1 Group Velocity

In quantum mechanics we deal with plane waves that are expressed as complex exponentials rather than sines and cosines. We first explain the mathematics of complex exponentials and Fourier transforms. We then go on to the idea of group velocity, which is the velocity at which a wave packet moves. We end with the definition of a special function of great importance in quantum mechanics called the Dirac delta function.

1.1 Mathematical Interlude

1.1.1 Euler's Equation

An important mathematical result is that

$$\exp(i\phi) = \cos(\phi) + i\sin(\phi). \tag{1}$$

This is called Euler's equation and may be demonstrated by comparing the Taylor expansions of both sides term by term. The Taylor expansion of the complex exponential is

$$\exp(i\phi) = 1 + (i\phi) + (i\phi)^2/2 + (i\phi)^3/6\ldots = 1 - \phi^2/2 + i(\phi - \phi^3/6)\ldots \tag{2}$$

which upon comparison with

$$\cos(\phi) = 1 - \phi^2/2\ldots \tag{3}$$

and

$$\sin(\phi) = \phi - \phi^3/6\ldots \tag{4}$$

shows that equation 1 is true. It is easy to show from equation 1 that

$$\cos\phi = \frac{\exp(i\phi) + \exp(-i\phi)}{2} \tag{5}$$

and

$$\sin\phi = \frac{\exp(i\phi) - \exp(-i\phi)}{2i}. \tag{6}$$

1.1.2 Fourier Transform

In this section we extend the ordinary Fourier series representation of a function in two ways, first by converting it into a series of complex exponentials, second by making it cover an infinite domain.

The ordinary Fourier series representation of a function $f(x)$ which is defined over $-L/2 \leq x \leq L/2$ is

$$f(x) = A_0 + \sum_{m=1}^{\infty} [A_m \cos(2\pi mx/L) + B_m \sin(2\pi mx/L)], \tag{7}$$

where the A_i and B_i are constants which depend on the form of the function. This representation turns out to be equivalent to

$$f(x) = \sum_{m=-\infty}^{\infty} C_m \exp(2\pi imx/L), \tag{8}$$

where $i = (-1)^{1/2}$ and the C_i form a possibly complex set of constants.

Equation (8) may be written

$$f(x) = C_0 + \sum_{m=1}^{\infty} [C_m \exp(2\pi imx/L) + C_{-m} \exp(-2\pi imx/L)]. \tag{9}$$

Using Euler's equation, this may be rewritten

$$\begin{aligned} f(x) = C_0 \quad + & \sum_{m=1}^{\infty} [(C_m + C_{-m}) \cos(2\pi mx/L) \\ & +i(C_m - C_{-m}) \sin(2\pi mx/L)]. \end{aligned} \tag{10}$$

This is equivalent to the ordinary Fourier series if we identify $A_0 = C_0$, $A_m = C_m + C_{-m}$, and $B_m = i(C_m - C_{-m})$.

The inverse transformation may be obtained by multiplying equation (8) by $\exp(-2\pi inx/L)$ and integrating over the domain $[-L/2, L/2]$. All terms in the sum are zero after integration except $m = n$, which means that we can solve the result for C_n:

$$C_n = \frac{1}{L} \int_{-L/2}^{L/2} f(x) \exp(-2\pi inx/L) dx. \tag{11}$$

We now redefine C_m in preparation for extension to an infinite domain. We first define $k_n = 2\pi n/L$ and $\Delta k = 2\pi/L$. We then write $\tilde{f}(k_m) =$

$(2\pi)^{1/2}C_m/\Delta k$, so that equations (8) and (11) become

$$f(x) = \frac{1}{(2\pi)^{1/2}} \sum_{m=-\infty}^{\infty} \tilde{f}(k_m) \exp(ik_m x)\Delta k \tag{12}$$

and

$$\tilde{f}(k_n) = \frac{1}{(2\pi)^{1/2}} \int_{-L/2}^{L/2} f(x) \exp(-ik_n x) dx. \tag{13}$$

Finally, we let $L \to \infty$ so that the difference Δk becomes the differential dk and the sum in equation (12) becomes an integral:

$$f(x) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} \tilde{f}(k) \exp(ikx) dk \tag{14}$$

and

$$\tilde{f}(k) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} f(x) \exp(-ikx) dx. \tag{15}$$

These equations are respectively the *inverse and forward Fourier transforms.* They show that any waveform can be expressed as a superposition of complex exponential plane waves. The parameter k is just the wavenumber, i. e., 2π over the wavelength, associated with each wave.

1.2 Plane Waves and Wave Packets

In quantum mechanics we must represent a plane wave by a complex exponential function rather than by a sine or a cosine. Thus,

$$\psi = \exp[i(kx - \omega t)] \tag{16}$$

represents the probability amplitude for a particle of definite wavenumber k and angular frequency ω. The phase speed of this wave is $v_\phi = \omega/k$. Notice that the probability of finding this particle at any point in space is $P = |\psi|^2 = 1$ — i. e., there is equal probability of finding the particle anywhere in the universe.

Quantum mechanical waves obey the *superposition principle*, i. e., if ψ_A and ψ_B are solutions to the quantum mechanical governing equations, then so is the arbitrary linear combination $A\psi_A + B\psi_B$, where A and B are constants.

Let us see what happens when two waves with slightly different wavenumber and angular frequency are added together. Suppose $\omega_{1,2} = \omega \pm \Delta\omega$ and $k_{1,2} = k \pm \Delta k$. The sum of these two waves becomes

$$\begin{aligned} \psi &= \exp[i(kx + \Delta kx - \omega t - \Delta\omega t)] + \exp[i(kx - \Delta kx - \omega t + \Delta\omega t)] \\ &= \exp[i(kx - \omega t)] \{\exp[i(\Delta kx - \Delta\omega t)] + \exp[-i(\Delta kx - \Delta\omega t)]\} \\ &= 2\exp[i(kx - \omega t)] \cos(\Delta kx - \Delta\omega t), \end{aligned} \tag{17}$$

and the probability distribution is

$$P = |\psi^2| = 4\cos^2(\Delta kx - \Delta\omega t). \tag{18}$$

Constructive and destructive interference between these two waves results in a pattern of peaks and valleys in the probability distribution. The peaks are called *wave packets*, and they move with a speed called the *group velocity*,

$$u = \frac{\Delta\omega}{\Delta k} \to \frac{d\omega}{dk}, \tag{19}$$

where in the rightmost expression we have taken the limit as Δk becomes very small.

Figure 1 shows the results of adding two sine waves together of slightly differing wavenumber. This isn't precisely the same as adding two complex exponentials, but is close enough for the purposes of illustration. Notice that the amplitude of the sum varies systematically with the phase relationship between the two waves, resulting in a series of wave packets, as described above.

In this example we have added only two plane waves together. If many waves of different wavelength and frequency are added together with the right amplitude and phase, one can obtain an isolated wave packet rather than the sequence of wave packets that we see here. Figure 2 shows an example in which 9 sine waves have been added together with wavenumbers ranging from 0.8 to 1.2

Physically, the wave packet represents a particle whose location has been restricted to some finite region, and the group velocity is the velocity with which this region moves. The group velocity depends on the functional relationship between the angular frequency and the wavenumber. For historical reasons this relationship is called the *dispersion relation*. Note that the phase and group velocities are only equal when the relationship between the frequency and wavenumber takes the form $\omega = v_\phi k$.

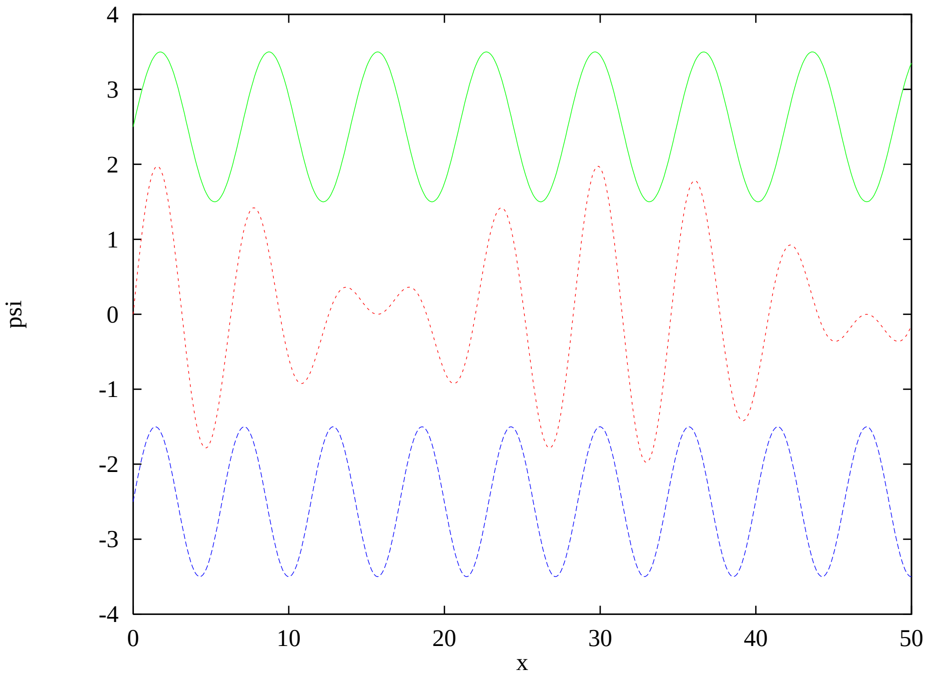

Figure 1: Example of adding two sine waves, the upper with $k = 0.9$ and the lower with $k = 1.1$. The middle plot shows the sum of the two.

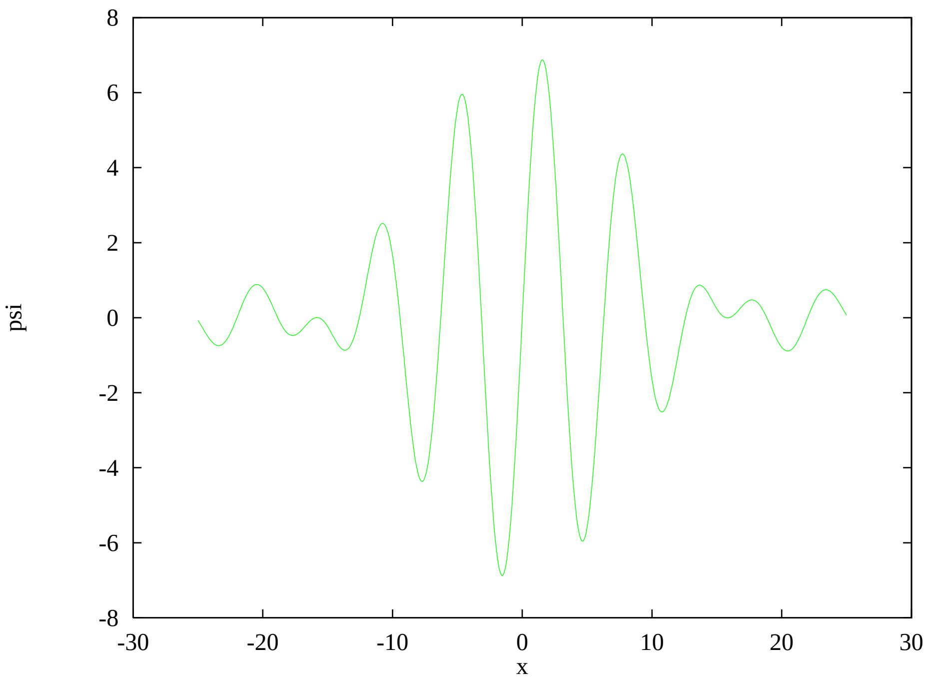

Figure 2: Example of adding nine sine waves with wavenumbers ranging from 0.8 to 1.2.

1.3 Integral Representation of a Wave Packet and Dirac Delta Function

We can represent a wave packet analytically as a superposition of an infinite number of plane waves by replacing the sum by an integral:

$$\psi(x,t) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} \phi(k) \exp[i(kx - \omega t)] dk. \tag{20}$$

If $\phi(k)$ doesn't oscillate rapidly, but has a peak at $k = k_0$ and approaches zero for larger and smaller values of k, we can estimate the group velocity in another way. Under these conditions the complex exponential in the integrand of equation (20) oscillates rapidly for most values of k. This oscillation causes the contribution of these regions to the integral to be small, because the positive and negative phases of the integrand tend to cancel. The only place where this isn't true is where the oscillation of the integrand isn't very rapid. This occurs near the point where

$$\frac{\partial}{\partial k}(kx - \omega t) = 0. \tag{21}$$

Expanding and rearranging this yields the condition

$$\left.\frac{\partial \omega}{\partial k}\right|_{k=k_0} = \frac{x}{t}. \tag{22}$$

The integral is the largest when this minimum in the oscillation of the complex exponential occurs near the peak in $\phi(k)$, which is why we have imposed the condition $k = k_0$.

The above result tells us that the wave packet $\psi(x,t)$ has the largest amplitude where $x = (\partial\omega/\partial k)_{k=k_0} t$, which simply indicates that the wave packet moves at velocity $(\partial\omega/\partial k)_{k=k_0}$. However, this is precisely the previously defined group velocity.

At time $t = 0$ equation (20) reduces to an ordinary inverse Fourier transform

$$\psi(x,0) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} \phi(k) \exp(ikx) dk, \tag{23}$$

which has an associated forward transform

$$\phi(k) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} \psi(x,0) \exp(-ikx) dx. \tag{24}$$

Substituting this into equation (20) and replacing x by x' to avoid confusion, we obtain

$$\psi(x,t) = \int_{-\infty}^{\infty} \left(\frac{1}{2\pi} \int_{-\infty}^{\infty} \psi(x',0) \exp(-ikx') dx' \right) \exp[i(kx - \omega t)] dk. \quad (25)$$

By interchanging the order of integration, we come up with an equation for $\psi(x,t)$ in terms of $\psi(x,0)$ and a function $K(x,t)$ which is independent of ψ:

$$\psi(x,t) = \int_{-\infty}^{\infty} K(x - x', t) \psi(x', 0) dx', \quad (26)$$

where

$$K(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp[ikx - i\omega(k)t] dk. \quad (27)$$

This function, called the *propagator*, depends only on the dispersion relation for the waves, $\omega(k)$, and contains all information needed to compute the evolution of a wave packet from its initial state at time $t = 0$ to an arbitrary time in the future.

For $t = 0$, K has a special behavior. At zero time we formally have

$$K(x,0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp(ikx). \quad (28)$$

This integral is undefined, which means that the interchange of the order of integration we made to obtain the propagator isn't mathematically justified. However, a sleazy mathematical trick allows us to obtain a definite value of K under these circumstances. If we replace ikx by $ikx - \epsilon|k|$, where ϵ is a small constant, then the integral in equation (28) becomes well defined and takes on the value $\epsilon/[\pi(x^2 + \epsilon^2)]$. This is plotted as a function of x for various values of ϵ in figure 3. Notice that as $\epsilon \to 0$, this function approaches zero everywhere except at $x = 0$, where it approaches infinity. Furthermore, notice that the x integral of the function is unity for all values of ϵ. In the limit as $\epsilon \to 0$ this function has a special name — it is called the *Dirac delta function*, written $\delta(x)$. Thus, for $t = 0$ we have $K(x,0) = \delta(x)$.

Let us return to equation (26) and set $t = 0$. We have

$$\psi(x,0) = \int_{-\infty}^{\infty} \delta(x - x') \psi(x', 0) dx'. \quad (29)$$

Thus, convoluting a Dirac delta function with any other function returns the original function back again. How does this work? Since the delta function

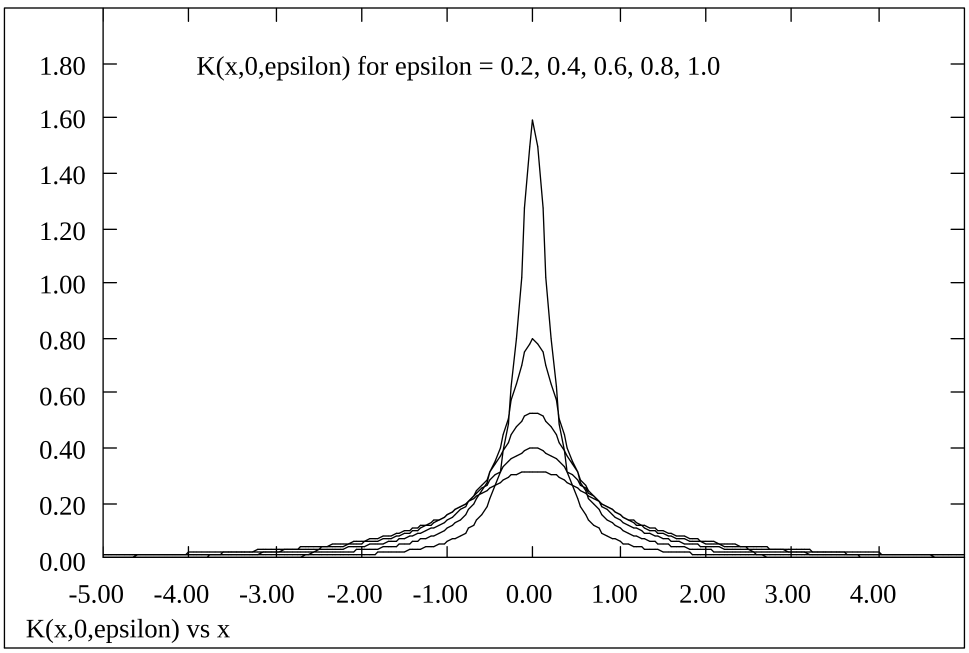

Figure 3: Plot of $\epsilon/[\pi(x^2+\epsilon^2)]$ for various values of ϵ. The smallest value of ϵ yields the highest peak.

$\delta(x - x')$ is zero everywhere except at $x' = x$, we can rewrite the above equation by substituting x for x' in $\psi(x', 0)$. This function becomes a constant as far as the integration goes, and it may therefore be extracted from the integral. Thus,

$$\psi(x, 0) = \psi(x, 0) \int_{-\infty}^{\infty} \delta(x - x') dx' = \psi(x, 0), \tag{30}$$

where the last step is justified because the integral of the Dirac delta function is unity.

Though the above analysis is slipshod, there exists a mathematically sound theory of functions such as the Dirac delta function, and all of the above results can be rigorously justified as long as $\psi(x', 0)$ is reasonably smooth.