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')

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

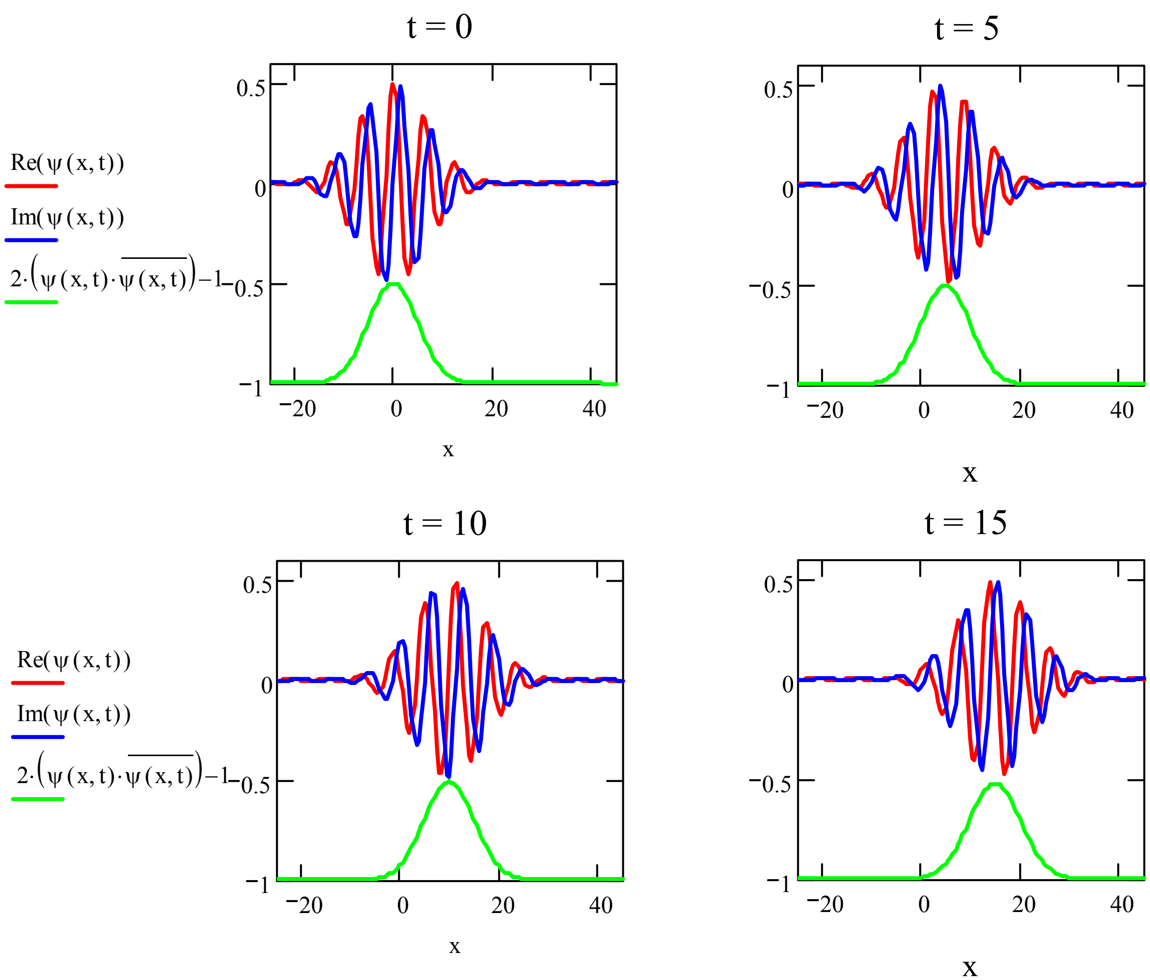
and now reusing the relation $k' = k - k_0$ we can write

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

[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



of the uncertainty principle. We shall discuss this in great detail in Lecture 29.

Let's now look at the time dependence of $\psi(x,t)$. With Eq. (9) we can now use Eq. (1) to write

$$\psi(x,t) = \frac{\psi_0 \sigma}{2\sqrt{\pi}} \int_{-\infty}^{\infty} dk\, e^{-(k-k_0)^2 \sigma^2/4}\; e^{i[k\,x - \omega(k)t]}, \tag{10}$$

keeping in mind that the dispersion relation $\omega(k)$ is given by Eq. (3). This looks complicated, so let's look at some graphs of $\psi(x,t)$ to see what is going on with this solution. The preceding figure, which contains snapshots of the video *SE Wavepacket 3.avi*, illustrates $\psi(x,t)$ as a function of time (for a positive value of k_0). Notice that the wave packet moves in the $+x$ direction with a constant velocity. Notice also that $\psi(x,t)$ is *not* simply a translation in time of the function $\psi(x,0)$. That is, the solution is not of the form $g(x - vt)$, where v is some velocity. This can be seen in the video by noticing that the center of the wave packet travels faster than any of the individual oscillation peaks.

II. The Group Velocity

We now want to determine the velocity of the propagating wave packet described by Eq. (10). Because this solution $\psi(x,t)$ can be thought of as having an average wave vector k_0, you might guess that the velocity is simply the phase velocity $v_{ph} = \omega(k)/k$ evaluated at the average wave vector k_0. That is, you might think that the packet's velocity is simply the velocity of the normal-mode traveling-wave solution

$$\psi_{k_0}(x,t) = \psi_0 e^{i[k_0 x - \omega(k_0)t]} = \psi_0 e^{ik_0[x - (\omega/k_0)t]}, \tag{11}$$

which propagates in the $+x$ direction at the phase velocity $v_{ph} = \omega(k_0)/k_0 = \hbar k_0/2m$. However, this is not correct!

To figure out the packet's velocity we must carefully analyze the propagating-pulse solution described by Eq. (10). This solution lends itself to some approximation because part of the integrand, $e^{-(k-k_0)^2 \sigma^2/4}$, is peaked at $k = k_0$, and for values of $|k - k_0| >> 2/\sigma$ this part of the integrand is nearly zero. The importance of this is that we only need to know what $\omega(k)$ is for $|k - k_0|$ less than a few times the width parameter $2/\sigma$. That is, we only need to know what $\omega(k)$ is for values of k close to k_0. If $\omega(k)$ is does not vary too much for these values of k, then it makes sense to approximate $\omega(k)$ by the first few terms of a Taylor series expansion about the point k_0. So we write

$$\omega(k) = \omega(k_0) + \omega'(k_0)(k - k_0) + \frac{1}{2}\omega''(k_0)(k - k_0)^2 + \ldots \tag{12}$$

If we now approximate $\omega(k)$ in Eq. (10) by the first two terms of the series, $\omega(k) \approx \omega(k_0) + \omega'(k_0)(k - k_0)$, then we obtain

$$\psi(x,t) \approx \frac{\psi_0 \sigma}{2\sqrt{\pi}} e^{-i[\omega(k_0) - \omega'(k_0)k_0]t} \int_{-\infty}^{\infty} dk\, e^{-(k-k_0)^2 \sigma^2/4}\, e^{ik[x - \omega'(k_0)t]} . \tag{13}$$

This looks rather messy, but the integral can be calculated exactly to yield

$$\psi(x,t) \approx \psi_0 e^{ik_0\{x - [\omega(k_0)/k_0]t\}}\, e^{-[x - \omega'(k_0)t]^2/\sigma^2} . \tag{14}$$

We can now easily see what is going on. This (approximate) solution is the product of the normal-mode traveling wave solution $\psi_{k_0}(x,t) = \psi_0 e^{ik_0\{x - [\omega(k_0)/k_0]t\}}$ (at the wave vector k_0), which travels at a speed equal to the phase velocity

$$v_{ph}(k) = \frac{\omega(k)}{k} \tag{15}$$

(evaluated at k_0) and a Gaussian "envelope" function $e^{-[x - \omega'(k_0)t]^2/\sigma^2}$, which travels at a speed equal to $\omega'(k_0)$. The derivative $\omega'(k)$ is known as the **group velocity**

$$v_{gr}(k) = \frac{d\omega(k)}{dk} \tag{16}$$

and so the envelope function, which describes the position of the packet, travels at the group velocity (evaluated at $k = k_0$). Note that the group and phase velocities are not necessarily equal. The group velocity is typically more important than the phase velocity because the average position of the particle is given by the peak of the envelope function.

With these definitions of phase and group velocities we can now write Eq. (14) as

$$\psi(x,t) \approx \psi_0 e^{ik_0(x - v_{ph}t)}\, e^{-(x - v_{gr}t)^2/a_x^2} , \tag{17}$$

where both v_{ph} and v_{gr} are evaluated at the wave vector k_0.

III. Application to the Schrödinger Equation

You may have noticed that nothing in the last section was necessarily directly related to the SE. That is, Eq. (17) can be applied to any situation where general solutions to the problem at hand can be described as a linear combination of harmonic, traveling-wave solutions that have a dispersion relation $\omega(k)$. The SE happens to be one of those situations; so let's apply the results of the last section to the SE. We simply need to know that for the SE the dispersion relation is

$$\omega(k) = \frac{\hbar k^2}{2m}. \qquad (18)$$

From Eq. (18) we obtain the phase and the group velocities $v_{ph}(k_0) = \hbar k_0/2m$ and $v_{gr}(k_0) = \hbar k_0/m$, respectively. Notice that the group velocity is twice the phase velocity. This explains the behavior of the pulse in the video, where the center of the pulse (which travels at v_{gr}) travels faster than any of the oscillation peaks (which travel at v_{ph}). With the interpretation that Eq. (10) describes a particle with an average momentum $p_0 = \hbar k_0$, we see that the group velocity corresponds to the result for a classical, nonrelativistic particle $v_{gr} = p_0/m$.

IV. Application to the Wave Equation

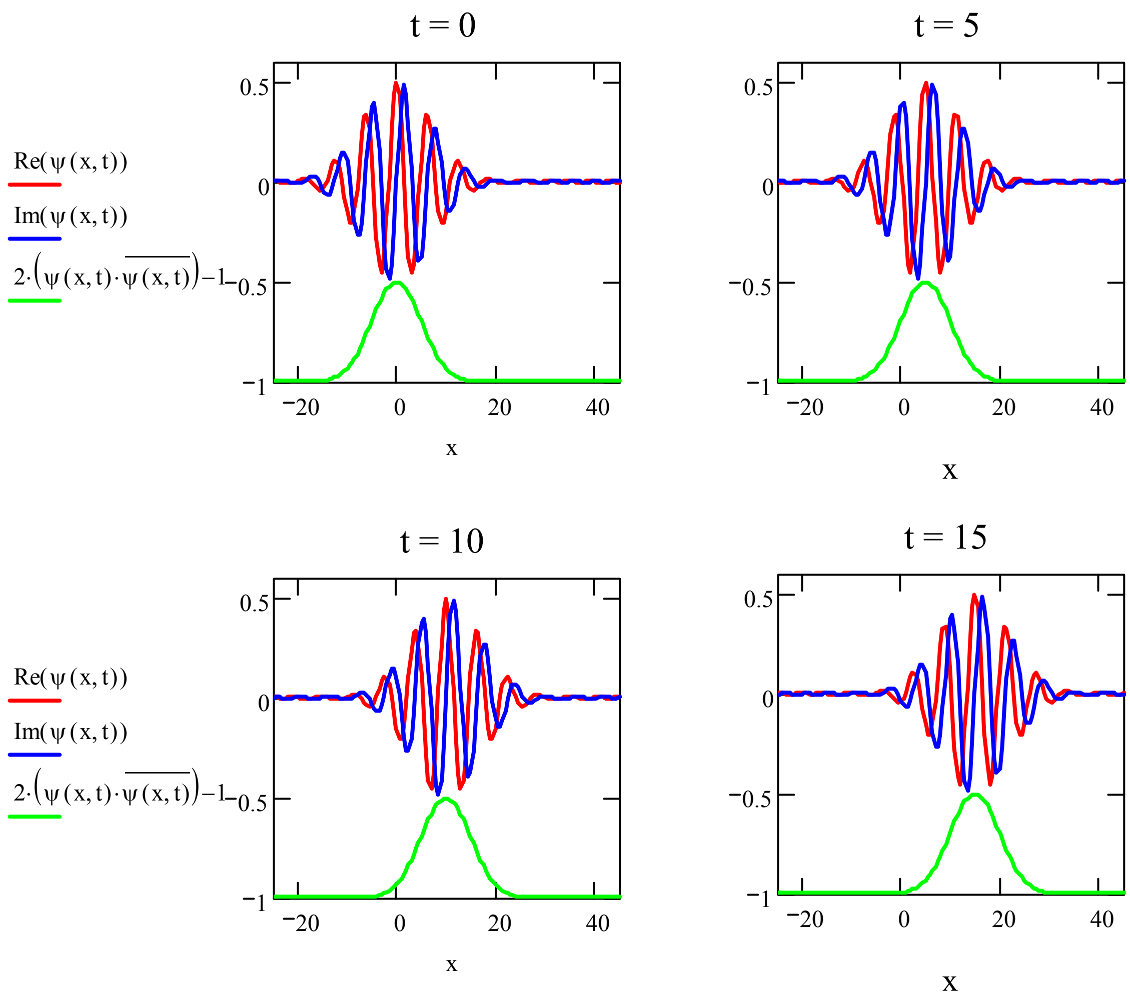
We can also apply the results of Sec. II to the wave equation. Because harmonic traveling waves can also be used as basis functions for solutions to the WE (see Lecture notes 21), we can also create a wave-packet solution to the WE of the form of Eq. (17). Again , we simply need to know the dispersion relation

$$\omega(k) = ck \qquad (19)$$

in order to calculate the phase and group velocities, which are thus $v_{ph}(k_0) = \omega(k_0)/k_0 = c$ and $v_{gr}(k_0) = \omega'(k_0) = c$, respectively. So in this case the two velocities are equal! Then the solution given by Eq. (17) becomes

$$\psi_{k_0}(x,t) = \psi_0 e^{ik_0(x-ct)} e^{-(x-ct)^2/a_x^2}. \qquad (20)$$

Notice that Eq. (20) is a function of $x - ct$, and as such is an *exact* solution to the wave equation, rather than an approximate solution (as it is for the SE). (Why is that?) The figure on the preceding page shows snapshots of the video *WE Wavepacket 1.avi*. In contrast to the SE solution both the center of the wave packet and the oscillation peaks travel at the same velocity, consistent with the solution being a function of $x - ct$.



Exercises

***27.1** Show that Eq. (13) follows from Eq. (10) with the linear Taylor's-series approximation described in the notes.

***27.2** Equation (12) is the Taylor's-series expansion of the dispersion relation about the point $k = k_0$. For the dispersion relation appropriate to the WE, find *all* terms in this expansion. Then argue why Eq. (20), is an exact solution to the WE.

****27.3 SE Approximate Solution**
(**a**) Calculate the integral on the rhs of Eq. (13) and show that Eq. (13) simplifies to Eq. (14). (Hint: Transform the integral to be the Fourier transform of a Gaussian, and then use the fact that the Fourier transform of e^{-x^2/σ^2} is $\frac{\sigma}{\sqrt{2}}e^{-k^2\sigma^2/4}$.)
(**b**) Show that Eq. (14) consistent with Eq. (5), the initial condition.

***27.4 EM Waves** For electromagnetic waves traveling in a dielectric material such as glass the dispersion relation is $\omega(k)=(c/n)k$, where n is the index of refraction, which is often assumed to be a constant.
(**a**) If n is indeed a constant, calculate the phase and group velocities for these waves.
(**b**) Often, however, the index of refraction depends upon the wave vector k. Assuming that $n(k)=n_0+n_1k$, find the phase and group velocities.
(**c**) For $n(k)$ given in (b) show that $v_{gr}=v_{ph}\left[1-n_1k/(n_0+n_1k)\right]$.

***27.5** Calculate $\psi^*\psi$ for the approximate wave function given by Eq. (17) and show that $\psi^*\psi$ travels at the group velocity v_{gr}.