

Chapter 3

The Wave Function

On the basis of the assumption that the de Broglie relations give the frequency and wavelength of some kind of wave to be associated with a particle, plus the assumption that it makes sense to add together waves of different frequencies, it is possible to learn a considerable amount about these waves without actually knowing beforehand what they represent. But studying different examples does provide some insight into what the ultimate interpretation is, the so-called Born interpretation, which is that these waves are ‘probability waves’ in the sense that the amplitude squared of the waves gives the probability of observing (or detecting, or finding – a number of different terms are used) the particle in some region in space. Hand-in-hand with this interpretation is the Heisenberg uncertainty principle which, historically, preceded the formulation of the probability interpretation. From this principle, it is possible to obtain a number of fundamental results even before the full machinery of wave mechanics is in place.

In this Chapter, some of the consequences of de Broglie’s hypothesis of associating waves with particles are explored, leading to the concept of the wave function, and its probability interpretation.

3.1 The Harmonic Wave Function

On the basis of de Broglie’s hypothesis, there is associated with a particle of energy E and momentum p , a wave of frequency f and wavelength λ given by the de Broglie relations Eq. (2.9). It more usual to work in terms of the angular frequency $\omega = 2\pi f$ and wave number $k = 2\pi/\lambda$ so that the de Broglie relations become

$$\omega = E/\hbar \quad k = p/\hbar. \quad (3.1)$$

With this in mind, and making use of what we already know about what the mathematical form is for a wave, we are in a position to make a reasonable guess at a mathematical expression for the wave associated with the particle. The possibilities include (in one dimension)

$$\Psi(x, t) = A \sin(kx - \omega t), \quad A \cos(kx - \omega t), \quad Ae^{i(kx - \omega t)}, \quad \dots \quad (3.2)$$

At this stage, we have no idea what the quantity $\Psi(x, t)$ represents physically. It is given the name the *wave function*, and in this particular case we will use the term harmonic wave function to describe any trigonometric wave function of the kind listed above. As

we will see later, in general it can take much more complicated forms than a simple single frequency wave, and is almost always a complex valued function.

In order to understand what information may be contained in the wave function, which will lead us toward gaining a physical understanding of what it might represent, we will turn things around briefly and look at what we can learn about the properties of a particle if we know what its wave function is.

First, given that the wave has frequency ω and wave number k , then it is straightforward to calculate the phase velocity v_p of the wave:

$$v_p = \frac{\omega}{k} = \frac{\hbar\omega}{\hbar k} = \frac{E}{p} = \frac{\frac{1}{2}mv^2}{mv} = \frac{1}{2}v. \quad (3.3)$$

Thus, given the frequency and wave number of a wave function, we can determine the speed of the particle from the phase velocity of its wave function, $v = 2v_p$. We could also try to learn from the wave function the position of the particle. However, the wave function above tells us nothing about where the particle is to be found in space. We can make this statement because this wave function is the same everywhere i.e. there is nothing whatsoever to distinguish Ψ at one point in space from any other, see Fig. (3.1).

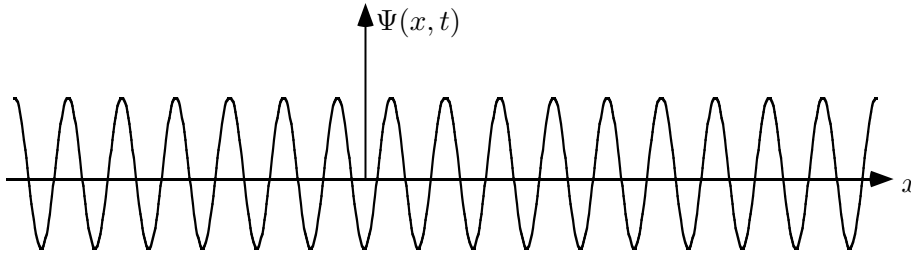


Figure 3.1: A wave function of constant amplitude and wavelength. The wave is the same everywhere and so there is no distinguishing feature that could indicate one possible position of the particle from any other.

Thus, this particular wave function gives no information on the whereabouts of the particle with which it is associated. So from a harmonic wave function it is possible to learn how fast a particle is moving, but not what the position is of the particle.

3.2 Wave Packets

From what was said above, a wave function constant throughout all space cannot give information on the position of the particle which suggests that a wave function that did not have the same amplitude throughout all space might be a candidate for a giving such information. In fact, since what we mean by a particle is a physical object that is confined to a highly localized region in space, ideally a point, it would be intuitively appealing to be able to devise a wave function that is zero or nearly so everywhere in space except for one localized region. It is in fact possible to construct, from the harmonic wave functions, a wave function which has this property. To show how this is done, we first consider what happens if we combine together two harmonic waves of very close frequency. The result is well-known: a ‘beat note’ is produced, i.e. periodically in space the waves add together in phase to produce a local maximum, while midway in between the waves will be totally out of phase and hence will destructively interfere. Each localized maximum is known

as a wave packet, so what is produced is a series of wave packets. Now suppose we add together a large number of harmonic waves with wave numbers k_1, k_2, k_3, \dots all lying in the range:

$$\bar{k} - \Delta k < k_n < \bar{k} + \Delta k \quad (3.4)$$

around a mean value \bar{k} , i.e.

$$\begin{aligned} \Psi(x, t) &= A(k_1) \cos(k_1 x - \omega_1 t) + A(k_2) \cos(k_2 x - \omega_2 t) + \dots \\ &= \sum_n A(k_n) \cos(k_n x - \omega_n t) \end{aligned} \quad (3.5)$$

where $A(k)$ is a function peaked about the mean value \bar{k} with a full width at half maximum of $2\Delta k$. (There is no significance to be attached to the use of cos functions here – the idea is simply to illustrate a point. We could equally well have used a sin function or indeed a complex exponential.) What is found is that in the limit in which the sum becomes an integral:

$$\Psi(x, t) = \int_{-\infty}^{+\infty} A(k) \cos(kx - \omega t) dk \quad (3.6)$$

all the waves interfere constructively to produce only a single beat note (in effect, the ‘beat notes’ or wave packets are infinitely far apart). In other words, the wave function so constructed is found to have essentially zero amplitude everywhere except for a *single* localized region in space, over a region of width $2\Delta x$, i.e. the wave function $\Psi(x, t)$ in this case takes the form of a single wave packet, see Fig. (3.2).

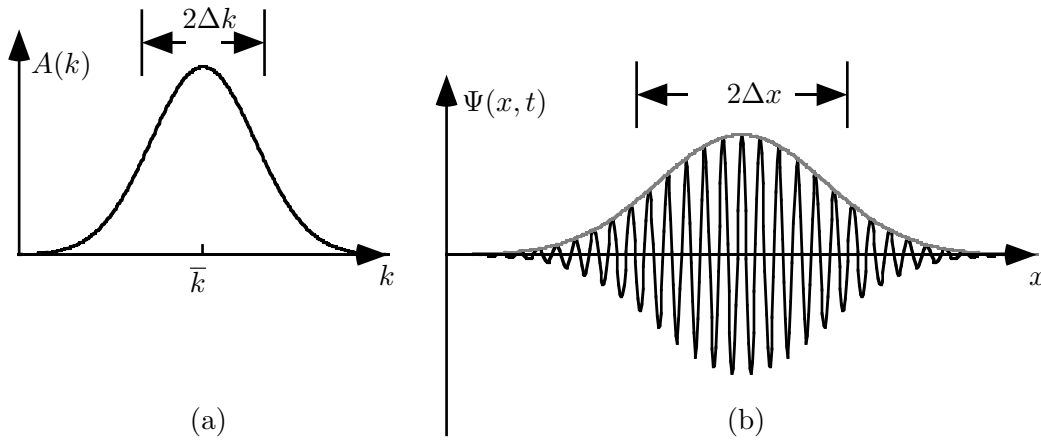


Figure 3.2: (a) The distribution of wave numbers k of harmonic waves contributing to the wave function $\Psi(x, t)$. This distribution is peaked about \bar{k} with a width of $2\Delta k$. (b) The wave packet $\Psi(x, t)$ of width $2\Delta x$ resulting from the addition of the waves with distribution $A(k)$. The oscillatory part of the wave packet (the ‘carrier wave’) has wave number \bar{k} .

This wave packet is clearly particle-like in that its region of significant magnitude is confined to a localized region in space. Moreover, this wave packet is constructed out of a group of waves with an average wave number \bar{k} , and so these waves could be associated in some sense with a particle of momentum $\bar{p} = \hbar\bar{k}$. If this were true, then the wave packet would be expected to move with a velocity of \bar{p}/m . This is in fact found to be the case, as the following calculation shows.

Because a wave packet is made up of individual waves which themselves are moving, though not with the same speed, the wave packet itself will move (and spread as well).

The speed with which the wave packet moves is given by its group velocity v_g :

$$v_g = \left(\frac{d\omega}{dk} \right)_{k=\bar{k}}. \quad (3.7)$$

This is the speed of the maximum of the wave packet i.e. it is the speed of the point on the wave packet where all the waves are in phase. Calculating the group velocity requires determining the relationship between ω to k , known as a dispersion relation. This dispersion relation is obtained from

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m}. \quad (3.8)$$

Substituting in the de Broglie relations Eq. (2.9) gives

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} \quad (3.9)$$

from which follows the dispersion relation

$$\omega = \frac{\hbar k^2}{2m}. \quad (3.10)$$

The group velocity of the wave packet is then

$$v_g = \left(\frac{d\omega}{dk} \right)_{k=\bar{k}} = \frac{\hbar\bar{k}}{m}. \quad (3.11)$$

Substituting $\bar{p} = \hbar\bar{k}$, this becomes $v_g = \bar{p}/m$. i.e. the packet is indeed moving with the velocity of a particle of momentum \bar{p} , as suspected.

This is a result of some significance, i.e. we have constructed a wave function of the form of a wave packet which is particle-like in nature. But unfortunately this is done at a cost. We had to combine together harmonic wave functions $\cos(kx - \omega t)$ with a range of k values $2\Delta k$ to produce a wave packet which has a spread in space of size $2\Delta x$. The two ranges of k and x are not unrelated – their connection is embodied in an important result known as the Heisenberg Uncertainty Principle.

3.3 The Heisenberg Uncertainty Principle

The wave packet constructed in the previous section obviously has properties that are reminiscent of a particle, but it is not entirely particle-like – the wave function is non-zero over a region in space of size $2\Delta x$. In the absence of any better way of relating the wave function to the position of the atom, it is intuitively appealing to suppose that where $\Psi(x, t)$ has its greatest amplitude is where the particle is most likely to be found, i.e. the particle is to be found somewhere in a region of size $2\Delta x$. More than that, however, we have seen that to construct this wavepacket, harmonic waves having k values in the range $(\bar{k} - \Delta k, \bar{k} + \Delta k)$ were adding together. These ranges Δx and Δk are related by the bandwidth theorem, which applies when adding together harmonic waves, which tell us that

$$\Delta x \Delta k \gtrsim 1. \quad (3.12)$$

Using $p = \hbar k$, we have $\Delta p = \hbar \Delta k$ so that

$$\Delta x \Delta p \gtrsim \hbar. \quad (3.13)$$

[A more rigorous derivation, based on a more precise definition of Δx and Δk leads to

$$\Delta x \Delta p \geq \frac{1}{2} \hbar \quad (3.14)$$

though we will mostly use the result Eq. (3.13).]

A closer look at this result is warranted. A wave packet that has a significant amplitude within a range $2\Delta x$ was constructed from harmonic wave functions which represent a range of momenta $\bar{p} - \Delta p$ to $\bar{p} + \Delta p$. We can say then say that the particle is likely to be found somewhere in the region $2\Delta x$, and given that wave functions representing a range of possible momenta were used to form this wave packet, we could also say that the momentum of the particle will have a value in the range $\bar{p} - \Delta p$ to $\bar{p} + \Delta p$. The quantities Δx and Δp are known as *uncertainties* for reasons that will become increasingly apparent, and the relation above Eq. (3.14) is known as the Heisenberg uncertainty relation for position and momentum. It tells us that we cannot determine, from knowledge of the wave function alone, the exact position and momentum of a particle at the same time. In the extreme case that $\Delta x = 0$, then the position uncertainty is zero, but Eq. (3.14) tells us that the uncertainty on the momentum is infinite, i.e. the momentum is entirely unknown. A similar statement applies if $\Delta p = 0$.

This conclusion flies in the face of our experience in the macroscopic world, namely that there is no problem, in principle, with knowing the position and momentum of a particle. Thus, we could then argue that our wave function idea is all very interesting, but that it is incomplete, that there is information missing. It is tempting to think that perhaps there is a prescription still to be found that will enable us to find the position and the momentum of the particle from the wave function, which amounts to saying that the wave function by itself does not give complete information on the state of the particle. Einstein fought vigorously for this position in a famous series of exchanges with Neils Bohr and others, i.e. that the wave function was not a complete description of ‘reality’, and that there was somewhere, in some sense, a repository of missing information that will remove the incompleteness of the wave function – so-called ‘hidden variables’. Unfortunately (for those who hold to his point of view) evidence has mounted, particularly in the past few decades, that the wave function (or its analogues in the more general formulation of quantum mechanics) does indeed represent the full picture – the most that can ever be known about a particle (or more generally any system) is what can be learned from its wave function. This means that the difficulty encountered above concerning not being able, in general, to pinpoint either the position or the momentum of a particle from knowledge of its wave function is not a reflection of any inadequacy on the part of experimentalists trying to measure these quantities, but is an irreducible property of the natural world. It is only at the macroscopic level where the uncertainties mentioned above become so small as to be experimentally unmeasurable that the effects of the uncertainty principle have no apparent effect.

The limitations implied by the uncertainty relation as compared to classical physics may give the impression that something has been lost, that the uncertainty principle is some sort of roadblock to obtaining complete information about a system. It is true that it seems that there is information about the physical world that is hidden from us,¹ at least on the basis of our classical physics expectations, which may then be seen as a cause for concern because of its implications that we cannot, even in principle, make exact predictions about the behaviour of any physical system. However, the view can be taken that the opposite is true, that the uncertainty principle is an indicator of greater freedom. In a sense, the uncertainty principle now makes it possible for a physical system to have a much broader

¹Or more alarming, the information may not even be there in the first place!

range of possible physical properties consistent with the smaller amount of information that is available about its properties. This leads to a greater richness in the properties of the physical world than could ever be found within classical physics.

3.3.1 The Size of an Atom

One important application of the uncertainty relation is to do with determining the size of atoms. Recall that classically atoms should not exist: the electrons must spiral into the nucleus, radiating away their excess energy as they do. However, if this were the case, then the situation would be arrived at in which the position and the momentum of the electrons would be known: stationary, and at the position of the nucleus. This is in conflict with the uncertainty principle, so it must be the case that the electron can spiral inward no further than an amount that is consistent with the uncertainty principle.

To see what the uncertainty principle does tell us about the behaviour of the electrons in an atom, consider as the simplest example a hydrogen atom. Here the electron is trapped in the Coulomb potential well due to the positive nucleus. We can then argue that if the electron cannot have a precisely defined position, then we can at least suppose that it is confined to a spherical (by symmetry) shell of radius a . Thus, the uncertainty Δx in x will be a , and similarly for the y and z positions. But, with the electron moving within this region, the x component of momentum, p_x , will, also by symmetry, swing between two equal and opposite values, p and $-p$ say, and hence p_x will have an uncertainty of $\Delta p_x \approx 2p$. By appealing to symmetry once again, the y and z components of momentum can be seen to have the same uncertainty.

By the uncertainty principle $\Delta p_x \Delta x \approx \hbar$, (and similarly for the other two components), the uncertainty in the x component of momentum will then be $\Delta p_x \approx \hbar/a$, and hence $p \approx \hbar/a$. The kinetic energy of the particle will then be

$$T = \frac{p^2}{2m} \approx \frac{\hbar^2}{2ma^2} \quad (3.15)$$

so including the Coulomb potential energy, the total energy of the particle will be

$$E \approx \frac{\hbar^2}{2ma^2} - \frac{e^2}{4\pi\epsilon_0 a}. \quad (3.16)$$

The lowest possible energy of the atom is then obtained by simple differential calculus. Thus, taking the derivative of E with respect to a and equating this to zero and solving for a gives

$$a \approx \frac{4\pi\epsilon_0 \hbar^2}{me^2} \approx 0.5 \text{ nm} \quad (3.17)$$

and the minimum energy

$$E_{\min} \approx -\frac{1}{2} \frac{me^4}{(4\pi\epsilon_0)^2 \hbar^2} \quad (3.18)$$

$$\approx -13.6 \text{ eV}. \quad (3.19)$$

The above values for atomic size and atomic energies are what are observed in practice. The uncertainty relation has yielded considerable information on atomic structure without knowing all that much about what a wave function is supposed to represent!

The exactness of the above result is somewhat fortuitous, but the principle is nevertheless correct: the uncertainty principle demands that there be a minimum size to an atom. If

a hydrogen atom has an energy above this minimum, it is free to radiate away energy by emission of electromagnetic energy (light) until it reaches this minimum. Beyond that, it cannot radiate any more energy. Classical EM theory says that it should, but it does not. The conclusion is that there must also be something amiss with classical EM theory, which in fact turns out to be the case: the EM field too must be treated quantum mechanically. When this is done, there is consistency between the demands of quantum EM theory and the quantum structure of atoms – an atom in its lowest energy level (the ground state) cannot, in fact, radiate – the ground state of an atom is stable.

Another important situation for which the uncertainty principle gives a surprising amount of information is that of the harmonic oscillator.

3.3.2 The Minimum Energy of a Simple Harmonic Oscillator

By using Heisenberg's uncertainty principle in the form $\Delta x \Delta p \approx \hbar$, it is also possible to estimate the lowest possible energy level (ground state) of a simple harmonic oscillator. The simple harmonic oscillator potential is given by

$$U = \frac{1}{2} m \omega^2 x^2 \quad (3.20)$$

where m is the mass of the oscillator and ω is its natural frequency of oscillation. This is a particularly important example as the simple harmonic oscillator potential is found to arise in a wide variety of circumstances such as an electron trapped in a well between two nuclei, or the oscillations of a linear molecule, or indeed in a manner far removed from the image of an oscillator as a mechanical object, the lowest energy of a single mode quantum mechanical electromagnetic field.

We start by assuming that in the lowest energy level, the oscillations of the particle have an amplitude of a , so that the oscillations swing between $-a$ and a . We further assume that the momentum of the particle can vary between p and $-p$. Consequently, we can assign an uncertainty $\Delta x = a$ in the position of the particle, and an uncertainty $\Delta p = p$ in the momentum of the particle. These two uncertainties will be related by the uncertainty relation

$$\Delta x \Delta p \approx \hbar \quad (3.21)$$

from which we conclude that

$$p \approx \hbar/a. \quad (3.22)$$

The total energy of the oscillator is

$$E = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 \quad (3.23)$$

so that roughly, if a is the amplitude of the oscillation, and $p \approx \hbar/a$ is the maximum momentum of the particle then

$$E \approx \frac{1}{2} \left(\frac{1}{2m} \frac{\hbar^2}{a^2} + \frac{1}{2} m \omega^2 a^2 \right) \quad (3.24)$$

where the extra factor of $\frac{1}{2}$ is included to take account of the fact that the kinetic and potential energy terms are each their maximum possible values.

The minimum value of E can be found using differential calculus i.e.

$$\frac{dE}{da} = \frac{1}{2} \left(-\frac{1}{m} \frac{\hbar^2}{a^3} + m \omega^2 a \right) = 0. \quad (3.25)$$

Solving for a gives

$$a^2 = \frac{\hbar}{m\omega}. \quad (3.26)$$

Substituting this into the expression for E then gives for the minimum energy

$$E_{\min} \approx \frac{1}{2}\hbar\omega. \quad (3.27)$$

A more precise quantum mechanical calculation shows that this result is (fortuitously) exactly correct, i.e. the ground state of the harmonic oscillator has a non-zero energy of $\frac{1}{2}\hbar\omega$.

It was Heisenberg's discovery of the uncertainty relation, and various other real and imagined experiments that ultimately lead to a fundamental proposal (by Max Born) concerning the physical meaning of the wave function. We shall arrive at this interpretation by way of the famous two slit interference experiment.