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. (2.11). It is 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

$$\omega = E/\hbar \qquad k = p/\hbar. \tag{3.1}$$

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)

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

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 fact, it turns out that the third possibility listed above is the appropriate wave function to associate with a free particle, but for the present we will work with real wave functions, if only because it gives us the possibility of visualizing their form while discussing their properties.

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In order to gain an understanding of what a wave function might represent, we will turn things around briefly and look at what we can learn about a particle if we know what its wave function is. We are implicitly bypassing here any consideration of whether we can understand a wave function as being a physical wave in the same way that a sound wave, a water wave, or a light wave are physical waves, i.e. waves made of some kind of physical 'stuff'. Instead, we are going to look on a wave function as something that gives us information on the particle it is associated with. To this end, we will suppose that the particle has a wave function given by $\Psi(x,t) = A\cos(kx - \omega t)$. Then, given that the wave has angular frequency ω and wave number k, it is straightforward to calculate the wave velocity, that is, the phase velocity v_p of the wave, which is just the velocity of the wave crests. This phase velocity is given by

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

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 more or less the same everywhere. For sure, the wave function is not *exactly* the same everywhere, but any feature that we might decide as being an indicator of the position of the particle, say where the wave function is a maximum, or zero, will not do: the wave function is periodic, so any feature, such as where the wave function vanishes, reoccurs an infinite number of times, and there is no way to distinguish any one of these repetitions from any other, see Fig. (3.1).

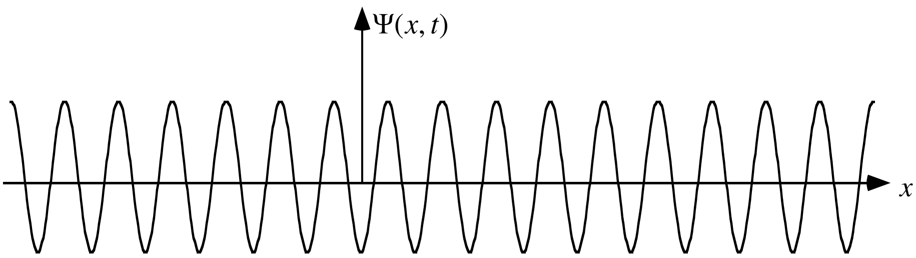

Figure 3.1: A wave function of constant amplitude and wavelength. The wave is the same everywhere and so there is no distinguishing feature that could indicate one possible position of the particle from any other.

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. This 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 whose wave numbers are very close together. 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

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midway in between the waves will be totally out of phase and hence will destructively interfere. This is illustrated in Fig. 3.2(a) where we have added together two waves $\cos(5x) + \cos(5.25x)$.

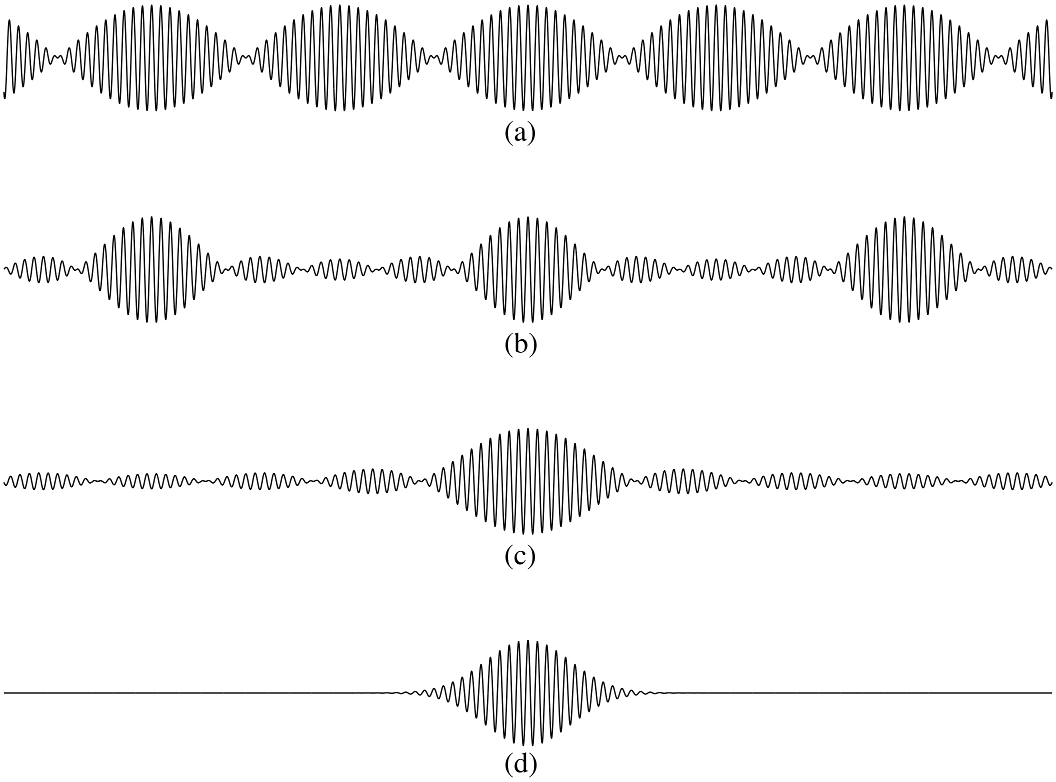

Figure 3.2: (a) Beat notes produced by adding together two cos waves: $\cos(5x) + \cos(5.25x)$.
(b) Combining five cos waves: $\cos(4.75x) + \cos(4.875x) + \cos(5x) + \cos(5.125x) + \cos(5.25x)$.
(c) Combining seven cos waves: $\cos(4.8125x) + \cos(4.875x) + \cos(4.9375x) + \cos(5x) + \cos(5.0625x) + \cos(5.125x) + \cos(5.1875x)$.
(d) An integral over a continuous range of wave numbers produces a single wave packet.

Now suppose we add five such waves together, as in Fig. 3.2(b). The result is that some beats turn out to be much stronger than the others. If we repeat this process by adding seven waves together, but now make them closer in wave number, we get Fig. 3.2(c), we find that most of the beat notes tend to become very small, with the strong beat notes occurring increasingly far apart. Mathematically, what we are doing here is taking a limit of a sum, and turning this sum into an integral. In the limit, we find that there is only one beat note – in effect, all the other beat notes become infinitely far away. This single isolated beat note is usually referred to as a wave packet.

We need to look at this in a little more mathematical detail, so suppose we add together a large number of harmonic waves with wave numbers $k_1, k_2, k_3, \ldots$ all lying in the range:

$$\bar{k} - \Delta k \lesssim k_n \lesssim \bar{k} + \Delta k \tag{3.4}$$

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

$$\begin{aligned}\Psi(x,t) =& A(k_1)\cos(k_1x - \omega_1 t) + A(k_2)\cos(k_2x - \omega_2 t) + \ldots\\ =& \sum_n A(k_n)\cos(k_nx - \omega_n t)\end{aligned} \tag{3.5}$$

where $A(k)$ is a function peaked about the 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:

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

all the waves interfere constructively to produce only a single beat note as illustrated in Fig. 3.2(d) above[1]. The wave function or wave packet 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. (3.3).

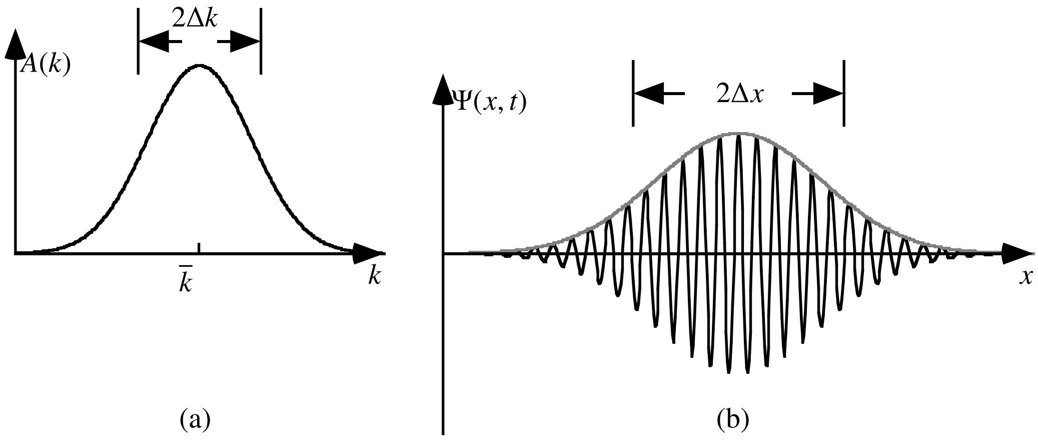

Figure 3.3: (a) The distribution of wave numbers k of harmonic waves contributing to the wave function $\Psi(x,t)$. This distribution is peaked about $\bar{k}$ with a width of $2\Delta k$. (b) The wave packet $\Psi(x,t)$ of width $2\Delta x$ resulting from the addition of the waves with distribution $A(k)$. 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:

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

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

$$E = \tfrac{1}{2}mv^2 = \frac{p^2}{2m}. \tag{3.8}$$

[1]In Fig. 3.2(d), the wave packet is formed from the integral

$$\Psi(x,0) = \frac{1}{4\sqrt{\pi}}\int_{-\infty}^{+\infty} e^{-((k-5)/4)^2}\cos(kx)\,dk.$$

Substituting in the de Broglie relations Eq. (2.11) gives

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} \tag{3.9}$$

from which follows the dispersion relation

$$\omega = \frac{\hbar k^2}{2m}. \tag{3.10}$$

The group velocity of the wave packet is then

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

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

3.3 The Heisenberg Uncertainty Relation

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

$$\Delta x \Delta k \gtrsim 1. \tag{3.12}$$

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

$$\Delta x \Delta p \gtrsim \hbar. \tag{3.13}$$

A closer look at this result is warranted. A wave packet that has a significant amplitude within a region of size $2\Delta x$ was constructed from harmonic wave functions which represent a range of momenta $\overline{p} - \Delta p$ to $\overline{p} + \Delta p$. 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 $\overline{p} - \Delta p$ to $\overline{p} + \Delta p$[2]. The quantities Δx and Δp are known as *uncertainties*, and the relation above Eq. (3.14) is known as the Heisenberg uncertainty relation for position and momentum.

All this is rather abstract. We do not actually 'see' a wave function accompanying its particle, so how are we to know how 'wide' the wave packet is, and hence what the uncertainty in position and momentum might be for a given particle, say an electron orbiting in an atomic nucleus, or the

[2]In fact, we can look on $A(k)$ as a wave function for k or, since $k = p/\hbar$ as effectively a wave function for momentum analogous to $\Psi(x, t)$ being a wave function for position.

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nucleus itself, or an electron in a metal or ...? The answer to this question is intimately linked with what has been suggested by the use above of such phrases as 'where the particle is most likely to be found' and so on, words that are hinting at the fundamental role of randomness as an intrinsic property of quantum systems, and role of probability in providing a meaning for the wave function.

To get a flavour of what is meant here, we can suppose that we have a truly vast number of identical particles, say 2×10^{26}, all prepared in some experiment so that they all have associated with them the same wave packet. For half these particles, we measure their position all at the same time, and for the other half we measure their momentum. What we find is that the results for the position are not all the same: they are spread out randomly around some average value, and the range over which they are spread is most conveniently measured by the usual tool of statistics: the standard deviation. This standard deviation in position turns out to be just the uncertainty Δx we introduced above in a non-rigorous manner. Similarly, the results for the measurement of momentum for the other half are randomly scattered around some average value, and the spread around the average is given by the standard deviation once again. This standard deviation in momentum we identify with the uncertainty Δp introduced above.

With uncertainties defined as standard deviations of random results, it is possible to give a more precise statement of the uncertainty relation, which is:

$$\Delta x \Delta p \geq \tfrac{1}{2}\hbar \tag{3.14}$$

but we will mostly use the result Eq. (3.13). The detailed analysis is left to much later (See Chapter ∞).

The Heisenberg relation has an immediate interpretation. 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 $\Delta p = 0$. In fact, this last possibility is the case for the example of a single harmonic wave function considered in Section 3.1. However, the uncertainty relation does not say that we cannot measure the position and the momentum at the same time. We certainly can, but we have to live with the fact that the results that are obtained will carry with them uncertainty by virtue of the uncertainty relation.

This conclusion that it is impossible for a particle to have zero uncertainty in both position *and* momentum at the same time flies in the face of our intuition, namely our belief that a particle moving through space will at any instant have a definite position and momentum which we can, in principle, measure to arbitrary accuracy. We could then feel quite justified in arguing that our wave function idea is all very interesting, but that it is not a valid description of the physical world, or perhaps it is a perfectly fine concept but that it is incomplete, that there is information missing from the wave function. Perhaps there is a prescription still to be found that will enable us to complete the picture: retain the wave function but add something further that will then not forbid our being able to measure the position and the momentum of the particle precisely and at the same time. This, of course, 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 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

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concerning not being able to pinpoint the position and 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. Nevertheless, at the macroscopic level the uncertainties mentioned above become so small as to be experimentally unmeasurable, so at this level the uncertainty relation has 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 nature has prevented us, to an extent quantified by the uncertainty principle, from having complete information about the physical world. To someone wedded to the classical deterministic view of the the physical world (and Einstein would have to be counted as one such person), it appears to be the case that there is information that is hidden from us. This may then be seen as a cause for concern because it implies 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 relation means it is possible for a physical system to have a much broader 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 Heisenberg microscope: the effect of measurement

The Heisenberg Uncertainty Relation is enormously general. It applies *without saying anything whatsoever about the nature of the particle, how it is prepared in an experiment, what it is doing, what it might be interacting with* . . . . It is clearly a profoundly significant physical result. But at its heart it is simply a mathematical statement about the properties of waves that flows from the assumed wave properties of matter plus some assumptions about the physical interpretation of these waves. There is little indication of what the *physics* might be that underlies it. One way to uncover what physics might be present is to study what takes place if we attempt to measure the position or the momentum of a particle. This is in fact the problem initially addressed by Heisenberg, and leads to a result that is superficially the same as 3.14, but, from a physics point of view, there is in fact a subtle difference between what Heisenberg was doing, and what Eq. (3.14) is saying.

Heisenberg's analysis was based on a *thought* experiment, i.e. an experiment that was not actually performed, but was instead analysed as a mental construct. From this experiment, it is possible to show, by taking account of the quantum nature of light and matter, that measuring the position of an electron results in an unavoidable, unpredictable change in its momentum. More than that, it is possible to show that if the particle's position were measured with ever increasing precision, the result was an ever greater disturbance of the particle's momentum. This is an outcome that is summarized mathematically by a formula essentially the same as Eq. (3.14).

In his thought experiment, Heisenberg considered what was involved in attempting to measure the position of a particle, an electron say, by shining light on the electron and observing the scattered light through a microscope. To analyse this measurement process, arguments are used which are a curious mixture of ideas from classical optics (the wave theory of light) and from the quantum theory of light (that light is made up of particles).

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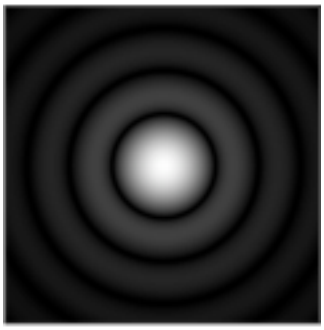

Figure 3.4: Airy disc diffraction pattern produced as image of a point object.

Classical optics enters the picture by virtue of the fact that in trying to measure the position of a *point* object using light, we must take into account the imprecision inherent in such a measurement. If a point object is *held fixed* (or is assumed to have infinite mass) and is illuminated by a steady beam of light, then the image of this object, as produced by a lens on a photographic image plate, is not itself a point — it is a diffraction pattern, a smeared out blob, brightest in the centre of the blob and becoming darker towards the edges (forming a so-called Airy disc). If there are two closely positioned point objects, then what is observed is two overlapping diffraction patterns. This overlap diminishes as the point objects are moved further apart until eventually, the edge of the central blob of one pattern will roughly coincide with the edge of the other blob. The separation d between the point objects for which this occurs can be shown to be given by

$$d = 2\frac{\lambda_l}{\sin\alpha} \tag{3.15}$$

where λ_l is the wavelength of the light, and 2α is the angle subtended at the lens by the object(s) (see Fig. (3.5)). This is a result that comes from the classical optics — it is essentially (apart from a factor of 2) the Rayleigh criterion for the resolution of a pair of images. For our purposes, we need to understand its meaning from a quantum mechanical perspective.

The quantum mechanical perspective arises because, according to quantum mechanics, a beam of light is to be viewed as a beam of individual particles, or photons. So, if we have a steady beam of light illuminating the fixed point object as before, then what we will observe on the photographic image plate is the formation of individual tiny spots, each associated with the arrival of a single photon. We would not see these individual photon arrivals with a normal every-day light source: the onslaught of photon arrivals is so overwhelming that all we see is the final familiar diffraction pattern. But these individual arrivals would be readily observed if the beam of light is weak, i.e. there is plenty of time between the arrival of one photon and the next. This gives rise to the question: we have individual particles (photons) striking the photographic plate, so where does the diffraction pattern come from? Answering this question goes to the heart of quantum mechanics. If we were to monitor where each photon strikes the image plate over a period of time, we find that the photons *strike at random*, more often in the centre, helping to build up the central bright region of the diffraction pattern, and more rarely towards the edges [3]. This probabilistic aspect of quantum mechanics we will study in depth in the following Chapter.

But what do we learn if we scatter just one photon off the point object? This photon will strike the image plate at some point, but we will have no way of knowing for sure if the point where the photon arrives is a point near the centre of the diffraction pattern, or near the edge of such a pattern or somewhere in between — we cannot reconstruct the pattern from just one photon hit! But what we can say is that if one photon strikes the image plate, for example at the point c (on Fig. 3.5), then this point could be anywhere between two extreme possibilities. We could argue that the point object was sitting at a, and the photon has scattered to the far right of the diffraction pattern that would be built up by many photons being scattered from a point object at position

[3] In fact, the formation of a diffraction pattern, from which comes the Rayleigh criterion Eq. (3.15) is itself a consequence of the $\Delta x\Delta p \geq \frac{1}{2}\hbar$ form of the uncertainty relation applied to the photon making its way through the lens. The position at which the photon passes through the lens can be specified by an uncertainty $\Delta x \approx$ half the width of the lens, which means that the photon will acquire an uncertainty $\Delta p \approx h/\Delta x$ in a direction parallel to the lens. This momentum uncertainty means that photons will strike the photographic plate randomly over a region whose size is roughly the width of the central maximum of the diffraction pattern.

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a (labelled A in Fig. 3.5), or we could argue at the other extreme that the point object was at b, and the photon reaching c has simply landed at the far left hand edge of the diffraction pattern (labelled B in Fig. 3.5) associated with a point particle sitting at b. Or the point object could be somewhere in between a and b, in which case c would be within the central maximum of the associated diffraction pattern. The whole point is that the arrival of the photon at c is not enough for us to specify with certainty where the point object was positioned when it scattered the photon. If we let $2\delta x$ be the separation between a and b, then the best we can say, after detecting one photon only, is that the point object that scattered it was somewhere in the region between a and b, i.e., we can specify the position of the point object only to an accuracy of $\pm\delta x$. The argument that leads to Eq. (3.15) applies here, so we must put $d = 2\delta x$ in Eq. (3.15) and hence we have

$$\delta x = \frac{\lambda_l}{\sin\alpha}. \tag{3.16}$$

Note that the δx introduced here is to be understood as the resolution of the microscope. It is a property of the *apparatus* that we are using to measure the position of the fixed point object and so is not the same as the uncertainty Δx introduced earlier that appears in Eq. (3.14), that being a property of the wave function of the particle.

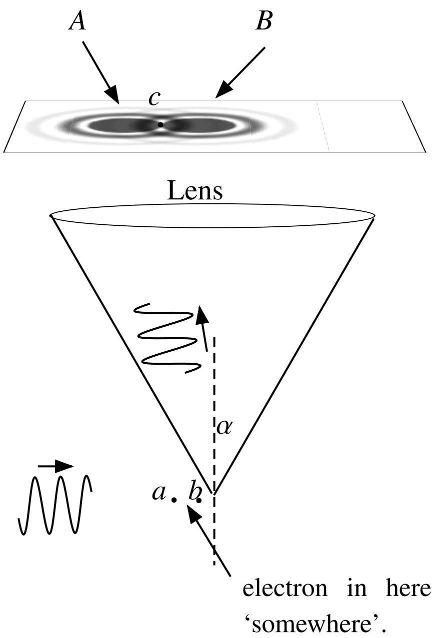

Figure 3.5: Diffraction images A and B corresponding to two extreme possible positions of a point object scattering a single photon that arrives at c. If one photon strikes the image plate, the point c where it arrives could be anywhere between two extreme possibilities: on the extreme right of the cenral maximum of a diffraction pattern (labelled A) built up by many photons scattered from a point object at position a, or on the extreme left of such a pattern (labelled B) built up by many photons being scattered from a point object at position b. With $2\delta x$ the separation beween a and b, the best we can say, after detecting one photon only, is that the object that scattered it was somewhere in the region between a and b, i.e., we can specify the position of the object only to an accuracy of $\pm\delta x$.

Now we turn to the experiment of interest, namely that of measuring the position of an electron presumably placed in the viewing range of the observing lens arrangement. In measuring its position we want to make sure that we disturb its position as little as possible. We can do this by using light whose intensity is as low as possible. Classically, this is not an issue: we can 'turn down' the light intensity to be as small as we like. But quantum mechanics gets in the way here. Given the quantum nature of light, the minimum intensity possible is that associated with the electron scattering only one photon. As we saw above, this single scattering event will enable us to determine the position of the electron only to an accuracy given by Eq. (3.16). But this photon will have a momentum $p_l = h/\lambda_l$, and when it strikes the electron, it will be scattered, and the electron will recoil. It is reasonable to assume that the change in the wavelength of the light as a result of the scattering is negligibly small, but what cannot be neglected is the change in the direction of motion of the photon. If it is to be scattered in a direction so as to pass through the lens, and as we do not know the path that the photon follows through the lens — we only see where it arrives on the image plate — the best we can say is that it has two extreme possibilities defined by the edge of the cone of half angle α. Its momentum can therefore change by any amount up to $\pm p_l \sin\alpha$. Conservation of momentum then tells us that the momentum of the electron has consequently undergone a change of the same amount. In other words, the electron has now undergone a change in its momentum of an amount that could be as large as $\pm p_l \sin\alpha$. Just how big a change has taken place is not known as we do not know the path followed by the photon through the lens — we only know where the photon landed. So the momentum of the electron after the measurement has been *disturbed* by an unknown amount that could be as large as $\delta p = p_l \sin\alpha$. Once again, this quantity δp is not the same as the uncertainty Δp introduced earlier that appears in Eq. (3.14). Nevertheless we find that

$$\delta p \approx p_l \sin\alpha = \frac{h\sin\alpha}{\lambda_l} = \frac{h}{\delta x}, \tag{3.17}$$

using Eq. (3.16) and hence

$$\delta x \delta p \approx h \tag{3.18}$$

which apart from a factor $\sim 4\pi$, which can be neglected here given the imprecise way that we have defined δx and δp, is very similar to the uncertainty relation, $\Delta x \Delta p \geq \frac{1}{2}\hbar$!!!! In fact, to add to the confusion, the quantities δx and δp are also often referred to as 'uncertainties', but their meaning, and the meaning of Eq. (3.18) is not quite the same as Eq. (3.14).

Firstly, the derivation of Eq. (3.18) was explicitly based on the study of a measurement process. This is quite different from the derivation of the superficially identical relation, $\Delta x \Delta p \geq \frac{1}{2}\hbar$, derived by noting certain mathematical properties of the shape of a wave packet. Here, the 'uncertainty' δx is the resolution of the measuring apparatus, and δp is the disturbance in the momentum of the electron as a consequence of the physical effects of a measurement having been performed. In contrast, the uncertainties Δx and Δp, and the associated uncertainty relation was *not* derived by analysing some measurement processes — it simply states a property of wavepackets. The uncertainty Δp in momentum does not come about as a consequence of a measurement of the position of the particle, or vice versa.

Thus there are (at least) two 'versions' of Heisenberg's uncertainty relation. Which one is the more valid? Heisenberg's original version, $\delta x \delta p \approx h$, (the measurement-disturbance based 'δ version') played a very important role in the early development of quantum mechanics, but it has been recognized that the physical arguments used to arrive at the result are not strictly correct: the argument is neither fully correct classically or fully correct quantum mechanically. It can also be argued that the result follows from the use of the Rayleigh criterion, a *definition* based purely on experimental convenience, to derive a quantum mechanical result. On the other hand, the later formulation of the uncertainty relation, $\Delta x \Delta p \geq \frac{1}{2}\hbar$ (the statistical or 'Δ version'), in which the uncertainties in position and momentum are, in a sense, understood to be present at the same time for a particle, can be put on a sound physical and mathematical foundation, and is now viewed as being the more fundamental version. However, the close similarity of the two forms of the uncertainty relation suggests that this is more than just a coincidence. In fact, it is possible to show that in many circumstances, the measurement based 'δ version' does follow from the 'Δ version'. In each such case, the argument has to be tailored to suit the physics of the specific measurement procedure at hand, whether it be waves and optics as here, or masses on springs, or gravitational fields or whatever. The physical details of the measurement process can then be looked on as nature's way of guaranteeing that the electron indeed acquires an uncertainty $\delta p \approx h/\delta x$ in its momentum if its position is measured with an uncertainty δx, while lurking in the background is the 'Δ version' of the uncertainty relation: in the example considered here, this describes how the uncertainty in the path followed by the photon through the lens leads to the formation of the diffraction pattern (see footnote 3 on p21). But the correspondence is not perfect — the two versions are not completely equivalent. No one has ever been able to show that Eq. (3.18) always follows from Eq. (3.14) for all and any measurement procedure, and for good reason.

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Einstein, Podolsky and Rosen showed that here are methods by which the position of a particle can be measured without physically interacting with the particle at all, so there is no prospect of the measurement disturbing the position of the particle.

Heisenberg's uncertainty principle has always been a source of both confusion and insight, not helped by Heisenberg's own shifting interpretation of his own work, and is still a topic that attracts significant research. The measurement-based 'δ version' has physical appeal as it seems to capture in an easily grasped fashion some of the peculiar predictions of quantum mechanics: measure the position of a particle to great accuracy, for instance, and you unavoidably thoroughly screw up its momentum. That performing an observation on a physical system can affect the system in an uncontrollably random fashion has been termed the 'observer effect', and is an aspect of quantum mechanics that has moved outside the purvey solely of quantum theory into other fields (such as sociology, for instance) involving the effects of making observations on other systems. But the statistical 'Δ version' is wholly quantum mechanical, and represents a significant constraint on the way physical systems can behave, and has remarkable predictive powers that belies the simplicity of its statement, as we will see in the next section.

3.3.2 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 $\Delta p_x \approx p$. 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

$$T = \frac{p^2}{2m} \approx \frac{\hbar^2}{2ma^2} \tag{3.19}$$

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

$$E \approx \frac{\hbar^2}{2ma^2} - \frac{e^2}{4\pi\epsilon_0 a}. \tag{3.20}$$

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

$$a \approx \frac{4\pi\epsilon_0\hbar^2}{me^2} \approx 0.5 \text{ nm} \tag{3.21}$$

and the minimum energy

$$E_{\min} \approx -\tfrac{1}{2}\frac{me^4}{(4\pi\epsilon_0)^2\hbar^2} \tag{3.22}$$

$$\approx -13.6 \text{ eV}. \tag{3.23}$$

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 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.

3.3.3 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

$$U = \tfrac{1}{2}m\omega^2x^2 \tag{3.24}$$

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

$$\Delta x\Delta p \approx \hbar \tag{3.25}$$

from which we conclude that

$$p \approx \hbar/a. \tag{3.26}$$

The total energy of the oscillator is

$$E = \frac{p^2}{2m} + \tfrac{1}{2}m\omega^2x^2 \tag{3.27}$$

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

$$E \approx \tfrac{1}{2}\left(\frac{1}{2m}\frac{\hbar^2}{a^2} + \tfrac{1}{2}m\omega^2a^2\right) \tag{3.28}$$

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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.

$$\frac{dE}{da} = \tfrac{1}{2}\left(-\frac{1}{m}\frac{\hbar^2}{a^3} + m\omega^2 a\right) = 0. \tag{3.29}$$

Solving for a gives

$$a^2 = \frac{\hbar}{m\omega}. \tag{3.30}$$

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

$$E_{\min} \approx \tfrac{1}{2}\hbar\omega. \tag{3.31}$$

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.

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