QUANTUM MECHANICS A (SPA 5319)

Introduction

(1) Arguments Leading to Schrödinger's Equation.

We will begin this module with a quick review of the basic ideas of quantum mechanics. Some of these you should have learned from Quantum Physics in your first year, but I will present them in my own way, adding some additional concepts as we proceed. Students often feel that Quantum Mechanics comes from thin air, but this is far from true: the theory was arrived at through an enormous intellectual struggle, driven by a truly remarkable range of experiments. Your first year of formal study and your own reading of the history of 20th century physics should by now have given you a full appreciation of how the ideas developed through physicists attempts to understand the experimental facts. Today there is no more successful theory in all of science, providing explanations for many long-standing as well as new mysteries of nature. One of the aims of this course is to show you some examples of these explanations; a second aim is to provide you with the concepts, language and techniques to enable you to carry out or understand simple applications of the theory; finally, I wish to lay down the groundwork for you to proceed further in the subject either on your own or in subsequent courses.

I will begin my simplified version of the story with Plancks idea that electromagnetic radiation is emitted and absorbed as quanta of energy,

$$E = h\nu = \hbar\omega \qquad \text{where} \qquad \hbar = h/2\pi\,. \tag{1}$$

He was reluctantly forced to this in his successful attempt to fit the new experiments (1900) of Lummer & Pringsheim and Rubens & Kurlbaum on black body radiation. It was Einstein (1905) who grasped the significance of the idea when he applied it to the photoelectric effect: Plancks quanta are particles of light, later named photons. His predictions were beautifully confirmed in Millikans experiments (1916). Comptons experiments (1923) on the scattering of X-rays by electrons provided an important step forward when he successfully explained his results by treating the X-rays as relativistic zero mass particles Einsteins photons colliding with electrons. Of course in this period of history Rutherfords nuclear atom and Bohrs model had added further puzzles which could not be solved by classical physics.

At this stage in the story electromagnetic radiation seems to be playing a dual role: in some experiments, such as interference and diffraction, it undoubtedly behaves like waves; in others it behaves like particles. These particles must be massless to travel at the velocity of light, with the momentum given by Einsteins relativistic formula:

$$\begin{aligned} E &= \sqrt{p^2c^2 + m^2c^4} && (2) \\ &= pc \qquad \text{for} \qquad m = 0 \qquad (\textit{i.e.} \text{ for photons}) && (3) \end{aligned}$$

If we combine this with Plancks formula $E = h\nu = \hbar\omega$ and use the expression $\nu = c/\lambda$ for the wavelength we discover an expression for the momentum in terms of wavelength,

$$p = \frac{h}{\lambda} = \hbar k \tag{4}$$

where $k = 2\pi/\lambda$ is the usual definition of wave number. In his doctoral thesis de Broglie (1923) made a very simple but profound conjecture: if waves can behave like particles, perhaps particles such as electrons, protons and even atoms can behave like waves. If so, what wavelength would they have? In his reasoning De Broglie understood clearly that some of the expressions above apply only to zero mass particles, so he took as his starting point the expression for all particles

$$p = \frac{h}{\lambda} = \hbar k \tag{5}$$

This gives a relation between the momentum p, a particle-like property, and a wave-like property, the wavelength λ (or equivalently the wave number, k). Once we accept this we can find the energy (or equivalently the angular frequency, ω, defined by $E = \hbar\omega$) from Einsteins relativistic formula for massive particles:

$$\begin{aligned} E &= \sqrt{p^2 + m^2c^4} && (6) \\ &= \hbar\omega && (7) \end{aligned}$$

Note that ω is defined by this expression by analogy with a photon. A plane monochromatic de Broglie wave, with wave number and frequency $\{k, \omega\}$ would therefore describe a beam of monoenergetic electrons with momentum and energy $\{p, E\}$ given by the boxed expressions. With this simple, even naive, idea de Broglie had made a definite experimentally verifiable prediction: diffraction and interference effects should be seen with beams of electrons, protons or even atoms; moreover the prediction was quantitative and could be experimentally tested in full detail. Indeed this was first done with electron beams by Davisson & Germer (1927) and completely independently by G.P. Thomson (1928); subsequent years have seen many confirmations using proton, neutron and atomic beams, leading to many practical uses in science and industry.

If matter can behave like waves, then one assumes that a monochromatic de Broglie waves amplitude $\Psi(x,t)$ can be represented by an expression just like that of classical running waves:

$$\Psi(x,t) = \cos(kx - \omega t) = \cos((px - Et)/\hbar) \tag{8}$$

or, in complex notation,

$$\Psi(x,t) = e^{i(kx-\omega t)} = e^{i(px-Et)/\hbar} \tag{9}$$

In both cases we have used de Broglies relations to translate the wave-like pair (k, ω) to the particle-like pair (p, E). At this juncture two questions immediately come to mind:

Question (1): What is the wave equation for de Broglie waves? Is it our old friend the classical wave equation?

$$\frac{\partial^2 \Psi}{\partial x^2} - \frac{1}{v^2}\frac{\partial^2 \Psi}{\partial t^2} = 0 \tag{10}$$

Question (2): What physical quantity does the wave function $\Psi(x,t)$ represent? In the case of sound waves it would represent the longitudinal displacement of the molecules from their equilibrium positions; for surface water waves or waves on a string it would be the transverse displacement of the waters surface or of the string; for electromagnetic waves it would stand for the components of the electric and magnetic fields constituting the wave.

Answer to Question (1): Assume the classical wave equation and ask for any of the above plane waves to be a solution. Substitution into the equation then gives the condition for Ψ to be a solution:

$$\left(-\frac{p^2}{\hbar^2} + \frac{1}{v^2}\frac{E^2}{\hbar^2}\right)\Psi(x,t) = 0 \tag{11}$$

Notice that this follows whichever of the above forms for Ψ, real or complex, we use. Since this equation must hold for all (x,t), the only possibility is that the bracketed factor vanish, leading to

$$\left(-\frac{p^2}{\hbar^2} + \frac{1}{v^2}\frac{E^2}{\hbar^2}\right) = 0 \tag{12}$$

i.e.

$$p^2 + \frac{1}{v^2}E^2 = 0 \tag{13}$$

or

$$E = pv \tag{14}$$

where we have taken the positive square root. This is only correct for a zero mass particle with $v = c$, but for a massive relativistic one we require $E^2 = p^2c^2 + m^2c^4$.

Its easy to see what modification is needed to get this relativistic formula: just add an extra term to generate m^4c^4 and replace v^2 by c^2,

$$\frac{\partial^2\Psi}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2\Psi}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\Psi = 0 \tag{15}$$

Substitution of our plane monochromatic Ψ then gives, as before,

$$\left(-\frac{p^2}{\hbar^2} + \frac{1}{c^2}\frac{E^2}{\hbar^2} - \frac{m^2c^2}{\hbar^2}\right) = 0 \tag{16}$$

ie.

$$-p^2 + \frac{1}{c^2}E^2 - m^2c^2 = 0 \tag{17}$$

or

$$E = \sqrt{p^2c^2 + m^2c^4} \tag{18}$$

where we have again taken the positive square root. This equation is indeed correct for a massive relativistic particle. It is known as the Klein-Gordon equation (1926) and is used in relativistic quantum mechanics[1]. But we are seeking a non-relativistic equation, where the rest mass energy is fixed and plays no role, so that the interesting part of a free particles energy is just its kinetic energy, henceforth also called E,

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} \tag{19}$$

Its clear that the wave equation that generates such an equation, by the substitution procedure we performed above, must have a double derivative in x to generate the p^2 factor, but only a single derivative in time to generate only one power of E. A minimally modified version of the wave equation is then:

$$\frac{\partial^2\Psi}{\partial x^2} + A\frac{\partial\Psi}{\partial t} = 0 \tag{20}$$

where A is a constant to be determined. Now we demand that our plane monochromatic free particle Ψ be a solution. We immediately see that the cos doesnt work as a solution because, although the spatial second derivative generates the cos again, the first time derivative generates a sin from the cos. However the complex exponential form is perfectly designed for the job because no matter how many derivatives we take we still generate only the exponential. Thus for $\Psi = \exp\{i(px - Et)/\hbar\}$ to be a solution we require:

$$\left(-\frac{p^2}{\hbar^2} - iA\frac{E}{\hbar}\right)\Psi(x,t) = \left(-\frac{p^2}{\hbar^2} - iA\frac{E}{\hbar}\right)e^{i(px-Et)/\hbar} = 0 \tag{21}$$

---

[1] The Klein-Gordon equation has its problems, however. It has negative energy solutions (the ± sign in taking the square root), which only get a proper interpretation in quantum field theory with creation and annihilation of particles and antiparticles.

Notice the appearance of the imaginary i. Thus for this Ψ to be a solution we require the factor in brackets to vanish,

$$-\frac{p^2}{\hbar^2} - iA\frac{E}{\hbar} = 0 \qquad \text{giving} \qquad E = -\frac{p^2}{iA\hbar} \tag{22}$$

To get the correct non-relativistic kinetic energy requires $iA\hbar = -2m$, or $A = 2mi/\hbar$, which gives the equation

$$\frac{\partial^2\Psi}{\partial x^2} + i\frac{2m}{\hbar}\frac{\partial\Psi}{\partial t} = 0 \tag{23}$$

or, multiplying by $\hbar^2/2m$ to make all terms have the dimensions of [energy][Ψ], we obtain the Schrödinger equation (1925) for a free non-relativistic particle of mass m:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = i\hbar\frac{\partial\Psi}{\partial t} \tag{24}$$

The final step is to determine the generalisation for the same particle moving in a potential field $V(x,t)$. As the energy is now kinetic plus potential energy, E=KE+PE, we need to obtain

$$E = \frac{1}{2}mv^2 + V(x,t) = \frac{p^2}{2m} + V(x,t)\,. \tag{25}$$

We immediately see that the above manipulations would give this expression with our complex Ψ if we simply added a term $V\Psi$:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x,t)\Psi(x,t) = i\hbar\frac{\partial\Psi}{\partial t} \qquad \text{TDSE} \tag{26}$$

This is the time-dependent Schrödinger equation (hereafter TDSE)[2] and plays the same fundamental role in quantum mechanics as Newtons Second law plays in classical mechanics: it determines the time evolution of the system and has the status of a postulate. It is assumed to be true but can never be proved to be true; because of its immensely successful application in understanding many experimental results, both qualitatively and quantitatively, we have every reason to accept it as an excellent approximation to the true law of Nature. The arguments I have given are only meant to provide some idea how one might have arrived at this equation through some reasoning process, to convince you that it does not simply come out of thin air. The actual historical process was in fact

---

[2] In 3-dimensions the TDSE is $-\frac{\hbar^2}{2m}\nabla^2\Psi(r,t) + V(r,t)\Psi(r,t) = i\hbar\partial\Psi(r,t)/\partial t$ or,written out fully in cartesian coordinates, with $r = (x,y,z)$,

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}\right) + V(r,t)\Psi(r,t) = i\hbar\frac{\partial\Psi(r,t)}{\partial t}.$$

rather more complicated and indirect!

(2) The Superposition principle.

In general there are many, often infinitely many, independent solutions, $\Psi_i(x,t)$, to the time-dependent Schrödinger equation. Because the TDSE is linear and homogeneous, any linear combination of these solutions is also a solution:

$$\Psi(x,t) = \sum_i c_i \Psi_i(x,t); \tag{27}$$

indeed, this is the most general solution, a fact familiar to you from your study of classical waves. This property is the source of the most unexpected (non-classical) aspects of quantum mechanics where particles behave like waves, can tunnel through forbidden barriers, where cats may be both alive and dead, and where so-called ghostly instantaneous interactions appear to take place over large distances. The interpretation (and sometimes, misinterpretation) of these phenomena arises from the physical interpretation of the wave function.

(3) The Born (or Probability) Interpretation of the Wave Function.

Answer to Question (2): The question of the physical significance of the wave function $\Psi(x,t)$ caused some considerable difficulties, and even today is not completely settled. It was Max Born (1926) who was finally led to the currently accepted and hugely successful Born interpretation or probability interpretation of the wave function:

In 1 dimension $|\Psi(x,t)|^2 dx$ is the probability that a measurement at time t of the particles position will yield a value between x and $x + dx$ (figure 1a).

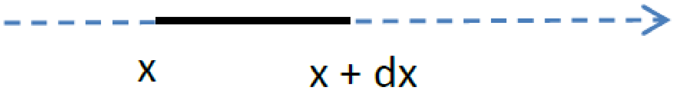

Figure 1a: *The Born interpretation in one dimension.*

In 3 dimensions $|\Psi(\mathbf{r},t)|^2 dV$ is the probability that a measurement at time t of the particles position will yield a value lying in the volume element dV at position $\mathbf{r}$, where $dV = d^3x = dxdydz$ in cartesian coordinates (figure 1b).

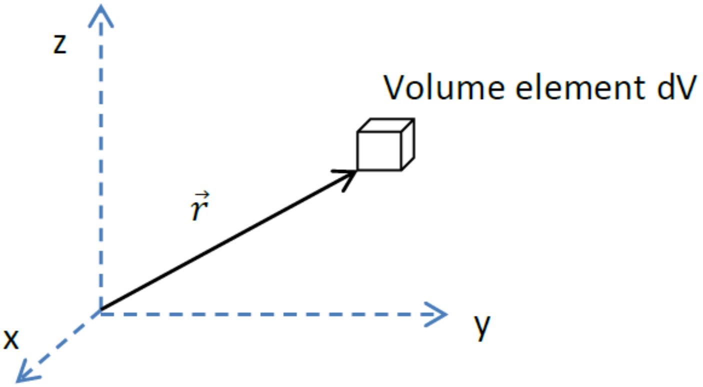

Figure 1b: *The Born interpretation in three dimensions.*

So, in general, the (always real) modulus squared of the complex wave function gives us a probability density function for the detection of a particle.

(4) The Time Independent Schrödinger Equation (TISE).

An important special case often encountered in elementary, as well as advanced applications of quantum mechanics is that of the time independent potential,

$$V(x,t) = V(x) \tag{28}$$

In this special case we can solve for the time dependence of the wave function $\Psi(x,t)$ by a mathematical technique known as separation of variables. The way to proceed is to notice that the time dependence and space dependence in the time-dependent Schrödinger equation (TDSE) can be put on different sides of the equation by searching for solutions of the form,

$$\Psi(x,t) = \psi(x)f(t) \tag{29}$$

where the factors $\psi(x)$ and $f(t)$ are to be found by demanding that this form be a solution to the TDSE. After dividing both sides of the equation by $\Psi(x,t) = \psi(x)f(t)$, then moving all functions of x to the left-hand side and all functions of t to the right-hand side, we obtain

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} + V(x) = i\hbar\frac{1}{f(t)}\frac{df(t)}{dt} \tag{30}$$

Now this equation must be true for all values of the independent variables x and t; this means that for any chosen t, we may choose x to have any value whatever, and the equation must still be satisfied. But the left-hand side of the equation is a function of x alone; the right a function of t alone. For them to be equal for any pair (x,t) whatever, they clearly cannot vary, i.e. they are constant[3]. Since both sides have the dimensions of $V(x)$, ie. of energy, we call this constant E:

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2}+V(x)=i\hbar\frac{1}{f(t)}\frac{df(t)}{dt}=E \qquad (31)$$

Thus, we obtain an easily solved equation for $f(t)$:

$$\frac{df}{dt}=-i\hbar Ef(t) \qquad (32)$$

which can be integrated to give

$$f(t)=Ae^{-iEt/\hbar} \qquad (33)$$

where A is the integration constant. We have now discovered the full time-dependence of the wave function:

$$\Psi(x,t)=\psi(x)e^{-iEt/\hbar}\,, \qquad (34)$$

where we have absorbed the constant A into $\psi(x)$. Going back to the separated equation above we also see that $\psi(x)$ must obey the time-independent Schrödinger equation (TISE):

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x) \qquad (35)$$

This equation has the form of an eigenvalue equation:

$$\hat{H}\psi(x)=E\psi(x) \qquad (36)$$

where $\hat{H}$ is a (differential) operator, the Hamiltonian operator,

$$\hat{H}=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x) \qquad (37)$$

The action of this operator on $\psi(x)$ is not to change the form of the function, but merely to multiply it by a constant E, the energy eigenvalue it extracts the energy when acting on $\psi(x)$. Of course, as only particular functions can be solutions to the TISE, depending on the value of E, we should really label these solutions with E,

$$\psi(x)=\psi_E(x) \qquad (38)$$

where $\psi_E(x)$ is known as the (energy) eigenfunction of the operator $\hat{H}$ belonging to the (energy) eigenvalue E. We will shortly discover that the Hamiltonian

---

[3] Choose a pair of values x, t for which the right-hand side equals the left. Now, keeping t fixed at this value, change x to any other value you like. Clearly if the left-hand side varies with x it will change its value and no longer be equal to the right side; so it must be a constant, and therefore so too must the right side since they are equal.

operator $\hat{H}$ is the operator representing energy in quantum mechanics, and its eigenvalues E are the only possible results of an energy measurement.

(5) Consequences of the Born Interpretation of the Wave Function.

The Born interpretation of the wave function is expressed above in terms of an infinitesimal portion dx of the x-axis; the probability of finding the particle between two points a and b separated by a finite distance is simply the sum of the probabilities,

$$P_{ab}(t) = \int_a^b |\Psi(x,t)|^2 dx \tag{39}$$

If a wave function $\Psi(x,t)$ describes the state of a single particle, then we are certain to find the particle somewhere, i.e. the probability for finding it anywhere on the x-axis is 1:

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1 \tag{40}$$

In three dimensions this becomes,

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\Psi(r,t)|^2 d^3x = 1 \tag{41}$$

This is known as the normalisation of the wave function: any proper single-particle wave function must be normalised (to 1).

The Born interpretation implies a profound change in our concept of measurement. The wave function is meant to encode all that we know about the system in quantum mechanics; the Born interpretation tells us that a measurement of position does not lead to a unique or definite result, but only to one of an infinite set of possible results. What is definite is the probability of obtaining a particular result; its just like throwing a dice: each throw of the dice yields a definite result, although we only know after the throw what the actual result is. A particular result (say a 5) has a probability of 1/6, and this is all we can say before the throw is made. Similarly, if we prepare the system in the quantum state $\Psi(x,t)$ then we can only predict the probability of a given result for a position measurement ($|\Psi(x,t)|^2 dx$ for the result to lie between x and $x + dx$); but once the measurement has been made then we know where the particle is at time t of the measurement.

Suppose we had computed the wave function and wished to check our calculation against experiment. The Born interpretation tells us that our wave function only allows us to predict probabilities. These probabilities can only be determined experimentally by doing very many (in principle infinitely many) repetitions of the measurement, each time preparing the system anew in the same state $\Psi(x,t)$ before repeating the measurement. This corresponds to the process of checking whether a dice is biassed, i.e. what the probabilities are for the various outcomes and whether they are equal: we would have to throw the dice infinitely many times and compare the relative frequencies of the different outcomes; these are proportional to the probabilities of the different outcomes and if they are equal, the dice is unbiassed. Preparation of the system is like throwing the dice; measuring position is like looking at the dice when its landed and noting the outcome. Just as with any repeated measurement, we can compute the average of all the individual measurements: the weight of each value of x is its probability, $|\Psi(x,t)|^2 dx$, and the average is obtained by summing over all the possibilities,

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\Psi(x,t)|^2 dx \tag{42}$$

Note that we did not divide by the integral of $|\Psi|^2$ because the wave function is normalised. The quantity $\langle x \rangle$ is often called the expectation value for x; it is usually written in an equivalent form resembling that for other quantum mechanical variables that are represented by operators where the order of factors is important:

$$\langle x \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) x \Psi(x,t) dx \tag{43}$$

The measurement process can either be performed as described above or by preparing an infinite number of identical replicas of the system, each in the same state Ψ, and measuring the position of every one; this collection of systems is known as an ensemble, and the interpretation of the wave function I have described is known as the ensemble interpretation of quantum mechanics. (A practical example of an ensemble is a beam of identical particles, all in the same state). This is usually called the Copenhagen interpretation because it was the one developed by Niels Bohr and his many collaborators, especially Heisenberg, in Copenhagen during the 1920s. You should particularly notice that this interpretation is rather careful not to identify Ψ with the state of a single system, but with an ensemble; Ψ is the outcome of a preparation process and is our tool for computing the probabilities of various results for individual measurements, and the expectation values obtained in ensemble measurements.

In an ensemble measurement of the particles position we measure many different values of x and compute their average $\langle x \rangle$. The quantity $|\Psi(x,t)|^2 dx$ gives the probability for the result of a single one of these measurements lying between x and $x + dx$; the expectation value $\langle x \rangle$ is then obtained by averaging all the individual results. Since individual results differ from each other, we would like to find a measure of the spread of these values about the mean. This is given by the variance or uncertainty Δx[4]:

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \tag{44}$$

where

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \Psi^* x^2 \Psi dx \tag{45}$$

We can interpret this as saying that the position of the particle is $\langle x \rangle \pm \Delta x$. I put this statement in quotation marks because it is not really the position of a single particle, but the average position of an ensemble of particles, each prepared in the state Ψ. We can usefully think of our particle in state Ψ as smeared out over this region $\langle x \rangle \pm \Delta x$, but you should be careful not to take this interpretation too literally. Physicists usually loosely identify Ψ as the state of an individual system; this works well enough in most situations, but is also a source of misconceptions in others.

Let me illustrate the trouble caused by saying the particle is literally in the state Ψ. Take the example of Youngs two-slit experiment using an electron beam. Let the wave function for the electron arriving at position x on the screen after going via slit 1 be Ψ_1; via slit 2 be Ψ_2. To explain why an electron beam produces interference at the screen we need to write the wave function as $\Psi = (\Psi_1 + \Psi_2)/\sqrt{2}$: the particle is equally likely to go through either slit. At the screen we measure the number of electrons arriving at each point, which is proportional to the probability of an electron arriving there[5]; this probability is proportional to

$$|\Psi|^2 = \frac{1}{2}|\Psi_1|^2 + |\Psi_2|^2| + 2\mathrm{Re}(\Psi_1^* \Psi_2)\,. \tag{46}$$

It is the cross-term - the real part, Re - which gives the constructive and destructive interference observed in the experiment; without the linear combination of both Ψ_1 and Ψ_2 there would be no interference. We are tempted to conclude that the state of a particle just before it arrives at the screen is in some sense both Ψ_1 and Ψ_2; has the particle gone through both slits, half through slit 1; the other half through slit 2? Surely not! The electron is not a particle that can be

---

[4] From laboratory measurements you may be familiar with the definition of the squared error as the result of taking the difference between each measurement and the mean, squaring, and then averaging:

$$\Delta x^2 \;=\; \langle ((\langle x \rangle x)^2 \rangle = \langle ((\langle x \rangle^2 - 2x\langle x \rangle + x^2)\rangle = \langle x \rangle^2 - 2\langle x \rangle\langle x \rangle + \langle x^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

This is therefore equivalent to the definition given in the text.

[5] Notice that the use of a beam amounts to an ensemble measurement of position on the screen; if we had sent just one electron through the apparatus it would have arrived somewhere on the screen, but on its own that would have told us virtually nothing about the probability distribution $|\Psi|^2$, and we would not have noticed the interference. Only by passing many electrons through the apparatus, either in an intense beam or one at a time, can we get to see the interference pattern.

broken up in that way: we have never seen such a division in any experiment and have good reasons to believe that this is impossible: lepton number conservation, quantisation of electric charge, no known particles with mass anywhere near one-half the electron mass[6]. What then should we say? In the Copenhagen version of quantum mechanics we refuse to identify Ψ as the actual state of a particular particle and so we avoid saying that it went through both slits or either slit; instead we take Ψ to represent the result of a preparation process (sending the particle into the apparatus) which tells us the possible outcomes and probabilites of a measurement process (detection at the screen); we cannot say which slit the particle went through because we did not carry out an appropriate measurement to investigate this - indeed we avoided doing so in order to measure an interference pattern on the screen. To experimentally determine detailed information about the wave function we must carry out an ensemble measurement, and so Ψ represents the entire ensemble rather than a single member of the ensemble. In practice we all loosely think of Ψ as representing the state of a single particle, although we have to be careful when doing so. You should be aware that this is a controversial aspect of quantum mechanics: there is so far no experiment contradicting the Copenhagen interpretation - and I believe it derives its power from the fact that is a rather conservative interpretation - but it makes many people uneasy. Both experimental and theoretical research continues to explore this crucial area of quantum mechanics.

(6) Physical Constraints on the Behaviour of the Wave Function: Boundary Conditions.

(1) All physical systems we study are localized in some finite region of space, so that the probability of finding the system at spatial infinity, $x \to \pm\infty$, is zero:

$$\lim_{x \to \mp\infty} \psi(x) = 0 \tag{47}$$

(2) As the probability interpretation requires that $\int |\psi(x)|^2 dx = 1$, which is finite, $\psi(x)$ must be square integrable. This says that not only must the wave function vanish at infinity (see (1) above) but it must vanish sufficiently rapidly. (e.g. $\psi \sim 1/\sqrt{x}$ would fail this test.)

(3) As $|\psi(x)|^2$ represents a physical probability density, it must have a unique value, ie. be single-valued. This is usually taken to imply that $\psi(x)$ be single-valued, although there are cases, such as spin-half particles electrons, protons,

---

[6] Also, if we tried to check whether the electron went through one or both slits by putting counters at the slits to detect the electron as it passed through on its way to the screen, quantum mechanics – in the form of Heisenbergs uncertainty relation – would show that the pattern on the screen is so smeared out as to remove any trace of interference.

quarks, etc. where the wave function is double-valued.

(4) $\psi(x)$ must be continuous everywhere, otherwise $|\psi(x)|^2$ would not have a unique value and could not represent a physical probability density.

(5) The derivative, $d\psi/dx$, must be continuous everywhere. This implies that there are no kinks in $\psi(x)$. If this were not the case then $d^2\psi/dx^2$ would be infinite, thereby contributing an infinite term to the Schrödinger equation where all other terms are finite. An exception to this rule occurs at points where the potential is infinite, such as the boundaries of the escape-proof box. But note that at such points the wave function itself must still be continuous because of its probability interpretation see (4) and so it only acquires a kink. At points where the potential is finite, but discontinuous, the second derivative of $\psi(x)$ will be discontinuous, although the first derivative will still remain continuous. At points where the wave function enters a classically forbidden region the second derivative changes sign this is a point of inflexion because the sign of $E - V(x)$ changes there.

(7) Potentials and Forces.

Before we launch into the detailed study of quantum effects in various idealised potentials we first discuss the physical meaning of potentials and the relationship between idealised and more realistic potentials. First recall the relation between force and potential: in one dimension the force in the x-direction is

$$F_x = -\frac{\partial V(x,t)}{\partial x}\,, \tag{48}$$

so the slope of the potential tells us how strong the force is. The potential shown in Figure 2a depicts an idealised potential with a vertical side where the slope is infinite and therefore so is the force. This cannot represent a physical potential, which must be continuous to give a finite force; of course it acts over zero distance and so does produce a finite effect on a particle. This potential therefore represents an idealisation of the more realistic potential illustrated in Figure 2b where the side now varies smoothly. The corresponding forces are shown in both figures: here the forces only act near the walls of and are zero elsewhere. These impulsive forces would act to confine a particle of low enough energy: if a (classical) particle approaches the step from the right it will feel a force pushing it back to the right (F_x positive): the particle has been accelerated to the right by interaction with the step. We say that the particle has been scattered by the potential. In quantum mechanics the quantum state of such a particle would be called a scattering state. When is an idealised potential with vertical sides a reasonable approximation to a more realistic smoothly varying one? To understand how to think about this question let us use our knowledge of the behaviour of a classical water wave when it meets an obstacle. Provided the obstacle is small enough, the wave will not be significantly affected by its presence, i.e. provided the wavelength λ is very much larger than the size of the obstacle. A quantum state in any well always has a characteristic oscillatory behaviour for which we can estimate its de Broglie wavelength λ: for an idealised potential with an abrupt edge replacing one with an edge varying more smoothly but still rapidly over a distance δx (Figure 3) we require

$$\lambda \gg \delta x \tag{49}$$

In this way, just as in the case of the water wave, the quantum state will not be changed significantly by using an abrupt potential approximation: the de Broglie wave will not notice the difference.

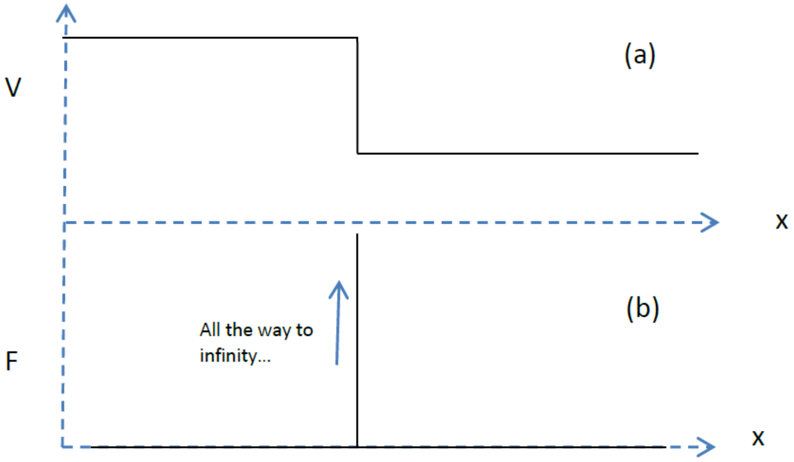

Figure 2: *An idelaised potential and resulting delta function force.*

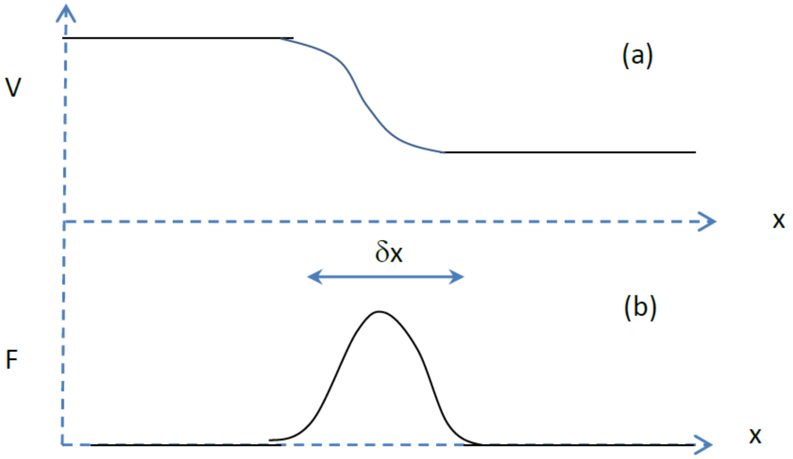

Figure 3: *A realistic potential and a corresonding finite magnitude force.*

(8) The Infinite Square Well (or the Escape-Proof Box) in 1-Dimension.

To remind you of the role played by the above conditions on the wave function, let us solve the familiar infinite square well problem. The potential $V(x)$ is time-independent, so the wave function for a given energy (energy eigenfunctions) have the form obtained in Section 4:

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar} \tag{50}$$

Our aim is to find the energy eigenvalues E and the corresponding eigenfunctions $\psi(x)$ by solving the time-independent Schrödinger equation (TISE):

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \tag{51}$$

For the infinite square well the particle of mass m is confined to the region $-L/2 < x < +L/2$; it cannot escape from that region because it cannot surmount the infinitely high potential barriers at the ends: $V(\pm L/2) = \infty$. Physically, this means there is zero probability of finding the particle outside the box; mathematically this is expressed as

$$\psi(x) = 0 \qquad \text{for} \qquad x \leq -L/2 \qquad \text{andfor} \qquad x \geq +L/2 \tag{52}$$

As the potential is constant inside the box we take $V(x) = 0$ there. The wave function inside the box is therefore given by solving the TISE:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \tag{53}$$

A simple rearrangement gives

$$\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x)\,, \tag{54}$$

where

$$k = \sqrt{\frac{2m}{\hbar^2}E}\,, \tag{55}$$

and is real because $E > 0$ (it cannot be less than the bottom of the well). Mathematically this differential equation is of the classical simple harmonic oscillator form and therefore the general solution is a linear combination of sin and cos[7],

$$\psi(x) = A\cos(kx) + B\sin(kx) \tag{56}$$

The boundary conditions at $x = \pm L/2$ determine the constants A, B and the energy eigenvalue. From Section 6 we know that the wave function must be

---

[7] We could equally well use complex exponentials $\psi(x) = ae^{ikx} + be^{-ikx}$. This is equivalent to our choice because its just a linear combination of the sin and cos. Our choice is more convenient for imposing the boundary conditions.

continuous everywhere: in particular, at $x = \pm L/2$ the wave function must vanish to match its value just outside the well[8]:

$$\begin{aligned} \psi(x = -kL/2) &= A\cos(kL/2) - B\sin(kL/2) = 0 && (57) \\ \psi(x = +kL/2) &= A\cos(kL/2) + B\sin(kL/2) = 0 && (58) \end{aligned}$$

Adding and subtracting these equations gives two simple conditions:

$$\begin{aligned} A\cos(kL/2) &= 0 && (59) \\ B\sin(kL/2) &= 0 && (60) \end{aligned}$$

To find all possible solutions we must explore all the possibilities; since the sin and cos cannot both vanish, there are just two cases:

(A) $A \neq 0$, $B = 0$: the second equation is then satisfied, while the first equation demands that $\cos(kL/2) = 0$, i.e. $kL/2 = n\pi/2$ for n odd; this gives energy quantisation:

$$\begin{aligned} E &= E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} \qquad \text{for} \qquad n = 1, 3, 5, && (61) \\ \psi_n(x) &= \sqrt{\frac{2}{L}} \cos(n\pi x/L) && (62) \end{aligned}$$

The constant $A = \sqrt{2/L}$ was determined by normalising the wave function.

(B) $B \neq 0$, $A = 0$: the first equation is then satisfied, while the second equation demands that $\sin(kL/2) = 0$, i.e. $kL/2 = n\pi/2$ for n even; this gives energy quantisation:

$$\begin{aligned} E &= E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} \qquad \text{for} \qquad n = 2, 4, 6, && (63) \\ \psi_n(x) &= \sqrt{\frac{2}{L}} \sin(n\pi x/L) && (64) \end{aligned}$$

The constant $B = \sqrt{2/L}$ was determined by normalising the wave function. The solutions are summarised in the following two pages.

A comment: Notice that the energy eigenstates $\psi_n(x)$ are either even functions of x, $\psi_n(x) = \sqrt{2/L}\cos(n\pi x/L)$, with $\psi_n(-x) = +\psi_n(x)$ or odd functions of x, $\psi_n(x) = \sqrt{2/L}\sin(n\pi x/L)$ with $\psi_n(-x) = -\psi_n(x)$. We say that the energy eigenstates have definite parity: even functions are called positive parity (or +1);

---

[8] We do not match the derivatives because the potential is infinite at $x = \pm L/2$: there is a kink in the wave function at these points. See Section 6 for a discussion.

odd functions negative parity (or -1). This is a consequence of the symmetry of the potential about our chosen origin $V(-x) = V(x)$ see later for a proof. If we had chosen our origin of coordinates not to be at the centre of the well (the symmetry point), but somewhere else such as the left-hand end of the well, this would have made the definite parity of the eigenstates less apparent (until we plotted them), although we can then use a single function to represent them all. Let us choose a new coordinate system x', with the well running from $x' = 0 \rightarrow L$. The relationship between our original coordinate system and this new one is,

$$x = x' - \frac{L}{2} \tag{65}$$

Substituting for x in our expressions for the eigenstates then yields,

$$\psi_n(x') = \sqrt{\frac{2}{L}} \sin(n\pi x'/L) \qquad \text{forall } n = 1, 2, 3, \tag{66}$$

Here we used the following identities,

$$\begin{aligned} \sin(n\pi x'/L - n\pi/2) &= \pm \sin(n\pi x'/L) \qquad \text{for n even} && (67) \\ \cos(n\pi x'/L - n\pi/2) &= \pm \sin(n\pi x'/L) \qquad \text{for n odd} && (68) \end{aligned}$$

We have then ignored the overall sign differences, as this does not change the physics, which only depends of $|\psi|^2$. This equivalent form of the eigenstates is used in Problems 2.

The eigenfunctions, $\Psi_n(x,t)$, specified by the quantum number n correspond to the energy eigenvalues

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad n = 1, 2, 3, \tag{69}$$

Note that the even functions of x (parity +1) have n odd; the odd functions (parity -1) have n even.

$$\begin{aligned} \Psi_1(x,t) &= \sqrt{\tfrac{2}{L}} \cos(\pi x/L) e^{-iE_1 t/\hbar} \qquad E_1 = \tfrac{{}^2\pi^2}{2mL^2} && (70) \\ \Psi_2(x,t) &= \sqrt{\tfrac{2}{L}} \sin(2\pi x/L) e^{-iE_2 t/\hbar} \qquad E_2 = \tfrac{4^2\pi^2}{2mL^2} && (71) \\ \Psi_3(x,t) &= \sqrt{\tfrac{2}{L}} \cos(3\pi x/L) e^{-iE_3 t/\hbar} \qquad E_3 = \tfrac{9^2\pi^2}{2mL^2} && (72) \\ \Psi_4(x,t) &= \sqrt{\tfrac{2}{L}} \sin(4\pi x/L) e^{-iE_4 t/\hbar} \qquad E_4 = \tfrac{16^2\pi^2}{2mL^2} && (73) \end{aligned}$$

There are several noteworthy general features of these eigenstates; we will encounter these throughout the course:

(1) The ground state (i.e. the lowest energy state, $n = 1$) has non-zero energy. This is a uniquely quantum mechanical effect - a consequence of Heisenbergs uncertainty principle for a localized particle. Can you show this?

(2) The eigenstates are either odd or even functions of x; i.e. $\psi(-x) = \pm\psi(x)$. Thus the ground state ($n = 1$) is even; the first excited state ($n = 2$) is odd; the second excited state ($n = 3$) is even; etc. We will discover later that this is a consequence of a symmetry of the potential, $V(-x) = V(x)$.

(3) Eigenstates corresponding to different energies are orthogonal:

$$\int_{-\infty}^{\infty} \psi_n^*(x)\psi_m(x)dx = 0 \qquad \text{for} \qquad n \neq m \tag{74}$$

Can you show this explicitly for a few of the infinite square well eigenstates[9]? We can combine this with the normalisation condition into the orthonormality condition:

$$\int_{-\infty}^{\infty} \psi_n^*(x)\psi_m(x)dx = \delta_{nm}\,, \tag{75}$$

where δ_{nm} is the Kronecker delta symbol ($= 1$ for $n = m$, $= 0$ for $n \neq m$).

(4) The most general solution, $\Psi(x,t)$, to the time-dependent Schrödinger equation (TDSE) for the infinite square well is a linear superposition of these eigenstates:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \Psi_n(x,t)\,, \tag{76}$$

where c_n are constants and the time-dependent energy eigenstates are

$$\Psi_n(x,t) = \psi_n(x)e^{-iE_nt/\hbar} \tag{77}$$

You may wonder about the physical significance of a state Ψ, which does not have a definite energy: what does it mean? This question is at the heart of quantum mechanics and will be addressed at various stages in the course.

(9) Momentum in Quantum Mechanics.

Our next task is to find a definition for the momentum variable in quantum mechanics. This may seem obvious because according to de Broglie, by analogy with a classical monochromatic plane wave, a free particle of momentum $p = \hbar k$ and energy $E = \hbar\omega$ has a wave function:

$$\Psi(x,t) = Ne^{i(kx-t)} = Ne^{i(px-Et)/\hbar} \tag{78}$$

---

[9] To perform the integrals use the trigonometric identities $\cos A \cos B = \frac{1}{2}(\cos(A-B) + \cos(A+B))$ and $\sin A \sin B = \frac{1}{2}(\cos(A-B) - \cos(A+B))$.

where N is a normalisation constant. So far so good; but we now face a difficulty: The de Broglie wave has a constant probability density, $|\Psi(x,t)|^2 = N^2$, presumably representing a particle (or particles) that are equally likely to be found anywhere in space, but is therefore not normalisable,

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = \infty \tag{79}$$

The de Broglie wave is actually an idealization, just as a plane monochromatic light wave is. To represent a more realistic situation such as a finite wave train or a particle localised in some finite region of space Δx say we need to construct a wave packet by superimposing infinitely many de Broglie waves of different wavelengths (or momenta). A typical wave packet will then have a whole range of wavelengths or momenta Δp, with a single de Broglie wave being a typical representative of those making up the packet. Now, we know that a wave packet made up from a superposition of a range of wave numbers Δk has a width Δx given by the bandwidth theorem:

$$\Delta k \Delta x \simeq \pi \tag{80}$$

Our quantum mechanical wave packet will have the same property, where $p = \hbar k$. Multiplying the bandwidth relation by $\hbar$ gives the uncertainty relation,

$$\Delta p \Delta x \simeq \pi \hbar \tag{81}$$

This is Heisenbergs uncertainty relation, which can be shown to have the precise form:

$$\Delta p \Delta x \geq \frac{\hbar}{2} \tag{82}$$

This is an expression of and a consequence of the wavelike nature of quantum mechanical particles. Since both the position and momentum of the wave packet do not have definite values, but have a spread, we call Δp and Δx the uncertainties in momentum and position.

Notice that we have already learned how to compute the position uncertainty from the wave function: we first compute the averages (or expectation values) $\langle x \rangle$ and $\langle x^2 \rangle$ and hence obtain the position uncertainty

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} \tag{83}$$

The natural question now arises: how might we compute from the wave function the corresponding momentum expectation values, $\langle p \rangle$ and $\langle p^2 \rangle$ and hence obtain the momentum uncertainty:

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} \qquad ? \tag{84}$$

The answer is surprising: just as $\langle x\rangle$ is given by the averaging procedure

$$\langle x\rangle = \int_{-\infty}^{\infty} \Psi^* x \Psi dx \,, \tag{85}$$

so the momentum average is obtained from

$$\langle p\rangle = \int_{-\infty}^{\infty} \Psi^* \hat{p} \Psi dx \,, \tag{86}$$

where $\hat{p}$ is a differential operator operating on the wave funtion to its right:

$$\hat{p} = -i\hbar \frac{\partial}{\partial x} \tag{87}$$

How can we possibly justify this apparently bizarre idea that a dynamical variable is represented by an operator? In the Quantum Mechanics B course this question will be studied in greater depth, but here we simply provide some evidence.

(a) For a single de Broglie wave this momentum operator $\hat{p}$ extracts its momentum: the de Broglie wave is an eigenstate of the momentum operator with eigenvalue p (not $\hat{p}$, note!):

$$\hat{p}\Psi(x,t) = -i\hbar \frac{\partial}{\partial x} e^{i(px-Et)/\hbar} = p e^{i(px-Et)/\hbar} \tag{88}$$

i.e.

$$\hat{p}\Psi(x,t) = p\Psi(x,t) \tag{89}$$

This seems eminently reasonable and makes equal sense when used to find the average momentum of a wave packet (see QMB).

(b) There is apparently no sign of the momentum p in the energy eigenstates for the infinite square well:

$$\Psi_n(x,t) = \sqrt{\frac{2}{L}} \cos(n\pi x/L) e^{-iE_n t/\hbar} \qquad n = 1, 3, 5, \tag{90}$$

but we can unscramble this by writing the cosine as a combination of complex exponentials and then combining these with the timedependent exponential to obtain a highly suggestive form:

$$\Psi_n(x,t) = \sqrt{\frac{2}{L}} \frac{1}{2} \left\{ e^{i(px-E_n t)/\hbar} + e^{i(-px-iE_n t)/\hbar} \right\} \tag{91}$$

where we have written

$$p = \frac{n\hbar\pi}{L} \tag{92}$$

We now recognise the two terms as de Broglie waves of momentum respectively $p = +n\hbar\pi/L$ running to the right and momentum $-p = -n\hbar\pi/L$ running to the left. They have equal amplitudes. You should now recall the normal models of vibration of a string fixed at its ends: there, too, you found that the standing waves (or normal modes) are made up of precisely the same superposition of running waves which reflect repeatedly from the fixed ends. They combine (interfere) to make a standing wave packet. Similarly, the eigenstates of the infinite square well the escapeproof box are wave packets made up from the superposition of just two de Broglie waves of equal and opposite momenta. The state itself does not have a definite momentum: it has a spread of two momenta $+p$ and $-p$, so its average momentum is zero and its momentum uncertainty is of order $\Delta p \simeq 2p$ or, equivalently,

$$\Delta p \simeq \frac{2n\hbar\pi}{L} \tag{93}$$

with

$$\langle p \rangle = 0 \tag{94}$$

Let us see if we can use our operator representation of momentum to confirm these reasonable estimates; success will be evidence in favour of our choice of the momentum operator. First the average for the n-th eigenstate:

$$\begin{aligned} \langle p \rangle &= \int_{-L/2}^{+L/2} \Psi^* \hat{p} \Psi dx\,, \qquad \text{(remember } \Psi = 0 \text{ outside the box)} && (95) \\ &= -i\hbar \frac{2}{L} \int_{-L/2}^{+L/2} \cos\left(\frac{n\pi}{L}x\right) \frac{\partial}{\partial x} \cos\left(\frac{n\pi}{L}x\right) dx && (96) \\ &= i\hbar \frac{2}{L} \frac{n\pi}{L} \int_{-L/2}^{+L/2} \cos\left(\frac{n\pi}{L}x\right) \sin\left(\frac{n\pi}{L}x\right) dx && (97) \end{aligned}$$

hence

$$\langle p \rangle = 0 \tag{98}$$

The integral vanishes because, (a) the integrand is odd, being a product of an even and odd function of x (cos and sin), and (b) the integration range is symmetric about zero ($-L/2 \to +L/2$). This confirms our expectation and suggests we are on the right track. Now for $\langle p^2 \rangle$:

$$\hat{p}^2 = -\hbar^2 \frac{\partial^2}{\partial x^2} \tag{99}$$

so

$$\begin{aligned}
\langle p^2 \rangle &= \int_{-\infty}^{\infty} \Psi^* \hat{p}^2 \Psi dx = -\hbar^2 \frac{2}{L} \int_{-L/2}^{+L/2} \cos\left(\frac{n\pi}{L}x\right) \frac{\partial^2}{\partial x^2} \cos\left(\frac{n\pi}{L}x\right) dx && (100)\\
&= \hbar^2 \frac{2}{L} \left(\frac{n\pi}{L}\right)^2 \int_{-L/2}^{+L/2} \cos^2\left(\frac{n\pi}{L}x\right) dx && (101)\\
&= \hbar^2 \frac{2}{L} \left(\frac{n\pi}{L}\right)^2 \frac{1}{2} \int_{-L/2}^{+L/2} \left(1 + \cos\left(\frac{2n\pi}{L}x\right)\right) dx && (102)\\
& \qquad\qquad\qquad\qquad (\text{as } \cos^2\theta = \frac{1}{2}(1 + \cos 2\theta)) \\
&= \hbar^2 \frac{2}{L} \left(\frac{n\pi}{L}\right)^2 \frac{1}{2} \left[x + \frac{L}{2n\pi} \sin\left(\frac{2n\pi}{L}x\right)\right]_{-L/2}^{+L/2} && (103)\\
&= \hbar^2 \frac{2}{L} \left(\frac{n\pi}{L}\right)^2 \frac{1}{2} [L + 0] \qquad (\text{as} \sin(\pm n\pi) = 0) && (104)
\end{aligned}$$

hence

$$\langle p^2 \rangle = \left(\frac{n\hbar\pi}{L}\right)^2 \tag{105}$$

Hence, finally we can compute the momentum uncertainty for the n-th eigenstate:

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{\left(\frac{n\hbar\pi}{L}\right)^2 - 0} \tag{106}$$

i.e.

$$\Delta p = \frac{n\hbar\pi}{L} \tag{107}$$

only differing by a factor 2 from our rough estimate given previously. We could now compute the position uncertainty Δx for this state, and check whether the result is consistent with Heisenbergs uncertainty relation for momentum and position. The results are:

$$\langle x \rangle = 0 \qquad (\text{as the integrand is odd in } x) \tag{108}$$

and

$$\langle x^2 \rangle = \frac{L^2}{4} \left(\frac{1}{3} - \frac{2}{n^{22}}\right) \tag{109}$$

so

$$\Delta x = \frac{L}{2} \sqrt{\frac{1}{3} - \frac{2}{n^2\pi^2}} \tag{110}$$

As the negative term in the square root is largest for $n = 1$ (remember n is odd here),

$$\Delta x \geq \frac{L}{2} \sqrt{\frac{1}{3} - \frac{2}{{}^2}} = 0.36\frac{L}{2} \tag{111}$$

We therefore obtain a result consistent with Heisenbergs uncertainty relation,

$$\Delta p \Delta x \geq 0.36\pi\frac{\hbar}{2} = 1.14\frac{\hbar}{2} > \frac{\hbar}{2} \qquad (112)$$

where we have used the fact that $n \geq 1$ for odd n to conclude that

$$\Delta p = \frac{n\hbar\pi}{L} \geq \frac{\hbar\pi}{L} \qquad (113)$$

As a useful way of studying and understanding the above you should repeat these calculations for the odd parity eigenstates of the escapeproof box:

$$\Psi_n(x,t) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)e^{-iE_n t/\hbar} \qquad n = 2, 4, 6, \qquad (114)$$

The results are identical except that for these negative parity states n is now even.

Notice how the position uncertainty depends only very weakly on n and approaches quite rapidly the value

$$\Delta x = \frac{L}{2}\sqrt{\frac{1}{3}} \simeq 0.3L \qquad (115)$$

As we would expect, it is some fraction of the size of the box to which the particle is confined it certainly couldnt be greater than L. Recall that the uncertainty tells us to think of the average position as

$$\langle x \rangle \pm \Delta x \qquad (116)$$

From experiments you have done in the laboratory you might expect to find the particle within the range $2\Delta x$ centred about the average $\langle x \rangle$ about 68% of the time. In fact this is nearly true the for the ground state ($n = 1$) where the figure is 65%; for $n = 2, 3, 4, 5, 6$ it is $56, 47, 51, 60, 62\%$. In fact only for a Gaussian distribution is the figure 68%, and the escapeproof probability distributions $|\Psi_n|^2$ are not Gaussian.

In contrast to the position uncertainty, the momentum uncertainty increases with n because the two superimposed de Broglie waves constituting the eigenstates have momenta proportional to $+n$ and $-n$; therefore their separation is proportional to $2n$. We already noted this before in our rough estimate of Δp;. Thus, as a reasonably good approximation, for the nth eigenstate,

$$\Delta p \Delta x \simeq n\left(\pi\sqrt{\frac{1}{3}}\right)\frac{\hbar}{2} = 1.8n\frac{\hbar}{2} > \frac{\hbar}{2} \qquad (117)$$

As always, this obeys Heisenbergs uncertainty relations.