Introduction to Quantum Mechanics

1. Electron Interference

Most textbooks of quantum mechanics start with Max Planck’s introduction of the “quantum” in the context of blackbody radiation in 1900. Let us break with tradition and start with the discussion of an experiment carried out in 1989. The experiment was done at the Hitachi Advanced Research Laboratory and Gakushuin University in Tokyo, by Tonomura et al.\(^1\) It consisted of a beam of electrons being split into two by an electric field, and then allowed to recombine, very similar to Young’s double slit experiment with light in which a beam of light is split into two by its passage through two closely spaced slits and allowed to recombine on a photographic plate. For convenience, let us call the apparatus a double-slit apparatus for electrons.

The results from this experiment, taken at various times, are shown in the figure. At first, only a few electrons have reached the photographic plate and no pattern is discernible. However, as time passes and more and more “events” are recorded, a definite pattern emerges. The pattern consists of light and dark bands which indicate that the electrons, after passing through (one of) the “slits,” prefer certain regions of the photographic plate and avoid the others.

We can perform a variation of the experiment, by blocking one of the “slits.” The result is that the pattern of alternating dark and bright bands disappears and is replaced by a single bright band directly across from the open slit. This could be considered proof that the electrons in the first experiment were passing through the slit that is now blocked. After all, if they were passing through the other slit, blocking the first one should have no effect on the pattern at all. However, repeating the experiment by closing the first slit and opening the second one leads to the same result: a single bright band directly across from the open slit’s position.

What we have done by this series of experiments is to show that the electrons on the first experiment were passing through both slits. Or have we? There is a possibility that when one of the slits is closed, we caused a traffic jam in the apparatus, similar to closing one of the two lanes of traffic on a busy highway. Even though a car does not use both lanes at once, blocking one lane does have an influence on the flow of traffic through the other!

The novelty of the Tonomura experiment was that this possibility could be completely ruled out. This was accomplished by allowing only one electron at a time in the apparatus. The advances in

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electronics and detection methods finally made this experiment, which could previously be “done” only in one’s imagination, a reality. Specifically, these scientists turned down the intensity of their electron source so low that the electron flux was about 1000 electrons per second. The electrons were calculated to have a speed of $10^8$ m/s, which meant that the electrons, if they were allowed to travel a large distance, would be separated from one another by an average distance of 100 km! In fact, the results shown in Fig. 1 were accumulated under these conditions. There appears to be no way around the conclusion that the electrons must pass through both slits at once! Otherwise, how could they be affected by the open or closed status of the slit through which they did not pass?

The interference of light can be explained only in terms of its wave properties. Therefore, the results of the electron experiment can be considered proof that electrons behave like waves. Louis de Broglie proposed just such a possibility in 1924, proposing that the wavelength of a particle with mass $m$ is

$$\lambda = \frac{h}{mv},$$

where $h$ is Planck’s constant. However, this brings up another difficulty. The electrons make tiny spots on the photographic plate at the point of their impact, clearly a characteristic of particles. If we assume that they are waves when they pass through the slits, how do they manage to turn back into particles at the instant they hit the photographic plate? As scientists, we should demand that any theory we formulate to explain this experiment should also explain how this transformation from wave to particle and vice versa is accomplished.

There is yet another possibility. Our understanding of nature is so completely conditioned by our everyday experience that we have assumed that the same rules that apply to marbles or mustard seeds should apply to electrons as well. Our experiments of first plugging one slit and then the other were based on the assumption that what happens at one slit should have no influence at all on the other. This is called the assumption of locality. If we drop the assumption of locality, we can admit the possibility that what happens at one slit can influence events at the other one, and we will no longer be forced to conclude that the electron was at two places at the same time.

Now, electrons are fairly insubstantial entities. Also, no one has ever seen an electron to know that it is really a particle. Surely, protons and neutrons, which are much more massive and more likely to behave unambiguously like particles, or atoms, which are definitely particles (we now have “visual” evidence, thanks to scanning tunneling microscopy’) will behave differently when subjected to similar experiments. These expectations were dashed in 1991. That year, reports of interference patterns generated using neutrons and atoms were published. These experiments were conducted under “single particle conditions,” i.e., conditions under which the possibility of interactions between the particles while they passed through the experimental apparatus, which could presumably result in “traffic jams,” is ruled out.

Locality has been one of the pillars of classical physics for a very long time. Now, it appears that a theory of matter that explains the results of these experiments must be either (a) one based on particles that have nonlocal interactions, i.e., are influenced by events occurring far from them (far in both space and time!), or (b) one based on waves that can be at two places at once. Either scenario is a departure from our everyday experience and forces us into unfamiliar territory.

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2 Of course, you know already about the de Broglie hypothesis and its experimental verification. However, the verification was done, by George Thompson in the UK and Davisson and Germer in the US, using the diffraction of high intensity electron beams, which allowed the possibility of “traffic jams.”

3 In 1990, Eigler and Schweizer created the IBM logo from xenon atoms by arranging the atoms one at a time using a scanning tunneling microscope. The photographs (see next page) clearly show the atoms as very localized spherical objects. See D.M. Eigler and E. K. Schweizer, Nature 344, 524 (1990).


The IBM logo created by Eigler and Schweizer from xenon atoms on a very cold nickel surface.

The neutron interference pattern obtained by Gähler and Zeilinger. The line is not a fit to the experimental data but, rather, the pattern predicted by quantum mechanics.

The atom interference pattern obtained by Carnal and Mlynek.
The wave mechanics of Schrödinger, first published in 1926 and now synonymous with quantum mechanics, belongs to the second category. Wave mechanics, or quantum mechanics, can exactly predict the results of the Tonomura experiment and the effects of closing one or the other slits. More recently, David Bohm has succeeded in formulating a theory that belongs to the first category which also leads to the same predictions as quantum mechanics. For the time being, we restrict ourselves to the more traditional quantum mechanics, as formulated by Schrödinger, Heisenberg, Born, Bohr, Pauli, and von Neumann and others.

2. The Quantum Mechanical “Explanation” of the Tonomura Experiment

Let us look at how quantum mechanics explains the results of the Tonomura experiment. The reason for the quotes around the word “explanation” above will become clear later.

The Schrödinger equation for a single particle in a one-dimensional Universe is

\[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V \psi = i\hbar \frac{\partial \psi}{\partial t}, \tag{1} \]

where \( m \) is the mass of the particle and \( V \) is the external potential acting on it. Now, in spite of the electric field used to split and recombine the electron beam, the electrons in the double slit experiment can be considered free particles, at least as a first approximation. Therefore, we may set \( V = 0 \). One possible solution to the equation is the traveling wave

\[ \psi(x,t) = A \exp \left[ i(kx - \omega t) \right], \tag{2} \]

where \( A \) is the amplitude of the wave, and \( k \) and \( \omega \) are constants yet to be determined. In terms of physical significance, the magnitude of \( k \) determines the “speed” with which the wave moves, its sign determines whether the wave is moving forward or backwards, and \( \omega \) is a non-negative number that gives the frequency of the wave. Substituting Eq. (2) into Eq. (1), the right hand side gives

\[ i\hbar \frac{\partial \psi}{\partial t} = \omega \hbar \psi, \tag{3} \]

while the left hand sides leads to

\[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = \frac{\hbar^2 k^2}{2m} \psi. \tag{4} \]

Since according to Eq. (1), Eqs. (3) and (4) are equal, we get

\[ k = \sqrt{\frac{2m \omega}{\hbar}}. \tag{5} \]

Thus, choosing a value for \( k \) determines the value of the other parameter, \( \omega \), in the wave function.

An even more intuitive picture of the wave is obtained if we replace the constants \( k \) and \( \omega \) with the wavelength and period of the wave. This can be done as follows: at time \( t = 0 \),

\[ \psi(x,0) = A e^{ikx}. \]

At the origin \( x = 0 \), \( \psi(0,0) = A \). By wavelength \( \lambda \), we mean the distance the wave must travel before its amplitude will return to the same value \( A \). Since \( e^{2\pi i} = 1 \), we can see that \( \psi = A \) when \( kx = k\lambda = 2\pi \). By similar arguments, we can show that the period \( \tau \) of the wave should satisfy \( \tau \omega = 2\pi \). Thus, we have

\[ \frac{k}{\lambda} = \frac{2\pi}{\hbar}; \quad \omega = \frac{2\pi}{\tau}, \tag{6} \]

which leads to
\[ \psi(x, t) = A \exp \left[ 2\pi i \left( \frac{x}{\lambda} - \frac{t}{\tau} \right) \right]. \]  

(7)

Now let us consider the double slit experimental set up shown in the figure below.

Let us denote the wave exiting slit 1 by \( \psi_1 \) and that exiting slit 2 by \( \psi_2 \). We are interested in the behavior of the total amplitude of the two waves when they reach the point \( P \) on the screen, at time \( t \). The total wave is

\[ \psi = \psi_1 + \psi_2 = A_1 \exp \left[ 2\pi i \left( \frac{x_1}{\lambda} - \frac{t}{\tau} \right) \right] + A_2 \exp \left[ 2\pi i \left( \frac{x_2}{\lambda} - \frac{t}{\tau} \right) \right] \]

\[ = \left[ A_1 e^{2\pi i x_1 / \lambda} + A_2 e^{2\pi i x_2 / \lambda} \right] e^{-2\pi it / \tau}. \]

This is a complex quantity, which takes on positive and negative values. Since negative values do not have physical significance when we are talking about the brightness (wave amplitude) of a certain spot on the screen, we may want to look at \( |\psi| \), which is a real, non-negative quantity. In fact, it is even easier to look at \( |\psi|^2 \). Recall that the “absolute value squared” of a complex number is obtained by multiplying it with its own complex conjugate, and that the complex conjugate is obtained by replacing all occurrences of “\( i \)” with “\( -i \).” Therefore,

\[ |\psi|^2 = \left[ A_1 e^{2\pi i x_1 / \lambda} + A_2 e^{2\pi i x_2 / \lambda} \right] \left[ A_1^* e^{-2\pi i x_1 / \lambda} + A_2^* e^{-2\pi i x_2 / \lambda} \right] \]

\[ = |A_1|^2 + |A_2|^2 + A_1^* A_2 e^{2\pi i (x_2 - x_1) / \lambda} + A_1 A_2^* e^{-2\pi i (x_2 - x_1) / \lambda}. \]

(8)

We may assume, without any loss of generality, that the amplitudes \( A_1 \) and \( A_2 \) are real. Then Eq. (8) simplifies to

\[ |\psi|^2 = A_1^2 + A_2^2 + 2A_1 A_2 \cos \left[ 2\pi \left( \frac{x_2 - x_1}{\lambda} \right) \right], \]

(9)

which describes the observed intensity variations, as shown in the figure below.
The left panel shows the amplitudes of $|A_1|^2$ and $|A_2|^2$ by themselves and the sum of the two. We have assumed that the amplitudes $A_1$ and $A_2$ behave like Gaussians when plotted as a function of $(x_1-x_2)/\lambda$. This is a reasonable assumption since, due to wave diffraction, the brightness would fall off rather gradually on either side of the bright band across from the slit. The right panel shows a plot of Eq. (9). The qualitative similarities to the neutron and atom diffraction patterns are immediately obvious. In fact, the line passing through the data points in the neutron diffraction experiment has no adjustable parameters but passes through all the experimental results perfectly.

Thus, quantum mechanics has spectacularly succeeded in explaining the rather puzzling results of the double slit experiments.

Or has it, really? After we compare Eq. (9) or similar relationships for $|\psi|^2$ with the experimental results and note the near perfect agreement, what have we learned? We still do not “understand” how these results come about. We still do not have an explanation of how an atom, which appears to be a particle in the IBM logo, turns into a wave as it passes through the slits and back to a particle again once it has passed through the slits. In fact, we do not know anything about what the particles do between the source and the screen. If we look back at the “explanation” (now I hope the reason for the “quotes” is clear), it is obvious that quantum mechanics deals with the wave functions rather than the particles themselves. Aside from the incorporation of its mass into the Schrödinger equation, the rest of the treatment does not rely on the particle at all but rather on the solution to the equation, $\psi$.

To understand what is going on in these experiments, let us look at experiments with photons, which are much easier to conduct (and, therefore, have been done many times over). Let us put photon detectors in each of the slits and conduct the experiment with a light source so dim that only one photon at a time enters the apparatus. Then, we find that the photons are detected at either one slit or the other but not both at the same time! These observations are consistent with particle behavior. Once again, the interference pattern on the screen is built up slowly, from individual events, one at a time.

Let us repeat the experiment with the following modification: we will keep slit 1 open and close slit 2 for half the time and then close slit 1 and open slit 2 for the remainder of the time. Since the order in which the photons pass through slit 1 and slit 2 should not matter (they were totally random in the first experiment) the pattern on the screen should be the same as in the first case. However, this is not the case. What we get looks like the sum of $|A_1|^2$ and $|A_2|^2$ on the previous page. If both slits are left open but the photon detector is placed only in one of them, so that we can tell which photon passes through which slit, again the interference pattern is not observed!

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6 The detectors will let the photons pass through unimpeded. We will skip the details because your instructor has no idea how to build one!
Indeed, it is quite impossible to visualize what is going on in these experiments. Whether we examine photons, electrons, neutrons or atoms, the complex patterns observed downstream from a pair of slits confound our intuitive understanding of particles. Quantum mechanics, of course, predicts the correct outcome in each of these cases (we will come back to the last experiment for more discussion later). Quantum mechanics thus provides us with the means to reproduce or predict the outcomes of experiments. It does this spectacularly well. On the other hand, it does not provide us with a better understanding of the results the same way classical mechanics provide us with an understanding of planetary motion or kinetic theory of gases provides us with an understanding of pressure and temperature. This often leads to a situation in quantum mechanics where, after all the mathematical simplifications, we are left with a result the meaning of which we then have to interpret.

This situation has led to two major camps among quantum physicists. One camp insists that the wave function $\psi$ contains all that can ever be known about the system under consideration and expecting anything more is foolish. After all, why should we humans demand that a fundamental theory of matter, which deals with exceedingly small entities such as electrons and neutrons, conform to our intuitive understanding of the world which is based on the behavior of massive objects like marbles and rocks? This camp generally maintains that quantum mechanics is a complete theory and provides us with all that we need to know, namely, the ability to accurately predict the outcomes of experiments. This camp is by far the overwhelming majority and claims the membership of some very impressive scientists, such as Bohr, Heisenberg, and Born. This is the traditional, “Copenhagen” school of quantum mechanics, or the quantum orthodoxy.

The other camp maintains that science should provide us with theories that explain what we observe, not theories that need to be interpreted. These physicists maintain that quantum mechanics is fine as a statistical theory of matter and makes perfect sense when applied to large ensembles of identically prepared systems. However, they continue to hold out hopes for a theory that explains the behavior of an individual electron or neutron in the double slit experiment. In this camp too we can count some impressive names: Einstein, de Broglie, Schrödinger, John Bell, and David Bohm.

Despite seventy-five years of progress in theory and experiments since the advent of modern quantum mechanics, we do not have a fundamentally better understanding of the behavior of atomic and subatomic particles other than to know that they steadfastly resist being explained in terms of our ordinary experiences. At the same time, quantum mechanics has been subjected to progressively more stringent tests and has passed each of them spectacularly well.

Given this state of affairs, we will restrict ourselves to Schrödinger’s quantum mechanics and see how we tackle problems of different types. Often in this process, you will start getting the funny feeling that although we are cranking out lots of equations, at the end of it all, things remain as cloudy as before. From what we have discussed here, you should remember that this feeling comes as part of the package when studying quantum mechanics. When, after many years of study, people finally say that they are “comfortable” with quantum mechanics, what they mean is not that they “understand” the behavior of quantum systems any better but, rather, that they have learned to live without that understanding! This is the nature of the quantum beast.

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7 The paper W. Heisenberg, Z. für Phys. 33, 879 (1925) on “matrix mechanics” is considered the first paper on modern quantum mechanics. The words “quantum mechanics” first appeared as the title of the paper M. Born, Z. für Phys. 33, 379 (1924) in which Born thanks his assistant, W. Heisenberg, for help with the calculations. The theories of the atom in existence before that time are now referred to as the “old quantum theory.”

8 I very highly and strongly recommend two books (I have received inspiration, words, and figures from these sources): The Infamous Boundary, by David Wick (Birkhäuser, Boston, 1995) and The Quantum Challenge, by G. Greenstein and A. G. Zajonc (Jones and Bartlett, Sudsbury, MA 1997) for very nice summaries of the historical development and the main questions that remain unanswered in quantum mechanics.
3. “Meaning” of the wave function

We have seen that quantum mechanics does not afford us the luxury of insights into the behavior of systems that obey its predictions. This brings up the question of what exactly the wave function stands for. There are many opinions but let us examine the most widely accepted one, which is due to the German scientist, Max Born. This “interpretation” actually pertains not to \( \psi \) itself but, rather, to \( |\psi|^2 \). The interpretation becomes quite clear from Eq. (9) and from the photograph of electron interference patterns on page 1. The pattern on the bottom panel of this photograph is built up from 70,000 individual electron impacts. It is clear that the electrons follow the pattern laid down by expressions like the one we derived in Eq. (9) for \( |\psi|^2 \). Therefore, we may say that the value of \( |\psi|^2 \) at a spot gives the probability for an electron to end up at that spot. If \( |\psi|^2 \) is large at a certain location, we expect that region to become “bright” with electron impacts after sufficient events have been accumulated. On the other hand, we would expect regions where \( |\psi|^2 \) is small to remain virtually free of electron impacts even at very long times. If we imagine a small element of length \( dx \) (or an area element \( dxdy \) in two dimensions or a volume element \( dx dy dz \) in three dimensions), the value of \( |\psi|^2 dx \) is the probability for finding an electron within that interval. The units of the wave function are such that quantities like \( |\psi|^2 dx \) are dimensionless. Since, for a three dimensional wave function \( |\psi|^2 \) will have to have dimensions of \( 1/\text{volume} \), the quantity \( |\psi|^2 \) by itself is called probability density or probability distribution.

This interpretation is obviously statistical in nature. It is also true that the probability distribution for the Tonomura experiment does not become evident until a large number of events have been accumulated. It is generally true that for quantum systems, a very large number of “measurements” are usually taken for each property of interest. Because of this, one would think that the view that quantum mechanics is a statistical theory of matter will be readily accepted by all. Unfortunately, that is not the case. The Copenhagen view vehemently denies the possibility that the statistical interpretation of \( |\psi|^2 \) implies that a deeper, non-statistical, theory exists from which quantum mechanics can be derived, just as the statistical kinetic theory of gases can be derived from classical mechanics applied to individual atoms and molecules of a gas. According to this view, the seemingly statistical nature of quantum mechanics arises from a fundamental limit that nature places on the accuracy of our measurements on quantum systems. This limit was discovered by Heisenberg, who set out to reconcile the tracks left by electrons in Wilson cloud chambers\(^9\) with the matrices of his own formulation of quantum mechanics and the waves of Schrödinger’s mechanics.

4. The Uncertainty Principle

There are a variety of ways to derive Heisenberg’s Uncertainty Principle. We will sketch one here and do a much more rigorous job when we discuss the mathematical tools of quantum mechanics. Heisenberg started out by asking how one would observe an electron in motion. To see an object, we rely on photons scattered off the object into our eyes, which then inform us of the object’s position. To accurately determine the electron’s position, we would need to use light of very short wavelength. So, Heisenberg proposed a thought (gedanken) experiment using a gamma ray microscope, shown in the figure. The impact of the photon of wavelength \( \lambda \) on the electron causes the electron to be scattered, which introduces a spread in the scattering angle of the photon. If the photon enters the microscope and is detected, the maximum

\(^9\) Cloud chambers contained air supersaturated with moisture so that ionizing particles such as electrons would leave a trail of water droplets in their wake, much like an airliner leaving vapor trails at high altitudes.
scattering angle is $\theta$, as shown in the figure. Since the light used has a finite wavelength, the spot created on the screen will have a finite extent. From the extent of this spot, it is possible to calculate the minimum uncertainty (or experimental error) in the measurement of the electron’s position. This is given by

$$\Delta x \approx \frac{\lambda}{\sin \theta}. \quad (10)$$

Now, the scattering also induces a spread in the momentum of the photon$^{10}$ since its direction of propagation after the collision with the electron is known only to within the angle $\theta$. This can be shown to be equal to

$$\Delta p \approx \frac{h}{\lambda} \sin \theta. \quad (11)$$

From Eq. (10) and (11), it is very easy to see that

$$\Delta x \Delta p \approx h. \quad (12)$$

Note that this equation is independent of all experimental parameters including the wavelength of the light and the aperture of the optics, implying that the product of the uncertainties in position and momentum can never be reduced to zero. This relationship, therefore, sets a fundamental limit on the accuracy of our measurements of positions and momenta of quantum particles. This does not, of course, mean that it is impossible to know the momentum or the position of a particle precisely. It simply means that in order to gain great accuracy in a momentum measurement, we should be willing to sacrifice all knowledge about the position of the particle, essentially giving up the right to call it a particle. On the other hand, if we wish to measure the position very precisely, we must tolerate a large uncertainty in the momentum, which is equivalent to abandoning the wave picture.$^{11}$ This scenario is illustrated in the figure above. Each of the shaded rectangular regions in this figure has the same area. However, the spread in the coordinate $x$ and in the momentum $p$ for each of them is different.

Although Bohr at first hated Heisenberg’s result, he eventually made it the basis for his “Complementarity” principle which, as far as anyone can tell,$^{12}$ means that one needs mutually conflicting pictures (such as wave and particle) to fully explain nature. However, these mutually conflicting pictures emerge from mutually exclusive experimental arrangements. So, for experiments in which the wave nature of matter is demonstrated, an explanation in terms of the particle nature is impossible, and vice versa. Neither picture contains the whole truth and so both are necessary. In practice, most physicists learn to think in terms of both at the same time, and we call these fuzzy things “wave packets.”

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$^{10}$ This can be treated like a collision of billiard balls, using classical mechanics. Experiments of Compton in 1922 established that photons and electrons undergo collisions in which the classical mechanical law of conservation of momentum is obeyed.

$^{11}$ The reason will become clear in the next few pages.

$^{12}$ Bohr wrote in English (so, translation is not the problem) but his style was such that he often left the meaning unclear. One passage he wrote as the final response to Einstein’s objections to the Copenhagen view –to which Einstein didn’t respond, thereby giving Bohr victory by default in the minds of most physicists– was completely incomprehensible to most people including Einstein. A few years later, Bohr admitted it didn't make any sense to him either! See Wick’s book (footnote 8) for a well-researched and balanced account of the Bohr-Einstein debates.
5. Quantum description of a particle: Wave packets and the superposition principle

There is one rather surprising thing about the Schrödinger equation: it is linear in $\psi$. The consequence of this is that waves corresponding to different values of the parameter $k$ (see Eq. 2; note that this also determines the value of $\omega$ through Eq. 5) can be added together to form new solutions of the Schrödinger equation. The values of $k$ and the amplitudes that make up such a “composite” wave can be chosen to give rise to a function whose highest amplitude occurs over a small range $\Delta x$. This is illustrated in the figure to the left. Such a composite wave is called a wave packet, and the method of its construction is called the superposition of waves.

Suppose we wish to construct a wave packet that has a specific shape at a particular value of time. This may be expressed as

$$\phi(x, t) = \sum_{k=-K}^{K} A(k) e^{i(kx-\omega t)t},$$  

(13)

where the $A(k)$ are the amplitudes. In general, we may wish to choose the values of $k$ from a continuous range rather than a discrete one. In that case, we would write

$$\phi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{i(kx-\omega t)} dk,$$

(14)

where the factor of $1/\sqrt{2\pi}$ is irrelevant for our discussion. Eq. (14) is called a Fourier transform, which transforms the integrand, which is a function of $k$, $x$, and $t$, to a function of just $x$ and $t$. The wave packet at $t = 0$ can be defined as

$$\phi(x, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{ikx} dk.$$  

(15)

In order to obtain the weight function $A(k)$, the following “inverse” Fourier transform is used:

$$A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(x, 0) e^{ikx} dx.$$  

(16)

Thus, we can choose the shape of the wave packet $\phi(x,0)$ and obtain the weight function from Eq. (16). Since the frequency $\omega$ is a function of $k$, the weight function $A(k)$ is sufficient to calculate the frequency-amplitude distribution of the wave packet or, in other words, the “spectrum” of the wave packet.

Let us consider a simple case where $A(k)$ is given by a function that has a maximum value at $k = k_0$, and smoothly falls off to half that value at $k = k_0 \pm \Delta k/2$. Now, we will construct a wave packet out of just three plane waves, with $k = k_0$, $k_0 + \Delta k/2$ and $k_0 - \Delta k/2$. Thus, we have

$$\phi(x, 0) = \frac{A(k_0)}{\sqrt{2\pi}} \left[ e^{ik_0 x} + \frac{1}{2} e^{i(k_0 + \Delta k/2)x} + \frac{1}{2} e^{i(k_0 - \Delta k/2)x} \right]$$  

(17)

$$= \frac{A(k_0)}{\sqrt{2\pi}} e^{ik_0 x} \left[ 1 + \cos \left( \frac{\Delta k}{2} x \right) \right].$$
Such a wave packet is shown in the figure to the left, in thick solid line, along with the three waves that make it up in dashed \((k_0+\Delta k)\), solid \((k_0)\), and dotted \((k_0-\Delta k)\) lines. It is clear from Eq. (17) that the wave packet has a maximum value at \(x = 0\). This is not surprising, since it is clear from the figure that all the waves making up the wave packet are perfectly in phase at this point. As we move away from this point in either direction, the magnitude of the wave packet decreases. This is because the waves that make up the wave packet are increasingly out of phase and interference effects set in. This becomes clear with the recognition that the amplitude of the wave packet goes exactly to zero at the two limits of \(x\) plotted in the figure. The interference between the wave with \(k = k_0\) and the two with \(k = k_0 \pm \Delta k\) becomes completely destructive when the argument of the cosine term is equal to \(\pm \pi\), i.e., when

\[
x = \pm \frac{2\pi}{\Delta k}.
\]

Therefore, the total distance along the \(x\)-coordinate from the point where the destructive interference is complete to the other is

\[
\Delta x = 2x = \frac{4\pi}{\Delta k},
\]

which, of course, leads to

\[
\Delta x \Delta k = 4\pi,
\]

an expression very similar to the Heisenberg Uncertainty principle. In fact, the similarity is no accident. Recall that according to Planck’s hypothesis, \(E = h\nu = \hbar \omega\). Also, for a free particle,

\[
E = \frac{1}{2}mv^2 = \frac{p^2}{2m}.
\]

Therefore, combining these two relationships and substituting for \(\omega\) from Eq. (5), we get

\[
\frac{\hbar^2k^2}{2m} = \frac{p^2}{2m},
\]

or \(k = p/\hbar\). Thus, Eq. (18) can be re-written as

\[
\Delta x \Delta p = 4\pi \hbar = 2\hbar,
\]

which is twice the value we obtained in Eq. (12). In fact, it is possible to construct wave packets for which the product \(\Delta x \Delta p\) is much larger or somewhat smaller than the limit in Eq. (19). However, it is impossible to construct a wave packet for which this product is smaller than \(\hbar\). In fact, a more accurate statement of the Uncertainty Principle is

\[
\Delta x \Delta p \geq \frac{\hbar}{2},
\]

which we will rigorously derive later in a much more general context.

The physical implications of the results obtained above are as follows: in order to describe a particle using waves, we need to construct a wave packet that has a rather small spread in the \(x\) direction, i.e., a small value of \(\Delta x\). However, in order to do this, we will need to add together waves that have large \(\Delta k\) or
\( \Delta p \). On the other hand, a wave extends over large regions of space, i.e., \( \Delta x \) is very large. This can be achieved only by keeping \( \Delta k \) very small. These comments help to clarify the statements made in connection with footnote 11. All of this is, of course, completely consistent with Bohr’s principle of the complementary relationship between position and momentum in quantum mechanics.

Let us now examine the time evolution of a wave packet. For simplicity, we will consider the wave packet given by Eq. (17) at \( t = 0 \). Noting again that the angular frequency \( \omega \) is dependent on \( k \), at time \( t \) we get

\[
\phi(x, t) = \frac{A(k)}{\sqrt{2\pi}} e^{\frac{i(k_0 - \Delta k)t}{2}} \left[ 1 + \cos \left( \frac{\Delta k}{2} x - \frac{\Delta \omega}{2} t \right) \right].
\]

The maximum of the wave packet has now moved from \( x = 0 \) to a value of \( x \) which makes the argument of the cosine term vanish. This point is, of course, at

\[
x(t) = \frac{\Delta \omega}{\Delta k} t = v_g t,
\]

where we have identified the ratio \( \Delta \omega / \Delta k \) as the group velocity, \( v_g \), of the wave packet. A more accurate definition is

\[
v_g = \left( \frac{d\omega}{dk} \right)_{k_0} = \frac{\hbar k_0}{m},
\]

where the second equality is readily obtained by using Eq. (5). Another useful quantity to introduce in this context is the phase velocity of a single wave, given by

\[
v_p = \frac{\omega}{k} = \frac{\hbar k}{2m}.
\]

Note that the definition of the group velocity is identical to the classical definition of velocity for a particle once the identification that \( p = \hbar k \) is made. This is an important result. This means that if we attempt to describe a particle using a wave packet whose \( \Delta x \) and \( \Delta k \) are negligible compared to the dimensions of the particle—in other words, try to describe a macroscopic system—we would get the result that the maximum of the wave packet obeys the laws of classical mechanics. Thus, quantum mechanics yields results that are compatible with classical mechanics when the particles under consideration become sufficiently large and/or massive. This is, of course, required in order for quantum mechanics to be an acceptable description of nature. This requirement is called the correspondence principle.

6. The time-independent Schrödinger equation: Stationary states

Consider the special case where a wave packet can be expressed in the form

\[
\phi(x, t) = e^{-i(kx - \omega t)} + e^{i(kx + \omega t)} = e^{i(kx + e^{-ikt})} e^{i\omega t} = 2 \cos(kx) e^{i\omega t}.
\]

The zero’s of such a wave occur whenever \( \cos(kx) = 0 \), i.e., at \( kx = \pm \pi / 2, \pm 3\pi / 2, \pm 5\pi / 2, \ldots \), regardless of the value of \( t \). In other words, these waves do not travel. The reason, of course, is that the positive and negative values of the momentum represented by \(+k\) and \(-k\), respectively, yield a wave packet of zero momentum. Such waves are called standing waves.
Standing waves can be substituted into the Schrödinger equation to eliminate its time dependence. We start with a standing wave which we express as

$$\phi(x, t) = \psi(x)e^{-i\omega t/\hbar}, \quad (24)$$

where we have used the definition of the angular frequency $$\omega$$ and the quantum hypothesis. Now, we substitute $$\phi(x, t)$$ into the Schrödinger equation to get

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \psi(x) \right] e^{-i\omega t/\hbar} = i\hbar \frac{\partial}{\partial t} \psi(x)e^{-i\omega t/\hbar}. \quad (25)$$

Since only the exponential term depends on time on the right hand side, we get

$$i\hbar \frac{\partial}{\partial t} \psi(x)e^{-i\omega t/\hbar} = E\psi(x)e^{-i\omega t/\hbar}. \quad (26)$$

Substituting this result back into Eq. (25) and eliminating the exponential term from both sides, we get the time-independent Schrödinger equation,

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)\psi(x) = E\psi(x). \quad (27)$$

For the next several weeks, we will be focusing on this equation and its solutions for various choices of the potential energy function $$V(x)$$. 