is independent of measurements performed on it, in quantum mechanics, the state of the quantum particle is intricately linked to measurements performed on it. We shall go back to the double slit experiment to illustrate this point. When

we measured which slit the electron passed through, that is when we measured its position, it stopped showing interference. The electron, before measurement, exhibited interference. After we carried out the measurement, it no longer showed interference. This shows that *measurement changed the state of the electron*. In general, measurement changes the state of a quantum particle, and its final state (after measurement) depends both on its initial state and the kind of measurement being performed. Do not be worried if the picture is not completely clear yet – to fully understand the process of measurement, we will have to know about operators and eigenvalues, which we will do in the next two sections.

1.1.2.4 Operators

The Born interpretation told us that we can obtain the probability of finding a quantum particle at any given point if we know its wavefunction. However, the wavefunction contains far more information than this. If you remember, the wavefunction was supposed to contain *all* the information about the quantum particle. How, then, do we extract this information from the wavefunction?

Since the wavefunction is a mathematical function, it is clear that we will be performing certain mathematical operations on it to get the information we desire. This mathematical operation must be different, depending on the specific kind of information – energy, momentum, position, etc. – we need to obtain. This, indeed, is the case.

Corresponding to every physically observable parameter (also called observables) of a quantum particle, such as position, momentum, energy, we have mathematical operators. The operators for certain common observables are listed below in Table 1.1, where i (iota) is the square root of negative unity and \hbar (h-cross or h-bar) is the reduced Planck’s constant.

To understand the use of these operators, let us imagine an experiment where we have a large number of quantum particles with the same wavefunction ψ . We wish to measure a particular observable, the mathematical operator corresponding to which is O . The outcome of each measurement is o . As the behaviour of

Table 1.1 Quantum mechanical operators corresponding to physical observables.

Observable	Operator
Position (x)	x
Momentum (\vec{p})	$-i\hbar\vec{\nabla}$
Energy (E)	$i\hbar\frac{\partial}{\partial t}$

quantum particles is probabilistic, measuring O for every particle will give a different outcome o . Looking back to our example of the double slit experiment, all the incoming electrons were exactly similar. However, when we start measuring which slit they pass through, sometimes we find that an electron passes through the upper slit and at other times through the lower slit. We can, therefore, only discuss the expectation value $\langle o \rangle$ after taking an average of all the measurements. This expectation value of the observable o is given as

$$\langle o \rangle = \frac{\int \int \int_{-\infty}^{\infty} \psi^* O \psi \, dx \, dy \, dz}{\int \int \int_{-\infty}^{\infty} \psi^* \psi \, dx \, dy \, dz} \quad (1.7)$$

The above equation tells us about the expectation value when we perform a large number of measurements, all on particles with the same wavefunction ψ . However, if we have only one particle, it would be useful to know the probability of obtaining a particular result. For us to know this, we must find the eigenfunctions of the operator in question.

1.1.2.5 Eigenfunctions

Let us recollect from the section on measurement (Section 1.1.2.3) that the state of a quantum particle changes upon measurement, and the final state is dependent on both the initial state and the kind of measurement being performed. However, there are certain very special states corresponding to every observable that do not change when it is measured. These special states are the eigenfunctions of that observable. If, for an operator O , the wavefunction ψ_o behaves as

$$O\psi_o = \lambda\psi_o \quad (1.8)$$

where λ is a constant, then ψ_o is an eigenfunction (also referred to as an eigenstate or an eigenvector) of the operator O and λ is the corresponding eigenvalue. Suppose that we measure the observable corresponding to the operator O on a particle having the wavefunction ψ_o . We will find the value of this observable to be λ . This can be proven by substituting the value of $O\psi_o$ from Equation (1.8) into Equation (1.7) that gave us the expectation value corresponding to any operator. Moreover, the wavefunction ψ_o will remain unchanged. Therefore, for a particle whose wavefunction is an eigenfunction of an observable, we can, with absolute certainty, state the result of measurement. To understand this, let us consider the energy operator (Table 1.1) as an example. Let us assume ψ_{E_i} ($i = 0, 1, 2, \dots$) to be the eigenfunctions of the energy operator, having eigenvalues E_i :

$$i\hbar \frac{\partial \psi_{E_i}}{\partial t} = E_i \psi_{E_i} \quad (1.9)$$

If we take a particle with wavefunction ψ_{E_i} , we *know* that its energy is E_i . There is no probability involved in this.

Furthermore, even if we have a wavefunction that is not an eigenfunction of the operator in question, the result of every measurement can *only* be one of the eigenvalues of the operator. Let us again take the energy operator as an example. Suppose that we measure the energy of a particle having a wavefunction Ψ that is *not* one of the eigenfunctions ψ_{E_i} of the operator. The result will *always* be one of the eigenvalues E_i . Note that every measurement will result in a *different* energy being observed each time. You will now say that once you have measured the energy, and it is found to be a particular E_i , you *know* the energy of the particle to be E_i . However, it was stated earlier in this section that we can only know (with absolute certainty) the energy of the eigenfunctions of an observable. Yet Ψ is not an eigenfunction of the energy operator. What happens is that, after measurement, the wavefunction Ψ “collapses” into the wavefunction ψ_{E_i} corresponding to the observed energy E_i . Remember that measurement changes the state of a quantum particle. Now we can say that *measuring an observable leads us to observe one of the eigenvalues of that observable, and the state of the quantum particle being measured changes to the corresponding eigenfunction.*

We now face the problem of finding the probability of this “collapse” into a particular eigenfunction. Linear algebra provides us with a very handy solution to this problem. Any general wavefunction can be written in terms of the eigenfunctions of an operator. Let us clarify this point. Every operator has a set of eigenfunctions. If we use a linear combination of all these eigenfunctions, we get a set of states that includes every possible state that the quantum particle can have. That is, every wavefunction can be decomposed into a linear superposition of the eigenfunctions of any given operator. Let us once again go back to the energy operator and its eigenfunctions that we discussed in Equation (1.9). *Any* general wavefunction Ψ can be written in terms of the eigenfunctions ψ_{E_i} of the energy operator as

$$\Psi = \sum a_i \psi_{E_i} \quad (1.10)$$

where a_i are coefficients corresponding to every wavefunction ψ_{E_i} and are complex numbers.

Unlike in the case of the eigenfunctions ψ_{E_i} , we cannot discuss the energy of this general particle as having wavefunction Ψ . It is a linear superposition of states ψ_{E_i} of different energies E_i . When the energy of this particle is measured, one obtains any one of the energies E_i , and the particle is found to be in the state ψ_{E_i} after the measurement. However, we cannot say that the particle had energy E_i because the measurement may very well have led to the observation of a different energy E_j . Now the state of the particle changes after measurement from

Ψ to ψ_{E_i} . The probability $P(\psi_{E_i})$ that the wavefunction Ψ collapses into a particular eigenfunction ψ_{E_i} can be written as

$$P(\psi_{E_i}) = |a_i|^2 \quad (1.11)$$

where a_i is the coefficient corresponding the eigenfunction ψ_{E_i} in the linear superposition shown in Equation (1.10).

1.1.3 Schrodinger's equation

1.1.3.1 Formulation of the equation

We have now understood what wavefunctions mean and how they behave when measured, yet we do not know how to find them for a particular physical situation, like an electron in a hydrogen atom. There must be some equations that have to be solved to give us these wavefunctions. Just as Maxwell's equations (when solved under an appropriate set of boundary conditions) give the equations for electromagnetic waves, an equation is needed that can be used to find the wavefunction of a quantum particle. This equation is called Schrodinger's equation. It is a quantum formulation of the statement that

$$\text{Total energy} = \text{kinetic energy} + \text{potential energy} \quad (1.12)$$

By using the operators listed in Section 1.1.2.4 (Table 1.1), we can write:

$$\text{Kinetic energy} = \frac{p^2}{2m} = -\frac{\hbar^2}{2m} \nabla^2 \quad (1.13a)$$

$$\text{Potential energy} = V(\vec{r}, t) \quad (1.13b)$$

$$\text{Total energy} = i\hbar \frac{\partial}{\partial t} \quad (1.13c)$$

which, when substituted into Equation (1.12), gives Schrodinger's equation:

$$-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}, t) = i\hbar \frac{\partial}{\partial t} \quad (1.14)$$

The above equation is in the form of operators of the individual energies. It needs to be operated upon the wavefunction ψ , giving the final form of the equation as

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = i\hbar \frac{\partial \psi}{\partial t} \quad (1.15)$$

The above equation is a partial differential equation, which has to be solved for ψ . The form of the potential $V(\vec{r}, t)$ and the boundary conditions will be different for different physical problems (e.g. a particle confined in a one-dimensional well, the tunnelling problem, the hydrogen atom, etc.), thus leading to different wavefunctions.

In Equation (1.15), we have introduced the time-dependent form of Schrodinger's equation. However, in most cases, we would be solving for energy eigenfunctions, which are stationary states and do not change with time. Therefore, the right-hand side of Equation (1.15) changes to $E\psi$, giving

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \tag{1.16}$$

This is the time-independent form of Schrodinger's equation, and it will be the building block for solving most elementary and slightly complex quantum problems. Additionally, most of the problems that are dealt with in this text are one dimensional. In this case, the time-independent Schrodinger equation (1.16) further simplifies to

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi \tag{1.17}$$

Using Schrodinger's equation, you can get some very important mathematical conditions that every wavefunction must obey [1]. These are:

1. The wavefunction must be continuous at each point in space.
2. The first derivative of the wavefunction must be continuous at each point in space, unless the potential V at the boundary in question is infinite.

1.1.3.2 Probability current

Our final aim is to model tunnel field-effect transistors (TFETs) for predicting their electric currents. We must keep this perspective in mind when we look at the quantum mechanical techniques that we are discussing. We know that electric current is a measure of the rate of flow of charge. These charges are either electrons or holes and their behaviour is best predicted by quantum mechanics. Therefore, we need to find a link between the electric current and the quantum mechanical behaviour of charge carriers.

Let us consider a single electron present inside a conducting wire. If we were to study the behaviour of this electron purely in terms of classical physics, we could find its position and velocity, and use this information to calculate the current in

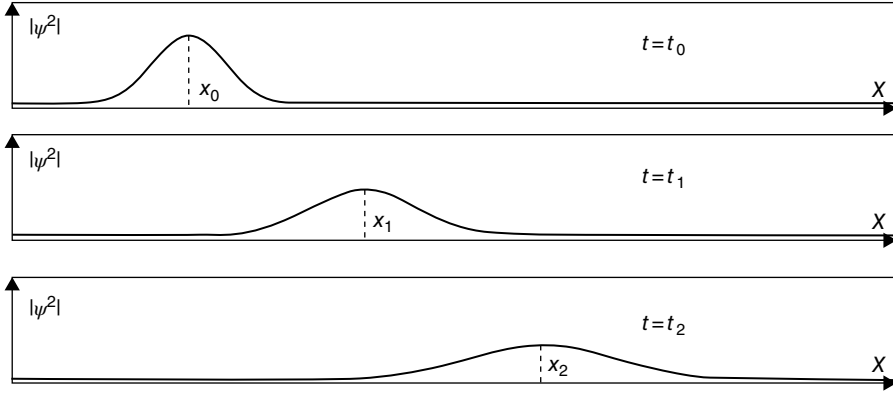


Figure 1.2 Probability density of a quantum particle moving from left to right, plotted at different points of time ($t_2 > t_1 > t_0$).

the wire. However, for an electron obeying the laws of quantum mechanics, we cannot specify its position – we can only find the probability of its presence at any point. From this point of view, what happens when an electron moves in a particular direction? The probability density $|\psi|^2$ of a quantum particle moving from left to right is plotted at various points of time in Figure 1.2. In terms of quantum mechanics, we might say that the probability of finding this particle is changing. In technical terms, there is now a probability current, which is the rate of flow of the probability of the quantum particle's presence. To calculate the electric current resulting from the flow of quantum particles, we need to find this probability current.

We know that the differential form of the continuity equation for charge is

$$\vec{\nabla} \cdot \vec{J} = -\frac{\partial \rho}{\partial t} \quad (1.18)$$

where \vec{J} is the current density and ρ is the charge density. In the case of a quantum particle, the same continuity equation holds, but with \vec{J} being the probability current and $\rho = \psi^* \psi$ being the probability density. We can use the left-hand side of the time-independent Schrodinger Equation (1.16) to give us the values of ψ and ψ^* . When these values of ψ and ψ^* are substituted in Equation (1.18), we can write the probability current \vec{J} as [1]

$$\vec{J} = \frac{i\hbar}{2m} \left(\psi \vec{\nabla} \psi^* - \psi^* \vec{\nabla} \psi \right) \quad (1.19)$$

1.2 Basic quantum physics problems

In this section, we will familiarise ourselves with certain basic problems of quantum mechanics. This would enable us to appreciate the concepts introduced that act as a bridge between the theoretical framework and the practical problem of tunnelling.

1.2.1 Free particle

The simplest quantum particle is a free particle – a particle that is completely unconstrained by any external potentials. This free particle is a basic building block for studying more complex quantum mechanical problems, just as we use the sine wave as a basic building block for representing complicated waves (by using Fourier series).

1.2.1.1 Wavefunction

As a free particle is unconstrained by any external potential, the term $V(\vec{r})$ in the time-independent Schrodinger equation (1.16) is zero at all points in space. Therefore, for a free particle, we can write

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E\psi \quad (1.20)$$

The solutions of Equation (1.20) are

$$\psi_{\pm} = Ae^{\pm ikx} \quad (1.21)$$

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad (1.22)$$

where k is referred to as the wave vector of the free particle and A is a complex constant. The general solution would be a linear superposition of ψ_+ and ψ_- :

$$\Psi = A'e^{ikx} + B'e^{-ikx} \quad (1.23)$$

where A' and B' are complex constants.

We find that there are two eigenvectors ψ_+ and ψ_- corresponding to a particular energy E – one with a plus sign and another with a minus sign in the exponential. Let us see what happens when we apply the momentum operator p_x (Table 1.1) to these wavefunctions:

$$p_x \psi_{\pm} = -i\hbar \frac{\partial \psi_{\pm}}{\partial x} = \pm \hbar k \psi_{\pm} \quad (1.24)$$

We find that the wavefunctions ψ_{\pm} are eigenfunctions of the momentum operator, with eigenvalues $\pm \hbar k$. This means that the particle corresponding to ψ_{+} has momentum in the positive x -direction, while ψ_{-} has momentum in the negative x -direction. Thus, ψ_{+} is a free particle moving forward with a momentum $\hbar k$ and ψ_{-} is a free particle moving backward with a momentum $\hbar k$.

Another important observation here is that the probability ρ (Equation (1.4)) of finding the particle at any location is uniform – the particle is fully dispersed in space. Therefore, we have

$$\rho = \psi^* \psi = |A|^2 \quad (1.25)$$

The fact that the particle is fully dispersed in space follows from Heisenberg's uncertainty principle. The momentum of either of the two wavefunctions ψ_{\pm} is known with complete certainty. Therefore, the uncertainty in the position of the particle is infinite.

1.2.1.2 Probability current

Using Equation (1.19), we can write the probability current for a free particle propagating along the positive x -axis as

$$J = \frac{\hbar k}{m} |A|^2 \quad (1.26)$$

Since $|A|^2$ is the probability density (Equation (1.25)) and $\hbar k$ is the momentum (Equation (1.24)) of the particle, the above equation can be rearranged to give

$$J = \frac{p}{m} \rho = v \rho \quad (1.27)$$

where $v = p/m$ is the velocity of the particle. We can now write the electric current density j as

$$j = qJ = qv\rho \quad (1.28)$$

In this section, we have discussed the behaviour of a completely unconstrained “free” particle. Let us now investigate the behaviour of a quantum particle that is bound to remain between two points – a particle in a box.

1.2.2 Particle in a one-dimensional box

The next problem we will deal with is a particle confined to move along an axis between two points. It cannot go beyond those two specified points. It is, therefore, referred to as a particle in a one-dimensional box. It is confined to remain within the

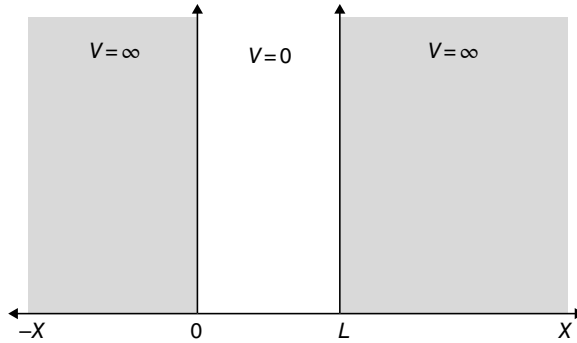


Figure 1.3 Particle in a one-dimensional box.

“box” (also referred to as an infinite potential well) with edges at $x = 0$ and $x = L$, as shown in Figure 1.3. The particle is completely free to move within these limits, implying that there is no external potential (i.e. $V = 0$) in the region $x \in (0, L)$. Outside these limits, there is an infinite potential barrier (i.e. $V = \infty$). Physically, this form of external potential ensures that the particle stays within the “box”. Since Schrodinger’s equation assumes different forms in different regions, its solution – the wavefunction – will also have different forms in different regions. We will, therefore, find the wavefunction separately for each region and then join these separate solutions to give the final solution. It is important to be familiar with this procedure since it will be used in this book, not just for solving Schrodinger’s equation but as a very important tool in the modelling of TFETs.

Now we know that the particle cannot be present in the regions $x \leq 0$ and $x \geq L$. Thus, in these regions, the probability of finding the electron is zero:

$$\rho = \psi^* \psi = 0 \tag{1.29}$$

This is only possible if $\psi = 0$ in these regions.

Let us now find the solution of Schrodinger’s equation within the box, where the form of Schrodinger’s equation is the same as that of the free particle (Equation (1.20)). However, we need to keep in mind the restrictions applied to a wavefunction, stated at the end of Section 1.1.3.1. The first condition is that the wavefunction must be continuous. Since the wavefunction is zero in the regions $x \leq 0$ and $x \geq L$, we get the following boundary conditions at the edges of our box:

$$\psi(0) = 0 \tag{1.30a}$$

$$\psi(L) = 0 \tag{1.30b}$$

The general solution of Equation (1.20) shown in Equation (1.23) can be written in the form of trigonometric functions as

$$\psi(x) = A \sin kx + B \cos kx \quad (1.31)$$

where A and B are complex constants and the wave vector k is

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad (1.32)$$

Applying the boundary conditions (1.30), we get

$$B = 0 \quad (1.33)$$

$$k_n L = n\pi \quad (1.34)$$

The subscript n has been added to k because Equation (1.34) shows that k is quantised and takes only certain fixed values. Using Equation (1.34) in (1.32) gives the possible values of energy E_n that the particle can have:

$$E_n = \frac{n^2 \hbar^2}{8mL^2} \quad (1.35)$$

and the wavefunction ψ_n corresponding the energy E_n is

$$\psi_n = A \sin \frac{n\pi x}{L} \quad (1.36)$$

The constant A is given by the normalisation condition (1.6):

$$A = \frac{1}{\sqrt{2L}} \quad (1.37)$$

The above wavefunctions (1.36) correspond to energy eigenstates, as we have solved the time-independent Schrodinger equation. A general wavefunction for a particle in a one-dimensional box would, therefore, be a superposition of these energy eigenstates:

$$\Psi = \sum a_n \psi_n \quad (1.38)$$

where a_n is the coefficient corresponding to the wavefunction ψ_n and is a complex number.

If we plot the wavefunctions of energy eigenstates for a particle in a one-dimensional box (Figure 1.4), we observe the same pattern as standing waves in a string.

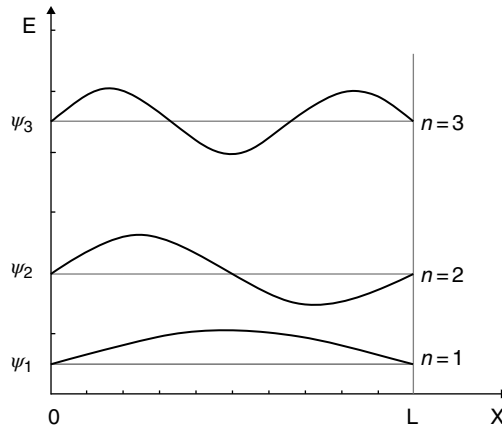


Figure 1.4 Energy eigenfunctions of a particle in a one-dimensional box.

Going back to classical physics, remember that a standing wave can be written as a superposition of two travelling waves. Therefore, we can represent the energy eigenstate of a particle in a one-dimensional box as a superposition of two free particle wavefunctions going in opposite directions:

$$\psi_n = \frac{1}{\sqrt{2L}} \sin k_n x = \frac{i}{\sqrt{2L}} (e^{-ik_n x} - e^{ik_n x}) \quad (1.39)$$

The first and second exponential terms in Equation (1.39) represent a free particle travelling in the negative and positive x -directions with momentum $\hbar k_n$, respectively. Therefore, if we take the expectation value (1.7) of their superposition, these momenta cancel each other and the expectation value of the momentum for ψ_n is zero.

Reference

- [1] D. J. Griffiths, *Introduction to Quantum Mechanics*, 2nd edn, Pearson Education, 2005.