CHAPTER OVERVIEW

2: Wave-Particle Duality

In classical mechanics, waves and particles are two completely distinct types of physical entity. Waves are continuous and spatially extended, whereas particles are discrete and have little or no spatial extent. However, in quantum mechanics, waves sometimes act as particles, and particles sometimes act as waves—this strange behavior is known as *wave-particle duality*. In this chapter, we shall examine how wave-particle duality shapes the general features of quantum mechanics.

2.1: Wavefunctions

A *wave* is defined as a disturbance in some physical system that is periodic in both space and time. In one dimension, a wave is generally represented in terms of a *wavefunction*: for instance,

$$\psi(x,t) = A\,\cos(k\,x - \omega\,t + \varphi), \tag{2.1.1}$$

where x is a position coordinate, t represents time, and A, k, $\omega > 0$. For example, if we are considering a sound wave then $\psi(x,t)$ might correspond to the pressure perturbation associated with the wave at position x and time t. On the other hand, if we are considering a light-wave then $\psi(x,t)$ might represent the wave's transverse electric field. As is well known, the cosine function, $\cos\theta$, is periodic in its argument, θ, with period 2π: in other words, $\cos(\theta+2\pi) = \cos\theta$ for all θ. The function also oscillates between the minimum and maximum values -1 and $+1$, respectively, as θ varies. It follows that the wavefunction (2.1.1) is periodic in x with period $\lambda = 2\pi/k$. In other words, $\psi(x+\lambda,t) = \psi(x,t)$ for all x and t. Moreover, the wavefunction is periodic in t with period $T = 2\pi/\omega$. In other words, $\psi(x,t+T) = \psi(x,t)$ for all x and t. Finally, the wavefunction oscillates between the minimum and maximum values $-A$ and $+A$, respectively, as x and t vary. The spatial period of the wave, λ, is known as its *wavelength*, and the temporal period, T, is called its *period*. Furthermore, the quantity A is termed the wave *amplitude*, the quantity k the *wavenumber*, and the quantity ω the wave *angular frequency*. Note that the units of ω are radians per second. The conventional wave *frequency*, in cycles per second (otherwise known as hertz), is $\nu = 1/T = \omega/2\pi$. Finally, the quantity φ, appearing in expression (2.1.1), is termed the *phase angle*, and determines the exact positions of the wave maxima and minima at a given time. In fact, the maxima are located at $k\,x - \omega\,t + \varphi = j\,2\pi$, where j is an integer. This follows because the maxima of $\cos\theta$ occur at $\theta = j\,2\pi$. Note that a given maximum satisfies $x = (j - \varphi/2\pi)\,\lambda + v\,t$, where $v = \omega/k$. It follows that the maximum, and, by implication, the whole wave, propagates in the positive x-direction at the velocity ω/k. Analogous reasoning reveals that

$$\psi(x,t) = A\,\cos(-k\,x - \omega\,t + \varphi) = A\,\cos(k\,x + \omega\,t - \varphi), \tag{2.1.2}$$

is the wavefunction of a wave of amplitude A, wavenumber k, angular frequency ω, and phase angle φ, that propagates in the negative x-direction at the velocity ω/k.

2.2: Plane-Waves

As we have just seen, a wave of amplitude A, wavenumber k, angular frequency ω, and phase angle φ, propagating in the positive x-direction, is represented by the following wavefunction:

$$\psi(x,t) = A\,\cos(k\,x - \omega\,t + \varphi). \tag{2.2.1}$$

This type of wave is conventionally termed a *one-dimensional plane-wave*. It is one-dimensional because its associated wavefunction only depends on the single Cartesian coordinate, x. Furthermore, it is a plane-wave because the wave maxima, which are located at

$$k\,x - \omega\,t + \varphi = j\,2\pi, \tag{2.2.2}$$

where j is an integer, consist of a series of parallel planes, normal to the x-axis, that are equally spaced a distance $\lambda = 2\pi/k$ apart, and propagate along the positive x-axis at the velocity $v = \omega/k$. These conclusions follow because Equation (2.2.2) can be rewritten in the form

$$x = d, \tag{2.2.3}$$

where $d = (j - \varphi/2\pi)\,\lambda + v\,t$. Moreover, as is well known, Equation (2.2.3) is the equation of a plane, normal to the x-axis, whose distance of closest approach to the origin is d.

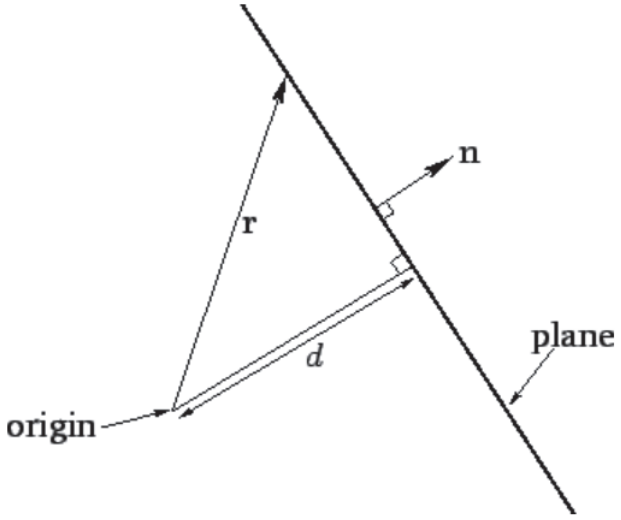

Figure 1: *The solution of* $\mathbf{n}\cdot\mathbf{r} = d$ *is a plane.*

The previous equation can also be written in the coordinate-free form

$$\mathbf{n}\cdot\mathbf{r} = d, \tag{2.2.4}$$

where $\mathbf{n} = (1,\,0,\,0)$ is a unit vector directed along the positive x-axis, and $\mathbf{r} = (x,\,y,\,z)$ represents the vector displacement of a general point from the origin. Because there is nothing special about the x-direction, it follows that if $\mathbf{n}$ is reinterpreted as a unit vector pointing in an arbitrary direction then Equation (2.2.4) can be reinterpreted as the general equation of a plane. As before, the plane is normal to $\mathbf{n}$, and its distance of closest approach to the origin is d. See Figure [f10.1]. This observation allows us to write the three-dimensional equivalent to the wavefunction (2.2.1) as

$$\psi(\mathbf{r},t) = A\,\cos(\mathbf{k}\cdot\mathbf{r} - \omega\,t + \varphi), \tag{2.2.5}$$

where the constant vector $\mathbf{k} = (k_x,\,k_y,\,k_z) = k\,\mathbf{n}$ is called the *wavevector*. The wave represented previously is conventionally termed a *three-dimensional plane-wave*. It is three-dimensional because its wavefunction, $\psi(\mathbf{r},t)$, depends on all three Cartesian coordinates. Moreover, it is a plane-wave because the wave maxima are located at

$$\mathbf{k}\cdot\mathbf{r} - \omega\,t + \varphi = j\,2\pi, \tag{2.2.6}$$

or

$$\mathbf{n}\cdot\mathbf{r} = (j-\varphi/2\pi)\,\lambda + v\,t, \tag{2.2.7}$$

where $\lambda = 2\pi/k$, and $v = \omega/k$. Note that the wavenumber, k, is the magnitude of the wavevector, $\mathbf{k}$: that is, $k \equiv |\mathbf{k}|$. It follows, by comparison with Equation (2.2.4), that the wave maxima consist of a series of parallel planes, normal to the wavevector, that are equally spaced a distance λ apart, and that propagate in the $\mathbf{k}$-direction at the velocity v. See Figure [f10.2]. Hence, the direction of the wavevector specifies the wave propagation direction, whereas its magnitude determines the wavenumber, k, and, thus, the wavelength, $\lambda = 2\pi/k$.

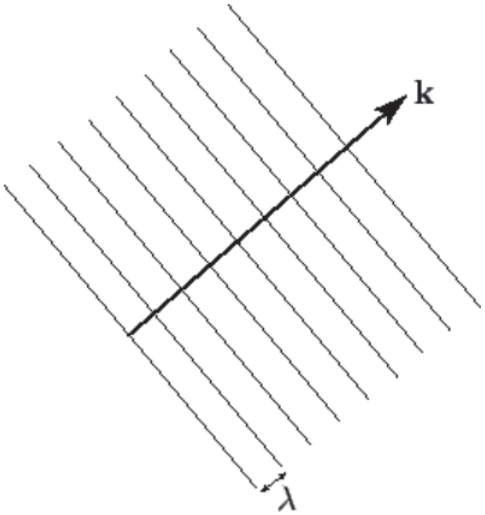

Figure 2: *Wave maxima associated with a three-dimensional plane wave.*

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2.3: Representation of Waves via Complex Functions

In mathematics, the symbol i is conventionally used to represent the square-root of minus one: in other words, one of the solutions of $\mathrm{i}^2 = -1$. Now, a *real number*, x (say), can take any value in a continuum of different values lying between $-\infty$ and $+\infty$. On the other hand, an *imaginary number* takes the general form $\mathrm{i}\,y$, where y is a real number. It follows that the square of a real number is a positive real number, whereas the square of an imaginary number is a negative real number. In addition, a general *complex number* is written

$$z = x + \mathrm{i}\,y, \tag{2.3.1}$$

where x and y are real numbers. In fact, x is termed the *real part* of z, and y the *imaginary part* of z. This is written mathematically as $x = \mathrm{Re}(z)$ and $y = \mathrm{Im}(z)$. Finally, the *complex conjugate* of z is defined $z^* = x - \mathrm{i}\,y$.

Just as we can visualize a real number as a point lying on an infinite straight-line, we can visualize a complex number as a point lying in an infinite plane. The coordinates of the point in question are the real and imaginary parts of the number: that is, $z \equiv (x,\, y)$. This idea is illustrated in Figure [f13.2]. The distance, $r = (x^2 + y^2)^{1/2}$, of the representative point from the origin is termed the *modulus* of the corresponding complex number, z. This is written mathematically as $|z| = (x^2 + y^2)^{1/2}$. Incidentally, it follows that $z\,z^* = x^2 + y^2 = |z|^2$. The angle, $\theta = \tan^{-1}(y/x)$, that the straight-line joining the representative point to the origin subtends with the real axis is termed the *argument* of the corresponding complex number, z. This is written mathematically as $\arg(z) = \tan^{-1}(y/x)$. It follows from standard trigonometry that $x = r\,\cos\theta$, and $y = r\,\sin\theta$. Hence, $z = r\,\cos\theta + \mathrm{i}\,r\sin\theta$.

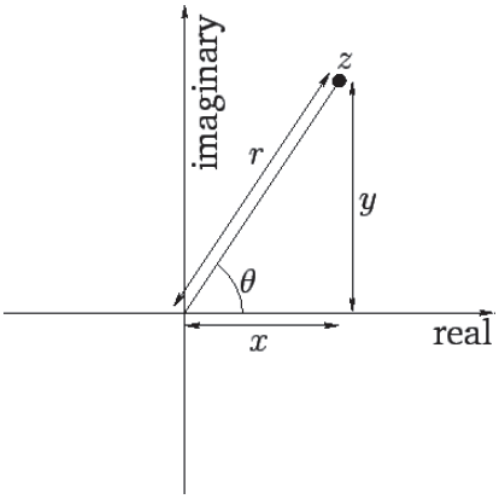

Figure 3: *Representation of a complex number as a point in a plane.*

Complex numbers are often used to represent wavefunctions. All such representations depend ultimately on a fundamental mathematical identity, known as *Euler's theorem*, that takes the form

$$\mathrm{e}^{\,\mathrm{i}\,\phi} \equiv \cos\phi + \mathrm{i}\,\sin\phi, \tag{2.3.2}$$

where ϕ is a real number. Incidentally, given that $z = r\,\cos\theta + \mathrm{i}\,r\,\sin\theta = r\,(\cos\theta + \mathrm{i}\,\sin\theta)$, where z is a general complex number, $r = |z|$ its modulus, and $\theta = \arg(z)$ its argument, it follows from Euler's theorem that any complex number, z, can be written

$$z = r\,\mathrm{e}^{\,\mathrm{i}\,\theta}, \tag{2.3.3}$$

where $r = |z|$ and $\theta = \arg(z)$ are real numbers.

A one-dimensional wavefunction takes the general form

$$\psi(x,t) = A\,\cos(k\,x - \omega\,t + \varphi), \tag{2.3.4}$$

where A is the wave amplitude, k the wavenumber, ω the angular frequency, and φ the phase angle. Consider the complex wavefunction

$$\psi(x,t) = \psi_0\, \mathrm{e}^{\,\mathrm{i}\,(k\,x-\omega\,t)}, \tag{2.3.5}$$

where ψ_0 is a complex constant. We can write

$$\psi_0 = A\, \mathrm{e}^{\,\mathrm{i}\,\varphi}, \tag{2.3.6}$$

where A is the modulus, and φ the argument, of ψ_0. Hence, we deduce that

$$\mathrm{Re}\left[\psi_0\, \mathrm{e}^{\,\mathrm{i}\,(k\,x-\omega\,t)}\right] = \mathrm{Re}\left[A\, \mathrm{e}^{\,\mathrm{i}\,\varphi}\, \mathrm{e}^{\,\mathrm{i}\,(k\,x-\omega\,t)}\right] = \mathrm{Re}\left[A\, \mathrm{e}^{\,\mathrm{i}\,(k\,x-\omega\,t+\varphi)}\right] = A\,\mathrm{Re}\left[\mathrm{e}^{\,\mathrm{i}\,(k\,x-\omega\,t+\varphi)}\right].$$

Thus, it follows from Euler's theorem, and Equation (2.3.4), that

$$\mathrm{Re}\left[\psi_0\, \mathrm{e}^{\,\mathrm{i}\,(k\,x-\omega\,t)}\right] = A\,\cos(k\,x-\omega\,t+\varphi) = \psi(x,t). \tag{2.3.7}$$

In other words, a general one-dimensional real wavefunction, (2.3.4), can be represented as the real part of a complex wavefunction of the form (2.3.5). For ease of notation, the "take the real part" aspect of the previous expression is usually omitted, and our general one-dimension wavefunction is simply written

$$\psi(x,t) = \psi_0\, \mathrm{e}^{\,\mathrm{i}\,(k\,x-\omega\,t)}. \tag{2.3.8}$$

The main advantage of the complex representation, (2.3.8), over the more straightforward real representation, (2.3.4), is that the former enables us to combine the amplitude, A, and the phase angle, φ, of the wavefunction into a single complex amplitude, ψ_0. Finally, the three-dimensional generalization of the previous expression is

$$\psi(\mathbf{r},t) = \psi_0\, \mathrm{e}^{\,\mathrm{i}\,(\mathbf{k}\cdot\mathbf{r}-\omega\,t)}, \tag{2.3.9}$$

where $\mathbf{k}$ is the wavevector.

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2.4: Classical Light-Waves

Consider a classical, monochromatic, linearly-polarized, plane light-wave, propagating through a vacuum in the x-direction. It is convenient to characterize a light-wave (which is, of course, a type of electromagnetic wave) by specifying its associated electric field. Suppose that the wave is polarized such that this electric field oscillates in the y-direction. (According to standard electromagnetic theory, the magnetic field oscillates in the z-direction, in phase with the electric field, with an amplitude which is that of the electric field divided by the velocity of light in vacuum.) Now, the electric field can be conveniently represented in terms of a *complex wavefunction*:

$$\psi(x,t) = \bar{\psi}\,\mathrm{e}^{\,\mathrm{i}\,(k\,x-\omega\,t)}. \tag{2.4.1}$$

Here, $\mathrm{i} = \sqrt{-1}$, k and ω are real parameters, and $\bar{\psi}$ is a complex wave amplitude. By convention, the physical electric field is the real part of the previous expression. Suppose that

$$\bar{\psi} = |\bar{\psi}|\,\mathrm{e}^{\,\mathrm{i}\,\varphi}, \tag{2.4.2}$$

where φ is real. It follows that the physical electric field takes the form

$$E_y(x,t) = \mathrm{Re}[\psi(x,t)] = |\bar{\psi}|\,\cos(k\,x-\omega\,t+\varphi), \tag{2.4.3}$$

where $|\bar{\psi}|$ is the amplitude of the electric oscillation, k the wavenumber, ω the angular frequency, and φ the phase angle. In addition, $\lambda = 2\pi/k$ is the wavelength, and $\nu = \omega/2\pi$ the frequency (in hertz).

According to standard electromagnetic theory , the frequency and wavelength of light-waves are related according to the well-known expression

$$c = \nu\,\lambda, \tag{2.4.4}$$

or, equivalently,

$$\omega = k\,c, \tag{2.4.5}$$

where $c = 3\times10^{8}\ \mathrm{m/s}$ is the velocity of light in vacuum. Equations (2.4.3) and (2.4.5) yield

$$E_y(x,t) = |\bar{\psi}|\,\cos(k\,[x-(\omega/k)\,t]+\varphi) = |\bar{\psi}|\,\cos(k\,[x-c\,t]+\varphi). \tag{2.4.6}$$

Note that E_y depends on x and t only via the combination $x-c\,t$. It follows that the wave maxima and minima satisfy

$$x - c\,t = \text{constant}. \tag{2.4.7}$$

Thus, the wave maxima and minima propagate in the x-direction at the fixed velocity

$$\frac{dx}{dt} = c. \tag{2.4.8}$$

An expression, such as Equation (2.4.5), that determines the wave angular frequency as a function of the wavenumber, is generally termed a *dispersion relation*. As we have already seen, and as is apparent from Equation (2.4.6), the maxima and minima of a plane-wave propagate at the characteristic velocity

$$v_p = \frac{\omega}{k}, \tag{2.4.9}$$

which is known as the *phase-velocity*. Hence, the dispersion relation (2.4.5) is effectively saying that the phase-velocity of a plane light-wave, propagating through a vacuum, always takes the fixed value c, irrespective of its wavelength or frequency.

From standard electromagnetic theory , the *energy density* (i.e., the energy per unit volume) of a plane light-wave is

$$U = \frac{E_y^{\,2}}{\epsilon_0}, \tag{2.4.10}$$

where $\epsilon_0 = 8.85\times10^{-12}\ \mathrm{F/m}$ is the *electrical permittivity of free space*. Hence, it follows from Equations (2.4.1) and (2.4.3) that

$$U \propto |\psi|^{\,2}. \tag{2.4.11}$$

Furthermore, a light-wave possesses linear momentum, as well as energy. This momentum is directed along the wave's direction of propagation, and is of density

$$G = \frac{U}{c}. \tag{2.4.12}$$

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2.5: Photoelectric Effect

The so-called *photoelectric effect*, by which a polished metal surface emits electrons when illuminated by visible and ultra-violet light, was discovered by Heinrich Hertz in 1887 . The following facts regarding this effect can be established via careful observation. First, a given surface only emits electrons when the frequency of the light with which it is illuminated exceeds a certain threshold value, which is a property of the metal. Second, the current of photoelectrons, when it exists, is proportional to the intensity of the light falling on the surface. Third, the energy of the photoelectrons is independent of the light intensity, but varies linearly with the light frequency. These facts are inexplicable within the framework of classical physics.

In 1905, Albert Einstein proposed a radical new theory of light in order to account for the photoelectric effect . According to this theory, light of fixed frequency ν consists of a collection of indivisible discrete packages, called *quanta*,[1] whose energy is

$$E = h\,\nu. \tag{2.5.1}$$

Here, $h = 6.6261 \times 10^{-34}$ J s is a new constant of nature, known as *Planck's constant*. Incidentally, h is called Planck's constant, rather than Einstein's constant, because Max Planck first introduced the concept of the quantization of light, in 1900, while trying to account for the electromagnetic spectrum of a black body (i.e., a perfect emitter and absorber of electromagnetic radiation) .

Suppose that the electrons at the surface of a metal lie in a potential well of depth W. In other words, the electrons have to acquire an energy W in order to be emitted from the surface. Here, W is generally called the *work function* of the surface, and is a property of the metal. Suppose that an electron absorbs a single quantum of light. Its energy therefore increases by $h\,\nu$. If $h\,\nu$ is greater than W then the electron is emitted from the surface with residual kinetic energy

$$K = h\,\nu - W. \tag{2.5.2}$$

Otherwise, the electron remains trapped in the potential well, and is not emitted. Here, we are assuming that the probability of an electron simultaneously absorbing two or more light quanta is negligibly small compared to the probability of it absorbing a single light quantum (as is, indeed, the case for sufficiently low-intensity illumination). Incidentally, we can calculate Planck's constant, and the work function of the metal, by simply plotting the kinetic energy of the emitted photoelectrons as a function of the wave frequency, as shown in Figure [f1]. This plot is a straight-line whose slope is h, and whose intercept with the ν-axis is W/h. Finally, the number of emitted electrons increases with the intensity of the light because the more intense the light, the larger the flux of light quanta onto the surface. Thus, Einstein's quantum theory is capable of accounting for all three of the previously mentioned observational facts regarding the photoelectric effect.

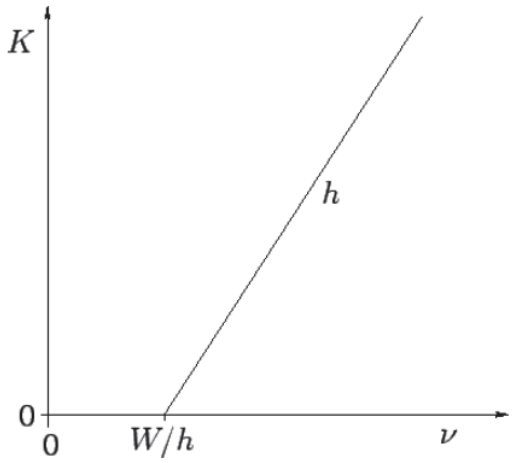

Figure 4: *Variation of the kinetic energy K of photoelectrons with the wave-frequency ν.*

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2.6: Quantum Theory of Light

According to Einstein's quantum theory of light, a monochromatic light-wave of angular frequency ω, propagating through a vacuum, can be thought of as a stream of particles, called *photons*, of energy

$$E = \hbar\,\omega, \tag{2.6.1}$$

where $\hbar = h/2\pi = 1.0546 \times 10^{-34}\,\mathrm{J\,s}$. Because classical light-waves propagate at the fixed velocity c, it stands to reason that photons must also move at this velocity. According to Einstein's special theory of relativity, only massless particles can move at the speed of light in vacuum . Hence, photons must be massless. Special relativity also gives the following relationship between the energy E and the momentum p of a massless particle ,

$$p = \frac{E}{c}. \tag{2.6.2}$$

Note that the previous relation is consistent with Equation (2.4.12), because if light is made up of a stream of photons, for which $E/p = c$, then the momentum density of light must be the energy density divided by c. It follows, from the previous two equations, that photons carry momentum

$$p = \hbar\,k \tag{2.6.3}$$

along their direction of motion, because $\omega/c = k$ for a light-wave. [See Equation (2.4.5).]

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2.7: Classical Interferences of Light Waves

Let us now consider the classical interference of light-waves. Figure [f2] shows a standard double-slit interference experiment in which monochromatic plane light-waves are normally incident on two narrow parallel slits that are situated a distance d apart. The light from the two slits is projected onto a screen a distance D behind them, where $D \gg d$.

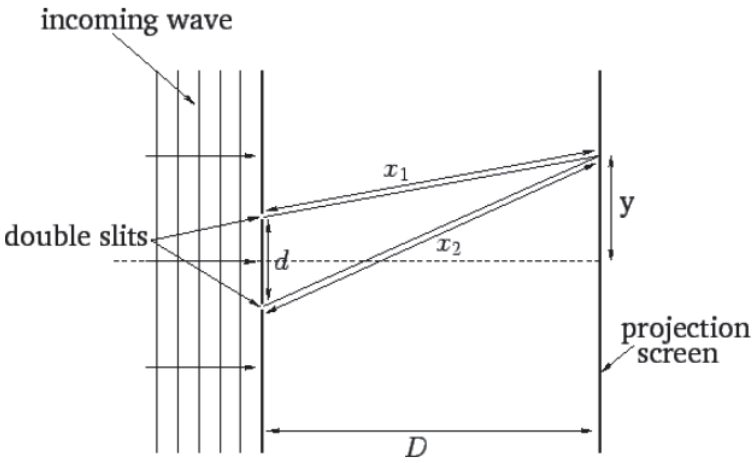


Figure 5: *Classical double-slit interference of light.*

Consider some point on the screen that is located a distance y from the centre-line, as shown in the figure. Light from the first slit travels a distance x_1 to get to this point, whereas light from the second slit travels a slightly different distance x_2. It is easily demonstrated that

$$\Delta x = x_2 - x_1 \simeq \frac{d}{D}\, y, \tag{2.7.1}$$

provided $d \ll D$. It follows from Equation (2.4.1), and the well-known fact that light-waves are superposible, that the wavefunction at the point in question can be written

$$\psi(y,t) \propto \psi_1(t)\, \mathrm{e}^{\,\mathrm{i}\, k\, x_1} + \psi_2(t)\, \mathrm{e}^{\,\mathrm{i}\, k\, x_2}, \tag{2.7.2}$$

where ψ_1 and ψ_2 are the wavefunctions at the first and second slits, respectively. However,

$$\psi_1 = \psi_2, \tag{2.7.3}$$

because the two slits are assumed to be illuminated by in-phase light-waves of equal amplitude. (Note that we are ignoring the difference in amplitude of the waves from the two slits at the screen, due to the slight difference between x_1 and x_2, compared to the difference in their phases. This is reasonable provided $D \gg \lambda$.) The intensity (that is, the energy flux) of the light at some point on the projection screen is approximately equal to the energy density of the light at this point times the velocity of light (provided that $y \ll D$). Hence, it follows from Equation (2.4.11) that the light intensity on the screen a distance y from the center-line is

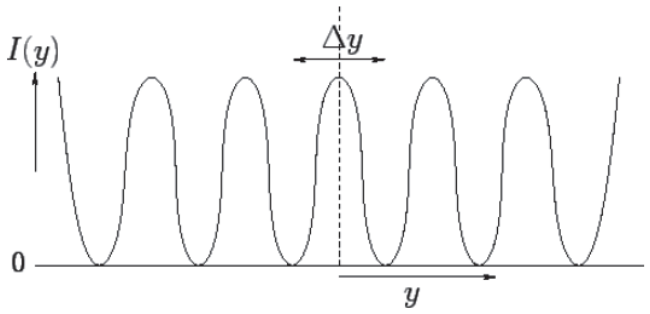
$$I(y) \propto |\psi(y,t)|^{\,2}. \tag{2.7.4}$$

Using Equations (2.7.1)–(2.7.4), we obtain

$$I(y) \propto \cos^2\left(\frac{k\,\Delta x}{2}\right) \simeq \cos^2\left(\pi\, \frac{d}{D\,\lambda}\, y\right). \tag{2.7.5}$$

Figure [f3] shows the characteristic interference pattern corresponding to the previous expression. This pattern consists of equally-spaced light and dark bands of characteristic width

$$\Delta y = \frac{D\,\lambda}{d}. \tag{2.7.6}$$



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2.8: Quantum Interference of Light

Let us now consider double-slit light interference from a quantum-mechanical point of view. According to quantum theory, light-waves consist of a stream of massless photons moving at the speed of light. Hence, we expect the two slits in Figure [f2] to be spraying photons in all directions at the same rate. Suppose, however, that we reduce the intensity of the light source illuminating the slits until the source is so weak that only a single photon is present between the slits and the projection screen at any given time. Let us also replace the projection screen by a photographic film that records the position where it is struck by each photon. If we wait a sufficiently long time that a great many photons have passed through the slits and struck the photographic film, and then develop the film, do we see an interference pattern which looks like that shown in Figure [f3]? The answer to this question, as determined by experiment , is that we see exactly the same interference pattern.

According to the previous discussion, the interference pattern is built up one photon at a time. In other words, the pattern is not due to the interaction of different photons. Moreover, the point at which a given photon strikes the film is not influenced by the points at which previous photons struck the film, given that there is only one photon in the apparatus at any given time. Hence, the only way in which the classical interference pattern can be reconstructed, after a great many photons have passed through the apparatus, is if each photon has a greater probability of striking the film at points where the classical interference pattern is bright, and a lesser probability of striking the film at points where the interference pattern is dark.

Suppose, then, that we allow N photons to pass through our apparatus, and then count the number of photons that strike the recording film between y and $y+\Delta y$, where Δy is a relatively small division. Let us call this number $n(y)$. The number of photons that strike a region of the film in a given time interval is equivalent to the intensity of the light illuminating that region of the film multiplied by the area of the region, because each photon carries a fixed amount of energy. Hence, in order to reconcile the classical and quantum viewpoints, we need

$$P_y(y) \equiv \lim_{N\rightarrow\infty}\left[\frac{n(y)}{N}\right] \propto I(y)\,\Delta y, \tag{2.8.1}$$

where $I(y)$ is given in Equation (2.7.5). Here, $P_y(y)$ is the probability that a given photon strikes the film between y and $y+\Delta y$. Note that $P_y \propto \Delta y$. In other words, the probability of a photon striking a region of the film of width Δy is directly proportional to this width. Actually, this is only true as long as Δy is relatively small. It is convenient to define a probability density, $P(y)$, which is such that the probability of a photon striking a region of the film of infinitesimal width dy is $P_y(y) = P(y)\,dy$. Now, Equation (2.8.1) yields $P_y(y) \propto I(y)\,dy$, which gives $P(y) \propto I(y)$. However, according to Equation (2.7.4), $I(y) \propto |\psi(y,t)|^2$. Thus, we obtain

$$P(y) \propto |\psi(y,t)|^2. \tag{2.8.2}$$

In other words, the probability density of a photon striking a given point on the film is proportional to the modulus squared of the wavefunction at that point. Another way of saying this is that the probability of a measurement of the photon's distance from the centerline, at the location of the film, yielding a result between y and $y+dy$ is proportional to $|\psi(y,t)|^2\,dy$.

Note that, in the quantum-mechanical picture, we can only predict the probability that a given photon strikes a given point on the film. If photons behaved classically then we could, in principle, solve their equations of motion and predict exactly where each photon was going to strike the film, given its initial position and velocity. This loss of determinancy in quantum mechanics is a direct consequence of wave-particle duality. In other words, we can only reconcile the wave-like and particle-like properties of light in a statistical sense. It is impossible to reconcile them on the individual particle level.

In principle, each photon that passes through our apparatus is equally likely to pass through one of the two slits. Can we determine through which slit a given photon passed? Suppose that our original interference experiment involves sending $N \gg 1$ photons through our apparatus. We know that we get an interference pattern in this experiment. Suppose that we perform a modified interference experiment in which we close off one slit, send $N/2$ photons through the apparatus, and then open the slit and close off the other slit, and send $N/2$ photons through the apparatus. In this second experiment, which is virtually identical to the first on the individual photon level, we know exactly which slit each photon passed through. However, the wave theory of light (which we expect to agree with the quantum theory in the limit $N \gg 1$) tells us that our modified interference experiment will not result in the formation of an interference pattern. After all, according to conventional wave theory, it is impossible to obtain a two-slit interference pattern from a single slit. Hence, we conclude that any attempt to measure through which slit each photon passes in our two-slit interference experiment results in the destruction of the interference pattern. It follows that, in the quantum-mechanical

version of the two-slit interference experiment, we must think of each photon as essentially passing through both slits simultaneously.

Contributors and Attributions

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2.9: Particles

Classical Particles

In this book, we are going to concentrate, almost exclusively, on the behavior of non-relativistic particles of non-zero mass (e.g., electrons). In the absence of external forces, such particles, of mass m, energy E, and momentum p, move classically in a straight-line with velocity

$$v = \frac{p}{m}, \tag{2.9.1}$$

and satisfy

$$E = \frac{p^2}{2\,m}. \tag{2.9.2}$$

Quantum Particles

Just as light-waves sometimes exhibit particle-like properties, it turns out that massive particles sometimes exhibit wave-like properties. For instance, it is possible to obtain a double-slit interference pattern from a stream of mono-energetic electrons passing through two closely-spaced narrow slits . The effective wavelength of the electrons can be determined by measuring the width of the light and dark bands in the interference pattern. [See Equation (2.7.6).] It is found that

$$\lambda = \frac{h}{p}. \tag{2.9.3}$$

The same relation is found for other types of particles. The previous wavelength is called the *de Broglie wavelength*, after Louis de Broglie, who first suggested that particles should have wave-like properties in 1923 . Note that the de Broglie wavelength is generally very small. For instance, that of an electron is

$$\lambda_e = 1.2 \times 10^{-9}\,[E(\text{eV})]^{-1/2}\,\text{m}, \tag{2.9.4}$$

where the electron energy is conveniently measured in units of electron-volts (eV). (An electron accelerated from rest through a potential difference of 1000 V acquires an energy of 1000 eV, and so on.) The de Broglie wavelength of a proton is

$$\lambda_p = 2.9 \times 10^{-11}\,[E(\text{eV})]^{-1/2}\,\text{m}. \tag{2.9.5}$$

Given the smallness of the de Broglie wavelengths of common particles, it is actually quite difficult to perform particle interference experiments. In general, in order to perform an effective interference experiment, the spacing of the slits must not be too much greater than the wavelength of the wave. Hence, particle interference experiments require either very low-energy particles (because $\lambda \propto E^{\,-1/2}$), or very closely-spaced slits. Usually the "slits" consist of crystals, which act a bit like diffraction gratings with a characteristic spacing of order the inter-atomic spacing (which is generally about 10^{-9} m).

Equation (2.9.3) can be rearranged to give

$$p = \hbar\, k, \tag{2.9.6}$$

which is exactly the same as the relation between momentum and wavenumber that we obtained earlier for photons. [See Equation ([e2.19b]).] For the case of a particle moving the three dimensions, the previous relation generalizes to give

$$\mathbf{p} = \hbar\, \mathbf{k}, \tag{2.9.7}$$

where $\mathbf{p}$ is the particle's vector momentum, and $\mathbf{k}$ its wavevector. It follows that the momentum of a quantum particle, and, hence, its velocity, is always parallel to its wavevector.

Because the relation ([e2.19b]) between momentum and wavenumber applies to both photons and massive particles, it seems plausible that the closely-related relation (2.6.1) between energy and wave angular frequency should also apply to both photons and particles. If this is the case, and we can write

$$E = \hbar\,\omega \tag{2.9.8}$$

for particle waves, then Equations (2.9.2) and (2.9.6) yield the following dispersion relation for such waves:

$$\omega = \frac{\hbar\, k^2}{2\, m}. \tag{2.9.9}$$

We saw earlier that a plane-wave propagates at the so-called phase-velocity,

$$v_p = \frac{\omega}{k}. \tag{2.9.10}$$

However, according to the previous dispersion relation, a particle plane-wave propagates at

$$v_p = \frac{p}{2\, m}. \tag{2.9.11}$$

Note, from Equation (2.9.1), that this is only half of the classical particle velocity. Does this imply that the dispersion relation (2.9.9) is incorrect? Let us investigate further.

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2.10: Wave-Packets

The previous discussion suggests that the wavefunction of a massive particle of momentum p and energy E, moving in the positive x-direction, can be written

$$\psi(x,t) = \bar{\psi}\,\mathrm{e}^{\,\mathrm{i}\,(k\,x-\omega\,t)}, \tag{2.10.1}$$

where $k = p/\hbar > 0$ and $\omega = E/\hbar > 0$. Here, ω and k are linked via the dispersion relation ([e2.38]). Expression ([e2.41]) represents a plane-wave whose maxima and minima propagate in the positive x-direction with the phase-velocity $v_p = \omega/k$. As we have seen, this phase-velocity is only half of the classical velocity of a massive particle.

From before, the most reasonable physical interpretation of the wavefunction is that $|\psi(x,t)|^{\,2}$ is proportional to the probability density of finding the particle at position x at time t. However, the modulus squared of the wavefunction ([e2.41]) is $|\bar{\psi}|^{\,2}$, which depends on neither x nor t. In other words, this wavefunction represents a particle that is equally likely to be found anywhere on the x-axis at all times. Hence, the fact that the maxima and minima of the wavefunction propagate at a phase-velocity that does not correspond to the classical particle velocity does not have any real physical consequences.

How can we write the wavefunction of a particle that is localized in x: that is, a particle that is more likely to be found at some positions on the x-axis than at others? It turns out that we can achieve this goal by forming a linear combination of plane-waves of different wavenumbers: in other words,

$$\psi(x,t) = \int_{-\infty}^{\infty} \bar{\psi}(k)\,\mathrm{e}^{\,\mathrm{i}\,(k\,x-\omega\,t)}\,dk. \tag{2.10.2}$$

Here, $\bar{\psi}(k)$ represents the complex amplitude of plane-waves of wavenumber k in this combination. In writing the previous expression, we are relying on the assumption that particle waves are superposable: that is, that it is always possible to add two valid wave solutions to form a third valid wave solution. The ultimate justification for this assumption is that particle waves satisfy a differential wave equation that is linear in ψ. As we shall see, in Section 1.15, this is indeed the case. Incidentally, a plane-wave that varies as $\exp[\,\mathrm{i}\,(k\,x-\omega\,t)]$ and has a negative k (but positive ω) propagates in the negative x-direction at the phase-velocity $\omega/|k|$. Hence, the superposition ([e2.42]) includes both forward and backward propagating waves.

There is a useful mathematical theorem, known as *Fourier's theorem* , which states that if

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \bar{f}\,(k)\,\mathrm{e}^{\,\mathrm{i}\,k\,x}\,dk, \tag{2.10.3}$$

then

$$\bar{f}\,(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)\,\mathrm{e}^{-\mathrm{i}\,k\,x}\,dx. \tag{2.10.4}$$

Here, $\bar{f}\,(k)$ is known as the *Fourier transform* of the function $f(x)$. We can use Fourier's theorem to find the k-space function $\bar{\psi}(k)$ that generates any given x-space wavefunction $\psi(x)$ at a given time.

For instance, suppose that at $t = 0$ the wavefunction of our particle takes the form

$$\psi(x,0) \propto \exp\left[\mathrm{i}\,k_0\,x - \frac{(x-x_0)^{\,2}}{4\,(\Delta x)^{\,2}}\right]. \tag{2.10.5}$$

Thus, the initial probability density of the particle is written

$$|\psi(x,0)|^{\,2} \propto \exp\left[-\frac{(x-x_0)^{\,2}}{2\,(\Delta x)^{\,2}}\right]. \tag{2.10.6}$$

This particular probability distribution is called a *Gaussian* distribution, and is plotted in Figure [f4]. It can be seen that a measurement of the particle's position is most likely to yield the value x_0, and very unlikely to yield a value which differs from x_0 by more than $3\,\Delta x$. Thus, Equation ([e2.45]) is the wavefunction of a particle that is initially localized around $x = x_0$ in some region whose width is of order Δx. This type of wavefunction is known as a *wave-packet*.

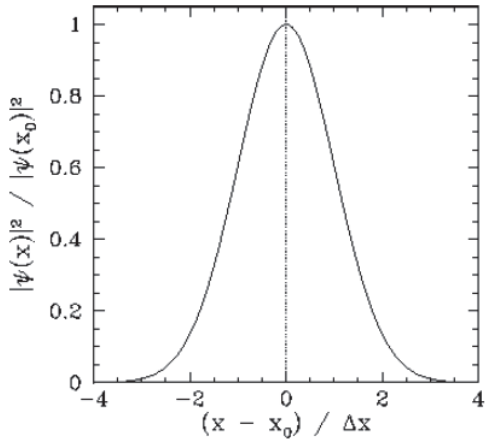

Figure 7: *A Gaussian probability distribution in x-space.*

According to Equation ([e2.42]),

$$\psi(x,0) = \int_{-\infty}^{\infty} \bar{\psi}(k)\, \mathrm{e}^{\,\mathrm{i}\,k\,x}\, dk. \tag{2.10.7}$$

Hence, we can employ Fourier's theorem to invert this expression to give

$$\bar{\psi}(k) \propto \int_{-\infty}^{\infty} \psi(x,0)\, \mathrm{e}^{-\mathrm{i}\,k\,x}\, dx. \tag{2.10.8}$$

Making use of Equation ([e2.45]), we obtain

$$\bar{\psi}(k) \propto \mathrm{e}^{-\mathrm{i}\,(k-k_0)\,x_0} \int_{-\infty}^{\infty} \exp\left[-\mathrm{i}\,(k-k_0)\,(x-x_0) - \frac{(x-x_0)^{\,2}}{4\,(\Delta x)^{\,2}}\right] dx. \tag{2.10.9}$$

Changing the variable of integration to $y = (x-x_0)/(2\,\Delta x)$, this reduces to

$$\bar{\psi}(k) \propto \mathrm{e}^{-\mathrm{i}\,k\,x_0} \int_{-\infty}^{\infty} \exp\bigl(-\mathrm{i}\,\beta\,y - y^{\,2}\bigr) dy, \tag{2.10.10}$$

where $\beta = 2\,(k-k_0)\,\Delta x$. The previous equation can be rearranged to give

$$\bar{\psi}(k) \propto \mathrm{e}^{-\mathrm{i}\,k\,x_0 - \beta^{\,2}/4} \int_{-\infty}^{\infty} \mathrm{e}^{-(y-y_0)^{\,2}}\, dy, \tag{2.10.11}$$

where $y_0 = -\mathrm{i}\,\beta/2$. The integral now just reduces to a number, as can easily be seen by making the change of variable $z = y - y_0$. Hence, we obtain

$$\bar{\psi}(k) \propto \exp\left[-\mathrm{i}\,k\,x_0 - \frac{(k-k_0)^{\,2}}{4\,(\Delta k)^{\,2}}\right], \tag{2.10.12}$$

where

$$\Delta k = \frac{1}{2\,\Delta x}. \tag{2.10.13}$$

If $|\psi(x)|^{\,2}$ is proportional to the probability density of a measurement of the particle's position yielding the value x then it stands to reason that $|\bar{\psi}(k)|^{\,2}$ is proportional to the probability density of a measurement of the particle's wavenumber yielding the value k. (Recall that $p = \hbar\,k$, so a measurement of the particle's wavenumber, k, is equivalent to a measurement of the particle's momentum, p). According to Equation ([e2.51]),

$$|\bar{\psi}(k)|^{\,2} \propto \exp\left[-\frac{(k-k_0)^{\,2}}{2\,(\Delta k)^{\,2}}\right]. \tag{2.10.14}$$

Note that this probability distribution is a Gaussian in k-space. [See Equation ([e2.46]) and Figure [f4].] Hence, a measurement of k is most likely to yield the value k_0, and very unlikely to yield a value which differs from k_0 by more than $3\,\Delta k$. Incidentally, a Gaussian is the only simple mathematical function in x-space that has the same form as its Fourier transform in k-space.

We have just seen that a Gaussian probability distribution of characteristic width Δx in x-space [see Equation ([e2.46])] transforms to a Gaussian probability distribution of characteristic width Δk in k-space [see Equation ([e2.53])], where

$$\Delta x\,\Delta k = \frac{1}{2}. \tag{2.10.15}$$

This illustrates an important property of wave-packets. Namely, if we wish to construct a packet that is very localized in x-space (i.e., if Δx is small) then we need to combine plane-waves with a very wide range of different k-values (i.e., Δk will be large). Conversely, if we only combine plane-waves whose wavenumbers differ by a small amount (i.e., if Δk is small) then the resulting wave-packet will be very extended in x-space (i.e., Δx will be large).

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2.11: Evolution of Wave-Packets

We have seen, in Equation ([e2.45]), how to write the wavefunction of a particle that is initially localized in x-space. Let us examine how this wavefunction evolves in time. According to Equation ([e2.42]), we have

$$\psi(x,t) = \int_{-\infty}^{\infty} \bar{\psi}(k)\, \mathrm{e}^{\,\mathrm{i}\,\phi(k)}\, dk, \tag{2.11.1}$$

where

$$\phi(k) = k\,x - \omega(k)\,t. \tag{2.11.2}$$

The function $\bar{\psi}(k)$ is obtained by Fourier transforming the wavefunction at $t=0$. [See Equations ([e2.42a]) and ([e2.51]).] According to Equation ([e2.53]), $|\bar{\psi}(k)|$ is strongly peaked around $k=k_0$. Thus, it is a reasonable approximation to Taylor expand $\phi(k)$ about k_0. Keeping terms up to second order in $k-k_0$, we obtain

$$\psi(x,t) \propto \int_{-\infty}^{\infty} \bar{\psi}(k)\, \exp\left[\mathrm{i}\left\{\phi_0 + \phi_0'\,(k-k_0) + \frac{1}{2}\,\phi_0''\,(k-k_0)^{\,2}\right\}\right], \tag{2.11.3}$$

where

$$\begin{aligned}
\phi_0 &= \phi(k_0) = k_0\,x - \omega_0\,t,\\
\phi_0' &= \frac{d\phi(k_0)}{dk} = x - v_g\,t,\\
\phi_0'' &= \frac{d^{\,2}\phi(k_0)}{dk^{\,2}} = -\alpha\,t,
\end{aligned}$$

with

$$\begin{aligned}
\omega_0 &= \omega(k_0),\\
v_g &= \frac{d\omega(k_0)}{dk},\\
\alpha &= \frac{d^{\,2}\omega(k_0)}{dk^{\,2}}.
\end{aligned}$$

Substituting from Equation ([e2.51]), rearranging, and then changing the variable of integration to $y = (k-k_0)/(2\,\Delta k)$, we get

$$\psi(x,t) \propto \mathrm{e}^{\,\mathrm{i}\,(k_0\,x-\omega_0\,t)} \int_{-\infty}^{\infty} \mathrm{e}^{\,\mathrm{i}\,\beta_1\,y-(1+\mathrm{i}\,\beta_2)\,y^{\,2}}\, dy, \tag{2.11.4}$$

where

$$\begin{aligned}
\beta_1 &= 2\,\Delta k\,(x - x_0 - v_g\,t),\\
\beta_2 &= 2\,\alpha\,(\Delta k)^{\,2}\,t.
\end{aligned}$$

Incidentally, $\Delta k = 1/(2\,\Delta x)$, where Δx is the initial width of the wave-packet. The previous expression can be rearranged to give

$$\psi(x,t) \propto \mathrm{e}^{\,\mathrm{i}\,(k_0\,x-\omega_0\,t)-(1+\mathrm{i}\,\beta_2)\,\beta^{\,2}/4} \int_{-\infty}^{\infty} \mathrm{e}^{-(1+\mathrm{i}\,\beta_2)\,(y-y_0)^{\,2}}\, dy, \tag{2.11.5}$$

where $y_0 = \mathrm{i}\,\beta/2$ and $\beta = \beta_1/(1+\mathrm{i}\,\beta_2)$. Again changing the variable of integration to $z = (1+\mathrm{i}\,\beta_2)^{1/2}\,(y-y_0)$, we get

$$\psi(x,t) \propto (1+\mathrm{i}\,\beta_2)^{-1/2}\, \mathrm{e}^{\,\mathrm{i}\,(k_0\,x-\omega_0\,t)-(1+\mathrm{i}\,\beta_2)\,\beta^{\,2}/4} \int_{-\infty}^{\infty} \mathrm{e}^{-z^{\,2}}\, dz. \tag{2.11.6}$$

The integral now just reduces to a number. Hence, we obtain

$$\psi(x,t) \propto \frac{\exp\left[\mathrm{i}\,(k_0\,x-\omega_0\,t) - (x-x_0-v_g\,t)^{\,2}\,\{1-\mathrm{i}\,2\,\alpha\,(\Delta k)^{\,2}\,t\}/(4\,\sigma^{\,2})\right]}{[1+\mathrm{i}\,2\,\alpha\,(\Delta k)^{\,2}\,t]^{1/2}}, \tag{2.11.7}$$

where

$$\sigma^2(t) = (\Delta x)^2 + \frac{\alpha^2 t^2}{4\,(\Delta x)^2}. \tag{2.11.8}$$

Note that the previous wavefunction is identical to our original wavefunction ([e2.45]) at $t = 0$. This justifies the approximation that we made earlier by Taylor expanding the phase factor $\phi(k)$ about $k = k_0$.

According to Equation ([exxx]), the probability density of our particle as a function of time is written

$$|\psi(x,t)|^2 \propto \sigma^{-1}(t) \exp\left[-\frac{(x - x_0 - v_g\,t)^2}{2\,\sigma^2(t)}\right]. \tag{2.11.9}$$

Hence, the probability distribution is a Gaussian, of characteristic width $\sigma(t)$, that peaks at $x = x_0 + v_g\,t$. The most likely position of our particle coincides with the peak of the distribution function. Thus, the particle's most likely position is given by

$$x = x_0 + v_g\,t. \tag{2.11.10}$$

It can be seen that the particle effectively moves at the uniform velocity

$$v_g = \frac{d\omega}{dk}, \tag{2.11.11}$$

which is known as the *group-velocity*. In other words, a plane-wave travels at the phase-velocity, $v_p = \omega/k$, whereas a wave-packet travels at the group-velocity, $v_g = d\omega/dt$. It follows from the dispersion relation ([e2.38]) for particle waves that

$$v_g = \frac{p}{m}. \tag{2.11.12}$$

However, it can be seen from Equation ([e2.31]) that this is identical to the classical particle velocity. Hence, the dispersion relation ([e2.38]) turns out to be consistent with classical physics, after all, as soon as we realize that individual particles must be identified with wave-packets rather than plane-waves. In fact, a plane-wave is usually interpreted as a continuous stream of particles propagating in the same direction as the wave.

According to Equation ([e2.70]), the width of our wave-packet grows as time progresses. Indeed, it follows from Equations ([e2.38]) and ([e2.64]) that the characteristic time for a wave-packet of original width Δx to double in spatial extent is

$$t_2 \sim \frac{m\,(\Delta x)^2}{\hbar}. \tag{2.11.13}$$

For instance, if an electron is originally localized in a region of atomic scale (i.e., $\Delta x \sim 10^{-10}$ m) then the doubling time is only about 10^{-16} s. Evidently, particle wave-packets (for freely-moving particles) spread very rapidly.

Note, from the previous analysis, that the rate of spreading of a wave-packet is ultimately governed by the second derivative of $\omega(k)$ with respect to k. [See Equations ([e2.64]) and ([e2.70]).] This explains why a functional relationship between ω and k is generally known as a dispersion relation—it governs how fast wave-packets disperse as time progresses. However, for the special case where ω is a linear function of k, the second derivative of ω with respect to k is zero, and, hence, there is no dispersion of wave-packets: that is, wave-packets propagate without changing shape. The dispersion relation ([e2.7]) for light-waves is linear in k. It follows that light pulses propagate through a vacuum without spreading. Another property of linear dispersion relations is that the phase-velocity, $v_p = \omega/k$, and the group-velocity, $v_g = d\omega/dk$, are identical. Thus, plane light-waves and light pulses both propagate through a vacuum at the characteristic speed $c = 3 \times 10^8$ m/s. Of course, the dispersion relation ([e2.38]) for particle waves is not linear in k. Hence, particle plane-waves and particle wave-packets propagate at different velocities, and particle wave-packets also gradually disperse as time progresses.

Heisenberg's Uncertainty Principle

According to the analysis contained in the previous two sections, a particle wave-packet that is initially localized in x-space with characteristic width Δx is also localized in k-space with characteristic width $\Delta k = 1/(2\,\Delta x)$. However, as time progresses, the width of the wave-packet in x-space increases, while that of the wave-packet in k-space stays the same. [After all, our previous analysis obtained $\psi(x,t)$ from Equation ([e2.56]), but assumed that $\bar{\psi}(k)$ was given by Equation ([e2.51]) at all times.] Hence, in general, we can say that

$$\Delta x \Delta k \gtrsim \frac{1}{2} \tag{2.11.14}$$

Furthermore, we can think of Δx and Δk as characterizing our uncertainty regarding the values of the particle's position and wavenumber, respectively.

A measurement of a particle's wavenumber, k, is equivalent to a measurement of its momentum, p, because $p = \hbar\, k$. Hence, an uncertainty in k of order Δk translates to an uncertainty in p of order $\Delta p = \hbar\, \Delta k$. It follows from the previous inequality that

$$\Delta x \Delta p \gtrsim \frac{\hbar}{2} \tag{2.11.15}$$

This is the famous *Heisenberg uncertainty principle*, first proposed by Werner Heisenberg in 1927 . According to this principle, it is impossible to simultaneously measure the position and momentum of a particle (exactly). Indeed, a good knowledge of the particle's position implies a poor knowledge of its momentum, and vice versa. Note that the uncertainty principle is a direct consequence of representing particles as waves.

It can be seen from Equations ([e2.38]), ([e2.64]), and ([e2.70]) that, at large t, a particle wavefunction of original width Δx (at $t = 0$) spreads out such that its spatial extent becomes

$$\sigma \sim \frac{\hbar\, t}{m\, \Delta x}. \tag{2.11.16}$$

It is easily demonstrated that this spreading is a consequence of the uncertainty principle. Because the initial uncertainty in the particle's position is Δx, it follows that the uncertainty in its momentum is of order $\hbar/\Delta x$. This translates to an uncertainty in velocity of $\Delta v = \hbar/(m\, \Delta x)$. Thus, if we imagine that parts of the wavefunction propagate at $v_0 + \Delta v/2$, and others at $v_0 - \Delta v/2$, where v_0 is the mean propagation velocity, then the wavefunction will spread as time progresses. Indeed, at large t, we expect the width of the wavefunction to be

$$\sigma \sim \Delta v\, t \sim \frac{\hbar\, t}{m\, \Delta x}, \tag{2.11.17}$$

which is identical to Equation ([espread]). Evidently, the spreading of a particle wavefunction must be interpreted as an increase in our uncertainty regarding the particle's position, rather than an increase in the spatial extent of the particle itself.

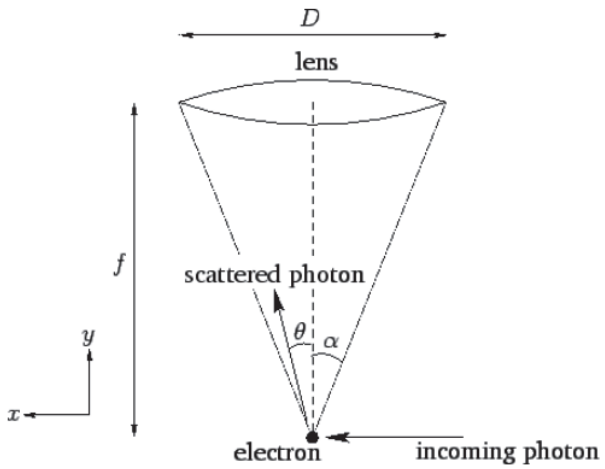

Figure 8: *Heisenberg's microscope.*

Figure [fh] illustrates a famous thought experiment known as *Heisenberg's microscope*. Suppose that we try to image an electron using a simple optical system in which the objective lens is of diameter D and focal-length f. (In practice, this would only be possible using extremely short-wavelength light.) It is a well-known result in optics that such a system has a minimum angular resolving power of λ/D, where λ is the wavelength of the light illuminating the electron . If the electron is placed at the focus of the lens, which is where the minimum resolving power is achieved, then this translates to a uncertainty in the electron's transverse position of

$$\Delta x \simeq f\, \frac{\lambda}{D}. \tag{2.11.18}$$

However,

$$\tan\alpha = \frac{D/2}{f}, \tag{2.11.19}$$

where α is the half-angle subtended by the lens at the electron. Assuming that α is small, we can write

$$\alpha \simeq \frac{D}{2\,f}, \tag{2.11.20}$$

so

$$\Delta x \simeq \frac{\lambda}{2\,\alpha}. \tag{2.11.21}$$

It follows that we can reduce the uncertainty in the electron's position by minimizing the ratio λ/α: that is, by employing short-wavelength radiation, and a wide-angle lens.

Let us now examine Heisenberg's microscope from a quantum-mechanical point of view. According to quantum mechanics, the electron is imaged when it scatters an incoming photon towards the objective lens. Let the wavevector of the incoming photon have the (x, y) components $(k, 0)$. See Figure [fh]. If the scattered photon subtends an angle θ with the center-line of the optical system, as shown in the figure, then its wavevector is written $(k\,\sin\theta, k\cos\theta)$. Here, we are ignoring any shift in wavelength of the photon on scattering—in other words, the magnitude of the $\mathbf{k}$-vector is assumed to be the same before and after scattering. Thus, the change in the x-component of the photon's wavevector is $\Delta k_x = k\,(\sin\theta - 1)$. This translates to a change in the photon's x-component of momentum of $\Delta p_x = \hbar\,k\,(\sin\theta - 1)$. By momentum conservation, the electron's x-momentum will change by an equal and opposite amount. However, θ can range all the way from $-\alpha$ to $+\alpha$, and the scattered photon will still be collected by the imaging system. It follows that the uncertainty in the electron's momentum is

$$\Delta p \simeq 2\,\hbar\,k\,\sin\alpha \simeq \frac{4\pi\,\hbar\,\alpha}{\lambda}. \tag{2.11.22}$$

Note that in order to reduce the uncertainty in the momentum we need to maximize the ratio λ/α. This is exactly the opposite of what we need to do to reduce the uncertainty in the position. Multiplying the previous two equations, we obtain

$$\Delta x\,\Delta p \sim h, \tag{2.11.23}$$

which is essentially the uncertainty principle.

According to Heisenberg's microscope, the uncertainty principle follows from two facts. First, it is impossible to measure any property of a microscopic dynamical system without disturbing the system somewhat. Second, particle and light energy and momentum are quantized. Hence, there is a limit to how small we can make the aforementioned disturbance. Thus, there is an irreducible uncertainty in certain measurements that is a consequence of the act of measurement itself.

Contributors and Attributions

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2.12: Schrodinger's Equation and Wavefunction Collapse

We have seen that the wavefunction of a free particle of mass m satisfies

$$\psi(x,t) = \int_{-\infty}^{\infty} \bar{\psi}(k)\, \mathrm{e}^{\,\mathrm{i}\,(k\,x-\omega\,t)}\, dk, \tag{2.12.1}$$

where $\bar{\psi}(k)$ is determined by $\psi(x,0)$, and

$$\omega(k) = \frac{\hbar\, k^{\,2}}{2\,m}. \tag{2.12.2}$$

It follows from Equation ([e2.78]) that

$$\frac{\partial \psi}{\partial x} = \int_{-\infty}^{\infty} (\mathrm{i}\,k)\, \bar{\psi}(k)\, \mathrm{e}^{\,\mathrm{i}\,(k\,x-\omega\,t)}\, dk, \tag{2.12.3}$$

and

$$\frac{\partial^{\,2}\psi}{\partial x^{\,2}} = \int_{-\infty}^{\infty} (-k^{\,2})\, \bar{\psi}(k)\, \mathrm{e}^{\,\mathrm{i}\,(k\,x-\omega\,t)}\, dk, \tag{2.12.4}$$

whereas

$$\frac{\partial \psi}{\partial t} = \int_{-\infty}^{\infty} (-\mathrm{i}\,\omega)\, \bar{\psi}(k)\, \mathrm{e}^{\,\mathrm{i}\,(k\,x-\omega\,t)}\, dk. \tag{2.12.5}$$

Thus,

$$\mathrm{i}\,\frac{\partial \psi}{\partial t} + \frac{\hbar}{2\,m}\,\frac{\partial^{\,2}\psi}{\partial x^{\,2}} = \int_{-\infty}^{\infty} \left(\omega - \frac{\hbar\, k^{\,2}}{2\,m}\right) \bar{\psi}(k)\, \mathrm{e}^{\,\mathrm{i}\,(k\,x-\omega\,t)}\, dk = 0, \tag{2.12.6}$$

where use has been made of the dispersion relation ([e2.79]). Multiplying through by $\hbar$, we obtain

$$\mathrm{i}\,\hbar\,\frac{\partial \psi}{\partial t} = -\frac{\hbar^{\,2}}{2\,m}\,\frac{\partial^{\,2}\psi}{\partial x^{\,2}}. \tag{2.12.7}$$

This expression is known as *Schrödinger's equation*, because it was first introduced by Erwin Schrödinger in 1926 . Schrödinger's equation is a linear, second-order, partial differential equation that governs the time evolution of a particle wavefunction, and is generally easier to solve than the integral equation ([e2.78]).

Of course, Equation ([e2.84]) is only applicable to freely-moving particles. Fortunately, it is fairly easy to guess the generalization of this equation for particles moving in some potential $V(x)$. It is plausible, from Equation ([e2.80]), that we can identify k with the differential operator $-\mathrm{i}\,\partial/\partial x$. Hence, the differential operator on the right-hand side of Equation ([e2.84]) is equivalent to $\hbar^{\,2}\,k^{\,2}/(2\,m)$. But, $p = \hbar\,k$. Thus, the operator is also equivalent to $p^{\,2}/(2\,m)$, which is just the energy of a freely-moving particle. However, in the presence of a potential $V(x)$, the particle's energy is written $p^{\,2}/(2\,m) + V$. Thus, it seems reasonable to make the substitution

$$-\frac{\hbar^{\,2}}{2\,m}\,\frac{\partial^{\,2}}{\partial x^{\,2}} \rightarrow -\frac{\hbar^{\,2}}{2\,m}\,\frac{\partial^{\,2}}{\partial x^{\,2}} + V(x). \tag{2.12.8}$$

This leads to the general (one-dimensional) form of Schrödinger's equation:

$$\mathrm{i}\,\hbar\,\frac{\partial \psi}{\partial t} = -\frac{\hbar^{\,2}}{2\,m}\,\frac{\partial^{\,2}\psi}{\partial x^{\,2}} + V(x)\,\psi. \tag{2.12.9}$$

Wavefunction Collapse

Consider an extended wavefunction, $\psi(x,t)$. According to our usual interpretation, $|\psi(x,t)|^{\,2}$ is proportional to the probability density of a measurement of the particle's position yielding the value x at time t. If the wavefunction is extended then there is a wide range of likely values that this measurement could give. Suppose that we make such a measurement, and obtain the value x_0. We now know that the particle is located at $x = x_0$. If we make another measurement immediately after the first one then common

sense tells us that we must obtain the same value, x_0, because the particle cannot have shifted position appreciably in an infinitesimal time interval. Thus, immediately after the first measurement, a measurement of the particle's position is certain to give the value x_0, and has no chance of giving any other value. This implies that the wavefunction must have collapsed to some sort of "spike" function located at $x = x_0$. This is illustrated in Figure [coll]. Of course, as soon as the wavefunction has collapsed, it starts to expand again, as discussed in Section 1.13. Thus, the second measurement must be made reasonably quickly after the first, in order to guarantee that the same result will be obtained.

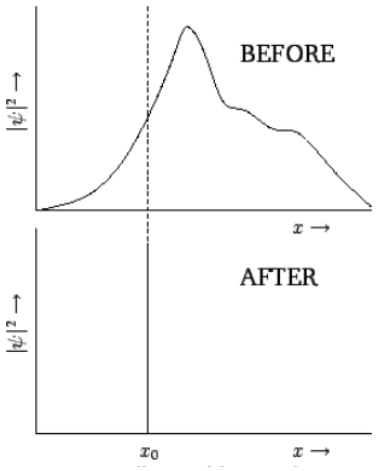

Figure 9: *Collapse of the wavefunction upon measurement of* x.

The previous discussion illustrates an important point in quantum mechanics. Namely, that the wavefunction of a particle changes discontinuously (in time) whenever a measurement is made. We conclude that there are two types of time evolution of the wavefunction in quantum mechanics. First, there is a smooth evolution that is governed by Schrödinger's equation. This evolution takes place between measurements. Second, there is a discontinuous evolution that takes place each time a measurement is made.

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2.13: Exercises

1. A He-Ne laser emits radiation of wavelength $\lambda = 633$ nm. How many photons are emitted per second by a laser with a power of 1 mW? What force does such laser exert on a body which completely absorbs its radiation?
2. The ionization energy of a hydrogen atom in its ground state is $E_{\rm ion} = 13.60$ eV (1 eV is the energy acquired by an electron accelerated through a potential difference of 1 V). Calculate the frequency, wavelength, and wavenumber of the electromagnetic radiation that will just ionize the atom.
3. The maximum energy of photoelectrons from aluminium is 2.3 eV for radiation of wavelength 2000,Angstorm), and 0.90 eV for radiation of wavelength 2580 Angstrom. Use this data to calculate Planck's constant, as well as the work function of aluminium.
4. Show that the de Broglie wavelength of an electron accelerated from rest across a potential difference V is given by
$$\lambda = 1.23 \times 10^{-9}\, V^{\,-1/2}\,{\rm m}, \tag{2.13.1}$$
where V is measured in volts.
5. If the atoms in a regular crystal are separated by 3×10^{-10} m demonstrate that an accelerating voltage of about $1.5\,{\rm kV}$ would be required to produce an electron diffraction pattern from the crystal.
6. The relationship between wavelength and frequency for electromagnetic waves in a waveguide is
$$\lambda = \frac{c}{\sqrt{\nu^{\,2} - {\nu_0}^2}}, \tag{2.13.2}$$
where c is the velocity of light in vacuum. What are the group- and phase-velocities of such waves as functions of ν_0 and λ?
7. Nuclei, typically of size 10^{-14} m, frequently emit electrons with energies of 1–10 MeV. Use the uncertainty principle to show that electrons of energy 1 MeV could not be contained in the nucleus before the decay.
8. A particle of mass m has a wavefunction
$$\psi(x,t) = A\,\exp\left[-a\left(\frac{m\,x^{\,2}}{\hbar} + {\rm i}\,t\right)\right], \tag{2.13.3}$$
where A and a are positive real constants. For what potential function $V(x)$ does ψ satisfy the Schrödinger equation?

1. Plural of *quantum*: Latin neuter of *quantus*: how much?↩

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CHAPTER OVERVIEW

3: Fundamentals of Quantum Mechanics

The previous chapter serves as a useful introduction to many of the basic concepts of quantum mechanics. In this chapter, we shall examine these concepts in a more systematic fashion. For the sake of simplicity, we shall concentrate on one-dimensional systems.

3.1: Schrodinger's Equation

Consider a dynamical system consisting of a single non-relativistic particle of mass m moving along the x-axis in some real potential $V(x)$. In quantum mechanics, the instantaneous state of the system is represented by a complex wavefunction $\psi(x,t)$. This wavefunction evolves in time according to Schrödinger's equation:

$$\mathrm{i}\,\hbar\,\frac{\partial\psi}{\partial t} = -\frac{\hbar^{\,2}}{2\,m}\,\frac{\partial^{\,2}\psi}{\partial x^{\,2}} + V(x)\,\psi. \tag{3.1.1}$$

The wavefunction is interpreted as follows: $|\psi(x,t)|^{\,2}$ is the probability density of a measurement of the particle's displacement yielding the value x. Thus, the probability of a measurement of the displacement giving a result between a and b (where $a<b$) is

$$P_{x\,\in\,a:b}(t) = \int_a^b |\psi(x,t)|^{\,2}\,dx. \tag{3.1.2}$$

Note that this quantity is real and positive definite.

3.2: Normalization of the Wavefunction

Now, a probability is a real number lying between 0 and 1. An outcome of a measurement that has a probability 0 is an impossible outcome, whereas an outcome that has a probability 1 is a certain outcome. According to Equation ([e3.2]), the probability of a measurement of x yielding a result lying between $-\infty$ and $+\infty$ is

$$P_{x\in -\infty:\infty}(t)=\int_{-\infty}^{\infty}|\psi(x,t)|^{\,2}\,dx. \tag{3.2.1}$$

However, a measurement of x must yield a value lying between $-\infty$ and $+\infty$, because the particle has to be located somewhere. It follows that $P_{x\in -\infty:\infty}=1$, or

$$\int_{-\infty}^{\infty}|\psi(x,t)|^{\,2}\,dx=1, \tag{3.2.2}$$

which is generally known as the *normalization condition* for the wavefunction.

For example, suppose that we wish to normalize the wavefunction of a Gaussian wave-packet, centered on $x=x_0$, and of characteristic width σ (see Section [s2.9]): that is,

$$\psi(x)=\psi_0\,\mathrm{e}^{-(x-x_0)^{\,2}/(4\,\sigma^{\,2})}. \tag{3.2.3}$$

In order to determine the normalization constant ψ_0, we simply substitute Equation ([e3.5]) into Equation ([e3.4]) to obtain

$$|\psi_0|^{\,2}\int_{-\infty}^{\infty}\mathrm{e}^{-(x-x_0)^{\,2}/(2\,\sigma^{\,2})}\,dx=1. \tag{3.2.4}$$

Changing the variable of integration to $y=(x-x_0)/(\sqrt{2}\,\sigma)$, we get

$$|\psi_0|^{\,2}\sqrt{2}\,\sigma\int_{-\infty}^{\infty}\mathrm{e}^{-y^{\,2}}\,dy=1. \tag{3.2.5}$$

However ,

$$\int_{-\infty}^{\infty}\mathrm{e}^{-y^{\,2}}\,dy=\sqrt{\pi}, \tag{3.2.6}$$

which implies that

$$|\psi_0|^{\,2}=\frac{1}{(2\pi\,\sigma^{\,2})^{1/2}}. \tag{3.2.7}$$

Hence, a general normalized Gaussian wavefunction takes the form

$$\psi(x)=\frac{e^{\,i\,\varphi}}{(2\pi\,\sigma^2)^{1/4}}e^{-(x-x_0)^2/(4\,\sigma^2)}, \tag{3.2.8}$$

where φ is an arbitrary real phase-angle.

It is important to demonstrate that if a wavefunction is initially normalized then it stays normalized as it evolves in time according to Schrödinger's equation. If this is not the case then the probability interpretation of the wavefunction is untenable, because it does not make sense for the probability that a measurement of x yields any possible outcome (which is, manifestly, unity) to change in time. Hence, we require that

$$\frac{d}{dt}\int_{-\infty}^{\infty}|\psi(x,t)|^{\,2}\,dx=0, \tag{3.2.9}$$

for wavefunctions satisfying Schrödinger's equation. The previous equation gives

$$\frac{d}{dt}\int_{-\infty}^{\infty}\psi^*\,\psi\,dx=\int_{-\infty}^{\infty}\left(\frac{\partial\psi^*}{\partial t}\,\psi+\psi^*\,\frac{\partial\psi}{\partial t}\right)\,dx=0. \tag{3.2.10}$$

Now, multiplying Schrödinger's equation by $\psi^*/(\mathrm{i}\,\hbar)$, we obtain

$$\psi^* \frac{\partial \psi}{\partial t} = \frac{\mathrm{i}\,\hbar}{2\,m}\,\psi^* \frac{\partial^2 \psi}{\partial x^2} - \frac{\mathrm{i}}{\hbar}\,V\,|\psi|^2. \tag{3.2.11}$$

The complex conjugate of this expression yields

$$\psi \frac{\partial \psi^*}{\partial t} = -\frac{\mathrm{i}\,\hbar}{2\,m}\,\psi \frac{\partial^2 \psi^*}{\partial x^2} + \frac{i}{\hbar}\,V\,|\psi|^2 \tag{3.2.12}$$

[because $(A\,B)^* = A^*\,B^*$, $A^{**} = A$, and $\mathrm{i}^* = -\mathrm{i}$].

Summing the previous two equations, we get

$$\frac{\partial \psi^*}{\partial t}\psi + \psi^*\frac{\partial \psi}{\partial t} = \frac{\mathrm{i}\hbar}{2\,m}\left(\psi^*\frac{\partial^2 \psi}{\partial x^2} - \psi\frac{\partial^2 \psi^*}{\partial t^2}\right) = \frac{\mathrm{i}\hbar}{2\,m}\frac{\partial}{\partial x}\left(\psi^*\frac{\partial \psi}{\partial x} - \psi\frac{\partial \psi^*}{\partial x}\right). \tag{3.2.13}$$

Equations ([e3.12]) and ([e3.15]) can be combined to produce

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\psi|^2\,dx = \frac{\mathrm{i}\,\hbar}{2\,m}\left[\psi^*\,\frac{\partial \psi}{\partial x} - \psi\,\frac{\partial \psi^*}{\partial x}\right]_{-\infty}^{\infty} = 0. \tag{3.2.14}$$

The previous equation is satisfied provided

$$|\psi| \rightarrow 0 \quad \text{as} \quad |x| \rightarrow \infty. \tag{3.2.15}$$

However, this is a necessary condition for the integral on the left-hand side of Equation ([e3.4]) to converge. Hence, we conclude that all wavefunctions that are *square-integrable* [i.e., are such that the integral in Equation ([e3.4]) converges] have the property that if the normalization condition ([e3.4]) is satisfied at one instant in time then it is satisfied at all subsequent times.

It is also possible to demonstrate, via very similar analysis to that just described, that

$$\frac{dP_{x\,\in\,a:b}}{dt} + j(b,t) - j(a,t) = 0, \tag{3.2.16}$$

where $P_{x\,\in\,a:b}$ is defined in Equation ([e3.2]), and

$$j(x,t) = \frac{\mathrm{i}\,\hbar}{2\,m}\left(\psi\,\frac{\partial \psi^*}{\partial x} - \psi^*\,\frac{\partial \psi}{\partial x}\right) \tag{3.2.17}$$

is known as the *probability current*. Note that j is real. Equation ([epc]) is a *probability conservation equation*. According to this equation, the probability of a measurement of x lying in the interval a to b evolves in time due to the difference between the flux of probability into the interval [i.e., $j(a,t)$], and that out of the interval [i.e., $j(b,t)$]. Here, we are interpreting $j(x,t)$ as the flux of probability in the $+x$-direction at position x and time t.

Note, finally, that not all wavefunctions can be normalized according to the scheme set out in Equation ([e3.4]). For instance, a plane-wave wavefunction

$$\psi(x,t) = \psi_0\,\mathrm{e}^{\,\mathrm{i}\,(k\,x - \omega\,t)} \tag{3.2.18}$$

is not square-integrable, and, thus, cannot be normalized. For such wavefunctions, the best we can say is that

$$P_{x\,\in\,a:b}(t) \propto \int_a^b |\psi(x,t)|^2\,dx. \tag{3.2.19}$$

In the following, all wavefunctions are assumed to be square-integrable and normalized, unless otherwise stated.

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3.3: Expectation Values (Averages) and Variances

We have seen that $|\psi(x,t)|^2$ is the probability density of a measurement of a particle's displacement yielding the value x at time t. Suppose that we make a large number of independent measurements of the displacement on an equally large number of identical quantum systems. In general, measurements made on different systems will yield different results. However, from the definition of probability (see Chapter [s2]), the mean of all these results is simply

$$\langle x\rangle = \int_{-\infty}^{\infty} x\,|\psi|^2\,dx. \tag{3.3.1}$$

Here, $\langle x\rangle$ is called the *expectation value* of x. (See Chapter [s2].) Similarly the expectation value of any function of x is

$$\langle f(x)\rangle = \int_{-\infty}^{\infty} f(x)\,|\psi|^2\,dx. \tag{3.3.2}$$

In general, the results of the various different measurements of x will be scattered around the expectation value, $\langle x\rangle$. The degree of scatter is parameterized by the quantity

$$\sigma_x^2 = \int_{-\infty}^{\infty} (x-\langle x\rangle)^2\,|\psi|^2\,dx \equiv \langle x^2\rangle - \langle x\rangle^2, \tag{3.3.3}$$

which is known as the *variance* of x. (See Chapter [s2].) The square-root of this quantity, σ_x, is called the *standard deviation* of x. (See Chapter [s2].) We generally expect the results of measurements of x to lie within a few standard deviations of the expectation value.

For instance, consider the normalized Gaussian wave-packet [see Equation ([eng])]

$$\psi(x) = \frac{\mathrm{e}^{\mathrm{i}\varphi}}{(2\pi\,\sigma^2)^{1/4}}\,\mathrm{e}^{-(x-x_0)^2/(4\,\sigma^2)}. \tag{3.3.4}$$

The expectation value of x associated with this wavefunction is

$$\langle x\rangle = \frac{1}{\sqrt{2\pi\,\sigma^2}}\int_{-\infty}^{\infty} x\,\mathrm{e}^{-(x-x_0)^2/(2\,\sigma^2)}\,dx. \tag{3.3.5}$$

Let $y = (x-x_0)/(\sqrt{2}\,\sigma)$. It follows that

$$\langle x\rangle = \frac{x_0}{\sqrt{\pi}}\int_{-\infty}^{\infty}\mathrm{e}^{-y^2}\,dy + \frac{\sqrt{2}\,\sigma}{\sqrt{\pi}}\int_{-\infty}^{\infty} y\,\mathrm{e}^{-y^2}\,dy. \tag{3.3.6}$$

However, the second integral on the right-hand side is zero, by symmetry. Hence, making use of Equation ([e3.8]), we obtain

$$\langle x\rangle = x_0. \tag{3.3.7}$$

Evidently, the expectation value of x for a Gaussian wave-packet is equal to the most likely value of x (i.e., the value of x that maximizes $|\psi|^2$).

The variance of x associated with the Gaussian wave-packet ([e3.24]) is

$$\sigma_x^2 = \frac{1}{\sqrt{2\pi\,\sigma^2}}\int_{-\infty}^{\infty}(x-x_0)^2\,\mathrm{e}^{-(x-x_0)^2/(2\,\sigma^2)}\,dx. \tag{3.3.8}$$

Let $y = (x-x_0)/(\sqrt{2}\,\sigma)$. It follows that

$$\sigma_x^2 = \frac{2\,\sigma^2}{\sqrt{\pi}}\int_{-\infty}^{\infty} y^2\,\mathrm{e}^{-y^2}\,dy. \tag{3.3.9}$$

However,

$$\int_{-\infty}^{\infty} y^2\,\mathrm{e}^{-y^2}\,dy = \frac{\sqrt{\pi}}{2}, \tag{3.3.10}$$

giving

$$\sigma_x^2 = \sigma^2. \tag{3.3.11}$$

This result is consistent with our earlier interpretation of σ as a measure of the spatial extent of the wave-packet. (See Section [s2.9].) It follows that we can rewrite the Gaussian wave-packet ([e3.24]) in the convenient form

$$\psi(x) = \frac{\mathrm{e}^{\,\mathrm{i}\,\varphi}}{(2\pi\,\sigma_x^2)^{1/4}}\,\mathrm{e}^{-(x-\langle x\rangle)^2/(4\,\sigma_x^2)}. \tag{3.3.12}$$

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3.4: Ehrenfest's Theorem

A simple way to calculate the expectation value of momentum is to evaluate the time derivative of $\langle x\rangle$, and then multiply by the mass m: that is,

$$\langle p\rangle = m\,\frac{d\langle x\rangle}{dt} = m\,\frac{d}{dt}\int_{-\infty}^{\infty} x\,|\psi|^{\,2}\,dx = m\int_{-\infty}^{\infty} x\,\frac{\partial|\psi|^{\,2}}{\partial t}\,dx. \tag{3.4.1}$$

However, it is easily demonstrated that

$$\frac{\partial|\psi|^{\,2}}{\partial t} + \frac{\partial j}{\partial x} = 0 \tag{3.4.2}$$

[this is just the differential form of Equation ([epc])], where j is the probability current defined in Equation ([eprobc]). Thus,

$$\langle p\rangle = -m\int_{-\infty}^{\infty} x\,\frac{\partial j}{\partial x}\,dx = m\int_{-\infty}^{\infty} j\,dx, \tag{3.4.3}$$

where we have integrated by parts. It follows from Equation ([eprobc]) that

$$\langle p\rangle = -\frac{\mathrm{i}\,\hbar}{2}\int_{-\infty}^{\infty}\left(\psi^*\,\frac{\partial\psi}{\partial x} - \frac{\partial\psi^*}{\partial x}\,\psi\right)dx = -\mathrm{i}\,\hbar\int_{-\infty}^{\infty}\psi^*\,\frac{\partial\psi}{\partial x}\,dx, \tag{3.4.4}$$

where we have again integrated by parts. Hence, the expectation value of the momentum can be written

$$\langle p\rangle = m\,\frac{d\langle x\rangle}{dt} = -\mathrm{i}\,\hbar\int_{-\infty}^{\infty}\psi^*\,\frac{\partial\psi}{\partial x}\,dx. \tag{3.4.5}$$

It follows from the previous equation that

$$\frac{d\langle p\rangle}{dt} = -\mathrm{i}\,\hbar\int_{-\infty}^{\infty}\left(\frac{\partial\psi^*}{\partial t}\,\frac{\partial\psi}{\partial x} + \psi^*\,\frac{\partial^{\,2}\psi}{\partial t\,\partial x}\right)dx = \int_{-\infty}^{\infty}\left[\left(\mathrm{i}\,\hbar\,\frac{\partial\psi}{\partial t}\right)^*\frac{\partial\psi}{\partial x} + \frac{\partial\psi^*}{\partial x}\left(\mathrm{i}\,\hbar\,\frac{\partial\psi}{\partial t}\right)\right]dx,$$

where we have integrated by parts. Substituting from Schrödinger's equation ([e3.1]), and simplifying, we obtain

$$\frac{d\langle p\rangle}{dt} = \int_{-\infty}^{\infty}\left[-\frac{\hbar^{\,2}}{2\,m}\frac{\partial}{\partial x}\left(\frac{\partial\psi^*}{\partial x}\,\frac{\partial\psi}{\partial x}\right) + V(x)\,\frac{\partial|\psi|^{\,2}}{\partial x}\right]dx = \int_{-\infty}^{\infty} V(x)\,\frac{\partial|\psi|^{\,2}}{\partial x}\,dx. \tag{3.4.6}$$

Integration by parts yields

$$\frac{d\langle p\rangle}{dt} = -\int_{-\infty}^{\infty}\frac{dV}{dx}\,|\psi|^{\,2}\,dx = -\left\langle\frac{dV}{dx}\right\rangle. \tag{3.4.7}$$

Hence, according to Equations ([e4.34x]) and ([e3.41]),

$$m\,\frac{d\langle x\rangle}{dt} = \langle p\rangle,$$
$$\frac{d\langle p\rangle}{dt} = -\left\langle\frac{dV}{dx}\right\rangle.$$

Evidently, the expectation values of displacement and momentum obey time evolution equations that are analogous to those of classical mechanics. This result is known as *Ehrenfest's theorem* .

Suppose that the potential $V(x)$ is slowly varying. In this case, we can expand dV/dx as a Taylor series about $\langle x\rangle$. Keeping terms up to second order, we obtain

$$\frac{dV(x)}{dx} = \frac{dV(\langle x\rangle)}{d\langle x\rangle} + \frac{dV^{\,2}(\langle x\rangle)}{d\langle x\rangle^{\,2}}\,(x-\langle x\rangle) + \frac{1}{2}\,\frac{dV^{\,3}(\langle x\rangle)}{d\langle x\rangle^{3}}\,(x-\langle x\rangle)^{\,2}. \tag{3.4.8}$$

Substitution of the previous expansion into Equation ([e3.43]) yields

$$\frac{d\langle p\rangle}{dt} = -\frac{dV(\langle x\rangle)}{d\langle x\rangle} - \frac{\sigma_x^2}{2}\,\frac{dV^{\,3}(\langle x\rangle)}{d\langle x\rangle^{\,3}}, \tag{3.4.9}$$

because $\langle 1\rangle = 1$, and $\langle x - \langle x\rangle\rangle = 0$, and $\langle (x-\langle x\rangle)^{\,2}\rangle = \sigma_x^2$. The final term on the right-hand side of the previous equation can be neglected when the spatial extent of the particle wavefunction, σ_x, is much smaller than the variation length-scale of the potential. In this case, Equations ([e3.42]) and ([e3.43]) reduce to

$$m\,\frac{d\langle x\rangle}{dt} = \langle p\rangle,$$
$$\frac{d\langle p\rangle}{dt} = -\frac{dV(\langle x\rangle)}{d\langle x\rangle}.$$

These equations are exactly equivalent to the equations of classical mechanics, with $\langle x\rangle$ playing the role of the particle displacement. Of course, if the spatial extent of the wavefunction is negligible then a measurement of x is almost certain to yield a result that lies very close to $\langle x\rangle$. Hence, we conclude that quantum mechanics corresponds to classical mechanics in the limit that the spatial extent of the wavefunction (which is typically of order the de Boglie wavelength) is negligible. This is an important result, because we know that classical mechanics gives the correct answer in this limit.

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3.5: Operators

An operator, O (say), is a mathematical entity that transforms one function into another: that is,

$$O(f(x)) \rightarrow g(x). \tag{3.5.1}$$

For instance, x is an operator, because $x\,f(x)$ is a different function to $f(x)$, and is fully specified once $f(x)$ is given. Furthermore, d/dx is also an operator, because $df(x)/dx$ is a different function to $f(x)$, and is fully specified once $f(x)$ is given. Now,

$$x\,\frac{df}{dx} \neq \frac{d}{dx}(x\,f)\,. \tag{3.5.2}$$

This can also be written

$$x\,\frac{d}{dx} \neq \frac{d}{dx}\,x, \tag{3.5.3}$$

where the operators are assumed to act on everything to their right, and a final $f(x)$ is understood [where $f(x)$ is a general function]. The previous expression illustrates an important point. Namely, in general, operators do not commute with one another. Of course, some operators do commute. For instance,

$$x\,x^{\,2} = x^{\,2}\,x. \tag{3.5.4}$$

Finally, an operator, O, is termed linear if

$$O(c\,f(x)) = c\,O(f(x)), \tag{3.5.5}$$

where f is a general function, and c a general complex number. All of the operators employed in quantum mechanics are linear.

Now, from Equations ([e3.22]) and ([e3.38]),

$$\langle x\rangle = \int_{-\infty}^{\infty} \psi^*\,x\,\psi\,dx,$$
$$\langle p\rangle = \int_{-\infty}^{\infty} \psi^*\left(-\mathrm{i}\,\hbar\,\frac{\partial}{\partial x}\right)\psi\,dx.$$

These expressions suggest a number of things. First, classical dynamical variables, such as x and p, are represented in quantum mechanics by linear operators that act on the wavefunction. Second, displacement is represented by the algebraic operator x, and momentum by the differential operator $-\mathrm{i}\,\hbar\,\partial/\partial x$: that is, \[\label{e3.54} p \equiv -{\rm i}\,\hbar\,\frac{\partial}{\partial x}.\]

Finally, the expectation value of some dynamical variable represented by the operator $O(x)$ is simply

$$\langle O\rangle = \int_{-\infty}^{\infty} \psi^*(x,t)\,O(x)\,\psi(x,t)\,dx. \tag{3.5.6}$$

Clearly, if an operator is to represent a dynamical variable that has physical significance then its expectation value must be real. In other words, if the operator O represents a physical variable then we require that $\langle O\rangle = \langle O\rangle^*$, or

$$\int_{-\infty}^{\infty} \psi^*\,(O\,\psi)\,dx = \int_{-\infty}^{\infty} (O\,\psi)^*\,\psi\,dx, \tag{3.5.7}$$

where O^* is the complex conjugate of O. An operator that satisfies the previous constraint is called an *Hermitian* operator. It is easily demonstrated that x and p are both Hermitian. The *Hermitian conjugate*, $O^\dagger$, of a general operator, O, is defined as follows:

$$\int_{-\infty}^{\infty} \psi^*\,(O\,\psi)\,dx = \int_{-\infty}^{\infty} (O^\dagger\,\psi)^*\,\psi\,dx. \tag{3.5.8}$$

The Hermitian conjugate of an Hermitian operator is the same as the operator itself: that is, $p^\dagger = p$. For a non-Hermitian operator, O (say), it is easily demonstrated that $(O^\dagger)^\dagger = O$, and that the operator $O + O^\dagger$ is Hermitian. Finally, if A and B are two operators, then $(A\,B)^\dagger = B^\dagger\,A^\dagger$.

Suppose that we wish to find the operator that corresponds to the classical dynamical variable $x\,p$. In classical mechanics, there is no difference between $x\,p$ and $p\,x$. However, in quantum mechanics, we have already seen that $x\,p \neq p\,x$. So, should we choose

$x\,p$ or $p\,x$? Actually, neither of these combinations is Hermitian. However, $(1/2)\,[x\,p+(x\,p)^\dagger]$ is Hermitian. Moreover, $(1/2)\,[x\,p+(x\,p)^\dagger] = (1/2)\,(x\,p+p^\dagger\,x^\dagger) = (1/2)\,(x\,p+p\,x)$, which neatly resolves our problem of the order in which to place x and p.

It is a reasonable guess that the operator corresponding to energy (which is called the Hamiltonian, and conventionally denoted H) takes the form

$$H \equiv \frac{p^2}{2\,m} + V(x). \tag{3.5.9}$$

Note that H is Hermitian. Now, it follows from Equation ([e3.54]) that

$$H \equiv -\frac{\hbar^2}{2\,m}\,\frac{\partial^2}{\partial x^2} + V(x). \tag{3.5.10}$$

However, according to Schrödinger's equation, ([e3.1]), we have

$$-\frac{\hbar^2}{2\,m}\,\frac{\partial^2}{\partial x^2} + V(x) = \mathrm{i}\,\hbar\,\frac{\partial}{\partial t}, \tag{3.5.11}$$

so

$$H \equiv \mathrm{i}\,\hbar\,\frac{\partial}{\partial t}. \tag{3.5.12}$$

Thus, the time-dependent Schrödinger equation can be written

$$\mathrm{i}\,\hbar\,\frac{\partial \psi}{\partial t} = H\,\psi. \tag{3.5.13}$$

Finally, if $O(x,p,E)$ is a classical dynamical variable that is a function of displacement, momentum, and energy then a reasonable guess for the corresponding operator in quantum mechanics is $(1/2)\,[O(x,p,H)+O^\dagger(x,p,H)]$, where $p = -\mathrm{i}\,\hbar\,\partial/\partial x$, and $H = \mathrm{i}\,\hbar\,\partial/\partial t$.

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3.6: Momentum Representation

Fourier's theorem (see Section [s2.9]), applied to one-dimensional wavefunctions, yields

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \bar{\psi}(k,t)\,\mathrm{e}^{+\mathrm{i}\,k\,x}\,dk,$$
$$\bar{\psi}(k,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \psi(x,t)\,\mathrm{e}^{-\mathrm{i}\,k\,x}\,dx,$$

where k represents wavenumber. However, $p = \hbar\,k$. Hence, we can also write

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\,\hbar}}\int_{-\infty}^{\infty} \phi(p,t)\,\mathrm{e}^{+\mathrm{i}\,p\,x/\hbar}\,dp,$$
$$\phi(p,t) = \frac{1}{\sqrt{2\pi\,\hbar}}\int_{-\infty}^{\infty} \psi(x,t)\,\mathrm{e}^{-\mathrm{i}\,p\,x/\hbar}\,dx,$$

where $\phi(p,t) = \bar{\psi}(k,t)/\sqrt{\hbar}$ is the momentum-space equivalent to the real-space wavefunction $\psi(x,t)$.

At this stage, it is convenient to introduce a useful function called the *Dirac delta-function*. This function, denoted $\delta(x)$, was first devised by Paul Dirac, and has the following rather unusual properties: $\delta(x)$ is zero for $x \neq 0$, and is infinite at $x = 0$. However, the singularity at $x = 0$ is such that

$$\int_{-\infty}^{\infty} \delta(x)\,dx = 1. \tag{3.6.1}$$

The delta-function is an example of what is known as a *generalized function*: that is, its value is not well defined at all x, but its integral is well defined. Consider the integral

$$\int_{-\infty}^{\infty} f(x)\,\delta(x)\,dx. \tag{3.6.2}$$

Because $\delta(x)$ is only non-zero infinitesimally close to $x = 0$, we can safely replace $f(x)$ by $f(0)$ in the previous integral (assuming $f(x)$ is well behaved at $x = 0$), to give

$$\int_{-\infty}^{\infty} f(x)\,\delta(x)\,dx = f(0)\int_{-\infty}^{\infty} \delta(x)\,dx = f(0), \tag{3.6.3}$$

where use has been made of Equation ([e3.64a]). A simple generalization of this result yields

$$\int_{-\infty}^{\infty} f(x)\,\delta(x-x_0)\,dx = f(x_0), \tag{3.6.4}$$

which can also be thought of as an alternative definition of a delta-function.

Suppose that $\psi(x) = \delta(x-x_0)$. It follows from Equations ([e3.65]) and ([e3.69]) that

$$\phi(p) = \frac{\mathrm{e}^{-ipx_0/\hbar}}{\sqrt{2\pi\hbar}} \tag{3.6.5}$$

Hence, Equation ([e3.64]) yields the important result

$$\delta(x-x_0) = \frac{1}{2\pi\,\hbar}\int_{-\infty}^{\infty} \mathrm{e}^{+\mathrm{i}\,p\,(x-x_0)/\hbar}\,dp. \tag{3.6.6}$$

Similarly,

$$\delta(p-p_0) = \frac{1}{2\pi\,\hbar}\int_{-\infty}^{\infty} \mathrm{e}^{+\mathrm{i}\,(p-p_0)\,x/\hbar}\,dx. \tag{3.6.7}$$

It turns out that we can just as easily formulate quantum mechanics using the momentum-space wavefunction, $\phi(p,t)$, as the real-space wavefunction, $\psi(x,t)$. The former scheme is known as the *momentum representation* of quantum mechanics. In the momentum representation, wavefunctions are the Fourier transforms of the equivalent real-space wavefunctions, and dynamical

variables are represented by different operators. Furthermore, by analogy with Equation ([e3.55]), the expectation value of some operator $O(p)$ takes the form

$$\langle O\rangle = \int_{-\infty}^{\infty} \phi^*(p,t)\, O(p)\, \phi(p,t)\, dp. \tag{3.6.8}$$

Consider momentum. We can write

$$\begin{aligned}\langle p\rangle &= \int_{-\infty}^{\infty} \psi^*(x,t)\left(-\mathrm{i}\,\hbar\,\frac{\partial}{\partial x}\right)\psi(x,t)\,dx\\ &= \frac{1}{2\pi\,\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\phi^*(p',t)\,\phi(p,t)\,p\,\mathrm{e}^{+\mathrm{i}\,(p-p')\,x/\hbar}\,dx\,dp\,dp',\end{aligned}$$

where use has been made of Equation ([e3.64]). However, it follows from Equation ([e3.72]) that

$$\langle p\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\phi^*(p',t)\,\phi(p,t)\,p\,\delta(p-p')\,dp\,dp'. \tag{3.6.9}$$

Hence, using Equation ([e3.69]), we obtain

$$\langle p\rangle = \int_{-\infty}^{\infty}\phi^*(p,t)\,p\,\phi(p,t)\,dp = \int_{-\infty}^{\infty} p\,|\phi|^2\,dp. \tag{3.6.10}$$

Evidently, momentum is represented by the operator p in the momentum representation. The previous expression also strongly suggests [by comparison with Equation ([e3.22])] that $|\phi(p,t)|^2$ can be interpreted as the probability density of a measurement of momentum yielding the value p at time t. It follows that $\phi(p,t)$ must satisfy an analogous normalization condition to Equation ([e3.4]): that is,

$$\int_{-\infty}^{\infty}|\phi(p,t)|^2\,dp = 1. \tag{3.6.11}$$

Consider displacement. We can write

$$\begin{aligned}\langle x\rangle &= \int_{-\infty}^{\infty}\psi^*(x,t)\,x\,\psi(x,t)\,dx\\ &= \frac{1}{2\pi\,\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\phi^*(p',t)\,\phi(p,t)\left(-\mathrm{i}\,\hbar\,\frac{\partial}{\partial p}\right)\mathrm{e}^{+\mathrm{i}\,(p-p')\,x/\hbar}\,dx\,dp\,dp'.\end{aligned}$$

Integration by parts yields

$$\langle x\rangle = \frac{1}{2\pi\,\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\phi^*(p',t)\,\mathrm{e}^{+\mathrm{i}\,(p-p')\,x/\hbar}\left(\mathrm{i}\,\hbar\,\frac{\partial}{\partial p}\right)\phi(p,t)\,dx\,dp\,dp'. \tag{3.6.12}$$

Hence, making use of Equations ([e3.72]) and ([e3.69]), we obtain

$$\langle x\rangle = \frac{1}{2\pi\,\hbar}\int_{-\infty}^{\infty}\phi^*(p)\left(\mathrm{i}\,\hbar\,\frac{\partial}{\partial p}\right)\phi(p)\,dp. \tag{3.6.13}$$

Evidently, displacement is represented by the operator

$$x \equiv \mathrm{i}\,\hbar\,\frac{\partial}{\partial p} \tag{3.6.14}$$

in the momentum representation.

Finally, let us consider the normalization of the momentum-space wavefunction $\phi(p,t)$. We have

$$\int_{-\infty}^{\infty}\psi^*(x,t)\,\psi(x,t)\,dx = \frac{1}{2\pi\,\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\phi^*(p',t)\,\phi(p,t)\,\mathrm{e}^{+\mathrm{i}\,(p-p')\,x/\hbar}\,dx\,dp\,dp'. \tag{3.6.15}$$

Thus, it follows from Equations ([e3.69]) and ([e3.72]) that

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2\, dx = \int_{-\infty}^{\infty} |\phi(p,t)|^2\, dp. \tag{3.6.16}$$

Hence, if $\psi(x,t)$ is properly normalized [see Equation ([e3.4])] then $\phi(p,t)$, as defined in Equation ([e3.65]), is also properly normalized [see Equation ([enormp])].

The existence of the momentum representation illustrates an important point. Namely, there are many different, but entirely equivalent, ways of mathematically formulating quantum mechanics. For instance, it is also possible to represent wavefunctions as row and column vectors, and dynamical variables as matrices that act upon these vectors.

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3.7: Heisenberg's Uncertainty Principle

Consider a real-space Hermitian operator, $O(x)$. A straightforward generalization of Equation ([e3.55a]) yields

$$\int_{-\infty}^{\infty} \psi_1^*\,(O\,\psi_2)\,dx = \int_{-\infty}^{\infty} (O\,\psi_1)^*\,\psi_2\,dx, \tag{3.7.1}$$

where $\psi_1(x)$ and $\psi_2(x)$ are general functions.

Let $f = (A - \langle A\rangle)\,\psi$, where $A(x)$ is an Hermitian operator, and $\psi(x)$ a general wavefunction. We have

$$\int_{-\infty}^{\infty} |f|^{\,2}\,dx = \int_{-\infty}^{\infty} f^*\,f\,dx = \int_{-\infty}^{\infty} [(A - \langle A\rangle)\,\psi]^{\,*}\,[(A - \langle A\rangle)\,\psi]\,dx. \tag{3.7.2}$$

Making use of Equation ([e3.84]), we obtain

$$\int_{-\infty}^{\infty} |f|^{\,2}\,dx = \int_{-\infty}^{\infty} \psi^*\,(A - \langle A\rangle)^{\,2}\,\psi\,dx = \sigma_A^{\,2}, \tag{3.7.3}$$

where $\sigma_A^{\,2}$ is the variance of A. [See Equation ([e3.24a]).] q4 Similarly, if $g = (B - \langle B\rangle)\,\psi$, where B is a second Hermitian operator, then

$$\int_{-\infty}^{\infty} |g|^{\,2}\,dx = \sigma_B^{\,2}, \tag{3.7.4}$$

Now, there is a standard result in mathematics, known as the *Schwartz inequality* , which states that

$$\left|\int_a^b f^*(x)\,g(x)\,dx\right|^{\,2} \leq \int_a^b |f(x)|^{\,2}\,dx \int_a^b |g(x)|^{\,2}\,dx, \tag{3.7.5}$$

where f and g are two general functions. Furthermore, if z is a complex number then

$$|z|^{\,2} = [\mathrm{Re}(z)]^{\,2} + [\mathrm{Im}(z)]^{\,2} \geq [\mathrm{Im}(z)]^{\,2} = \left[\frac{1}{2\,\mathrm{i}}\,(z - z^*)\right]^{\,2}. \tag{3.7.6}$$

Hence, if $z = \int_{-\infty}^{\infty} f^*\,g\,dx$ then Equations ([e3.86])–([e3.89]) yield

$$\sigma_A^{\,2}\,\sigma_B^{\,2} \geq \left[\frac{1}{2\,\mathrm{i}}\,(z - z^*)\right]^{\,2}. \tag{3.7.7}$$

However,

$$z = \int_{-\infty}^{\infty} [(A - \langle A\rangle)\,\psi]^{\,*}\,[(B - \langle B\rangle)\,\psi]\,dx = \int_{-\infty}^{\infty} \psi^*\,(A - \langle A\rangle)\,(B - \langle B\rangle)\,\psi\,dx, \tag{3.7.8}$$

where use has been made of Equation ([e3.84]). The previous equation reduces to

$$z = \int_{-\infty}^{\infty} \psi^*\,A\,B\,\psi\,dx - \langle A\rangle\,\langle B\rangle. \tag{3.7.9}$$

Furthermore, it is easily demonstrated that

$$z^* = \int_{-\infty}^{\infty} \psi^*\,B\,A\,\psi\,dx - \langle A\rangle\,\langle B\rangle. \tag{3.7.10}$$

Hence, Equation ([e3.90]) gives

$$\sigma_A^{\,2}\,\sigma_B^{\,2} \geq \left(\frac{1}{2\,\mathrm{i}}\langle[A, B]\rangle\right)^{\,2}, \tag{3.7.11}$$

where

$$[A, B] \equiv A\,B - B\,A. \tag{3.7.12}$$

Equation ([e3.94]) is the general form of *Heisenberg's uncertainty principle* in quantum mechanics. It states that if two dynamical variables are represented by the two Hermitian operators A and B, and these operators do not commute (i.e., $A\,B \neq B\,A$), then it is impossible to simultaneously (exactly) measure the two variables. Instead, the product of the variances in the measurements is always greater than some critical value, which depends on the extent to which the two operators do not commute.

For instance, displacement and momentum are represented (in real-space) by the operators x and $p \equiv -\mathrm{i}\,\hbar\,\partial/\partial x$, respectively. Now, it is easily demonstrated that

$$[x, p] = \mathrm{i}\,\hbar. \tag{3.7.13}$$

Thus,

$$\sigma_x\,\sigma_p \geq \frac{\hbar}{2}, \tag{3.7.14}$$

which can be recognized as the standard displacement-momentum uncertainty principle (see Section [sun]). It turns out that the minimum uncertainty (i.e., $\sigma_x\,\sigma_p = \hbar/2$) is only achieved by Gaussian wave-packets (see Section [s2.9]): that is,

$$\psi(x) = \frac{\mathrm{e}^{+ip_0 x/\hbar}}{\left(2\pi\sigma_x^2\right)^{1/4}}\,\mathrm{e}^{-(x-x_0)^2/4\sigma_x^2} \tag{3.7.15}$$

$$\phi(p) = \frac{\mathrm{e}^{-\mathrm{i}px_0/\hbar}}{\left(2\pi\sigma_p^2\right)^{1/4}}\,\mathrm{e}^{-(p-p_0)^2/4\sigma_p^2} \tag{3.7.16}$$

where $\phi(p)$ is the momentum-space equivalent of $\psi(x)$.

Energy and time are represented by the operators $H \equiv \mathrm{i}\,\hbar\,\partial/\partial t$ and t, respectively. These operators do not commute, indicating that energy and time cannot be measured simultaneously. In fact,

$$[H, t] = \mathrm{i}\,\hbar, \tag{3.7.17}$$

so

$$\sigma_E\,\sigma_t \geq \frac{\hbar}{2}. \tag{3.7.18}$$

This can be written, somewhat less exactly, as

$\Delta E \Delta t \gtrsim \hbar$ are the uncertainties in energy and time, respectively. The previous expression is generally known as the *energy-time uncertainty principle*.

For instance, suppose that a particle passes some fixed point on the x-axis. Because the particle is, in reality, an extended wave-packet, it takes a certain amount of time, Δt, for the particle to pass. Thus, there is an uncertainty, Δt, in the arrival time of the particle. Moreover, because $E = \hbar\,\omega$, the only wavefunctions that have unique energies are those with unique frequencies: that is, plane-waves. Because a wave-packet of finite extent is made up of a combination of plane-waves of different wavenumbers, and, hence, different frequencies, there will be an uncertainty ΔE in the particle's energy that is proportional to the range of frequencies of the plane-waves making up the wave-packet. The more compact the wave-packet (and, hence, the smaller Δt), the larger the range of frequencies of the constituent plane-waves (and, hence, the large ΔE), and vice versa.

To be more exact, if $\psi(t)$ is the wavefunction measured at the fixed point as a function of time then we can write

$$\psi(t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \chi(E)\mathrm{e}^{-iEt/\hbar}\,dE \tag{3.7.19}$$

In other words, we can express $\psi(t)$ as a linear combination of plane-waves of definite energy E. Here, $\chi(E)$ is the complex amplitude of plane-waves of energy E in this combination.

By Fourier's theorem, we also have

$$\chi(E) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \psi(t)\mathrm{e}^{+iEt/\hbar}\,dt \tag{3.7.20}$$

For instance, if $\psi(t)$ is a Gaussian then it is easily shown that $\chi(E)$ is also a Gaussian: that is,

$$\psi(t) = \frac{\mathrm{e}^{-iE_0 t/\hbar}}{\left(2\pi\sigma_t^2\right)^{1/4}}\mathrm{e}^{-(t-t_0)^2/4\sigma_t^2} \tag{3.7.21}$$

$$\chi(E) = \frac{\mathrm{e}^{+iEt_0/\hbar}}{\left(2\pi\sigma_E^2\right)^{1/4}}\mathrm{e}^{-(E-E_0)^2/4\sigma_E^2} \tag{3.7.22}$$

where $\sigma_E\,\sigma_t = \hbar/2$. As before, Gaussian wave-packets satisfy the minimum uncertainty principle $\sigma_E\,\sigma_t = \hbar/2$. Conversely, non-Gaussian wave-packets are characterized by $\sigma_E\,\sigma_t > \hbar/2$.

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3.8: Eigenstates and Eigenvalues

Consider a general real-space operator, $A(x)$. When this operator acts on a general wavefunction $\psi(x)$ the result is usually a wavefunction with a completely different shape. However, there are certain special wavefunctions which are such that when A acts on them the result is just a multiple of the original wavefunction. These special wavefunctions are called *eigenstates*, and the multiples are called *eigenvalues*. Thus, if

$$A\,\psi_a(x) = a\,\psi_a(x), \tag{3.8.1}$$

where a is a complex number, then ψ_a is called an eigenstate of A corresponding to the eigenvalue a.

Suppose that A is an Hermitian operator corresponding to some physical dynamical variable. Consider a particle whose wavefunction is ψ_a. The expectation of value A in this state is simply [see Equation ([e3.55])]

$$\langle A\rangle = \int_{-\infty}^{\infty} \psi_a^*\, A\,\psi_a\, dx = a\int_{-\infty}^{\infty} \psi_a^*\,\psi_a\, dx = a, \tag{3.8.2}$$

where use has been made of Equation ([e3.107]) and the normalization condition ([e3.4]). Moreover,

$$\langle A^2\rangle = \int_{-\infty}^{\infty} \psi_a^*\, A^2\,\psi_a\, dx = a\int_{-\infty}^{\infty} \psi_a^*\, A\,\psi_a\, dx = a^{\,2}\int_{-\infty}^{\infty} \psi_a^*\,\psi_a\, dx = a^{\,2}, \tag{3.8.3}$$

so the variance of A is [cf., Equation ([e3.24a])]

$$\sigma_A^{\,2} = \langle A^2\rangle - \langle A\rangle^2 = a^{\,2} - a^{\,2} = 0. \tag{3.8.4}$$

The fact that the variance is zero implies that every measurement of A is bound to yield the same result: namely, a. Thus, the eigenstate ψ_a is a state that is associated with a unique value of the dynamical variable corresponding to A. This unique value is simply the associated eigenvalue.

It is easily demonstrated that the eigenvalues of an Hermitian operator are all real. Recall [from Equation ([e3.84])] that an Hermitian operator satisfies

$$\int_{-\infty}^{\infty} \psi_1^*\,(A\,\psi_2)\, dx = \int_{-\infty}^{\infty} (A\,\psi_1)^*\,\psi_2\, dx. \tag{3.8.5}$$

Hence, if $\psi_1 = \psi_2 = \psi_a$ then

$$\int_{-\infty}^{\infty} \psi_a^*\,(A\,\psi_a)\, dx = \int_{-\infty}^{\infty} (A\,\psi_a)^*\,\psi_a\, dx, \tag{3.8.6}$$

which reduces to [see Equation ([e3.107])]

$$a = a^*, \tag{3.8.7}$$

assuming that ψ_a is properly normalized.

Two wavefunctions, $\psi_1(x)$ and $\psi_2(x)$, are said to be *orthogonal* if

$$\int_{-\infty}^{\infty} \psi_1^*\,\psi_2\, dx = 0. \tag{3.8.8}$$

Consider two eigenstates of A, ψ_a and $\psi_{a'}$, which correspond to the two different eigenvalues a and a', respectively. Thus,

$$A\,\psi_a = a\,\psi_a,$$
$$A\,\psi_{a'} = a'\,\psi_{a'}.$$

Multiplying the complex conjugate of the first equation by $\psi_{a'}$, and the second equation by ψ_a^*, and then integrating over all x, we obtain

$$\int_{-\infty}^{\infty} (A\,\psi_a)^*\,\psi_{a'}\,dx = a\int_{-\infty}^{\infty}\psi_a^*\,\psi_{a'}\,dx,$$
$$\int_{-\infty}^{\infty} \psi_a^*\,(A\,\psi_{a'})\,dx = a'\int_{-\infty}^{\infty}\psi_a^*\,\psi_{a'}\,dx.$$

However, from Equation ([e3.111]), the left-hand sides of the previous two equations are equal. Hence, we can write

$$(a-a')\int_{-\infty}^{\infty}\psi_a^*\,\psi_{a'}\,dx = 0. \tag{3.8.9}$$

By assumption, $a\neq a'$, yielding

$$\int_{-\infty}^{\infty}\psi_a^*\,\psi_{a'}\,dx = 0. \tag{3.8.10}$$

In other words, eigenstates of an Hermitian operator corresponding to different eigenvalues are automatically orthogonal.

Consider two eigenstates of A, ψ_a and ψ'_a, that correspond to the same eigenvalue, a. Such eigenstates are termed *degenerate*. The previous proof of the orthogonality of different eigenstates fails for degenerate eigenstates. Note, however, that any linear combination of ψ_a and ψ'_a is also an eigenstate of A corresponding to the eigenvalue a. Thus, even if ψ_a and ψ'_a are not orthogonal, we can always choose two linear combinations of these eigenstates that are orthogonal. For instance, if ψ_a and ψ'_a are properly normalized, and

$$\int_{-\infty}^{\infty}\psi_a^*\,\psi'_a\,dx = c, \tag{3.8.11}$$

then it is easily demonstrated that

$$\psi''_a = \frac{|c|}{\sqrt{1-|c|^2}}\left(\psi_a - c^{-1}\,\psi'_a\right) \tag{3.8.12}$$

is a properly normalized eigenstate of A, corresponding to the eigenvalue a, that is orthogonal to ψ_a. It is straightforward to generalize the previous argument to three or more degenerate eigenstates. Hence, we conclude that the eigenstates of an Hermitian operator are, or can be chosen to be, mutually orthogonal.

It is also possible to demonstrate that the eigenstates of an Hermitian operator form a complete set : that is, any general wavefunction can be written as a linear combination of these eigenstates. However, the proof is quite difficult, and we shall not attempt it here.

In summary, given an Hermitian operator A, any general wavefunction, $\psi(x)$, can be written

$$\psi = \sum_i c_i\,\psi_i, \tag{3.8.13}$$

where the c_i are complex weights, and the ψ_i are the properly normalized (and mutually orthogonal) eigenstates of A: that is,

$$A\,\psi_i = a_i\,\psi_i, \tag{3.8.14}$$

where a_i is the eigenvalue corresponding to the eigenstate ψ_i, and

$$\int_{-\infty}^{\infty}\psi_i^*\,\psi_j\,dx = \delta_{ij}. \tag{3.8.15}$$

Here, δ_{ij} is called the *Kronecker delta-function* , and takes the value unity when its two indices are equal, and zero otherwise.

It follows from Equations ([e3.123]) and ([e3.125]) that

$$c_i = \int_{-\infty}^{\infty}\psi_i^*\,\psi\,dx. \tag{3.8.16}$$

Thus, the expansion coefficients in Equation ([e3.123]) are easily determined, given the wavefunction ψ and the eigenstates ψ_i. Moreover, if ψ is a properly normalized wavefunction then Equations ([e3.123]) and ([e3.125]) yield

$$\sum_i |c_i|^2 = 1. \tag{3.8.17}$$

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3.9: Measurement

Suppose that A is an Hermitian operator corresponding to some dynamical variable. By analogy with the discussion in Section [scoll], we expect that if a measurement of A yields the result a then the act of measurement will cause the wavefunction to collapse to a state in which a measurement of A is bound to give the result a. What sort of wavefunction, ψ, is such that a measurement of A is bound to yield a certain result, a? Well, expressing ψ as a linear combination of the eigenstates of A, we have

$$\psi = \sum_i c_i \, \psi_i, \tag{3.9.1}$$

where ψ_i is an eigenstate of A corresponding to the eigenvalue a_i. If a measurement of A is bound to yield the result a then

$$\langle A \rangle = a, \tag{3.9.2}$$

and

$$\sigma_A^{\,2} = \langle A^2 \rangle - \langle A \rangle = 0. \tag{3.9.3}$$

Now, it is easily seen that

$$\langle A \rangle = \sum_i |c_i|^{\,2} \, a_i,$$
$$\langle A^2 \rangle = \sum_i |c_i|^{\,2} \, a_i^{\,2}.$$

Thus, Equation ([e4.130]) gives

$$\sum_i a_i^{\,2} \, |c_i|^{\,2} - \left(\sum_i a_i \, |c_i|^{\,2} \right)^2 = 0. \tag{3.9.4}$$

Furthermore, the normalization condition yields

$$\sum_i |c_i|^{\,2} = 1. \tag{3.9.5}$$

For instance, suppose that there are only two eigenstates. The previous two equations then reduce to $|c_1|^{\,2} = x$, and $|c_2|^{\,2} = 1 - x$, where $0 \leq x \leq 1$, and

$$(a_1 - a_2)^2 \, x \, (1 - x) = 0. \tag{3.9.6}$$

The only solutions are $x = 0$ and $x = 1$. This result can easily be generalized to the case where there are more than two eigenstates. It follows that a state associated with a definite value of A is one in which one of the $|c_i|^{\,2}$ is unity, and all of the others are zero. In other words, the only states associated with definite values of A are the eigenstates of A. It immediately follows that the result of a measurement of A must be one of the eigenvalues of A. Moreover, if a general wavefunction is expanded as a linear combination of the eigenstates of A, like in Equation ([e4.128]), then it is clear from Equation ([e4.131]), and the general definition of a mean, that the probability of a measurement of A yielding the eigenvalue a_i is simply $|c_i|^{\,2}$, where c_i is the coefficient in front of the ith eigenstate in the expansion. Note, from Equation ([e4.134]), that these probabilities are properly normalized: that is, the probability of a measurement of A resulting in any possible answer is unity. Finally, if a measurement of A results in the eigenvalue a_i then immediately after the measurement the system will be left in the eigenstate corresponding to a_i.

Consider two physical dynamical variables represented by the two Hermitian operators A and B. Under what circumstances is it possible to simultaneously measure these two variables (exactly)? Well, the possible results of measurements of A and B are the eigenvalues of A and B, respectively. Thus, to simultaneously measure A and B (exactly) there must exist states which are simultaneous eigenstates of A and B. In fact, in order for A and B to be simultaneously measurable under all circumstances, we need all of the eigenstates of A to also be eigenstates of B, and vice versa, so that all states associated with unique values of A are also associated with unique values of B, and vice versa.

Now, we have already seen, in Section 1.8, that if A and B do not commute (i.e., if $A\,B \neq B\,A$) then they cannot be simultaneously measured. This suggests that the condition for simultaneous measurement is that A and B should commute.

Suppose that this is the case, and that the ψ_i and a_i are the normalized eigenstates and eigenvalues of A, respectively. It follows that

$$(A\,B - B\,A)\,\psi_i = (A\,B - B\,a_i)\,\psi_i = (A - a_i)\,B\,\psi_i = 0, \tag{3.9.7}$$

or

$$A\,(B\,\psi_i) = a_i\,(B\,\psi_i). \tag{3.9.8}$$

Thus, $B\,\psi_i$ is an eigenstate of A corresponding to the eigenvalue a_i (though not necessarily a normalized one). In other words, $B\,\psi_i \propto \psi_i$, or

$$B\,\psi_i = b_i\,\psi_i, \tag{3.9.9}$$

where b_i is a constant of proportionality. Hence, ψ_i is an eigenstate of B, and, thus, a simultaneous eigenstate of A and B. We conclude that if A and B commute then they possess simultaneous eigenstates, and are thus simultaneously measurable (exactly).

Continuous Eigenvalues

In the previous two sections, it was tacitly assumed that we were dealing with operators possessing discrete eigenvalues and square-integrable eigenstates. Unfortunately, some operators—most notably, x and p—possess eigenvalues that lie in a continuous range and non-square-integrable eigenstates (in fact, these two properties go hand in hand). Let us, therefore, investigate the eigenstates and eigenvalues of the displacement and momentum operators.

Let $\psi_x(x, x')$ be the eigenstate of x corresponding to the eigenvalue x'. It follows that

$$x\,\psi_x(x, x') = x'\,\psi_x(x, x') \tag{3.9.10}$$

for all x. Consider the Dirac delta-function $\delta(x - x')$. We can write

$$x\,\delta(x - x') = x'\,\delta(x - x'), \tag{3.9.11}$$

because $\delta(x - x')$ is only non-zero infinitesimally close to $x = x'$. Evidently, $\psi_x(x, x')$ is proportional to $\delta(x - x')$. Let us make the constant of proportionality unity, so that

$$\psi_x(x, x') = \delta(x - x'). \tag{3.9.12}$$

It is easily demonstrated that

$$\int_{-\infty}^{\infty} \delta(x - x')\,\delta(x - x'')\,dx = \delta(x' - x''). \tag{3.9.13}$$

Hence, $\psi_x(x, x')$ satisfies the orthonormality condition

$$\int_{-\infty}^{\infty} \psi_x^*(x, x')\,\psi_x(x, x'')\,dx = \delta(x' - x''). \tag{3.9.14}$$

This condition is analogous to the orthonormality condition ([e3.125]) satisfied by square-integrable eigenstates. Now, by definition, $\delta(x - x')$ satisfies

$$\int_{-\infty}^{\infty} f(x)\,\delta(x - x')\,dx = f(x'), \tag{3.9.15}$$

where $f(x)$ is a general function. We can thus write

$$\psi(x) = \int_{-\infty}^{\infty} c(x')\,\psi_x(x, x')\,dx', \tag{3.9.16}$$

where $c(x') = \psi(x')$, or

$$c(x') = \int_{-\infty}^{\infty} \psi_x^*(x, x')\,\psi(x)\,dx. \tag{3.9.17}$$

In other words, we can expand a general wavefunction $\psi(x)$ as a linear combination of the eigenstates, $\psi_x(x, x')$, of the displacement operator. Equations ([e4.144]) and ([e4.145]) are analogous to Equations ([e3.123]) and ([e3.126]), respectively, for

square-integrable eigenstates. Finally, by analogy with the results in Section 1.9, the probability density of a measurement of x yielding the value x' is $|c(x')|^2$, which is equivalent to the standard result $|\psi(x')|^2$. Moreover, these probabilities are properly normalized provided $\psi(x)$ is properly normalized [cf., Equation ([e3.127])]: that is,

$$\int_{-\infty}^{\infty} |c(x')|^2\, dx' = \int_{-\infty}^{\infty} |\psi(x')|^2\, dx' = 1. \tag{3.9.18}$$

Finally, if a measurement of x yields the value x' then the system is left in the corresponding displacement eigenstate, $\psi_x(x,x')$, immediately after the measurement. That is, the wavefunction collapses to a "spike-function", $\delta(x-x')$, as discussed in Section [scoll].

Now, an eigenstate of the momentum operator $p \equiv -\mathrm{i}\,\hbar\,\partial/\partial x$ corresponding to the eigenvalue p' satisfies

$$-\mathrm{i}\,\hbar\,\frac{\partial \psi_p(x,p')}{\partial x} = p'\,\psi_p(x,p'). \tag{3.9.19}$$

It is evident that

$$\psi_p(x,p') \propto \mathrm{e}^{+\mathrm{i}\,p'\,x/\hbar}. \tag{3.9.20}$$

We require $\psi_p(x,p')$ to satisfy an analogous orthonormality condition to Equation ([e4.143]): that is,

$$\int_{-\infty}^{\infty} \psi_p^*(x,p')\,\psi_p(x,p'')\,dx = \delta(p'-p''). \tag{3.9.21}$$

Thus, it follows from Equation ([e3.72]) that the constant of proportionality in Equation ([e4.148]) should be $(2\pi\,\hbar)^{-1/2}$: that is,

$$\psi_p(x,p') = \frac{\mathrm{e}^{+\mathrm{i}\,p'\,x/\hbar}}{(2\pi\,\hbar)^{1/2}}. \tag{3.9.22}$$

Furthermore, according to Equations ([e3.64]) and ([e3.65]),

$$\psi(x) = \int_{-\infty}^{\infty} c(p')\,\psi_p(x,p')\,dp', \tag{3.9.23}$$

where $c(p') = \phi(p')$ [see Equation ([e3.65])], or

$$c(p') = \int_{-\infty}^{\infty} \psi_p^*(x,p')\,\psi(x)\,dx. \tag{3.9.24}$$

In other words, we can expand a general wavefunction $\psi(x)$ as a linear combination of the eigenstates, $\psi_p(x,p')$, of the momentum operator. Equations ([e4.152]) and ([e4.153]) are again analogous to Equations ([e3.123]) and ([e3.126]), respectively, for square-integrable eigenstates. Likewise, the probability density of a measurement of p yielding the result p' is $|c(p')|^2$, which is equivalent to the standard result $|\phi(p')|^2$. The probabilities are also properly normalized provided $\psi(x)$ is properly normalized [cf., Equation ([e3.83])]: that is,

$$\int_{-\infty}^{\infty} |c(p')|^2\, dp' = \int_{-\infty}^{\infty} |\phi(p')|^2\, dp' = \int_{-\infty}^{\infty} |\psi(x')|^2\, dx' = 1. \tag{3.9.25}$$

Finally, if a mesurement of p yields the value p' then the system is left in the corresponding momentum eigenstate, $\psi_p(x,p')$, immediately after the measurement.

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3.10: Stationary States

An eigenstate of the energy operator $H \equiv \mathrm{i}\,\hbar\,\partial/\partial t$ corresponding to the eigenvalue E_i satisfies

$$\mathrm{i}\,\hbar\,\frac{\partial \psi_E(x,t,E_i)}{\partial t} = E_i\,\psi_E(x,t,E_i). \tag{3.10.1}$$

It is evident that this equation can be solved by writing

$$\psi_E(x,t,E_i) = \psi_i(x)\,\mathrm{e}^{-\mathrm{i}\,E_i\,t/\hbar}, \tag{3.10.2}$$

where $\psi_i(x)$ is a properly normalized stationary (i.e., non-time-varying) wavefunction. The wavefunction $\psi_E(x,t,E_i)$ corresponds to a so-called *stationary state*, because the probability density $|\psi_E|^2$ is non-time-varying. Note that a stationary state is associated with a unique value for the energy. Substitution of the previous expression into Schrödinger's equation ([e3.1]) yields the equation satisfied by the stationary wavefunction:

$$\frac{\hbar^2}{2\,m}\,\frac{d^2\psi_i}{dx^2} = [V(x) - E_i]\,\psi_i. \tag{3.10.3}$$

This is known as the *time-independent Schrödinger equation*. More generally, this equation takes the form

$$H\,\psi_i = E_i\,\psi_i, \tag{3.10.4}$$

where H is assumed not to be an explicit function of t. Of course, the ψ_i satisfy the usual orthonormality condition:

$$\int_{-\infty}^{\infty} \psi_i^*\,\psi_j\,dx = \delta_{ij}. \tag{3.10.5}$$

Moreover, we can express a general wavefunction as a linear combination of energy eigenstates:

$$\psi(x,t) = \sum_i c_i\,\psi_i(x)\,\mathrm{e}^{-\mathrm{i}\,E_i\,t/\hbar}, \tag{3.10.6}$$

where

$$c_i = \int_{-\infty}^{\infty} \psi_i^*(x)\,\psi(x,0)\,dx. \tag{3.10.7}$$

Here, $|c_i|^2$ is the probability that a measurement of the energy will yield the eigenvalue E_i. Furthermore, immediately after such a measurement, the system is left in the corresponding energy eigenstate. The generalization of the previous results to the case where H has continuous eigenvalues is straightforward.

If a dynamical variable is represented by some Hermitian operator A that commutes with H (so that it has simultaneous eigenstates with H), and contains no specific time dependence, then it is evident from Equations ([e4.157]) and ([e4.158]) that the expectation value and variance of A are time independent. In this sense, the dynamical variable in question is a constant of the motion.

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3.11: Exercises

1. Monochromatic light with a wavelength of $6000\,\text{Å}$ passes through a fast shutter that opens for 10^{-9} sec. What is the subsequent spread in wavelengths of the no longer monochromatic light?
2. Calculate $\langle x\rangle$, $\langle x^2\rangle$, and σ_x, as well as $\langle p\rangle$, $\langle p^2\rangle$, and σ_p, for the normalized wavefunction

$$\psi(x) = \sqrt{\frac{2\,a^3}{\pi}}\,\frac{1}{x^2+a^2}. \tag{3.11.1}$$

   Use these to find $\sigma_x\,\sigma_p$. Note that $\int_{-\infty}^{\infty} dx/(x^2+a^2) = \pi/a$.
3. Classically, if a particle is not observed then the probability of finding it in a one-dimensional box of length L, which extends from $x=0$ to $x=L$, is a constant $1/L$ per unit length. Show that the classical expectation value of x is $L/2$, the expectation value of x^2 is $L^2/3$, and the standard deviation of x is $L/\sqrt{12}$.
4. Demonstrate that if a particle in a one-dimensional stationary state is bound then the expectation value of its momentum must be zero.
5. Suppose that $V(x)$ is complex. Obtain an expression for $\partial P(x,t)/\partial t$ and $d/dt\int P(x,t)\,dx$ from Schrödinger's equation. What does this tell us about a complex $V(x)$?
6. $\psi_1(x)$ and $\psi_2(x)$ are normalized eigenfunctions corresponding to the same eigenvalue. If

$$\int_{-\infty}^{\infty} \psi_1^*\,\psi_2\,dx = c, \tag{3.11.2}$$

   where c is real, find normalized linear combinations of ψ_1 and ψ_2 that are orthogonal to (a) ψ_1, (b) $\psi_1+\psi_2$.
7. Demonstrate that $p = -\mathrm{i}\,\hbar\,\partial/\partial x$ is an Hermitian operator. Find the Hermitian conjugate of $a = x + \mathrm{i}\,p$.
8. An operator A, corresponding to a physical quantity α, has two normalized eigenfunctions $\psi_1(x)$ and $\psi_2(x)$, with eigenvalues a_1 and a_2. An operator B, corresponding to another physical quantity β, has normalized eigenfunctions $\phi_1(x)$ and $\phi_2(x)$, with eigenvalues b_1 and b_2. The eigenfunctions are related via

$$\begin{aligned}\psi_1 &= (2\,\phi_1 + 3\,\phi_2)/\sqrt{13},\\ \psi_2 &= (3\,\phi_1 - 2\,\phi_2)/\sqrt{13}.\end{aligned}$$

   α is measured and the value a_1 is obtained. If β is then measured and then α again, show that the probability of obtaining a_1 a second time is $97/169$.
9. Demonstrate that an operator that commutes with the Hamiltonian, and contains no explicit time dependence, has an expectation value that is constant in time.
10. For a certain system, the operator corresponding to the physical quantity A does not commute with the Hamiltonian. It has eigenvalues a_1 and a_2, corresponding to properly normalized eigenfunctions

$$\begin{aligned}\phi_1 &= (u_1+u_2)/\sqrt{2},\\ \phi_2 &= (u_1-u_2)/\sqrt{2},\end{aligned}$$

    where u_1 and u_2 are properly normalized eigenfunctions of the Hamiltonian with eigenvalues E_1 and E_2. If the system is in the state $\psi=\phi_1$ at time $t=0$, show that the expectation value of A at time t is

$$\langle A\rangle = \left(\frac{a_1+a_2}{2}\right) + \left(\frac{a_1-a_2}{2}\right)\cos\left(\frac{[E_1-E_2]\,t}{\hbar}\right). \tag{3.11.3}$$

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