Chapter 5. Wave Properties of Matter

Notes:

- *Most of the material in this chapter is taken from Thornton and Rex, Chapter 5, and "The Feynman Lectures on Physics – Vol. I" by R. P. Feynman, R. B. Leighton, and M. Sands, Chapter 37 (1963, Addison-Wesley).*

5.1 The Wave Character of Matter

The road that led to the advent Bohr's atomic model was sparked by a series of bold ideas and discoveries that allowed physicist to make significant leaps in their interpretation of experimental data and understanding of the microscopic world. As we have seen, it all started with Planck's quantization idea to solve the blackbody radiation problem, followed by Einstein's theory of the particle-like behaviour of light to explain the photoelectric effect, and then Bohr's radical view of the atom with the introduction of stationary states and the quantization of the electron's orbital angular momentum. In the years that followed not only was the quantum nature of the atom gaining in acceptance, but the *wave-particle duality* of radiation, introduced by Einstein, was also firmly established. Indeed, further evidence was provided by the confirmation that X-rays, which behaved like particles in Compton scattering, were just a shorter (than light) wavelength realization of electromagnetic radiation. This was established with their diffraction through crystalline structures, which provided the right aperture sizes for these short wavelengths (approximately $10^{-11}-10^{-8}\,\mathrm{m}$).

It should therefore not be too surprising that the next major step forward came with another bold and revolutionary idea, this time provided the French physicist **Louis V. de Broglie** (1892-1987). Being fully aware of the pioneering work of Einstein on the photoelectric effect, de Broglie extended the notion of wave-particle duality to matter. In a nutshell he postulated that just as a particle (the photon) of energy $E = hc/\lambda$ is ascribed to electromagnetic radiation of wavelength λ a massive particle such as the electron is assigned a *de Broglie wavelength*

$$\lambda = \frac{h}{p}, \tag{5.1}$$

with p the particle's momentum. It is important to realize that the attribution of a wavelength to a massive particle implies that it should behave as a wave under some conditions. For example, it should be possible to verify this wavelike behaviour when performing a diffraction experiment. Of course, there was no experimental evidence of any sort at the time to justify such an assertion; de Broglie's proposition was bold indeed.

To understand how a massive particle could exhibit wavelike properties, or even better, how a wave could "behave" as a particle we must first review the notions of phase and group velocities.

5.1.1 Phase and Group Velocities

We already know from the material covered in Section 1.1.2 of Chapter 1 that the solution to the one-dimensional wave equation

$$\frac{\partial^2 \psi_1}{\partial x^2} - \frac{1}{v_\mathrm{p}^2}\frac{\partial^2 \psi_1}{\partial t^2} = 0 \tag{5.2}$$

is of the type

$$\psi_1(x,t) = A_1 \cos(k_1 x - \omega_1 t), \tag{5.3}$$

when $\omega_1 = k_1 v_\mathrm{p}$. It should be clear, however, that any other similar functions with potentially different values for the wave number and frequency would also satisfy this equation. For example, two waves ψ_1 and ψ_2 could combine to give

$$\begin{aligned}\psi(x,t) &= \psi_1(x,t) + \psi_2(x,t)\\ &= A\cos(k_1 x - \omega_1 t) + A\cos(k_2 x - \omega_2 t)\\ &= 2A\cos\left(\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t\right)\cos\left(\frac{\Sigma k}{2}x - \frac{\Sigma\omega}{2}t\right),\end{aligned} \tag{5.4}$$

where we used $2\cos(a)\cos(b) = \cos(a-b) + \cos(a+b)$ with $\Delta k = k_1 - k_2$, $\Sigma k = k_1 + k_2$, $\Delta\omega = \omega_1 - \omega_2$, and $\Sigma\omega = \omega_1 + \omega_2$. If we consider the case where the differences Δk and $\Delta\omega$ are much smaller than the respective summations Σk and $\Sigma\omega$, then we find that the resulting wave is composed as a "carrier" $\cos\left[(\Sigma k\, x - \Sigma\omega\, t)/2\right]$, which varies rapidly with time and position, multiplied by a slowly varying "envelope" $\cos\left[(\Delta k\, x - \Delta\omega\, t)/2\right]$. An example of this is shown in Figure 1. We find in general that the carrier travels at the *phase velocity*

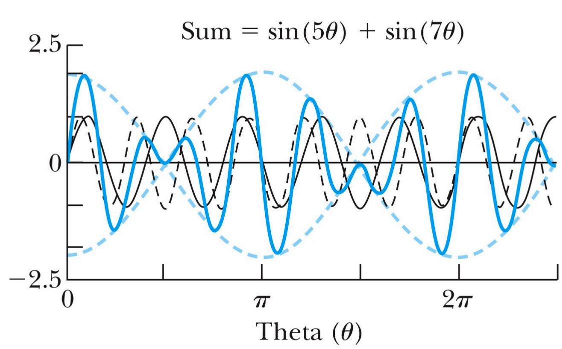


Figure 1 – An example of the sum of two waves that can be described as the product of an envelope and a carrier.

$$v_{\mathrm{p}}=\frac{\Sigma\omega}{\Sigma k}=\frac{\omega_1}{k_1}=\frac{\omega_2}{k_2}, \tag{5.5}$$

while the envelope travels at the so-called *group velocity*

$$v_{\mathrm{g}}=\frac{\Delta\omega}{\Delta k}, \tag{5.6}$$

which is in general different from the phase velocity. Evidently, this process can be extended to an arbitrary number of waves. Before we do so, we will replace our cosine function with a complex exponential

$$e^{\pm j\theta}=\cos(\theta)\pm j\sin(\theta), \tag{5.7}$$

with $j\equiv\sqrt{-1}$ the imaginary number. It is straightforward to verify that this function is also a solution of equation (5.2) when $\theta=kx-\omega t$. As we will see later on, the complex exponential is a fundamental function for the description of quantum mechanical systems.

[1]We then generalize the solution of the wave equation for a discrete set of waves to the summation

$$\psi(x,t)=\sum_n A_n e^{j(k_n x-\omega_n t)}, \tag{5.8}$$

which is known as the *Fourier series* of $\psi(x,t)$. In the case of a continuum of waves equation (5.8) is replaced by the *(inverse) Fourier transform*, which we can write as

$$\psi(x,t)=\int_{-\infty}^{\infty} A(k)e^{j(kx-\omega t)}\,dk \tag{5.9}$$

when we allow the frequency to be a function of the wave number. Such functions $\psi(x,t)$ that consist of superposition of waves are commonly called *wave packets*.

Now, let us write the following Taylor series

$$\omega(k)=\omega_0+\left.\frac{d\omega}{dk}\right|_{k_0}(k-k_0)+\cdots \tag{5.10}$$

where k_0 and ω_0 are "center" or reference values. We can alternatively turn the problem around and evaluate the amplitudes $A(k)$ from $\psi(x,t)$ with (the *Fourier transform* of

[1] The material contained between equations (5.8) and (5.17) is mathematically advanced, and you will ***not*** be tested on it.

$\psi(x,t)$)

$$A(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\psi(x,0)e^{-jkx}\,dx. \tag{5.11}$$

Inserting equation (5.10) into (5.9) we have

$$\begin{aligned}\psi(x,t)&\simeq\frac{e^{j\left[k_0(d\omega/dk)|_{k_0}-\omega_0\right]t}}{\sqrt{2\pi}}\int_{-\infty}^{\infty}A(k)e^{j\left[x-t(d\omega/dk)|_{k_0}\right]k}\,dk\\&\simeq\psi\left(x-t\left.\frac{d\omega}{dk}\right|_{k_0},0\right)e^{j\left[k_0(d\omega/dk)|_{k_0}-\omega_0\right]t}.\end{aligned} \tag{5.12}$$

It follows from this equation that, apart from the phase factor on the right, the initial wave located at $x-t\left[d\omega/dk\right]\!\big|_{k_0}$ when $t=0$ travels, with its shape seemingly unaltered, at the *group velocity*

$$v_{\mathrm{g}}=\left.\frac{d\omega}{dk}\right|_{k_0}. \tag{5.13}$$

to become the wave $\psi(x,t)$ at a later time t at position x. Incidentally, we find that equation (5.13) is a generalization of equation (5.6).

Example

To make things clearer let us consider a wave packet that is highly localized in space

$$\psi(x,t)=\varphi(x)e^{j(k_0x-\omega_0t)}, \tag{5.14}$$

with the envelope

$$\varphi(x)=\begin{cases}B, & \text{for } |x|<\Delta x\\ 0, & \text{for } |x|>\Delta x.\end{cases} \tag{5.15}$$

We now use equation (5.11) to calculate the “spectrum” associated with $\psi(x,t)$

$$
\begin{aligned}
A(k) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \varphi(x) e^{jk_0 x} e^{-jkx}\, dx \\
&= \frac{B}{\sqrt{2\pi}} \int_{-\Delta x}^{\Delta x} e^{-j(k-k_0)x}\, dx \\
&= \frac{2B}{\sqrt{2\pi}} \frac{\sin\left[(k-k_0)\Delta x\right]}{(k-k_0)}.
\end{aligned} \tag{5.16}
$$

Since the first zeros of $A(k)$ happen at $|k-k_0| \equiv \Delta k = \pi/\Delta x$, we find the following relation

$$
\Delta k \Delta x \sim 1. \tag{5.17}
$$

Equation (5.17) is a mathematical statement of the so-called *wave-train uncertainty*, which is also central to quantum mechanics.

5.1.2 The de Broglie Waves

The idea behind de Broglie's proposition to assign a wavelike nature to massive particle rested on the hypothesis that, perhaps, it can be associated with a highly localized wave packet in space. For example, in our previous example we can think of the envelope $\varphi(x)$ as defining the shape and extent of a particle in space, which would be moving with the group velocity v_{g} according to equation (5.13) (i.e., given a *dispersion relation* specifying $\omega = \omega(k)$).

Following de Broglie's reasoning we assign to massive particles some of the same attributes that hold for electromagnetic waves (and photons) since we assume that they can also be described with waves. For example, considering the group velocity we write

$$
\begin{aligned}
v_{\mathrm{g}} &= \frac{d\omega}{dk} \\
&= \frac{d(\hbar\omega)}{d(\hbar k)} \\
&= \frac{dE}{dp},
\end{aligned} \tag{5.18}
$$

with E and p the energy and momentum, respectively. Evidently, this relation is verified for photons and we therefore enforce it for massive particle as well. The needed relation between these two quantities is found in special relativity through

$$
E^2 = p^2c^2 + m^2c^4. \tag{5.19}
$$

We then have that $2E\,dE = 2pc^2 dp$ and therefore

$$v_{\mathrm{g}} = \frac{pc^2}{E}. \tag{5.20}$$

But we also know from special relativity, however, that

$$\begin{aligned} E &= \gamma mc^2 \\ p &= \gamma mv, \end{aligned} \tag{5.21}$$

with $v = dx/dt$ the "classical" speed of the particle and $\gamma = \left(1 - v^2/c^2\right)^{-1/2}$ the Lorentz factor. It follows that $v_{\mathrm{g}} = v$ and we find that idea of assigning a wave-particle duality to massive particle is consistent with special relativity. The particle can then be assign a wavelength through

$$\begin{aligned} p &= \hbar k \\ &= \hbar \frac{2\pi}{\lambda} \\ &= \frac{h}{\lambda}. \end{aligned} \tag{5.22}$$

Since we know from diffraction theory that a wave will show interference behaviour when incident on slits of a grating of dimension comparable to its wavelength (see Prob. 3 of the First Assignment), we should expect from de Broglie's theory that the same would apply to a massive particle. Needless to say that such an expectation was very counterintuitive at the time he made this prediction.

Exercises

1. Calculate the de Broglie wavelength of (a) a tennis ball of mass 57 g travelling at 25 m/s and (b) an electron with kinetic energy of 50 eV.

Solution.

We use equation (5.22) for these calculations. (a) For the tennis ball

$$\lambda = \frac{h}{p} = \frac{6.62 \times 10^{-34}\,\mathrm{J \cdot s}}{0.057\ \mathrm{kg} \cdot 25\ \mathrm{m/s}} = 4.7 \times 10^{-34}\,\mathrm{m}, \tag{5.23}$$

and (b) for the electron

$$\begin{aligned}\lambda &= \frac{h}{p}\\ &= \frac{h}{\sqrt{2mK}} = \frac{hc}{\sqrt{2\left(mc^2\right)K}}\\ &= \frac{1240\ \text{eV}\cdot\text{nm}}{\sqrt{2\cdot 511\times 10^3\ \text{eV}\cdot 50\ \text{eV}}} = 0.17\ \text{nm}.\end{aligned} \tag{5.24}$$

It should be clear from these numbers that, although there is little chance it could be possible to find or fabricate a slit or a grating sufficiently small to diffract a tennis ball, a 50 eV electron should effectively interfere when passing through a crystal (as for X-rays) since the interatomic distance compares well to the corresponding de Broglie wavelength.

5.1.3 Quantization of the Atomic Orbital Angular Momentum

We saw in Chapter 3 that one of the fundamental postulates introduced by Bohr to explain the hydrogen atom was the notion that the orbital angular momentum of the electron on a stationary state was quantized to multiples of the Planck constant $\hbar$ (see the fourth postulate in Sec. 3.3). This postulate can easily be shown to be consistent the introduction of the de Broglie wavelength, if we assume that a stationary state can only be achieved when conditions necessary to obtain a standing wave are met.

This is reasonable since a standing wave reflects a state that is, in a way, unchanging or stationary. For electromagnetic waves we know from our discussion of the blackbody in Chapter 2 (see Sec. 2.3.1) that a standing wave is made-up of two counter-propagating waves, when the length over which the waves are propagating is a multiple of the (half-) wavelength. For the electron matter wave (i.e., it is very important to realize that we are not talking about electromagnetic or acoustic waves) if we apply a similar condition

$$2\pi r = n\lambda, \tag{5.25}$$

with r the radius of the orbit and n a positive integer, then inserting equation (5.22) for the wavelength we find

$$2\pi r = \frac{nh}{p} \tag{5.26}$$

or with $\mathbf{L} = \mathbf{r}\times\mathbf{p}$ for the angular momentum

$$L = n\hbar. \tag{5.27}$$

We thus find that Bohr's angular momentum quantization is encompassed within de Broglie's postulate on the existence of matter waves.

Exercises

2. (Ch. 5, Prob. 6, in Thornton and Rex.) Calculate the de Broglie wavelength of a typical nitrogen molecule on a hot summer day ($37^\circ\mathrm{C}$). Compare this with the diameter of the molecule (less than 1 nm).

Solution.

We know from out calculations leading to equation (1.47) in Chapter 1 that according to classical statistical mechanics the mean kinetic energy K of a particle of mass m at temperature T equals $3kT/2$. If we choose $v_{\mathrm{rms}} \equiv \sqrt{\langle v^2 \rangle}$, then

$$mv_{\mathrm{rms}} = \sqrt{3mkT} = 2.45 \times 10^{-23}\,\mathrm{kg} \cdot \mathrm{m/s}. \tag{5.28}$$

As this is the value for the momentum, the de Broglie wavelength is

$$\lambda = \frac{h}{mv_{\mathrm{rms}}} = 2.7 \times 10^{-11}\,\mathrm{m}, \tag{5.29}$$

which represents approximately 3% of the size of the molecule.

3. (Ch. 5, Prob. 11, in Thornton and Rex.) Determine the de Broglie wavelength of a particle of mass m and kinetic energy K. Do this for both (a) a relativistic and (b) a nonrelativistic particle.

Solution.

We must first understand that the kinetic energy is defined relativistically such that the total energy is given by $E = K + mc^2$. This is justified by the expansion of the first of equations (5.21) with a Taylor series in $(v/c)^2$

$$\begin{aligned} E &= \gamma mc^2 \\ &= mc^2\left[1 - \left(\frac{v}{c}\right)^2\right]^{-1/2} \\ &= mc^2\left[1 + \frac{1}{2}\left(\frac{v}{c}\right)^2 + \cdots\right] \\ &= mc^2 + \frac{1}{2}mv^2 + \cdots \end{aligned} \tag{5.30}$$

In the weakly relativistic case we can write $K \simeq mv^2/2 \ll mc^2$ and we therefore find that $E \simeq K + mc^2$, which is in agreement with the aforementioned definition. But the fully relativistic equation for the (square of) energy can also be written as $E^2 = p^2c^2 + m^2c^4$, and we can write

$$\begin{aligned} pc &= \left[E^2 - \left(mc^2\right)^2\right]^{1/2} \\ &= \left[\left(K + mc^2\right)^2 - \left(mc^2\right)^2\right]^{1/2} \\ &= \left[K^2 + 2Kmc^2\right]^{1/2}. \end{aligned} \tag{5.31}$$

(a) Thus, for a relativistic particle the de Broglie wavelength is

$$\lambda = \frac{h}{p} = \frac{hc}{\sqrt{K^2 + 2Kmc^2}}. \tag{5.32}$$

(b) For a nonrelativistic particle we have

$$\begin{aligned} \lambda &= \frac{hc}{\sqrt{K^2 + 2Kmc^2}} \\ &\simeq \frac{hc}{\sqrt{2Kmc^2}} \\ &\simeq \frac{h}{\sqrt{2mK}}. \end{aligned} \tag{5.33}$$

5.1.4 Experimental Evidence for Matter Waves – Electron Scattering

We already mentioned that diffraction of X-rays through crystalline structures had been important in establishing their wavelike properties. Because of the closeness in values for the separation between adjacent fundamental planes in a crystal, which act in a way similar to the slits in a grating, and the de Broglie wavelength of the electron, crystals are also perfectly suited to test the potential existence of matter waves.

The diffraction equation needed to understand diffraction through crystals is very similar

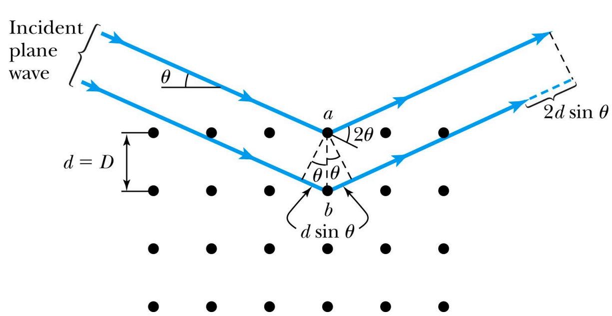


Figure 2 – The diffraction of waves off the adjacent planes of a crystalline structure.

to that derived in Prob. 3 of the first assignment when studying the diffraction of electromagnetic waves through a grating. The small difference between the two equations that characterize these processes can be discerned with Figure 2. We see that, just as for a grating, the outgoing (or reflected) waves in a crystal have an extra optical path $nd\sin(\theta)$ depending on the position n of the scattering plane (the upper most plane has $n = 0$ in the figure, the angle between the incident and scattered waves is 2θ, and the distance between adjacent planes is d). However, it is also seen that the incident waves further acquire the same corresponding phase retardation, which therefore doubles the value of the extra optical path to $2nd\sin(\theta)$ for a scattering off plane n. The equation that specifies the locations of maxima for crystalline diffraction differs accordingly from that for gratings (see equation (3.3) in the first assignment) such that

$$n\lambda = 2d\sin(\theta), \tag{5.34}$$

with n an integer. Equation (5.34) is also refereed to as *Bragg's law*.

The wavelike nature of the electron was first made evident in 1925 from scattering measurements off large nickel crystals by **Clinton J. Davisson** (1881-1958) and **Lester H. Germer** (1896-1971) of Bell Telephone Laboratory. In their experiment, they were able to measure the angle of maximum diffracted intensity as a function of the incident electron's kinetic energy (and therefore of the de Broglie wavelength through equation (5.32)). Their results were in almost perfect agreement with de Broglie's prediction as they obtained $\lambda = 0.165$ nm (compare with the calculations leading to equation (5.24)). Their results were soon corroborated by a series of experiments conducted by **George P. Thomson** (1892-1975), the son of J. J. Thomson who had previously discovered the electron.

5.2 Wave-Particle Duality

We are thus left with the seemingly contradicting picture where both radiation and particles can take on the character of a wave or that of a particle depending on the situation… But how can this be so? Why and how a physical entity (e.g., an electric field or an electron) can present both characters? This is a deep and important question about the nature of physics in general that is still debated. But we can bring some sort of sense to it by considering Young's double-slit diffraction experiment.

The general set-up for this experiment is shown in Figure 3, where waves are incident on a grating made of two narrow slits located some large distance away from a detector screen. When both slits are unobstructed an interference pattern is measured. This is readily calculated using the results of Prob. 3 in the first assignment when $N = 2$. The intensity thus measured becomes

$$I_{12}(\theta) = \frac{I_0}{4}\frac{\sin^2\left[kd\sin(\theta)\right]}{\sin^2\left[kd\sin(\theta)/2\right]}, \tag{5.35}$$

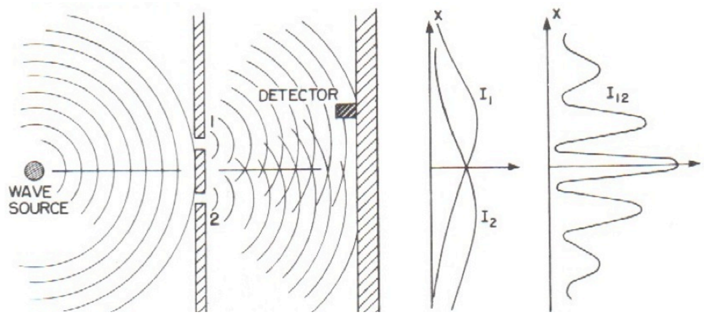


Figure 3 - Young's double-slit experiment. Waves are incident on a grating made of two slits located some large distance away from a detector screen. When both slits are unobstructed an interference pattern (I_{12} curve on the far-right) is measured, while broad intensity profiles are detected when one slit is blocked (I_1 and I_2 curves).

with I_0 the maximum intensity detected at $\theta = 0$ (i.e., in the middle of the detector screen). This result is, of course, typical and is measured whenever the incident waves are electromagnetic in nature, for example. On the other hand, the broad and smooth profiles $I_1(\theta)$ or $I_2(\theta)$ are observed when slit 2 or 1 are, respectively, blocked. These intensities do not possess an interference pattern at all. In fact, it is important to realize that $I_{12}(\theta) \neq I_1(\theta) + I_2(\theta)$ but rather[2]

$$I_{12}(\theta) = I_1(\theta) + I_2(\theta) + 2\sqrt{I_1(\theta) I_2(\theta)} \cos\left[kd\sin(\theta)\right] \tag{5.36}$$

in general. Again, this is typical behaviour for a wave.

We now ask the question as to what would a pre-de Broglie physicist have expected to result from these experiments when effected on particles? It is easier to first consider the case where one slit is covered at a time, when $I_1(\theta)$ or $I_2(\theta)$ are measured. The big difference from the previous experiment on waves is that with both slits unobstructed our physicist would *not* expect to obtain equation (5.36) but rather

$$I_{12}(\theta) = I_1(\theta) + I_2(\theta). \tag{5.37}$$

Indeed, this is what one would measure *today* if the double-slit experiment were performed with incident macroscopic massive particles (e.g., bullets of some sort) instead of waves. Of course, we know from our previous discussion of the Davisson-Germer

[2] Equation (5.36) can be recovered from equation (5.35) by using equations (3.16) of Chapter 3 and multiplying both the numerator and denominator of equation (5.36) by $1 - \cos\left[kd\sin(\theta)\right]$ and setting $I_1 = I_2 = I_0/4$ (since equation (5.35) assumes that I_1 and I_2 are constant and equal for any value of θ, which is approximately true when $\theta \ll 1$).

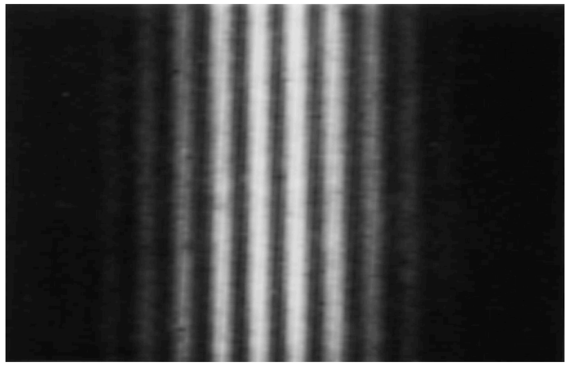


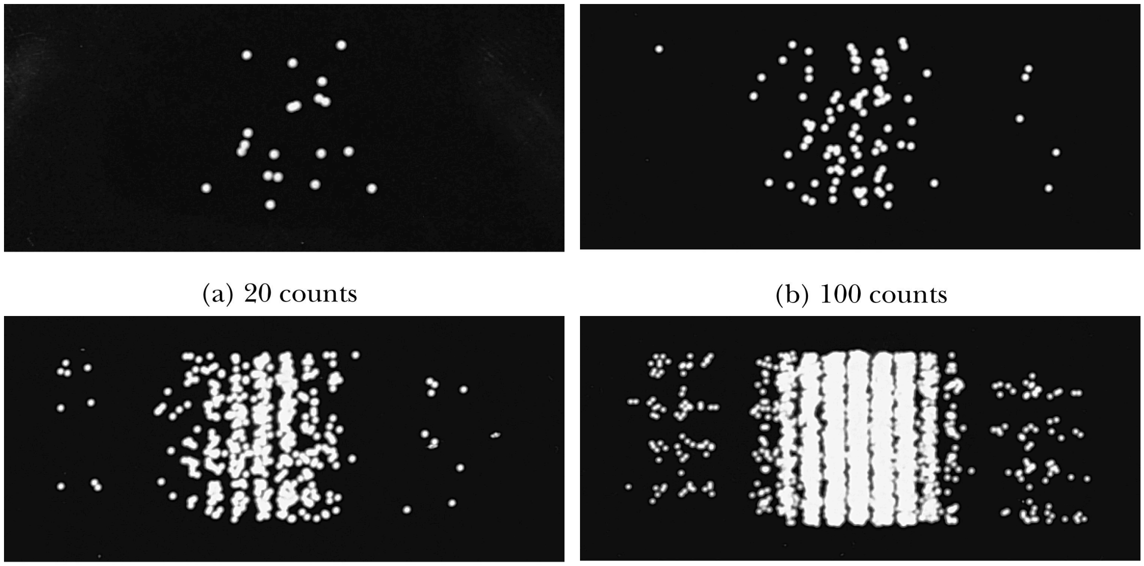
Figure 4 – Result of a Young double-slit experiment on electrons. The wavelike character of the detected intensity is clear, in agreement with de Broglie's theory.

experiment that such expectations for elementary particles (e.g., electrons) will not be realized. Indeed, modern versions of the Young double-slit experiment give similar results for electromagnetic radiation or massive particles. Such an example is shown in Figure 4 where the interference pattern detected for a high flux of incident electrons is similar to what is measured with photons. This maybe counterintuitive or shocking, but that is the way nature is. Both electrons and photons exhibit wave *and* particle characters! But that is not all…

The results of the Young's double-slit experiment discussed so far and exemplified in Figure 4 all assume that a large number of electrons or photons (or whatever type particle chosen for the experiment) are impinging on the grating. Something interesting happens if the intensity of the incident wave is greatly reduce such that, say, only one photon (or electron) is detected every second or so. We may perhaps intuitively expect that the interference pattern of Figure 4 would still be detected at a correspondingly lower intensity. But this is not what is observed. Instead, the interference wave pattern is not measured at once but is built up as more and more particles are detected. That is, it is very important to note that in quantum mechanics *one never measures waves, but only particles*. As we will see later, although a quantum mechanical system (or a particle) can be interpreted as evolving like a wave, the outcome of an experiment will always yield a particle (e.g., a photon or an electron). Therefore in the case of Young's double-slit experiment with a weak incident wave, the interference pattern will be similar to what would be observed with a strong incident wave but it would take a much longer time before becoming well defined on the detector screen. This phenomenon is made apparent in Figure 5.

Furthermore, we also note that *we can never predict where on the screen a particle will be detected. We can only assign a probability with which it may be measured at a given position on the screen*. In the case of the Young's double-slit experiment this probability is proportional to the intensity of the final interference wave pattern.

The wave-particle duality is intrinsic to quantum mechanics and is such that one type of behaviour seems to exclude the other. The previous statement on the evolution of a



(a) 20 counts (b) 100 counts

(c) 500 counts (d) ~4000 counts

Figure 5 – Computer simulation of Young's double-slit experiment for light or electron where the incident wave is of very low intensity. The interference pattern builds up slowly with time as particles are detected. That is, one particle does not show the interference pattern but contributes to it with all the other particles measured.

system being represented by a wave and a measurement by the detection of a particle is such an example. It is also found, as we will soon discuss, that any attempt to determine, say, the position of a particle as it is evolving (as a wave) will invariably suppress any interference pattern. This is because the measurement of the position brings the particle aspect into play, as previously stated. Bohr has addressed this issue through his *principle of complementarity*, which states that:

It is not possible to describe physical observables simultaneously in terms of particles and waves.

By *physical observables* Bohr meant measurable quantities such as position, momentum, velocity, energy that are likely to be the result of an experiment.

Exercises

4. In the Young's double-slit experiment 50 keV electrons impinged on slits of width 500 nm separated by a distance of $d = 2000$ nm. The observation screen was located $\ell = 350$ mm beyond the slit. What is the distance between the first two maxima?

Solution.

We know from equation (5.35) that the locations of maxima follow the relation

$$d\sin(\theta) = n\lambda. \tag{5.38}$$

The first maximum for $n=0$ is at $\theta=0$, while the second for $n=1$ has

$$\sin(\theta)=\frac{\lambda}{d}. \tag{5.39}$$

The de Broglie wavelength is given by equation (5.32)

$$\begin{aligned}\lambda&=\frac{h}{p}=\frac{hc}{\sqrt{K^2+2Kmc^2}}\\&=\frac{1240\text{ eV}\cdot\text{nm}}{\sqrt{(50{,}000\text{ eV})^2+2\cdot 50{,}000\text{ eV}\cdot 511{,}000\text{ eV}}}\\&=5.36\times10^{-3}\text{nm}.\end{aligned} \tag{5.40}$$

From equation (5.38) we then find

$$\sin(\theta)=\frac{5.36\times10^{-3}\text{nm}}{2000\text{ nm}}=2.68\times10^{-6}. \tag{5.41}$$

Finally, the corresponding distance on the screen is

$$\begin{aligned}y&=\ell\tan(\theta)\simeq\ell\theta\\&\simeq 350\text{ mm}\cdot 2.68\times10^{-6}\\&\simeq 938\text{ nm}.\end{aligned} \tag{5.42}$$

5. (Ch. 5, Prob. 35, in Thornton and Rex.) You want to design a Young's double slit experiment that does not require magnification of the interference pattern in order to be seen. Let the two slits separated by $d=2000$ nm. Assume that you can discriminate visually between maxima that are as little as $y=0.3$ mm apart. You have at your disposal a laboratory that allows the screen to be placed $\ell=80$ cm away from the slits. What energy electrons will you require? Do you think such low-energy electrons will represent a problem? Explain.

Solution.

Let us make the small angle approximation $\tan(\theta)\simeq\sin(\theta)\simeq\theta$, and therefore

$$\theta\simeq\frac{y}{\ell}=\frac{0.3\text{ mm}}{800\text{ mm}}=3.75\times10^{-4}, \tag{5.43}$$

and from equation (5.39)

$$\lambda \simeq d\theta = 2000 \text{ nm} \cdot 3.75 \times 10^{-4} = 0.75 \text{ nm}. \tag{5.44}$$

The momentum of the electrons is then

$$p = \frac{h}{\lambda} = \frac{hc}{\lambda c} = \frac{1240 \text{ eV·nm}}{\left(0.75 \text{ nm}\right)c} = 1.653 \text{ keV}/c, \tag{5.45}$$

and their kinetic energy

$$\begin{aligned} K &= E - mc^2 \\ &= \sqrt{p^2c^2 + mc^2} - mc^2 \\ &= \sqrt{\left(1.653 \text{ keV}\right)^2 + \left(511 \text{ keV}\right)^2} - 511 \text{ keV} \\ &= 2.67 \text{ eV}. \end{aligned} \tag{5.46}$$

Such low energies will present problems, because low-energy electrons take longer to move through the region of the electric field that is needed to accelerate and put them in motion toward the slits. They will thus be more susceptible to suffer deflection by stray electric fields.

5.3 The Heisenberg Inequality

We have already seen in the example of the rectangular wave packet in Section 5.1.1 that there is an inherent uncertainty in the determination of the wavelength (or wave vector $k = 2\pi/\lambda$) of a wave when observed over a finite spatial extent. For the case of the rectangular wave packet we found that

$$\Delta k \cdot \Delta x \simeq \pi. \tag{5.47}$$

In Problem 10 of the second assignment it will be shown that for a Gaussian wave packet $\Delta k \cdot \Delta x = 1/2$. A rigorous quantum mechanical analysis would show that value for the product of the uncertainties in wavenumber and position is a minimum, and we therefore write $\Delta k \cdot \Delta x \geq 1/2$.

Although equation (5.47) was derived for waves in general, we can readily apply it to quantum physics by combining it with equation (5.1) for the de Broglie wavelength such that

$$
\begin{aligned}
\Delta k \cdot \Delta x &= \Delta\left(\frac{2\pi}{\lambda}\right) \cdot \Delta x \\
&= \Delta\left(\frac{2\pi p}{h}\right) \cdot \Delta x \\
&= \frac{1}{\hbar}\left(\Delta p \cdot \Delta x\right).
\end{aligned} \tag{5.48}
$$

When considering the previous quantum mechanical result specifying the minimum value achievable for this product we can write the so-called *Heisenberg inequality*

$$
\Delta p \cdot \Delta x \geq \frac{\hbar}{2}. \tag{5.49}
$$

Equation is also commonly called the Heisenberg *uncertainty principle*. Although this last appellation may convey some sort of mythical aura, our previous analysis should make it clear that such inequality will apply whenever waves enter the picture. That is, the Heisenberg inequality is simply the wave train uncertainty applied to particles and waves generally.

It is important to realize that equation (5.49) *apply to the position and linear momentum in a given direction*. That is, in the case considered here the uncertainties in momentum and position are both along the x-axis; similar relations exist for the y and z directions. *This inequality does not apply, however, when dealing with a position and linear momentum of different orientations*. More precisely, there is no lower limit to the product of, say, $\Delta p_x \cdot \Delta y$ or $\Delta p_z \cdot \Delta x$; both these products can be equal to zero.

Finally, we note that the wave train uncertainty does not only apply to uncertainties in wave number and position but also to frequency and time. This will be easily understood by reconsidering the earlier example of the rectangular wave packet but by now observing it at a fixed position (instead of a given time) over and interval of time. That is, we consider the wave packet

$$
\psi(x,t) = \varphi(t)\, e^{j(k_0 x - \omega_0 t)}, \tag{5.50}
$$

with the envelope

$$
\varphi(t) = \begin{cases} B, & \text{for } |t| < \Delta t \\ 0, & \text{for } |t| > \Delta t. \end{cases} \tag{5.51}
$$

There also exists a pair of Fourier transform between time and frequency defined with

$$\begin{aligned}\psi(x,t) &= \int_{-\infty}^{\infty} A(\omega) e^{j(kx-\omega t)}\, d\omega \\ A(\omega) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(0,t) e^{j\omega t}\, dt,\end{aligned} \tag{5.52}$$

which when going through the same type of calculations as before yields

$$A(\omega) = \frac{2B}{\sqrt{2\pi}} \frac{\sin\left[(\omega-\omega_0)\Delta t\right]}{(\omega-\omega_0)}. \tag{5.53}$$

We can therefore write $|\omega - \omega_0| \equiv \Delta\omega \simeq \pi/\Delta t$ and we once again recover the wave train uncertainty. Since we know from Planck, Einstein, and de Broglie that $E = \hbar\omega$, then we can write $\Delta E \cdot \Delta t \simeq \pi\hbar$ in this case, but in general

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2}. \tag{5.54}$$

Exercises

6. In the Young double-slit experiment we seek to determine through which slit the electrons responsible for the wave interference pattern go through. To do so, the experimenter sets up a radiation source incident on one of the two slits with the hope that a photon will scatter off an electron when it goes through the slit (see Figure 6). The detection, or the absence of detection, of a scattered photon would then inform us of which slit an electron detected on the screen would have gone through on its way to the detector. Use the Heisenberg inequality to show that the interference pattern will be made to vanish whenever such detection technique is used.

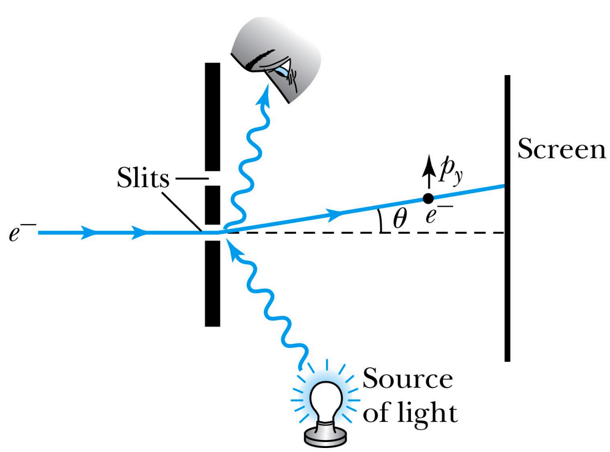


Figure 6 – The set-up for determining through which slit do electrons pass in the Young's double-slit experiment.

Solution.

To be able to discern which slit an electron has gone through we must use photons with a wavelength short enough to allow us to discriminate a vertical position with a precision of approximately half the distance d between the two slits. That is, the uncertainty in the vertical position must be such that

$$\Delta y < \frac{d}{2}. \tag{5.55}$$

From the wave train uncertainty, the photon wavelength is $\lambda \approx \Delta y$. According to the Heisenberg inequality (i.e., equation (5.49)) there will be an associated uncertainty in the vertical momentum of the photon given by

$$\Delta p_y \geq \frac{\hbar}{2\Delta y} = \frac{\hbar}{d}. \tag{5.56}$$

Also, as a photon scatters off an electron it will change the latter's momentum by approximately the same amount (because of the requirement of conserving the total linear momentum of the system). If the electron was incident on the slit with a momentum $p_x = h/\lambda_\text{e}$, according to de Broglie, then there will be an angular deviation $\Delta\theta$ on its path to the detector screen compared to when it does not interact with a photon. We can therefore write

$$\begin{aligned}\Delta\theta &\simeq \frac{\Delta p_y}{p_x} \geq \frac{\hbar}{d} \cdot \frac{\lambda_\text{e}}{h} \\ &\geq \frac{\lambda_\text{e}}{2\pi d}.\end{aligned} \tag{5.57}$$

However, we know from equation (5.35) that the first minimum in a Young double-slit experiment will happen at $\sin(\theta_\text{min}) \simeq \theta_\text{min} = \lambda_\text{e}/2d$, when the system is unperturbed by photons incident on the electrons. We then find that, approximately, $\theta_\text{min} \leq \Delta\theta$ and the interference pattern will be destroyed (or at least strongly affected) by the presence of the scattered photons.

We conclude that the determination of which slit the electron goes through destroys the wave interference pattern. This is in line with Bohr's principle of complementarity and the statement that quantum mechanical systems evolve as waves and are detected as particles. That is, in the experiment considered here scattering photons off electrons is de facto a measuring process, which reveals the particle characteristics of electrons and destroys any wavelike pattern.

5.4 Wave Function, Probability, and the Copenhagen Interpretation of Quantum Mechanics

We saw when considering diffraction gratings or more simply the double-slit experiment, in Section 5.2, that we could express the intensity $I_{12}(\theta)$ of the interference wave detected at the screen with equations (5.35) or (5.36). For example, if the incident wave were electromagnetic in nature, then this intensity would be related to the square of the electric field at the detector through

$$I_{12}(\theta) = \varepsilon_0 c \left\langle E_{12}^2(\theta) \right\rangle, \tag{5.58}$$

where $\langle \cdots \rangle$ denotes a time average. Considering this equation within the context of wave-particle duality, where photons are detected at the screen when the intensity of the electromagnetic waves is very low, the outcome of the experiment would be as shown in Figure 5 with the interference wave pattern slowly emerging out as time elapses and more and more photons are detected, as previously discussed. Alternatively, we could equate the measured intensity at a given position θ on the screen with the number of photons $N(\theta)$ per unit time per unit area (i.e., the *flux*) detected. More precisely, we write we also have

$$I_{12}(\theta) = N(\theta)\hbar\omega, \tag{5.59}$$

with ω the angular frequency of the photons.

The comparison of equations (5.58) and (5.59) now makes clearer or previous statement that "*the probability with which a particle may be detected is proportional to the intensity of the interference wave pattern*." The probability in this case would be proportional to $N(\theta)$ the number of photons detected (per unit time per unit area), which in turn is proportional to the square of the (electromagnetic) wave amplitude $\left\langle E_{12}^2(\theta) \right\rangle$. This interpretation seems natural for photons in view of the a priori known existence of the "classical" electromagnetic wave associated to them. But what can we say about electrons or other massive particles?

For massive particles we rely on the de Broglie's idea of matter wave, which we now denote by $\psi(\mathbf{r},t)$, generally composed of several independent waves to form a wave packet. From now on we will refer to $\psi(\mathbf{r},t)$ as the *wave function*. While the electric field $\mathbf{E}(\mathbf{r},t)$ obeys the electromagnetic wave equation (recall the one-dimensional form given by equation (1.24) in Chapter 1), the wave function for a particle will obey a different wave equation, i.e., the *Schrödinger equation*. Although we will more formally introduce this equation in the next chapter, we list here some the main attributes of the wave function.

First, the wave function $\psi(\mathbf{r},t)$ will in general be complex (in the mathematical sense) with $\psi^*(\mathbf{r},t)$ its *complex conjugate*. That is, if we write

$$\psi(\mathbf{r},t)=\psi_{\mathrm{re}}(\mathbf{r},t)+j\psi_{\mathrm{im}}(\mathbf{r},t), \tag{5.60}$$

with two real functions $\psi_{\mathrm{re}}(\mathbf{r},t)$ and $\psi_{\mathrm{im}}(\mathbf{r},t)$ for the *real* and *imaginary* parts, respectively, then

$$\psi^*(\mathbf{r},t)=\psi_{\mathrm{re}}(\mathbf{r},t)-j\psi_{\mathrm{im}}(\mathbf{r},t). \tag{5.61}$$

The amplitude of the wave function varies with position and time, and is given by its value at any given point and instant. We define the probability of finding the particle at a position $\mathbf{r}$ in a volume d^3r (for example, $d^3r = dx\,dy\,dz$ in Cartesian coordinates) at time t with

$$P(\mathbf{r},t)d^3r=\left|\psi(\mathbf{r},t)\right|^2 d^3r, \tag{5.62}$$

where $\left|\psi(\mathbf{r},t)\right|^2=\psi(\mathbf{r},t)\psi^*(\mathbf{r},t)$ is the square of the norm of the wave function. Because a particle has a probability of one of being detected somewhere in space at any given time we must have

$$\begin{aligned}\int_{-\infty}^{\infty}P(\mathbf{r},t)d^3r &= \int_{-\infty}^{\infty}\left|\psi(\mathbf{r},t)\right|^2 d^3r\\ &=1.\end{aligned} \tag{5.63}$$

For example, in the double-slit experiment a particle will be detected somewhere on the screen with certainty. It is then said that the wave function is *normalized*. We thus see that the classical picture with which one determines the position of a particle through a function of time $\mathbf{r}(t)$ for the coordinates must be abandoned in quantum mechanics, where only probabilities can be calculated. This probabilistic interpretation of the wave function is due to **Max Born** (1882-1970).

As will become clearer as we progress in our study, the mathematical formalism based on the wave function and the Schrödinger equation has been very successful in accounting for quantum phenomena. Indeed, it is safe to state that quantum mechanics is the most successful physics theory in accurately predicting the outcomes of experiments. Although we cannot properly address this issue at the level of our discussion, it is important to understand that there is, however, no universal consensus regarding its interpretation. The mainstream interpretation of quantum mechanics is based on the so-called *Copenhagen Interpretation* developed mainly at Bohr's Institute for Theoretical Physics by Bohr himself and **Werner Heisenberg** (1901-1976) soon after the latter published his theory of quantum mechanics in 1926.[3] The Copenhagen interpretation is based on the application of the following three elements, which we have already studied in detail,

1. The Heisenberg inequality.
2. Bohr's complementarity principle.
3. Born's statistical interpretation based on probabilities calculated through the square of the norm of the wave function.

This interpretation basically asserts that we should not ask how nature works, but that the outcome of measurements is the only physical reality that is available to us. For this reason, the Copenhagen interpretation of quantum mechanics is sometimes (sarcastically) referred to as the "shut up and calculate!" approach…

5.5 A First Application – The Particle in a Box

Let us apply our notions of quantum mechanics to the simple problem of a particle of mass m confined inside a one-dimensional "box" of size ℓ. We want to show that the energy of the particle is quantized, and determine the probability of finding the particle at a position x at, say, time $t=0$ when in a given state (i.e., energy). To do so, we first express the wave function $\psi(x,t)$ as a wave packet using the Fourier series expansion given by equation (5.8)

$$\begin{aligned}\psi(x,0) &= \sum_{n=-\infty}^{\infty} A_n e^{jk_n x} \\ &= A_0 + \sum_{n=1}^{\infty}\left[B_n \cos(k_n x) + C_n \sin(k_n x)\right],\end{aligned} \tag{5.64}$$

where A_n, B_n, and C_n are potentially complex coefficients and we have transformed the infinite summation over complex exponentials with a finite summation on sine and cosine functions.[4] Since the particle is confined to the interior of the box, it must be that the probability of finding it outside of it is zero. That is, we have $\psi(0,0)=0$, $A_0=0$ and, because $\cos(0)=1$, $B_n=0$. It therefore follows that

$$\psi(x,0) = \sum_{n=1}^{\infty} C_n \sin(k_n x). \tag{5.65}$$

It is also the case that $\psi(\ell,0)=0$, which imposes the further condition

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[3] **Erwin Schrödinger** (1887-1961) independently published his own version of quantum mechanics based on wave functions at approximately the same time (this is the formulation we will use). Heisenberg and Schrödinger are widely regarded as the fathers of the modern theory of quantum mechanics.

[4] Verify that it is possible to do so, and that $B_n = A_n + A_{-n}$ and $C_n = j(A_n - A_{-n})$.

$$k_n \ell = n\pi, \tag{5.66}$$

or

$$\lambda_n = \frac{2\ell}{n}. \tag{5.67}$$

We now calculate the energy of the particle using the de Broglie wave-particle duality

$$\begin{aligned} E_n &= \frac{p_n^2}{2m} = \frac{h^2}{2m\lambda_n^2} \\ &= n^2 \frac{h^2}{8m\ell^2}. \end{aligned} \tag{5.68}$$

We therefore find that the energy of the particle is quantized with the integer n.

To calculate probabilities for finding the particles at different position inside the box we must determine what the C_n coefficients are, which we do by normalizing the wave function. We therefore write, using equation (5.66),

$$\begin{aligned} \int_0^\ell \left|\psi(x,0)\right|^2 dx &= \int_0^\ell \sum_{n=1}^\infty \sum_{m=1}^\infty C_n C_m^* \sin\left(n\pi \frac{x}{\ell}\right) \sin\left(m\pi \frac{x}{\ell}\right) dx \\ &= \frac{1}{2} \sum_{n=1}^\infty \sum_{m=1}^\infty C_n C_m^* \int_0^\ell \left\{ \cos\left[(n-m)\pi \frac{x}{\ell}\right] - \cos\left[(n+m)\pi \frac{x}{\ell}\right] \right\} dx \\ &= 1. \end{aligned} \tag{5.69}$$

We find, however, that this equation is greatly simplified because both n and m are integers. That is, we have

$$\int_0^\ell \cos\left[(n-m)\pi \frac{x}{\ell}\right] dx = \begin{cases} 0, & \text{for } n \neq m \\ \ell, & \text{for } n = m, \end{cases} \tag{5.70}$$

while

$$\int_0^\ell \cos\left[(n+m)\pi \frac{x}{\ell}\right] dx = 0 \tag{5.71}$$

always since $n + m \geq 2$. Combining the last three equations we then find

$$\sum_{n=1}^\infty \left|C_n\right|^2 = \frac{2}{\ell}. \tag{5.72}$$

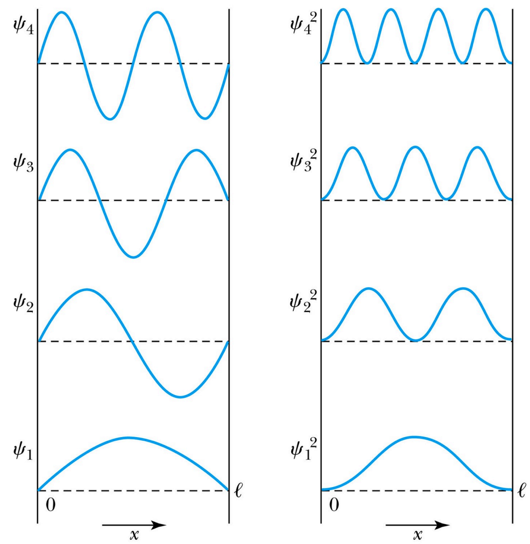

Figure 7 – The first four modes for a particle confined to a one-dimensional box. The amplitudes of the wave functions are on the left and the probability densities are on the right.

Equation (5.72) is a general constraint that relates the amplitudes of the different modes (i.e., the waves associated with different values of n) that compose the wave function. Usually, a quantum mechanical system will be "prepared" in a given state or combination of states and then is left to evolve before measurements are made. We cannot, at this point, say anything about the evolution of a system, as this would require using the Schrödinger equation, which we have yet to study. We can still, however, investigate the *probability density* that a particle has to be at a position x if it is assumed to be in a single state of energy E_n. In that case we write

$$\begin{aligned}\psi(x,0) &= \psi_n(x) \\ &= \sqrt{\frac{2}{\ell}}\sin\left(n\pi\frac{x}{\ell}\right).\end{aligned} \tag{5.73}$$

The probability density is then simply given by

$$\begin{aligned}P(x,0) &= \left|\psi_n(x)\right|^2 \\ &= \frac{2}{\ell}\sin^2\left(n\pi\frac{x}{\ell}\right).\end{aligned} \tag{5.74}$$

We therefore find, as shown in Figure 7 for the first four modes, that the probability of finding the particle varies with position in the box.

Exercises

7. As we will see in the next chapter, when a quantum mechanical system initially prepared at $t=0$ in a stationary state $\psi_n(\mathbf{r})$ of energy E_n is allowed to evolve according to the Schrödinger wave equation, then we find that it does so according to the following relation

$$\varphi_n(\mathbf{r},t)=\psi_n(\mathbf{r})e^{-jE_nt/\hbar}. \tag{5.75}$$

Let us then consider a particle of mass m in a one-dimensional box of length ℓ when the initial state is composed of the superposition of two stationary states

$$\psi(x,0)=\frac{1}{\sqrt{2}}\left[\psi_m(x)+\psi_n(x)\right], \tag{5.76}$$

with $m\neq n$, and allowed to evolve to a time t where measurements are effected to determine the position and energy of the particle. As before, the mathematical form of the stationary states is given by

$$\psi_n(x)=C\sin\left(n\pi\frac{x}{\ell}\right), \tag{5.77}$$

with C a real coefficient common to both states.

(a) Calculate the probability density of finding the particle at location x at time t. Is it equal to $\left[\left|\psi_m(x)\right|^2+\left|\psi_n(x)\right|^2\right]\Big/2$? Explain.

(b) What is the energy of the particle at time t ?

Solution.

(a) From equations (5.75) and (5.76) we can write

$$\begin{aligned}\psi(x,t)&=\frac{1}{\sqrt{2}}\left[\psi_m(x)e^{-jE_mt/\hbar}+\psi_n(x)e^{-jE_nt/\hbar}\right]\\&=\frac{1}{\sqrt{2}}e^{-jE_mt/\hbar}\left[\psi_m(x)+\psi_n(x)e^{-j(E_n-E_m)t/\hbar}\right].\end{aligned} \tag{5.78}$$

The general form for the probability density of finding the particle at location x at time t is therefore

$$\begin{aligned}\left|\psi(x,t)\right|^2 &= \frac{1}{\sqrt{2}} e^{-jE_m t/\hbar}\left[\psi_m(x)+\psi_n(x)e^{-j(E_n-E_m)t/\hbar}\right] \\ &\quad\times\frac{1}{\sqrt{2}} e^{jE_m t/\hbar}\left[\psi_m^*(x)+\psi_n^*(x)e^{j(E_n-E_m)t/\hbar}\right] \\ &= \frac{1}{2}\left\{\left|\psi_m(x)\right|^2+\left|\psi_n(x)\right|^2+2\psi_m(x)\psi_n(x)\cos\left[\left(E_n-E_m\right)t/\hbar\right]\right\},\end{aligned} \tag{5.79}$$

where we have taken into account the fact that $\psi_n(\mathbf{r})$ is real. Evidently, this probability density is different from $\left[\left|\psi_m(x)\right|^2+\left|\psi_n(x)\right|^2\right]/2$, which is the sum of the densities for states m and n. We find that there is a cross-term that brings oscillations with time at the frequency of $\left(E_n-E_m\right)/\hbar$. This is the same type of interference term that we saw in the double-slit experiment, for example.

To completely determine the probability density we have to calculate the coefficient C, which is accomplished through the normalization of the initial wave function. We thus write

$$\begin{aligned}\int_0^\ell\left|\psi(x,0)\right|^2 dx &= \frac{1}{2}\left[\int_0^\ell\left|\psi_m(x)\right|^2 dx+\int_0^\ell\left|\psi_n(x)\right|^2 dx\right] \\ &= \frac{C^2}{2}\left[\int_0^\ell \sin^2\left(m\pi\frac{x}{\ell}\right)dx+\int_0^\ell \sin^2\left(n\pi\frac{x}{\ell}\right)dx\right] \\ &= \frac{C^2\ell}{2},\end{aligned} \tag{5.80}$$

and therefore

$$C=\sqrt{\frac{2}{\ell}}. \tag{5.81}$$

The probability density of finding the particle at location x at time t is therefore

$$\begin{aligned}\left|\psi(x,t)\right|^2 = \frac{1}{\ell}\Big\{&\sin^2\left(m\pi\frac{x}{\ell}\right)+\sin^2\left(n\pi\frac{x}{\ell}\right) \\ &+2\sin\left(m\pi\frac{x}{\ell}\right)\sin\left(n\pi\frac{x}{\ell}\right)\cos\left[\left(E_n-E_m\right)t/\hbar\right]\Big\}.\end{aligned} \tag{5.82}$$

(b) We cannot give a definite value for the energy of the particle at any given time but only a probability for the two possible values. That is, we must ask ourselves what are the probabilities that the particle be in states m and n? For example, the energy of the particle will be E_m when it is in state m, etc. From equations (5.77) and (5.78) we find that the two states $\psi_m(x)$ and $\psi_n(x)$ contribute equally to the amplitude of the total wave function $\psi(x,t)$. Their contributions being $1/\sqrt{2}$, the probability of finding the particle in either state is the same at $1/2$. Accordingly, the energy of the particle is equally likely (at 0.5 probability) to be E_m or E_n.