A Propagating Wave Packet – The Group Velocity

Overview and Motivation: Last time we looked at a solution to the Schrödinger equation (SE) with an initial condition $\psi(x,0)$ that corresponds to a particle initially localized near the origin. We saw that $\psi(x,t)$ broadens as a function of time, indicating that the particle becomes more delocalized with time, but with an average position that remains at the origin. To extend that discussion of a localized wave (packet) here we look at a propagating wave packet. The two key things that we will discuss are the velocity of the wave packet (this lecture) and its spreading as a function of time (next lecture). As we shall see, both of these quantities are intimately related to the dispersion relation $\omega(k)$. This discussion has applications whenever we have localized, propagating waves, including solutions to the SE and the wave equation (WE).

Key Mathematics: Taylor series expansion of the dispersion relation $\omega(k)$ will be central in understanding how the dispersion relation is related to the properties of a propagating wave packet. The Fourier transform is again key because the localized wave packet will be described as a linear combination of harmonic waves.

I. A Propagating Schrödinger-Equation Wave Packet

In the last lecture we found the formal solution to the initial value problem for the free particle SE, which can be written as

$$\psi(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dk\,C(k)\,e^{i[kx-\omega(k)t]}, \tag{1}$$

where the coefficients $C(k)$ are the Fourier transform of the initial condition $\psi(x,0)$,

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

and the dispersion relation (for the SE) is given by

$$\omega(k)=\frac{\hbar k^2}{2m}. \tag{3}$$

The example that we previously considered was for the initial condition

$$\psi(x,0)=\psi_0 e^{-x^2/\sigma^2}. \tag{4}$$

We saw that for increasing positive time $\psi(x,t)$ becomes broader (vs x), but its average position remains at the origin. So, *on average* the particle is motionless, but there is increasing probability that it will be found further away from the origin as t increases.

So you might ask, what initial condition would describe a particle initially localized at the origin, but propagating with some average velocity? Well, here is one answer:

$$\psi(x,0) = \psi_0 e^{ik_0 x} e^{-x^2/\sigma^2} . \tag{5}$$

As will be demonstrated below, you may think of k_0 as some average wave vector (or momentum $\hbar k_0$ through deBroglie's relation $p = \hbar k$) associated with the state $\psi(x,t)$.

As we did in the last lecture, let's find an expression for $\psi(x,t)$. We start by using Eq. (2) to calculate $C(k)$, so we have

$$C(k) = \frac{\psi_0}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, e^{-x^2/\sigma^2} \; e^{-i(k-k_0)x} . \tag{6}$$

This almost looks like the Fourier transform of a Gaussian, which we can calculate.[1] Indeed, we can make it be the Fourier transform of a Gaussian if define the variable $k' = k - k_0$, so that the rhs of Eq. (6) becomes

$$\frac{\psi_0}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, e^{-x^2/\sigma^2} \; e^{-ik'x} . \tag{7}$$

This equals the Gaussian (in the variable k')

$$\frac{\psi_0 \sigma}{\sqrt{2}} e^{-k'^2 \sigma^2/4} , \tag{8}$$

and now reusing the relation $k' = k - k_0$ we can write

$$C(k) = \frac{\psi_0 \sigma}{\sqrt{2}} e^{-(k-k_0)^2 \sigma^2/4} . \tag{9}$$

[1] As we stated in the last lecture, the Fourier transform of the Gaussian e^{-x^2/σ^2} is another Gaussian $\frac{\sigma}{\sqrt{2}} e^{-k^2\sigma^2/4}$.

Note that if $k_0 = 0$, then we obtain $C(k) = \left(\psi_0\sigma/\sqrt{2}\right)e^{-k^2\sigma^2/4}$, the result from the last lecture.

Equation (9) tells us several important things. Recall that we are describing the state $\psi(x,t)$ as a linear combination of normal-mode traveling-wave states $e^{i[kx-\omega(k)t]}$, each of which is characterized by the wavevector $k = 2\pi/\lambda$ and phase velocity $v_{ph} = \omega(k)/k = \hbar k/2m$. As Eq. (1) indicates, the function $C(k)$ is the amplitude (or coefficient) associated with the state with wavevector k. As Eq. (9) indicates, the coefficients $C(k)$ are described by a Gaussian centered at the wave vector k_0. Thus, you may think of the state $\psi(x,t)$ as being characterized by an average wave vector k_0. The width of the function $C(k)$, with width parameter $2/\sigma$, is also key to describing the state $\psi(x,t)$. Because this width parameter is inversely proportional to the localization (characterized by σ) of the initial wave function $\psi(x,0)$, we see that a more localized wave function $\psi(x,0)$ requires a broader distribution (characterized by $2/\sigma$) of (normal-mode) states in order to describe it. Insofar as momentum is equal to $\hbar k$, this inverse relationship between the widths of $\psi(x,0)$ and $C(k)$ is the essence