Free particle waves

So, we have confirmed the idea that matter behaves like waves, but what is the nature of these waves, and how do we describe them. Let’s begin with a free particle, that is, a particle moving in one dimension with no force acting on it, therefore with no potential changes. We start by writing a function that will describe the dynamics of the wave, what we will henceforth refer to as the wavefunction:

$$\Psi(x, t) = \sin(kx - \omega t)$$

This function describes an oscillating wave with wavelength $$\lambda = 2\pi/k$$ and frequency $$\nu = \omega/2\pi$$. Let us try to extract the dynamics of the particle from this function. There are zeros of this function whenever $$(kx-\omega t)=\pi n$$ or whenever $$x_n=\pi n/k+\omega t/k$$. The velocity of these zeros is $$v = \frac{d}{dt}(x_n) = \frac{\omega}{k} = \frac{2\pi\nu}{2\pi/\lambda} = \nu\lambda$$ as we expect for the relationship between the velocity, wavelength and frequency.

But, let’s now go back to the de Broglie relationship between the wavelength and momentum, and the Einstein relationship between the energy and the frequency: $$p = \frac{h}{\lambda}$$ and $$E = h\nu$$. Then $$\nu\lambda = (E/h)(h/p) = E/p = (\frac{1}{2})mv^2/mv = \frac{1}{2}v$$. This gives us the puzzling result that the group velocity (the velocity of the group of waves) is $$\frac{1}{2}$$ of the particle velocity!? So, how can we reasonable describe the particle with such a wavefunction? Well, there is another problem with the wavefunction that we initially chose, that is that there is no defined spatial extent. There are an infinite number of zeros, or, if we choose, an infinite number of maxima. So it would be a stretch to call this a particle wavefunction – something that intuitively we would expect to describe a localized particle moving with velocity $$v$$.

We make one step towards creating a wave packet. Let’s look at the sum of two wavefunctions, one with a slightly different wavelength and frequency:

$$\Psi(x, t) = \Psi_1(x, t) + \Psi_2(x, t)$$

$$\Psi_1(x, t) = \sin(kx - \omega t)$$

$$\Psi_2(x, t) = \sin((k + dk)x - (\omega + d\omega)t)$$

using $$\sin A + \sin B = 2\cos[(A-B)/2]\sin[(A+B)/2]$$, then

$$\Psi(x, t) = 2\cos\left(\frac{dk}{2}x - \frac{d\omega}{2}t\right)\sin\left(\frac{2k + dk}{2}x - \frac{2\omega + d\omega}{2}t\right)$$

$$= 2\cos\left(\frac{dk}{2}x - \frac{d\omega}{2}t\right)\sin(kx - \omega t)$$

where the last step is a simplification from the fact that $$d\omega<<2\omega$$ and $$dk<<2k$$. Looking at this wavefunction, we can see that it is the same sin function, moderated by a changing
amplitude (cos function). From the figure below we see now larger “packets of waves” with wavelengths \(1/\kappa\) moving with velocity \(g = d\omega/d\kappa\).

So, now we have two distinct velocities for the wavefunction: 1) the wave velocity \(w = \omega/k\), and 2) the group velocity \(g = d\omega/d\kappa\). If we now return to the de Broglie relationships: \(\omega = 2\pi E/h\) and \(k = 2\pi/\lambda = 2\pi p/h\), then \(d\omega = 2\pi dE/h\) and \(dk = 2\pi dp/h\). This gives us for the group velocity, \(g = d\omega/dk = dE/dp\). Using \(E = mv^2/2\) and \(p = mv\), \(dE = mv dv\) and \(dp = mv dv\) or, \(dE/dp = v\).

OK, so now we have that the group velocity for the wavefunction is the same as the particle velocity, but what about localization? We still have an infinite number of these “groups” moving at \(v\). The next step we make is to sum more waves together. The figure below shows seven different waves with different \(\kappa (k/2\pi) = 9, 10 \ldots 15\). The amplitude and phase of each wave has been chosen such that all the waves are in phase at \(x = 0\) and that the sum of all the waves \(\Psi = \sum_k \Psi_k\) (shown at the bottom) gives a packet of particular width and shape. Notice that there is still a repeated pattern at the right side of the plot of the sum.
If we were to extend this process using the exact same k-range (i.e. \( k = 9-15 \)) but with a greater number of k values (say, \( k = 9, 9.5, 10, 10.5, \ldots 14.5, 15 \)) one would find that the width of the packet centered around \( x = 0 \) would remain the same, but the distance between the repeated patterns would increase, and the amplitude of the oscillations between the repeated patterns would diminish. We could continue this process of subdividing the k-space and adding waves and we will find that as the number of waves in this interval goes to infinity, the number of packets that are left goes to one. Instead of a sum of waves, we could now write this as an integral:

\[
Ψ(x, t) = \int_{-\infty}^{\infty} \phi(k) \sin(\omega t - \omega t) dk
\]

where \( \phi(k) \) now represents the relative amplitude of the waves in the integral.

OK, so now we have a wavefunction that is localized (is non-zero over a limited x-range), travels with a group velocity equal to that of a moving particle, \( v \). But we have arrived at this wave description at a price. In order to make the packet spatial dimension increasingly small, we must increase the range of the k-values that we include. Hence, if we want a localized wave packet around some very small x-value \( a \) (in the figure below), then we must include a large range in the wave number \( k \). Hence, if we make many measurements of the position, \( x \), we find a small uncertainty, whereas if we make the same measurements in the momentum (related to the wave number by the de Broglie relationships), we find a large uncertainty. This is a direct consequence of wave mechanics.

Conversely, if we don’t limit the position of the particle (read: packet), then the wavenumbers will cover a limited range and the uncertainty in \( x \) will be large, with the corresponding uncertainty in momentum small. This is the basis for the Heisenberg Uncertainty Principle which we will discuss in more detail later.
There is one additional novelty that comes with the wave nature of our treatment of particles. Since we have many wave numbers now in our packet, the evolution of this wave packet with time is not what we might expect for a classical particle. Even though at some time we have a narrow wave packet, the spread in momentum will cause the packet to grow with time.

We will return to the free particle later, once we have a better understanding of what exactly we mean when we talk about “particle waves”.