CHAPTER III
The Solution of the Free-Particle Wave Equation

Introduction

In the last two chapters, we have demonstrated that the probability of finding a particle somewhere in space should be related to the absolute magnitude squared of the wave-function solution to Schrödinger's equation. We also demonstrated that for this interpretation to be valid, the wavefunction should be normalizable (square-integrable). We defined the expectation value (ensemble average) of the location of a particle and the particle's momentum, and demonstrated that the measurements of position and momentum in classical physics are related to the corresponding expectation values of the position and momentum, and we showed that the time-derivative of the expectation value of momentum was consistent with Newton's second law.

In this chapter we wish to investigate even further the nature of the solution to Schrödinger's equation. We will develop the most general solution to Schrödinger's equation which is consistent with the description of a single free particle localized within some region of space at time $t = 0$, and demonstrate how this general solution varies in time and space. In so doing, we will discover the very important Heisenberg uncertainty principle, so fundamental to quantum physics, which relates the measurement of the position of a particle to the measurement of the momentum of that same particle.

The General Solution to Schrödinger's Equation

We want to consider the one-dimensional *time-dependent* Schrödinger equation for a particle under the influence of a potential energy $V(x)$ which is a function of the position of the particle. This equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\,\Psi(x,t)\;+\;V(x)\,\Psi(x,t)\;=\;i\hbar\frac{\partial}{\partial t}\,\Psi(x,t) \tag{3.1}$$

where $\Psi(x,t)$ is the time-dependent wavefunction, and m is the mass of the particle. As we have already pointed out, if the potential energy function is *not* explicitly a function of time, it is possible to separate the Schrödinger equation so that we have the dependence on position separated from its dependence upon time.

To do this we assume that $\Psi(x,t)$ can be written as a function of position only, $\psi(x)$, times a function of time only, $T(t)$, so that

$$\Psi(x,t) = \psi(x)T(t) \tag{3.2}$$

The Schrödinger equation then becomes:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)T(t)\;+\;V(x)\,\psi(x)T(t) = i\hbar\frac{\partial}{\partial t}\,\psi(x)T(t) \tag{3.3}$$

Now the partial with respect to position does not act upon $T(t)$ and the partial with respect to time does not operate on $\psi(x)$, so that this can be written

$$T(t)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)\right)+V(x)\,\psi(x)T(t)=\psi(x)\left(i\hbar\frac{\partial}{\partial t}\,T(t)\right) \tag{3.4}$$

Dividing both sides of this equation by $\psi(x)T(t)$ we obtain

$$\frac{1}{\psi(x)}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)\right)+V(x)\;=\;\frac{1}{T(t)}\left(i\hbar\frac{\partial}{\partial t}\,T(t)\right) \tag{3.5}$$

The left-hand side of this equation is a function of the position alone, while the right-hand-side of this equation is a function of time alone. For this equation to be valid for *all possible combinations of times and positions*, it should be obvious that both sides of this equation must be set equal to some arbitrary (undetermined) constant! We will let this constant be η. This leaves us with two differential equations which must be solved:

$$\frac{1}{\psi(x)}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)\right)+V(x)\;=\eta \tag{3.6}$$

and

$$\frac{1}{T(t)}\left(i\hbar\frac{\partial}{\partial t}\,T(t)\right)=\eta \tag{3.7}$$

The solution of the temporal equation is relatively easy. Rewriting Equ.3.7 we have

$$i\hbar\frac{\partial}{\partial t}\,T(t)=\eta\,T(t) \tag{3.8}$$

or

$$\frac{\partial}{\partial t}\,T(t)=\;-\frac{i}{\hbar}\eta\,T(t) \tag{3.9}$$

the solution of which is

$$T(t)=Ce^{-i\eta t/\hbar} \tag{3.10}$$

where C is some arbitrary constant. Now since $\Psi(x,t)$ is given by the product of $\psi(x)$ and $T(t)$, we can set the constant C equal to unity and let any necessary adjustments be made by changing the constants that will occur in the solution of the spatial equation. This means that the general solution to Schrodinger's time-dependent equation has the form

$$\Psi(x,t)=\psi(x)e^{-i\eta t/\hbar} \tag{3.11}$$

where $\psi(x)$ is the solution to the time-independent Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)+V(x)\,\psi(x)\;=\eta\,\psi(x) \tag{3.12}$$

In the last chapter, we showed that the momentum can be expressed in terms of a differential operator acting on a position-dependent wave function according to equation

$$\widehat{p} = -i\hbar\frac{\partial}{\partial x} \tag{3.13}$$

The square of this operator is given by

$$\widehat{p}^2 = -\hbar^2\frac{\partial^2}{\partial x^2} \tag{3.14}$$

so that the time-independent Schrödinger equation can be written in the form

$$\left(\frac{\widehat{p}^2}{2m} + V(x)\right)\psi(x) = \eta\,\psi(x) \tag{3.15}$$

We also pointed out that the position operator is just the variable x, so we can write this last equation as

$$\left(\frac{\widehat{p}^2}{2m} + V(\widehat{x})\right)\psi(x) = \eta\,\psi(x) \tag{3.16}$$

where you should remember that η is just an arbitrary separation constant. The left side of this last equation looks like the sum of the kinetic and potential energy of the particle, so we associate this operator with the Hamiltonian of the system. For conservative systems, the Hamiltonian is simply the total energy of that system. Thus, this last equation can be written in operator form as

$$\widehat{H}\psi(x) = \eta\psi(x) \tag{3.17}$$

which is in the form of an *eigenvalue* equation. The expectation value of the Hamiltonian operator

$$\langle\widehat{H}\rangle = \int_{-\infty}^{+\infty}\psi^*(x)\widehat{H}\psi(x)\,dx = \eta\int_{-\infty}^{+\infty}\psi^*(x)\psi(x)\,dx = \eta \tag{3.18}$$

is equal to the separation constant, so we will associate the separation constant with a symbol representing the total energy of the system, $\eta = E$.

Thus, the time-independent Schrödinger equation appears to be just a statement of the conservation of total mechanical energy, provided we write the momentum as a differential operator, and associate the separation constant η with the total energy E. Because of this association, we will write the time-dependent solution in the form

$$\Psi(x,t) = \psi(x)e^{-i\omega t} \tag{3.19}$$

where $\omega = \eta/\hbar = E/\hbar$ is consistent with the Einstein relationship between frequency and total energy for a particle. Everything we have said so far is totally general. We now want to examine the special case where the particle is in a region where the potential energy is constant.

Schrödinger's Equation for a Free Particle and Its Solutions

In this section we will examine the general solution to Schrödinger's equation for a *free* particle - i.e., one which moves in a region of space where the potential energy is constant (and the force is zero). For simplicity, we let this constant potential energy be zero. We have already demonstrated that the most general solution to Schrödinger's equation is of the form

$$\Psi(x,t) = \psi(x)e^{-i\omega t} \tag{3.20}$$

where $\psi(x)$ must satisfy Schrödinger's time-independent equation. For the case of a free particle, this time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\psi(x) \tag{3.21}$$

where $E = \hbar\omega$. Multiplying this last equation by $-2m/\hbar^2$ gives

$$\frac{\partial^2\psi(x)}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi(x) = -k^2\psi(x) \tag{3.22}$$

where $k = 2mE/\hbar^2$ is a constant. Notice that this constant energy is just equal to the kinetic energy in a region of space where the potential energy is constant. We assume that the solution to this differential equation is of the form

$$\psi(x) = Ae^{\lambda x} \tag{3.23}$$

and find that this is indeed a solution to this equation, provided that

$$\lambda = \pm ik \tag{3.24}$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$. Now k is *real* if $E > 0$, and *pure imaginary* if $E < 0$. In the case were $E < 0$, we write

$$k = \sqrt{\frac{2mE}{\hbar^2}} = \sqrt{-\frac{2m|E|}{\hbar^2}} = i\kappa \tag{3.25}$$

where $\kappa = \sqrt{2m|E|/\hbar^2}$ is real.

The possible solutions, then, are

$$\psi(x) = Ae^{+ikx} + Be^{-ikx} \qquad \text{for } E > 0 \tag{3.26}$$

$$\psi(x) = Ce^{+\kappa x} + De^{-\kappa x} \qquad \text{for } E < 0 \tag{3.27}$$

These solutions to Schrödinger's equation are general in nature, with the coefficients to be determined by specific boundary conditions, and by the normalization condition.

Total Energy Less than Zero Everywhere Let us first consider the case where the total energy is less than zero ($E < 0$). In the region where $x > 0$, equation 3.27 will blow up as x

$\rightarrow +\infty$, unless $C = 0$; likewise, if $x < 0$, it will blow up as $x \rightarrow -\infty$, unless $D = 0$. Thus, in order for the wave function solution to be normalizable, equation 3.27 must be written

$$\psi(x) = Ce^{+\kappa x} \qquad \text{for } E < 0,\ x < 0 \tag{3.28}$$

and

$$\psi(x) = De^{-\kappa x} \qquad \text{for } E < 0,\ x > 0 \tag{3.29}$$

Continuity of the Wave Function

There are two additional conditions we must also impose on these wave functions for them to be physically meaningful. The first is that *the wave function must be a continuous, single-valued function*. This requirement is simply an extension of the fact that the wave function is related to the probability. If the probability of finding a particle at a particular location x is to be single-valued (i.e., if there cannot be two different values for the probability at a single location), then the wave function must be continuous. If there is a boundary between two regions in which the solutions to Schrödinger's equation differ (this is often associated with a point where there is a change in potential energy), the wave function must be continuous across that boundary so that it remains single-valued.

For our free-particle solution, the requirement that the wave function be continuous means that $C = D$ at $x = 0$, so we can write the last two equations in the form

$$\psi(x) = Ce^{-\kappa |x|} \qquad \text{for } E < 0 \tag{3.30}$$

A plot of this function is shown below. The wavefunction is continuous at the point $x = 0$, but the derivative of this function is obviously not continuous at the point $x = 0$.

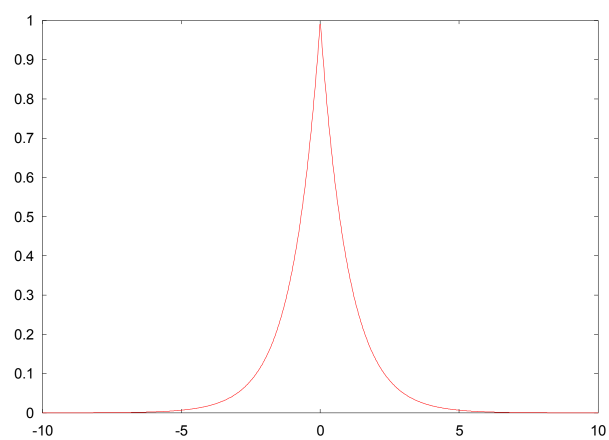


Fig. 3.1 Wave function solution for a free particle with $E < 0$.

Continuity of the First Derivative of the Wave Function

In addition to the requirement that the wave function be continuous, the Schrödinger equation imposes a restriction on the *first derivative* of the wave function at any boundary. This can be demonstrated by integrating the Schrödinger equation with respect to x over a small interval $\Delta\epsilon$ which encloses the boundary

$$-\frac{\hbar^2}{2m}\int_{x_o-\epsilon}^{x_o+\epsilon}\frac{\partial^2\psi(x)}{\partial x^2}\,dx+\int_{x_o-\epsilon}^{x_o+\epsilon}V(x)\psi(x)\,dx=E\int_{x_o-\epsilon}^{x_o+\epsilon}\psi(x)\,dx \tag{3.31}$$

The term on the right side of this last equation is a constant times the integral of the wavefunction over some finite interval. If we take the limit as $\Delta\epsilon \to 0$ this integral (the area under the function between $x_o - \epsilon$ and $x_o + \epsilon$) must go to zero, since the function is a finite, continuous, single-valued function. The integral on the far left is an integral of the second derivative of the wave function, and must be equivalent to first derivative of the wave function. This gives, in the limit as $\Delta\epsilon \to 0$

$$\lim_{\Delta\epsilon\to 0}\left.\frac{\partial\psi(x)}{\partial x}\right|_{x_o-\epsilon}^{x_o+\epsilon}=\lim_{\Delta\epsilon\to 0}\frac{2m}{\hbar^2}\int_{x_o-\epsilon}^{x_o+\epsilon}V(x)\psi(x)\,dx \tag{3.32}$$

Now the integral of the potential energy function times the wave function can be represented by the diagram below. The integral is just the area under the curve defined by the product of the potential energy function and the wave function. The wave function must be finite, continuous, and single-valued, but the potential energy function may exhibit discontinuities. As long as the potential energy function has only a finite number of finite steps (i.e., it is “piecewise-continuous”), the integral of the product of the potential energy function and the wave function remains finite. In the limit as $\Delta\epsilon \to 0$ this integral (the area under the curve between $x - \epsilon$ and $x + \epsilon$) will go to zero, requiring that *the first derivative of the wave function solution to Schrödinger's equation be continuous at a boundary* *so long as the potential energy function is piecewise-continuous.*

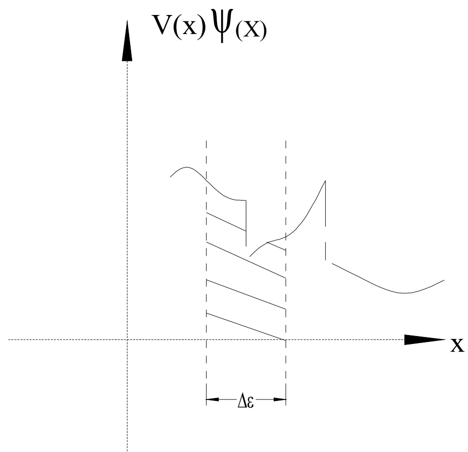


Fig. 3.2 A plot of the product of the potential energy function and the wavefunction. The integral of this product is the area under the curve. In the limit as $\Delta\epsilon \to 0$, this area goes to zero.

Now, we will carry out the operations defined in the last equation. The solution for the free particle where $E < 0$ is given by

$$\psi(x) = Ce^{+\kappa x} \qquad \text{for } E < 0,\ x < 0 \tag{3.33}$$

$$\psi(x) = Ce^{-\kappa x} \qquad \text{for } E < 0,\ x > 0 \tag{3.34}$$

At the point $x = -\epsilon$, the derivative is given by

$$+\kappa Ce^{-\kappa\epsilon} \tag{3.35}$$

and at the point $x = +\epsilon$, the derivative is given by

$$-\kappa Ce^{-\kappa\epsilon} \tag{3.36}$$

The requirement that the derivative be continuous (at the point $x = 0$) means that these two equations must be equal in the limit as $\epsilon \to 0$, or

$$+\kappa C = -\kappa C \tag{3.37}$$

Now, since $\kappa = \sqrt{2mE/\hbar^2}$ is generally not zero (unless $E = 0$), this last equation requires that $C = 0$. This is just the null solution and is not normalizable. This simply means that no physical solution exists for the case where $E < 0$ everywhere! This makes sense because the total energy for a free particle is just the kinetic energy which, classically, can never be less than zero. This does not mean, however, that a solution does not exist if there are finite regions where $E < 0$ and other regions where $E > 0$.

Total Energy Greater than Zero Everywhere We next consider the case where the total energy is greater that zero ($E > 0$). The wave function solution to the time-independent Schrödinger equation is

$$\psi(x) = Ae^{+ikx} + Be^{-ikx} \qquad \text{for } E > 0 \tag{3.38}$$

which is a sinusoidal solution and does not blow up as $x \to \pm\infty$. The time-dependent solution to this equation is

$$\Psi(x,t) = \left(Ae^{+ikx} + Be^{-ikx}\right)e^{-i\omega t} \quad \text{for } E > 0 \tag{3.39}$$

which can be written in the form

$$\Psi(x,t) = Ae^{+i(kx-\omega t)} + Be^{-i(kx+\omega t)} \tag{3.40}$$

The first term of this solution is just the equation of a plane wave of well-defined energy (or wavelength, since $k = 2\pi/\lambda$) traveling in the $+x$ direction. This can be seen by using Euler's equation and writing

$$e^{i(kx-\omega t)} = \cos(kx - \omega t) + i\sin(kx - \omega t) \tag{3.41}$$

If we look at the cosine function we can move along with the wave by chosing to ride along at a point of constant phase. Choosing the point where the phase angle is zero, we obtain

$$kx - \omega t = 0 \qquad \Rightarrow \qquad x = \left(\frac{\omega}{k}\right)t = v_{phase}t \tag{3.42}$$

Likewise, the second term in equation 3.40 represents a plane wave of the same well-defined energy traveling in the $-x$ direction. If this wave function is to represent a *single* particle moving through space, it cannot be moving in *both* directions at the same time, so we have to choose either A or B to be zero. This means that *the solution for a free particle can be written in the form of a traveling plane wave*

$$\Psi(x,t) = Ae^{+i(kx-\omega t)} \tag{3.43}$$

where

$$k \equiv \pm\frac{\sqrt{2mE}}{\hbar}, \qquad \text{with} \begin{cases} k > 0 \Rightarrow & \text{traveling to the right} \\ k < 0 \Rightarrow & \text{traveling to the left} \end{cases} \tag{3.44}$$

We can also express this solution in the form of sines and cosines, using Euler's equation

$$\Psi(x,t) = A[\cos(kx-\omega t) + i\sin(kx-\omega t)] \tag{3.45}$$

Now, to see if this is a reasonable solution to Schrödinger's equation, we examine the probability function and find that

$$\Psi^*(x,t)\Psi(x,t) = |\Psi(x,t)|^2 = |A|^2 \tag{3.46}$$

which means that the probability density of finding a particle is constant everywhere. But this means that the wave function *is not normalizable*! The reason the wave function is not normalizable is that the sine and cosine functions have no *end* - i.e., they do not go to zero as $x \to \pm\infty$. We must, therefore, truncate these functions somehow in order to produce a wave function solution to Schrödinger's equation which represents the motion of a single, free particle in space.

This problem is the same as that encountered in classical wave theory when we wish to describe sound or light *waves* in a more or less *localized* sense. As an example, consider a clap of thunder which is a relatively localized (in time) acoustical pulse. If we were to analyze such a clap, we would find that the sound is composed of a large number of different frequencies (as can be demonstrated by the electrical noise picked up on the radio *at all frequencies*). Likewise, a pulse of light emitted from a pulsed laser is somewhat localized in space and time. The answer to this normalization problem lies in the application of Fourer series and integrals. As we will demonstrate in the next two sections, *any* periodic or non-periodic waveform can be expressed in terms of a complex Fourier series or Fourier integral (i.e., a combination of harmonic waveforms).

> Note: We can sometimes get around the problem of normalization if we examine some finite region of space and develop our equations in terms of the probability current density. One can show (problem 2.6) that the probability current density for a traveling wave is given by
>
> $$j = \pm|A|^2\frac{\hbar k}{m}$$
>
> The term $\hbar k/m$ is just the equivalent of the classical velocity of a particle, and A is the amplitude of the wave function. Notice that the units of A must be $1/\sqrt{L}$

where L is some length, since $\int \Psi^* \Psi \, dx = 1$. This means that the units of j must be $(1/L)(L/t) = (1/t)$. This means we can let $|A|^2 = N/L$, represent the number of particles per unit length (the number of particles per unit volumn in one-dimension). Thus, the units of j correspond to the number of particles passing a given point x per unit time. Since j is not a function of the position or the time, this means that the traveling wave equation represented by a sine of cosine wave represents a situation where the number of particles per second passing a particular location is independent of time or position along the x-axis.

Fourier Series

One can show that *any* periodic function, no matter how bizarre, can be expressed mathematically in terms of an infinite series of sines and cosines. Thus, for a function $f(\theta)$, which is periodic with period 2π, such that

$$f(\theta + 2\pi) = f(\theta) \tag{3.47}$$

we can always express $f(\theta)$ in terms of the infinite series:

$$\begin{aligned} f(\theta) = \frac{1}{2}a_o + a_1 \cos\theta + a_2 \cos 2\theta + a_3 \cos 3\theta + \cdots \\ + b_1 \sin\theta + b_2 \sin 2\theta + b_3 \sin 3\theta + \cdots \end{aligned} \tag{3.48}$$

where the coefficients are chosen so that the Fourier series actually reproduces the waveform of interest in the interval $0 < \theta < 2\pi$.

Now it turns out that the Fourier series can also be expressed in terms of complex notation, since both the sine and the cosine function can be expressed in terms of complex exponentials. Using Euler's relations, we have

$$\sin n\theta = \frac{e^{in\theta} - e^{-in\theta}}{2i} \quad \text{and} \quad \cos n\theta = \frac{e^{in\theta} + e^{-in\theta}}{2} \tag{3.49}$$

If we substitute these expressions into the equation above, we can write the Fourier series expansion of a periodic function $f(\theta)$ in the form:

$$f(\theta) = \sum_{n=-\infty}^{+\infty} c_n \, e^{in\theta} \tag{3.50}$$

Notice here that the sum is from *negative infinity* to *positive infinity*, and that the constant term arises when you set $n = 0$. This method of representing the Fourier series is often a bit simpler to use. Again, we must determine the correct values of the constants, c_n, to represent the desired function. These coefficients can be found by using the orthogonality relationships for the exponentials:

$$\int_{-\pi}^{+\pi} e^{i(m-n)\theta} \, d\theta = 2\pi \, \delta_{mn} \tag{3.51}$$

where the integral is over a *period* 2π.

Problem 3.1 Prove the orthogonality relationship

$$\int_{-\pi}^{+\pi} e^{i(m-n)\theta}\, d\theta = 2\pi\, \delta_{mn}$$

If we multiply both sides of equation (3.50) by $e^{-im\theta}$ and integrate from $-\pi$ to $+\pi$ we obtain:

$$\int_{-\pi}^{+\pi} e^{-im\theta}\, f(\theta)\, d\theta = \sum_{n=-\infty}^{+\infty} c_n \int_{-\pi}^{+\pi} e^{i(n-m)\theta}\, d\theta \tag{3.52}$$
$$= \sum_{n=-\infty}^{+\infty} c_n\, 2\pi\, \delta_{mn} = 2\pi\, c_m$$

The coefficients, c_n, are, therefore, given by:

$$c_n = \frac{1}{2\pi} \int_{-\pi}^{+\pi} f(\theta)\, e^{-in\theta}\, d\theta \tag{3.53}$$

This whole proceedure can also be written in terms of some spatial displacement, x, by expressing the angle θ in terms of x. Thus, we let $\theta = 2\pi x/P$, where P is the spacial period. It is, however, even more convenient to write this as $\theta = \pi x/\xi$, where $\xi = P/2$, or one half the spatial period. In this case, we can write $f(\pi x/\xi) = f(x)$, where

$$f(x + 2\xi) = f(x) \tag{3.54}$$

We can, therefore, express $f(x)$ in terms of the infinite series:

$$f(x) = \frac{1}{2} a_o + a_1 \cos \pi x/\xi + a_2 \cos 2\pi x/\xi + a_3 \cos 3\pi x/\xi + \cdots \tag{3.55}$$
$$+ b_1 \sin \pi x/\xi + b_2 \sin 2\pi x/\xi + b_3 \sin 3\pi x/\xi + \cdots$$

or, in complex notation,

$$f(x) = \sum_{n=-\infty}^{+\infty} c_n\, e^{in\pi x/\xi} \tag{3.56}$$

Again we must determine the constants c_n which will give us our desired function! The orthogonality relationships for the exponentials can be expressed in terms of the spatial displacement, x, by the equation:

$$\int_{-\xi}^{+\xi} e^{i(m-n)\pi x/\xi}\, dx = 2\xi\, \delta_{mn} \tag{3.57}$$

Multiplying both sides of equation (3.56) by $e^{-im\pi x/\xi}$ and integrating from $-\xi$ to $+\xi$ we obtain:

$$\int_{-\xi}^{+\xi} e^{-im\pi x/\xi} f(x)\,dx = \sum_{n=-\infty}^{+\infty} c_n \left[\int_{-\xi}^{+\xi} e^{i(n-m)\pi x/\xi}\,dx \right] \tag{3.58}$$
$$= \sum_{n=-\infty}^{+\infty} c_n\, 2\xi\, \delta_{mn} = 2\xi\, c_m$$

Thus the coefficients c_n are given by:

$$c_n = \frac{1}{2\xi} \int_{-\xi}^{+\xi} e^{-in\pi x/\xi} f(x)\,dx \tag{3.59}$$

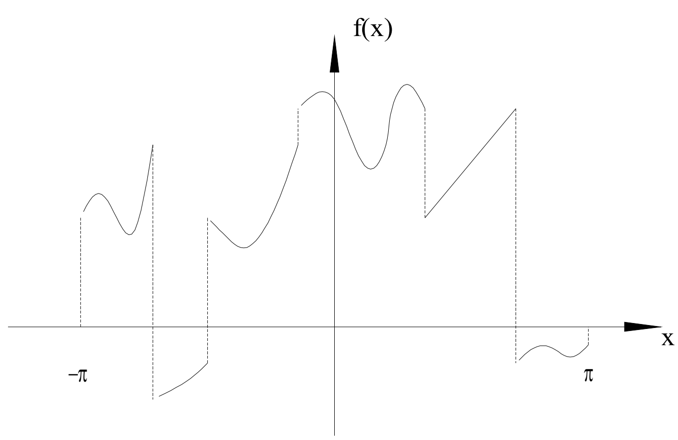
where 2ξ is the period!

DIRICHLET CONDITIONS

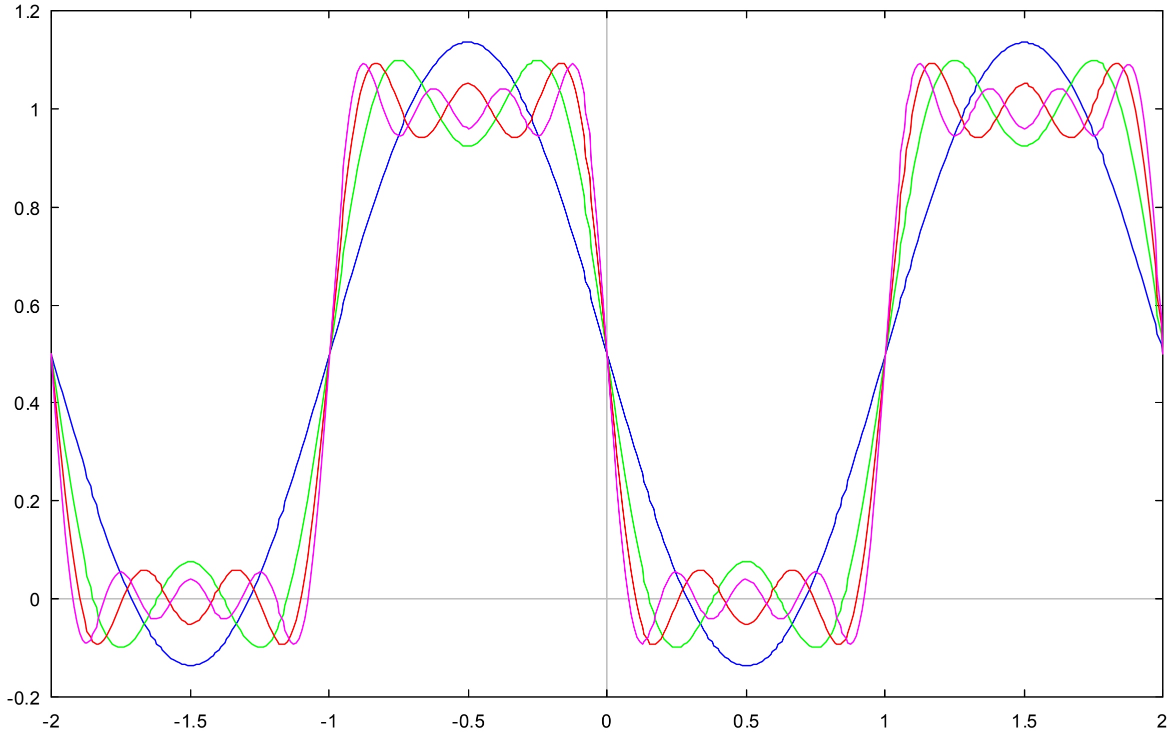
We have demonstrated that a Fourier series can be found for a periodic function $f(x)$, but we must ask under what conditions this series actually converges to that function. Dirichlet's theorem states that:

> *If f(x) is periodic in 2π, and if between $-\pi$ and π it is single-valued, has a finite number of maximum and minimum values, and a finite number of discontinuities, and if*
>
> $$\int_{-\pi}^{+\pi} |f(x)|\,dx$$
>
> *is finite, then the Fourier series converges to f(x) at all the points where f(x) is continuous; at jumps the Fourier series converges to the midpoint of the jump.*

An example of a function which satisfies the Dirichlet condition is shown below.



The figure below illustrates how the Fourier series converges to a square-wave function. Notice that the Fourier series is equal to the midpoint of a discontinuity, and that *there is an overshoot in the Fourier series at a discontinuity which does not go away as we add more and more terms*! This is called the Gibbs phenomena.



Problem 3.2 Expand in a complex Fourier series the periodic function $f(x)$ which is defined in the interval $0 < x < 2L$ by the relation:

$$f(x) = \begin{cases} 0 & 0 < x < L \\ 1 & L < x < 2L \end{cases}$$

[If this were a periodic function in time, it would correspond to a square wave of one volt. The terms of the Fourier series would then correspond to the different a-c frequencies which are combined in this "square wave" voltage, and the magnitude of the Fourier coefficients would indicate the relative importance of the various frequencies.] Show that the solution can be written as:

$$f(x) = \frac{1}{2} - \frac{2}{\pi}\left[\sin\frac{\pi x}{L} + \frac{1}{3}\sin\frac{3\pi x}{L} + \frac{1}{5}\sin\frac{5\pi x}{L} + \cdots\right]$$

Problem 3.3 When a guitar string is plucked, it generally does not oscillate with a single frequency, unless it is plucked in a very particular way. If we assume that the string is plucked in the center (displaced from equilibrium a distance δ), but remains fixed on each end, then we can determine the frequency components by performing a Fourier series expansion to describe the initial waveform of the string! Assume the length of the string is L, and express the functional form of this plucked string by expanding the waveform in terms of a complex Fourier expansion [the waveform will look something like a roof top]. In addition, write the expansion in terms of sines and/or cosines. The result you get will depend upon the particular coordinate system you use, and *upon your choice of the periodic function*. Choose a coordinate system so that one end is located at $x = 0$, while the other end is at $x = L$, and show that the expansion can be written in terms of $sines$ or $cosines$, depending upon the form of the wave function chosen. [In one case, you will have a series of roof tops, all above the $y = 0$ line; in the other, you will have a function that looks like a triangular sine wave with both positive and negative values of y, but the negative values are outside the region of interest].

Fourier Integrals and the Dirac Delta Function

The question now arises: What do we do about wave functions which are not periodic, and which cannot be made to look periodic? In addition, we have noticed that periodic functions can be formed from a discrete set of frequencies, i.e., not all frequencies are needed to give a certain periodic function. An expansion of the concept of the Fourier series allows us to treat any wave function whatsoever, whether it is periodic or not, and also to include all possible frequencies.

The complex Fourier expansion of a function which is periodic with period 2ξ is given by

$$f(x) = \sum_{n=-\infty}^{+\infty} c_n \, e^{in\pi x/\xi} \tag{3.60}$$

where c_n can be determined from:

$$c_n = \frac{1}{2\xi}\int_{-\xi}^{+\xi} e^{-in\pi x'/\xi} \, f(x') \, dx' \tag{3.61}$$

Now if we substitute this last equation into the previous one, we have

$$f(x) = \sum_{n=-\infty}^{+\infty} \left[\frac{1}{2\xi}\int_{-\xi}^{+\xi} e^{-in\pi x'/\xi} \, f(x') \, dx' \right] e^{in\pi x/\xi} \tag{3.62}$$

If we now let $k_n = n\pi/\xi$, and $\Delta k = k_{n+1} - k_n = \pi/\xi$, so that $\xi = \pi/\Delta k$, we have

$$f(x) = \sum_{n=-\infty}^{+\infty} \left[\frac{\Delta k}{2\pi} \int_{-\pi/\Delta k}^{\pi/\Delta k} e^{-ikx'} \, f(x') \, dx' \right] e^{ikx} \tag{3.63}$$

and, in the limit as $\Delta k \to 0$, $\Delta k \to dk$ and $\pi/\Delta k \to \infty$, and $\sum \to \int$, giving,

$$f(x) = \int_{-\infty}^{+\infty} \left[\frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-ikx'} f(x') \, dx' \right] e^{ikx} \, dk \tag{3.64}$$

Notice that the term in brackets is a function of k only, which we will call $g(k)$. Thus, we can write $f(x)$ as

$$f(x) = \int_{-\infty}^{+\infty} g(k)\, e^{ikx}\, dk \ , \tag{3.65}$$

where

$$g(k) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} f(x)\, e^{-ikx} dx \ . \tag{3.66}$$

These equations define the Fourier transform and its inverse. This transform is valid for *any* type of function $f(x)$, periodic or not, and also allows for all possible values of the frequency (since $k = 2\pi/\lambda = 2\pi\nu/c$). Since these last two equations are nearly symmetric except for the factor $1/2\pi$, it is a common practice to slightly alter our definitions in order to make these two equations more nearly alike. (It is important to check how a text defines the transform and it's inverse because this is not always done in the same way!) Thus, we will *define* the Fourier transform and its inverse by the equations:

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} g(k)\, e^{ikx}\, dk \ , \tag{3.67}$$

and

$$g(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} f(x)\, e^{-ikx}\, dx \ . \tag{3.68}$$

Now in order for these two equations to actually be useful we require consistency in our definition. That is, if we substitute the equation for $g(k)$ back into the first equation

$$f(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} f(x')\, e^{-ikx'} dx' \right] e^{ikx}\, dk \tag{3.69}$$

we must still get an equality. Now if we change the order of integration, we get

$$f(x) \ = \ \frac{1}{2\pi}\int_{-\infty}^{+\infty} f(x') \left[\int_{-\infty}^{+\infty} e^{ik(x-x')}\, dk \right] dx' \tag{3.70}$$

and, in order for the right-hand-side of this equation to be $f(x)$, we require that the integral in the braces be a very special integral indeed. We require that the integral over all k be equal to 2π *only* at the point $x = x'$ and zero everywhere else! We write this in a special notation:

$$\int_{-\infty}^{+\infty} e^{ik(x-x')}\, dk \ = \ 2\pi\, \delta(x - x') \tag{3.71}$$

where $\delta(x - x')$ is called the *Dirac delta function.* This function can be thought of as a function which is zero everywhere except where the argument is zero, and at this single point, it is equal to ∞, but in such a way that the area under the curve is unity! This definition enables us to write:

$$f(x) \;=\; \frac{1}{2\pi}\int_{-\infty}^{+\infty} f(x')\,[2\pi\,\delta(x-x')]\;\,dx' \tag{3.72}$$

or

$$f(x) \;=\; \int_{-\infty}^{+\infty} f(x')\,\delta(x-x')\;\,dx' \tag{3.73}$$

As we stated above, the Dirac delta function can be thought of as a special function that forces the integrand to take on the value where the argument of the delta function equals to zero. This is equivalent to the equation

$$f(0) \;=\; \int_{-\infty}^{+\infty} f(x)\,\delta(x)\;\,dx \tag{3.74}$$

These last two equations can be considered the *definition* of the Dirac delta function. From this basic definition, one can derive (by using a change of variables in most cases) the following relationships:

$$\begin{aligned} x\delta(x-a) &= a\delta(x-a) \\ \delta(-x) &= \delta(x) \\ \delta(ax) &= \frac{1}{\mid a \mid}\;\delta(x) \qquad \text{for } a \neq 0 \\ \int f(x)\,\delta'(x)\,dx \;&=\; -f'(0) \end{aligned} \tag{3.75}$$

As an example of the utility of the Dirac delta function we will derive an extremely important relationship, known as *Parseval's theorem*:

$$\int_{-\infty}^{+\infty} f^*(x)f(x)dx \;=\int_{-\infty}^{+\infty} g^*(k)g(k)dk \tag{3.76}$$

which relates the absolute magnitude squared of the wave function to the absolute magnitude squared of the Fourier transform of the wave function. We can verify this last equation by using the Dirac delta function, as follows:

$$\int_{-\infty}^{+\infty} f^*(x)f(x)dx = \int_{-\infty}^{+\infty}\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} g^*(k)e^{+ikx}dk\right]\left[\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} g(k')e^{-ik'x}dk'\right]dx \tag{3.77}$$

$$\int_{-\infty}^{+\infty} f^*(x) f(x) dx = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} g^*(k) g(k') e^{+i(k-k')x} dk\, dk' dx \tag{3.78}$$

$$\int_{-\infty}^{+\infty} f^*(x) f(x) dx = \iint_{-\infty}^{+\infty} g^*(k) g(k') \delta(k-k')\, dk\, dk' \tag{3.79}$$

$$\int_{-\infty}^{+\infty} f^*(x) f(x) dx = \int_{-\infty}^{+\infty} g^*(k) g(k) dk \tag{3.80}$$

This equation illustrates the fact that *normalizing the function* $f(x)$ *simultaneously normalizes the function* $g(k)$.

Fourier Transforms and the Free-Particle Wave Equation

Earlier in this chapter we pointed out that the localized nature of a pulse might serve as a wave-like representation of a particle, and that such a representation required the use of Fourier analysis. We postulate, therefore, that a possible solution to Schrödinger's equation which could represent a single, localized particle might be expressed in the form

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{ikx}\, dk \tag{3.81}$$

where $\psi(x)$ is the Fourier integral expansion of the wavefunction, and where

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(x)\, e^{-ikx}\, dx \tag{3.82}$$

is the inverse transform of $\psi(x)$. Now the function $\phi(k)$ can also be expressed as $\phi(p)$ since $p = \hbar k$, and we will discover in what follows, that the function $\phi(p)$ is the probability amplitude for measuring a particular value of the momentum. Because of *Parseval's theorem*, we know that if we normalize the position wave function $\psi(x)$ we will automatically normalize the momemtum wave function $\phi(p)$. In addition, all the consequences arising from the normalization of the position wave function also apply to the momentum wave function.

Although the idea of forming a wave-packet from the sinusoidal solutions to Schrödinger's equation may seem reasonable, we must now determine if a wave function of this form will in fact satisfy the Schrödinger equation for a free particle, and thus be an acceptable solution to our problem. To do this, we assume, even though the equations above are not explicitly time dependent, that these equations are valid at any particular instant of time, or, more generally,

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k,t)\, e^{ikx}\, dk\ . \tag{3.83}$$

We now insert this wave function into the Schrödinger equation for a free particle and determine if this equation is indeed a valid solution. This give us

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k,t)\, e^{ikx}\, dk\right] = i\hbar\,\frac{\partial}{\partial t}\left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k,t)\, e^{ikx}\, dk\right] \tag{3.84}$$

The partial derivatives can be moved into the intergrals to obtain

$$-\frac{\hbar^2}{2m}\left[\int_{-\infty}^{+\infty} -k^2\phi(k,t)\, e^{ikx}\, dk\right] = i\hbar\left[\int_{-\infty}^{+\infty} \frac{\partial}{\partial t}\phi(k,t)\, e^{ikx}\, dk\right] \tag{3.85}$$

where you should notice that $\phi(k,t)$ is *not* a function of x. Moving the constants into the integrals gives

$$\int_{-\infty}^{+\infty} \frac{\hbar^2 k^2}{2m}\phi(k,t)\, e^{ikx}\, dk = \int_{-\infty}^{+\infty} i\hbar\frac{\partial}{\partial t}\phi(k,t)\, e^{ikx}\, dk \tag{3.86}$$

which will always be valid if the integrands are equal, or if

$$\frac{\hbar^2 k^2}{2m}\phi(k,t) = i\hbar\frac{\partial}{\partial t}\phi(k,t) \tag{3.87}$$

We can solve this equation to obtain

$$\phi(k,t) = \phi(k,0)e^{-i\hbar^2k^2t/2m\hbar} = \phi(k,0)e^{-i\omega t} \tag{3.88}$$

where $\omega = E/\hbar$, and where $E = \hbar^2k^2/2m = p^2/2m$.

This last equation means that the solution to Schrödinger's equation for a free particle can always be written in the form

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k,0)\, e^{ikx-i\omega t}\, dk\ . \tag{3.89}$$

where $\phi(k,0)$ is some arbitrary function that depends upon the initial conditions of the problem and where $\omega = \hbar^2k^2/2m$. Now at time $t=0$, we get *back* the Fourier transform

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k,0)\, e^{ikx}\, dk \tag{3.90}$$

We can, therefore, determine the function $\phi(k,0)$ from the Fourier transform of $\Psi(x,0)$

$$\phi(k,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0)\, e^{-ikx}\, dx \ . \tag{3.91}$$

Thus, *we have the tools to determine the wave function $\Psi(x,t)$ at any time t if we know the wave function $\Psi(x,0)$ at time $t = 0$. From Parseval's theorem, we also know that the required normalization condition on the wave function $\Psi(x,0)$ imposes a similar normalization condition on the function $\phi(k,0)$, and once the wavefunction is normalized, it remains normalized for all time.*

We can express the equations above in terms of the momentum and the energy by using the fact that $p = \hbar k$, and $E = \hbar\omega$. (Remember that the deBroglie relationship between wave-like and particle-like phenomena is $p = h/\lambda$.) The general solution to Schrödinger's equation can thus be written as

$$\Psi(x,t) = \frac{1}{\hbar\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(p,0)\, e^{i(p/\hbar)x - i(E/\hbar)t}\, dp\,, \tag{3.92}$$

where

$$\phi(p,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0)\, e^{-ipx/\hbar}\, dx\,. \tag{3.93}$$

and where we must always remember that the energy $E = \hbar\omega$ is in general a function of the momentum. Again, to make these two equations more symmetric, we will divide the $\hbar$ between these two equations (using the flexibility of normalization to allow us to absorb constants into the wave functions) so that we have the two equations:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \phi(p,0)\, e^{i(p/\hbar)x - i(E/\hbar)t}\, dp \tag{3.94}$$

$$\phi(p,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \Psi(x,0)\, e^{-ipx/\hbar}\, dx$$

The Interpretation of $\phi(p,t)$

Now, let's look at a few examples. First we will consider the case where the initial momentum of a particle is well defined, i.e., the case where the particle has a definite value of the momentum, p_o. Mathematically, we can express this by saying that the function $\phi(p,0)$ is given by

$$\phi(p,0) = \mathcal{A}\delta(p - p_{\mathrm{o}}) \tag{3.95}$$

where $\mathcal{A}$ is some constant. The wave function which is a solution to Schrödinger's equation is therefore given by

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \mathcal{A}\delta(p - p_o)\, e^{i(p/\hbar)x - i(E/\hbar)t}\, dp\,. \tag{3.96}$$

or

$$\psi(x,t) = \frac{\mathcal{A}}{\sqrt{2\pi\hbar}}\, e^{i(p_o/\hbar)x - i(E_o/\hbar)t} \tag{3.97}$$

where $E_o = p_o^2/2m$ for a free particle. But this is just the equation of a plane wave, which we already know is not normalizable and *implies a constant density everywhere*. The only way we can represent a *localized* distribution of particles is to make use of the equation

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \phi(p,0)\, e^{i(p/\hbar)x - i(E/\hbar)t}\, dp\,. \tag{3.98}$$

where $\phi(p,0)$ cannot be associated with one single, well-defined momentum, but must be associated with a *distribution* in the value of the momentum of the particle. [One might think of this by considering a group of particles, and assuming each particle might have a slightly different momentum - however, this must be applicable to a *single* particle as well, so our interpretation must be consistent with a description of a single particle.] We might, therefore, interpret the function $|\phi(p,t)|^2$ as the *probability density for measuring a particular value of momentum* p *at a particular time* t. If this is true, then $\phi(p,t)$ must be the *momentum probability amplitude for measuring a particular value of momentum,* in direct correspondence with the interpretation of $\psi(x,t)$ as the probability amplitude for measuring a particular value of position, x, as some time t.

As further justification for this association, let's look again at the expectation value of the momentum. This is given by

$$\langle p \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t) \left(-i\hbar \frac{\partial}{\partial x} \right) \Psi(x,t)\, dx \tag{3.99}$$

Each of the wave functions of position and time can be written as

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \phi(p,t) e^{ipx/\hbar}\, dp \tag{3.100}$$

However, in order to keep the various parameters identifiable, we will use p for the dummy variable in the second integral and p' for the dummy variable in the first integral. The partial derivative acts only on the integrand, so that

$$-i\hbar \frac{\partial}{\partial x} \Psi(x,t) = \frac{-i\hbar}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \phi(p,t) \frac{ip}{\hbar} e^{ipx/\hbar}\, dp \tag{3.101}$$

Now writing the expectation value of p using the momentum representation we obtain

$$\langle p\rangle = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dp' \phi^*(p',t)e^{+ip'x/\hbar}\int_{-\infty}^{+\infty} dp\,\phi(p,t)pe^{ipx/\hbar} \tag{3.102}$$

Rearranging terms and integrating first over position, we obtain

$$\langle p\rangle = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dpdp'\phi^*(p',t)\,p\,\phi(p,t)\int_{-\infty}^{+\infty} e^{i(p-p')x/\hbar}\,dx \tag{3.103}$$

Recall that we defined the Dirac delta function as

$$\delta(k-k') = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{i(k-k')x}\,dx \tag{3.104}$$

which is equivalent to

$$\delta(p-p') = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} e^{i(p-p')x/\hbar}\,dx \tag{3.105}$$

This means that the expectation value of the momentum can be written as

$$\langle p\rangle = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} dpdp'\phi^*(p',t)\,p\,\phi(p,t)\,\delta(p-p') \tag{3.106}$$

Integrating over p', the delta function gives zero everywhere except where $p' = p$, so we are left with

$$\langle p\rangle = \int_{-\infty}^{+\infty} dp\,\phi^*(p,t)\,p\,\phi(p,t) \tag{3.107}$$

Notice that this equation for the expectation value of momentum has the same form as the expression

$$\langle x\rangle = \int_{-\infty}^{+\infty} dx\ \psi^*(x,t)\,x\,\psi(x,t) \tag{3.108}$$

for the expectation value of the position. This would seem to indicate that the wave function solutions $\Psi(x,t)$ are wave functions which represent the probability amplitude in position, while $\phi(p,t)$ are wave functions which represent the probability amplitude in momentum. The wave functions $\Psi(x,t)$ are often described as being the wave functions in position space, while the wave functions $\phi(p,t)$ are described as being the wave functions in momentum space. Thus, *the momentum operator* $\widehat{\mathrm{p}}$ *in momentum space is just the variable* p, *just like the position operator* $\widehat{x}$ *in position space is just the variable* x.

Now let's find an expression for the position operator $\widehat{x}$ in momentum space. To do that we start with the expectation value of position and write

$$\langle x\rangle = \int_{-\infty}^{+\infty} dx\ \Psi^*(x,t)\,x\,\Psi(x,t) \tag{3.109}$$

and then use the general expression for $\Psi(x,t)$ in terms of the momentum

$$\langle x \rangle = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dp\, \phi^*(p,t)\; e^{-i(p/\hbar)x}(x) \int_{-\infty}^{+\infty} dp'\; \phi(p',t)\; e^{+i(p'/\hbar)x} \tag{3.110}$$

The variable x can be carried into the last integral, since it is independent of p'. And this variable can be written as a parital with respect to momentum, as in the next equation

$$\langle x \rangle = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dp\, \phi^*(p,t)\; e^{-i(p/\hbar)x} \int_{-\infty}^{+\infty} dp'\; \phi(p',t)\left[\frac{\hbar}{i}\frac{\partial}{\partial p'}\;\left(e^{+i(p'/\hbar)x}\right)\right] \tag{3.111}$$

The last integral in the equation above can be integrated by parts to give

$$\begin{aligned}\int_{-\infty}^{+\infty} \phi(p',t)\left[\frac{\hbar}{i}\frac{\partial}{\partial p'}\;\left(e^{+i(p'/\hbar)x}\right)\right] dp' \;=\; &-\int_{-\infty}^{+\infty}\left[\frac{\hbar}{i}\frac{\partial}{\partial p'}(\phi(p',t)\,)\right]\left(e^{+i(p'/\hbar)x}\right)\,dp' \\ &+\phi(p',t)\left(e^{+i(p'/\hbar)x}\right)\Big|_{-\infty}^{+\infty}\end{aligned} \tag{3.112}$$

Because the momentum wave function $\phi(p',t)$ must be normalizable, this function must go to zero faster than $1/p'$, so that the last term in the expression above must be zero. Thus, we are left with an expression for the expectation value of x given by

$$\langle x \rangle = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dp\, \phi^*(p,t)\; e^{-i(p/\hbar)x} \int_{-\infty}^{+\infty} dp'\;\left[i\hbar\frac{\partial}{\partial p'}(\phi(p',t)\,)\right]\left(e^{+i(p'/\hbar)x}\right) \tag{3.113}$$

Now, if we reorder the way in which we take the integral, we obtain

$$\langle x \rangle = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dp\,dp'\phi^*(p,t)\;\left(i\hbar\frac{\partial}{\partial p'}\right)\;\phi(p',t)\int_{-\infty}^{+\infty} dx\, e^{-i(p-p')x/\hbar} \tag{3.114}$$

The last integral in the equation above is equal to $2\pi\hbar\,\delta(p-p')$, giving

$$\langle x \rangle = \int_{-\infty}^{+\infty} dp\,dp'\phi^*(p,t)\;\left(i\hbar\frac{\partial}{\partial p'}\right)\;\phi(p',t)\,\delta(p-p') \tag{3.115}$$

or, integrating over p' first, we obtain

$$\langle x \rangle = \int_{-\infty}^{+\infty} dp\,\phi^*(p,t)\;\left(i\hbar\frac{\partial}{\partial p}\right)\;\phi(p,t) \tag{3.116}$$

This last equation can be expressed in the form

$$\langle x\rangle = \int_{-\infty}^{+\infty} dp\, \phi^*(p,t)\, \widehat{x}\, \phi(p,t) \tag{3.117}$$

where $\widehat{x} = i\hbar(\partial/\partial p)$ is the position operator in momentum representation.

<u>**Commutation of Operators**</u>

Since both the momentum and postition operators may need to be expressed in terms of partial derivatives, we will need to take special care when we deal with the products of operators. For example, let's consider the product of the position and the mometum operators operating on a position dependent wavefunction

$$\widehat{xp}\,\psi(x) = x\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x) = -i\hbar x\frac{\partial\psi(x)}{\partial x} \tag{3.118}$$

The product of these same two operators operating in reverse order gives

$$\widehat{px}\,\psi(x) = \left(-i\hbar\frac{\partial}{\partial x}\right)x\,\psi(x) = -i\hbar\left[\psi(x) + x\frac{\partial\psi(x)}{\partial x}\right] \tag{3.119}$$

These two operations are clearly not the same. If we take the difference between these two operations we obtain

$$(\widehat{xp} - \widehat{px})\,\psi(x) = i\hbar\,\psi(x) \tag{3.120}$$

We define the *commutation operator* for x and p by the equation

$$[\widehat{x},\widehat{p}] = \widehat{xp} - \widehat{px} \tag{3.121}$$

so that equation (3.120) can be written as

$$[\widehat{x},\widehat{p}] = i\hbar$$

Two operators are said to commute when the commutation operator is equal to zero, i.e., when the order of operation of the two operators is insignificant. They are said to be non-commuting when the commutator is non-zero, i.e., when the order of operation is significant. It is interesting to consider that the non-commutation of the position and momentum operators arises because $\hbar$ is finite! In classical physics (where energy levels, etc., can be considered as continuous), we would expect these two operators to commute.

The commutation operation we have just introduced is significant for two reasons: 1) This commutation operation is related to the uncertainty principle! If the commutator of two operators is not zero, then there exists an uncertainty relationship between the two observables associated with these operators. 2) The commutation relationship is *independent of representation*! One obtains the same result whether you work in position representation or momentum representation!

Introduction to The Heisenberg Uncertainty Relation

To gain a better picture of how $\psi(x,0)$ and $\phi(p,0)$ are related to one another, we will consider a function which would represent a particle localized in space (with some uncertainty Δx. We will choose the wave function $\psi(x,0)$ so that

$$\psi(x,0) = \begin{cases} \dfrac{1}{\sqrt{\Delta x}} & \text{if } |x| < \dfrac{\Delta x}{2} \\ 0 & \text{if } |x| > \dfrac{\Delta x}{2} \end{cases} \tag{3.122}$$

The Fourier transform of this function

$$\phi(p{,}0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \psi(x{,}0)\; e^{-ipx/\hbar}\; dx\;. \tag{3.123}$$

gives

$$\phi(p,0) = \frac{2(\hbar/p)}{\sqrt{2\pi\hbar\Delta x}} \sin(p\Delta x/2\hbar) \tag{3.124}$$

Notice that this last equation is zero when $p\Delta x/2\hbar = n\pi$, or where $p = n2\pi\hbar/\Delta x$ so that as Δx *decreases*, the value of p where $\phi(p,0) = 0$ *increases*. If we define the uncertainty in p as the *width* of the function $\phi(p,0)$ (i.e., the distance between the first zeros of the function) then $\Delta p = 4\pi\hbar/\Delta x$ [or $\Delta p \Delta x = 4\pi\hbar = 2h$]. Thus, as $\psi(x,0)$ becomes more localized (i.e., as Δx gets smaller) then $\phi(p,0)$ becomes more spread out. This is the basic nature of the Heisenberg uncertainty relation (although at this point we have not been very precise in our definition of uncertainty). A more exact statement of the Heisenberg uncertainty principle will be developed later.

This position-momentum uncertainty is a natural consequence of using Fourier transforms to produce a localized wave packet (a necessity if we want to describe the motion of a *particle). Our mathematical model seems to imply that the more precisely we know x, at time $t = 0$, the less precisely we know p at time $t = 0$, and vise versa*!

Problem 3.4 Consider the wave function

$$\Psi(x,t) = Ae^{-\lambda|x|}e^{-i\omega t}$$

Determine the Fourier transform in momentum space of this wave function at time $t = 0$ [i.e., the momentum distribution function $\phi(p,0)$] and the normalization constant A. Comment on how the momentum distribution function varys with very large values of λ, and with very small values of λ? How does this relate to the Heisenberg uncertainty principle?

Traveling Waves and the Spreading of a Gaussian Wave Packet

We now want to examine how our mathematical description of the wave function for a free particle changes in space and time (as it should for a free particle moving through space). Our general solution for the free-particle Schrödinger's equation is

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k,0)\, e^{ikx - i\omega t}\, dk\ . \tag{3.125}$$

where

$$\phi(k,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(x,0)\, e^{-ikx}\, dx \tag{3.126}$$

Since $\omega = E/\hbar$, and $k = p/\hbar$, and since E and p are generally related in some fashion, we note that, in general, $\omega = \omega(k)$. This is just the simple relationship between the frequency of the wave and the wavelength. For *photons* this relationship (derived from the fact that $E = pc$) is very simple

$$\omega = kc \quad \Rightarrow \quad v_{ph} = c = \omega/k = \lambda\nu \tag{3.127}$$

where c is the speed of light in a vacuum, and is a constant. This gives

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k,0)\, e^{ik(x - v_{ph}t)}\, dk\ . \tag{3.128}$$

which is just the equation for the propagation of plane waves *whose phase velocities remain constant as the waves propagate.*

For particles, however, the relationship is not so simple. Relativistically, the equation for the energy $E^2 = p^2c^2 + m_o^2c^4$ gives the expression

$$\omega = \sqrt{k^2c^2 + \frac{m_o^2c^4}{\hbar^2}} \tag{3.129}$$

Classically, the energy reduces to $E = m_o c^2 + p^2/2m + \cdots$, and, since $E = \hbar\omega$, this reduces to

$$\omega = \frac{m_o c^2}{\hbar} + \frac{(\hbar k)^2}{2m} \tag{3.130}$$

In neither case do we obtain the simple relationship ω/k = constant. However, we know that *the general form of the wave function which must describe particles is given by*

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k,0)\, e^{ikx - i\omega(k)t}\, dk\ . \tag{3.131}$$

where $\omega(k)$ is an appropriate function of k. Unlike the equation for photons, the plane-wave components of this equation do not travel at the same speed. This causes them to interfere in a complicated manner which gives rise to an interference *envelope*. We now want to examine this last equation in greater detail to see if it does, indeed, give a reasonable description of what is observed in nature.

To make this example as concrete as possible, we will assume that $\phi(k,0)$ is a simple function of the form

$$\phi(k,0) = \gamma e^{-\alpha(k-k_o)^2} \tag{3.132}$$

This is a Gaussian function which is peaked (with a maximum value of γ) about the value $k = k_o$ and which has a *width* associated with the constant parameter α. (The size of α determines how faster $\phi(k)$ falls off as k moves away from k_o.) Since the function $\phi(k,0)$ is the probability amplitude for finding a particular value of k (and thus of p) we see that α is a measure of the uncertainty in a measurement of the momentum. We will give a more precise definition of this uncertainty later.

From Parseval's theorem, we know that if the function $\phi(k,0)$ satisfies the normalization condition, then the wave function $\psi(x,0)$ will automatically be normalized. The normalization condition,

$$\int_{-\infty}^{+\infty} \phi^*(k,0)\phi(k,0)dk = 1 \tag{3.133}$$

fixes the area of the function $\phi(k,0)$, and demands that γ and α are related by the equation

$$\gamma = \left[\frac{2\alpha}{\pi}\right]^{1/4} \tag{3.134}$$

Since we may not generally know the functional form of ω (or since it may be very complicated), we will expand $\omega(k)$ about the point $k = k_o$ using a Taylor series:

$$\omega(k) = \omega(k_o) + \left.\frac{\partial\omega}{\partial k}\right|_{k_o} (k-k_o) + \frac{1}{2!}\left.\frac{\partial^2\omega}{\partial k^2}\right|_{k_o} (k-k_o)^2 + \cdots \tag{3.135}$$

This equation will give us good results as long as k is not much different from k_o. Thus, the equation for our wave function having a Gaussian momentum distribution becomes:

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \gamma\, e^{-\alpha(k-k_o)^2}\, e^{i(kx-\omega(k)t)}\, dk \tag{3.136}$$

where the exponential term is given by

$$e^{i(kx-\omega t)} = exp\left\{ i\left[kx - \omega(k_o)t - \left.\frac{\partial\omega}{\partial k}\right|_{k_o} t\,(k-k_o) + \cdots \right.\right.$$
$$\left.\left. - \frac{1}{2!}\left.\frac{\partial^2\omega}{\partial k^2}\right|_{k_o} t\,(k-k_o)^2 + \cdots \right]\right\} \tag{3.137}$$

Where we originally had the term k in our integral equation, we now have the combination $(k - k_o)$ everywhere *except* in the term kx. If we add and subtract the term $k_o x$ in the exponential and group the terms appropriately we will have

$$e^{i(kx-\omega t)} = exp\left\{[+ik_o x] + i\left[(k-k_o)x - \omega_o t - \left.\frac{\partial\omega}{\partial k}\right|_{k_o} t\,(k-k_o) + \cdots \right.\right.$$
$$\left.\left. - \frac{1}{2!}\left.\frac{\partial^2\omega}{\partial k^2}\right|_{k_o} t\,(k-k_o)^2 + \cdots \right]\right\} \tag{3.138}$$

We now introduce the symbols $k' = (k - k_o)$ and $\beta = \frac{1}{2!}\left.\frac{\partial^2\omega}{\partial k^2}\right|_{k_o}$ and write this last expression as

$$e^{i(kx-\omega t)} = exp\left\{ + ik_o x - \omega_o t\right\}$$
$$\times\ exp\left\{ + ik'\left(x - \left.\frac{\partial\omega}{\partial k}\right|_{k_o} t\right) - i\beta k'^2 t + \cdots \right]\right\} \tag{3.139}$$

We recognize the term $(\partial\omega/\partial k)_{k_o}$ as a *velocity* term for this waveform in analogy with the phase velocity of a plane wave. We call this velocity term the *group velocity*. We will see in what follows that the term containing β determines the "spread" in the wave packet as a function of time. [In those cases where $k' = (k - k_o)$ is small, the term with β is very small and quite often negligible.]

With these substitutions, our integral expression becomes

$$\psi(x,t) = \frac{\gamma}{\sqrt{2\pi}}\, e^{i(k_o x - \omega_o t)} \int_{-\infty}^{+\infty} e^{-\alpha k'^2}\, e^{i[k'(x - v_g t) - \beta k'^2 t + \cdots]}\, dk' \tag{3.140}$$

where we have changed the integration variable from $dk \to dk'$ [$= d(k - k_o) = dk$, since k_o is a constant], and where we have factored out the terms γ and $exp\left\{ + ik_o x - \omega_o t\right\}$ which are *not* functions of k'.

We are now in a position to evaluate the integral. The integral can be written in the form of a generalized Gaussian integral (see Appendix 2.C) of order zero

$$J_o = \int_{-\infty}^{+\infty} e^{-ax^2 - bx}\, dx \tag{3.141}$$

where a and b are complex constants. The solution of this integral is

$$J_{\mathrm{o}} = \sqrt{\frac{\pi}{a}}\;\; e^{b^2/4a} \tag{3.142}$$

Therefore, we rewrite our integral representing $\psi(x,t)$ by grouping together powers of k' to obtain

$$\psi(x,t) \;=\; \frac{\gamma}{\sqrt{2\pi}}\, e^{i(k_{\mathrm{o}}x-\omega_{\mathrm{o}}t)} \int_{-\infty}^{+\infty} e^{-[\alpha+i\beta t]\,k'^2-[-i(x-v_g t)]\,k'}\; dk' \tag{3.143}$$

from which we see that $a=[\alpha+i\beta t]$ and $b=[-i(x-v_g t)]$, giving as our solution to the wave function

$$\psi(x,t) \;=\; \frac{\gamma}{\sqrt{2\pi}}\, e^{i(k_{\mathrm{o}}x-\omega_{\mathrm{o}}t)} \left\{ \sqrt{\frac{\pi}{\alpha+i\beta t}}\;\; e^{-(x-v_g t)^2/4[\alpha+i\beta t]} \right\} \tag{3.144}$$

$$\psi(x,t) \;=\; e^{ik_{\mathrm{o}}[x-(\omega_{\mathrm{o}}/k_{\mathrm{o}})t]} \left\{ \frac{\gamma}{\sqrt{2(\alpha+i\beta t)}}\;\; e^{-(x-v_g t)^2/4[\alpha+i\beta t]} \right\} \tag{3.145}$$

Thus, for the special case where $\phi(k)$ is a Gaussian function, peaked around the value $k=k_{\mathrm{o}}$, the traveling wave function corresponding to this looks like a *plane wave* with a *phase* velocity $v_{ph}=\omega_{\mathrm{o}}/k_{\mathrm{o}}$, and with an amplitude given by the expression within the curly brackets, { }. We say that this plane wave is *amplitude modulated*. That is, the amplitude of the sine waves vary with position and time in such a way that we have a Gaussian wave *packet* which moves with a speed given by v_g. The width of this packet as well as its amplitude changes with time, due to the presence of the constant β.

The probability density for finding a particle at a point x at time t is given by the square of the magnitude of $\psi(x,t)$, or $|\psi(x,t)|^2$ which gives

$$P(x,t) = \frac{\gamma^2}{2}\,\frac{1}{\sqrt{\alpha+i\beta t}} \;\times\; \frac{1}{\sqrt{\alpha-i\beta t}}\; exp\left\{ -\,\frac{(x-v_g t)^2}{4(\alpha+i\beta t)} - \frac{(x-v_g t)^2}{4(\alpha-i\beta t)} \right\} \tag{3.146}$$

$$P(x,t) = \frac{\gamma^2/2}{\sqrt{\alpha^2+\beta^2t^2}}\; exp\left\{ -\,\frac{1}{4}(x-v_g t)^2 \left[\frac{1}{\alpha+i\beta t} + \frac{1}{\alpha-i\beta t}\right] \right\} \tag{3.147}$$

$$P(x,t) = \frac{\gamma^2/2}{\sqrt{\alpha^2+\beta^2t^2}}\, exp\left\{ \frac{-\alpha(x-v_gt)^2}{2[\alpha^2+\beta^2t^2]} \right\} \tag{3.148}$$

$$P(x,t) = \frac{\gamma^2/2}{\sqrt{\alpha^2+\beta^2t^2}}\, exp\left\{ -\frac{(x-v_gt)^2}{2[\alpha^2+\beta^2t^2]/\alpha} \right\} \tag{3.149}$$

or, using the normalization condition requirement for γ, we have

$$P(x,t) = \frac{1}{\sqrt{2\pi}\sqrt{[\alpha^2+\beta^2t^2]/\alpha}}\, exp\left\{ -\frac{(x-v_gt)^2}{2[\alpha^2+\beta^2t^2]/\alpha} \right\} \tag{3.150}$$

The equation shows that the probability density is in the form of a Gaussian

$$G(z) = A(\epsilon)\, e^{-z^2/\epsilon} \tag{3.151}$$

The maximum of this function $[A(\epsilon)]$ occurs when $z = 0$. Thus the maximum point of our function occurs when $x - v_gt = 0$, or when $x = v_gt$! This implies that the peak of the probability function travels at a speed equal to the group velocity v_g. In addition, since the Gaussian is symmetric about the point $z = 0$, the *average value of x is the point where $x = v_gt$*!

From this equation we see that *the probability density of finding a particle at a location x at a time t changes as a function of time. The probability density is peaked where z $=$ x $-$ v$_g$t $=$ 0; and thus we see that the peak moves in the positive-x direction with a speed equal to v$_g$. For a "free particle" where $\hbar\omega = \hbar^2k^2/2m$ the group velocity is given by*

$$v_g = \left.\frac{\partial\omega}{\partial k}\right|_{k_o} = \frac{\hbar k_o}{m} = \frac{p_o}{m} \tag{3.152}$$

which is the classical velocity of a free particle!

Problem 3.5 For surface tension waves in shallow water, the relation between frequency and wavelength is given by

$$\nu = \sqrt{\frac{2\pi T}{\rho\lambda^3}}$$

where T is the surface tension and ρ is the density. Determine the phase velocity and the group velocity for these surface tension waves.

The width of a Gaussian can be determined by noticing that the Gaussian function decreases to $1/e$ of its maximum value when $z^2/\epsilon = 1$, or when $z = \pm\sqrt{\epsilon}$. Thus, the full width of the Gaussian is given by the equation

$$\delta z = 2\ \sqrt{\epsilon} = 2\sqrt{2(\alpha^2 + \beta^2 t^2)/\alpha} \tag{3.153}$$

which varies as a function of time, getting wider *as time progresses in either the positive or negative direction*! We see that the width of the peak depends upon α, a function of the original width of the function $\phi(k)$, and upon β. [We have used the symbol δx for the width of the function x to differentiate it from the more precise definition of the uncertainty of a measurement Δx, which we will discuss in more detail later.]

At time $t = 0$, the width is a *minimum,* and is given by

$$\delta z_{\text{o}} = 2\sqrt{2\alpha} \tag{3.154}$$

[Notice that this is the width which the 'packet' would maintain if $\beta = 0$.] Now α is a measure of the width of the momentum distribution function $\phi(k)$,

$$\phi(k) = \gamma\ e^{-\alpha(k-k_{\text{o}})^2} = \gamma e^{-k'^2/(1/\alpha)} \tag{3.155}$$

From what we have just done, we see that the width of that function is given by

$$\delta k' = \delta k = 2\sqrt{1/\alpha} \tag{3.156}$$

which gives

$$\delta k \times \delta z_{\text{o}} = 2\sqrt{1/\alpha}\ \times\ 2\sqrt{2\alpha}\ =\ 4\sqrt{2} \tag{3.157}$$

and we see that if δk is large, then δz_{o} is small, and vise versa!

A more precise definition of the uncertainty in x, which we will designate by Δx, is given by the *root-mean square* (rms) *deviation from the mean*, or

$$\Delta x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle} \tag{3.158}$$

which can also be written as

$$\Delta x^2 = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 \tag{3.159}$$

Since we understand $\psi(x,t)$ to be the probability amplitude, and $\mid \psi(x,t) \mid^2$ to be the probability density, then we know that the *average* of any function $f(x)$ is given by

$$\langle f(x) \rangle = \int_{-\infty}^{+\infty} f(x)\ \psi^*(x,t)\psi(x,t)\ dx = \int_{-\infty}^{+\infty} f(x)\ P(x,t)\ dx \tag{3.160}$$

which gives, for the uncertainty in x,

$$\Delta x = \quad \left[\int_{-\infty}^{+\infty} (x - x_{\text{o}})^2 P(x,t) dx \right]^{1/2} \tag{3.161}$$

Since the probability density for the location of our particle, $P(x,t)$, is symmetric about the peak, the average of x is just the peak value, i.e., the value where $x = v_g t$. Thus, $x_o = v_g t$, so that we can write $P(x,t)$ as

$$\begin{aligned} P(x,t) &= \frac{1}{\sqrt{2\pi}\sqrt{[\alpha^2+\beta^2t^2]/\alpha}}\, exp\left\{ -\frac{(x-v_gt)^2}{2[\alpha^2+\beta^2t^2]/\alpha} \right\} \\ &= A(\epsilon)e^{-(x-x_o)^2/\epsilon} \end{aligned} \tag{3.162}$$

where

$$A(\epsilon) = \frac{1}{\sqrt{2\pi}\sqrt{[\alpha^2+\beta^2t^2]/\alpha}} \tag{3.163}$$

and

$$\epsilon = 2[\alpha^2+\beta^2t^2]/\alpha \tag{3.164}$$

Now we are in a position to evaluate the uncertainty in x:

$$\Delta x = \left[A(\epsilon)\int_{-\infty}^{+\infty} (x-x_o)^2 e^{-(x-x_o)^2/\epsilon} dx \right]^{1/2} \tag{3.165}$$

$$\Delta x = \left[A(\epsilon)\int_{-\infty}^{+\infty} z^2 e^{-(1/\epsilon)z^2} dz \right]^{1/2} \tag{3.166}$$

which is a Gaussian integral and can easily be evaluated to give

$$\Delta x = \left[A(\epsilon)\,\frac{1}{2}\,\sqrt{\pi}\,(1/\epsilon)^{-3/2} \right]^{1/2} \tag{3.167}$$

or, plugging in for $A(\epsilon)$ and ϵ

$$\Delta x = \left[\frac{1}{\sqrt{2\pi}\sqrt{[\alpha^2+\beta^2t^2]/\alpha}}\,\frac{\sqrt{\pi}}{2}\,\left[\frac{1}{2[\alpha^2+\beta^2t^2]/\alpha}\right]^{-3/2} \right]^{1/2} \tag{3.168}$$

$$\Delta x = \left\{ \left[\frac{1}{2[\alpha^2+\beta^2t^2]/\alpha}\right]^{1/2} \frac{1}{2} \left[\frac{1}{2[\alpha^2+\beta^2t^2]/\alpha}\right]^{-3/2} \right\}^{1/2} \tag{3.169}$$

or

$$\boxed{\Delta x = \sqrt{\frac{[\alpha^2+\beta^2t^2]}{\alpha}}} \tag{3.170}$$

This is the expression for any arbitrary time t, *but for the special case where* $t = 0$*,* it reduces to

$$\boxed{\Delta x_o = \sqrt{\alpha} \qquad (3.171)}$$

where the subscript denotes that this is for time $t = 0$.

If we consider a traveling wavepacket, the width of that packet can be expressed as

$$\Delta x = \sqrt{\frac{[\Delta x_o^4 + \beta^2 t^2]}{\Delta x_o^2}} = \Delta x_o \sqrt{1 + \frac{\beta^2 t^2}{\Delta x_o^4}} \tag{3.172}$$

The relative spread of the wavepacket, then, is given by

$$\frac{\Delta x}{\Delta x_o} = \sqrt{1 + \frac{\beta^2 t^2}{\Delta x_o^4}} \tag{3.173}$$

For cases where βt is very small relative to the original width of the wavepacket, the spread of the wavepacket is negligible.

We determine Δk in the same way beginning with

$$\Delta k = \left[\int_{-\infty}^{+\infty} (k - k_o)^2 \mid \phi(k,t) \mid {}^2 dk \right]^{1/2} \tag{3.174}$$

where

$$\mid \phi(k,t) \mid {}^2 = \gamma^2 e^{-2\alpha(k-k_o)^2} = \sqrt{2\alpha/\pi}\, e^{-2\alpha(k-k_o)^2} \tag{3.175}$$

Notice that the time dependence in $\phi(k,t)$ cancels, so that the uncertainty in momentum is time independent! The uncertainty in k then becomes

$$\Delta k = \left[\sqrt{2\alpha/\pi} \int_{-\infty}^{+\infty} (k - k_o)^2 e^{-2\alpha(k-k_o)^2} dk \right]^{1/2} \tag{3.176}$$

or

$$\Delta k = \left[\sqrt{2\alpha/\pi} \int_{-\infty}^{+\infty} z^2 e^{-2\alpha z^2} dz \right]^{1/2} \tag{3.177}$$

which evaluates to give

$$\Delta k = \left[\sqrt{2\alpha/\pi}\, \frac{1}{2}\, \sqrt{\pi}\, (2\alpha)^{-3/2} \right]^{1/2} \tag{3.178}$$

or,

$$\boxed{\Delta k = \frac{1}{2\sqrt{\alpha}}} \tag{3.179}$$

and, utilizing our previous result of $\Delta x_o = \sqrt{\alpha}$, we have the Heisenberg uncertainty relation

$$\boxed{\Delta k_o \Delta x_o = \tfrac{1}{2}} \tag{3.180}$$

where the subscripts denote the uncertainties at time $t = 0$. If we write this in terms of the momentum, we have and relation

$$\boxed{\Delta p_o \Delta x_o = \frac{\hbar}{2}} \tag{3.181}$$

At any time other than $t = 0$ the position distribution function is wider than at $t = 0$, so that the general Heisenberg uncertainty principle becomes

$$\Delta p \Delta x \geq \frac{\hbar}{2} \tag{3.182}$$

where the equality holds *only for the minimum width of* <u>*Gaussian*</u> *wave packets.*

Problem 3.6 Radioactive materials typically emit electrons in the energy range of 1-10 MeV. The energies of electrons which orbit the nucleus are typically in the energy range of 10's of eV or less. In the early days of nuclear physics many scientist thought that these high-energy electrons were somehow “trapped” in the unstable nuclei associated with radioactive decay. Show that the Heisenberg uncertainty condition rules out the possibility that electrons can exist within a nucleus of the size of 10^{-14} m. Thus, the electrons are somehow “produced” when a proton changes to a neutron, or vice versa.

The fact that $P(x,t)$ is a function which spreads out in time indicates the necessity of interpreting this as a probability function. The particle itself does not get **larger** in time, but rather **the ability to predict where the particle will be at a later time** changes with time such that the uncertainty in location of the particle increases with time!

Since the spreading of the wave packet with time is not a classical phenomenon, this spreading in the probability function must remain very small for macroscopic objects even for long periods of time (for example the orbits of the planets are very well known). In order to get a better understanding of the nature of the spreading we will look again at the source of the spreading. The spreading is a result of the presence of the constant β in the exponential which arises in the expansion of $\omega(k)$. If the part of $\psi(x,t)$ which contained this term were small enough to be ignored, there would be no appreciable spreading. Thus if the term

$$\beta {k'}^2 t = \frac{1}{2!} \left.\frac{\partial^2 \omega}{\partial k^2}\right|_{k_o} (k - k_o)^2 \, t \ll 1 \tag{3.183}$$

then there will be no appreciable spreading. One way of looking at this is to ask how long the system can progress before the spreading becomes significant. This would mean that the time during which the system is being observed must be such that

$$t \ll t_o = \left[\frac{1}{2!} \left. \frac{\partial^2 \omega}{\partial k^2} \right|_{k_o} (k - k_o)^2 \right]^{-1} \tag{3.184}$$

where t_o is the characteristic time for spreading of the wave packet. Let's see what this means for classical (non-relativistic) particles in potential-free regions of space. In this case we have

$$E = \frac{p^2}{2m} \;\Rightarrow\; \hbar\omega = \frac{\hbar^2 k^2}{2m} \;\Rightarrow\; \omega = \frac{\hbar k^2}{2m} \tag{3.185}$$

from which we can obtain the group velocity

$$v_g = \frac{d\omega}{dk} = \frac{\hbar k}{m} = \frac{p}{m} = v_{\text{particle}} \tag{3.186}$$

and

$$\beta = \frac{1}{2!} \left. \frac{\partial^2 \omega}{\partial k^2} \right|_{k_o} = \frac{\hbar}{2m} \tag{3.187}$$

or, since $k = p/\hbar$,

$$t_o = \left[\frac{1}{2!} \left. \frac{\partial^2 \omega}{\partial k^2} \right|_{k_o} (k - k_o)^2 \right]^{-1} = \left[\frac{\hbar}{2m} \frac{(p - p_o)^2}{\hbar^2} \right]^{-1} = \left[\frac{(p - p_o)^2}{2m\hbar} \right]^{-1} \tag{3.188}$$

Thus, we have for a free particle

$$t_o = \frac{2m\hbar}{(p - p_o)^2} = \frac{2m\hbar}{(\Delta p)^2} \tag{3.189}$$

where we interpret t_o in an *average* sense and so use the uncertainty in p as determined from the momentum distribution. This last equation can be written in two revealing forms:

(1) in terms of the energy, since $p^2/2m = E$

$$t_o = \frac{\hbar}{(\Delta p)^2/2m} = \frac{\hbar}{\Delta E} \tag{3.190}$$

(2) in terms of the initial uncertainty in position, using the approximate uncertainty principle $\Delta p \Delta x \geq \hbar/2$

$$t_o = \frac{2m\hbar}{(\Delta p)^2} \;\Rightarrow\; t_o \leq \frac{2m\hbar}{(\hbar/2\Delta x)^2} = \frac{2m(2\Delta x)^2}{\hbar} = \frac{8m(\Delta x)^2}{\hbar} \tag{3.191}$$

Let's see how this works out for a couple of simple examples. If we attempt to determine the location of a small 1 mg object to an uncertainty of 1 millimeter (1×10^{-3} meters), then

$$t_o = \frac{8(1 \times 10^{-6}\, kg)(1 \times 10^{-3}\, m)^2}{1.055 \times 10^{-34}\, J - sec} = 7.583 \times 10^{22} \text{ seconds}$$

This means that no significant spreading of the wave packet would occur for this situation within the lifetime of the universe! (One year is 3.156×10^7 seconds, and the age of the universe is estimated to be about 15 billion years old, so that the age of the universe in seconds is approzimately 4.734×10^{17} seconds.) However, if we attempted to locate *an electron* with a similar precision, then

$$t_o = \frac{8(9.11 \times 10^{-31}\, kg)(1 \times 10^{-3}\, m)^2}{1.055 \times 10^{-34}\, J - sec} = 6.908 \times 10^{-2} \text{ seconds}$$

This means that there would be no significant spreading of the wave packet within about 70 milliseconds. If we try to locate an electron to within the dimensions of an atom, we obtain

$$t_o = \frac{8(9.11 \times 10^{-31}\, kg)(1 \times 10^{-10}\, m)^2}{1.055 \times 10^{-34}\, J - sec} = 6.908 \times 10^{-16} \text{ seconds}$$

and significant spreading is seen to occur almost instantaneously.

Problem 3.7 A beam of electons is to be fired over a distance of 10^4 km. If the size of the initial packet is 10^{-3}m, what will be its size upon arrival, if its kinetic energy is (a) 13.6 eV; (b) 100 MeV? [Remember that the relationship between the kinetic energy and the momentum is not given by $p^2/2m$ for a relativistic particle.]
