A Propagating Wave Packet – Group Velocity Dispersion

Overview and Motivation: In the last lecture we looked at a localized solution $\psi(x,t)$ to the 1D free-particle Schrödinger equation (SE) that corresponds to a particle moving along the x axis (at a constant velocity). We found an approximate solution that has two velocities associated with it, the phase velocity and the group velocity. However, the approximate solution did not exhibit an important feature of the full solution – that the localization (i.e., width) of the wave packet changes with time. In this lecture we discuss this property of propagating, localized solutions to the SE.

Key Mathematics: The next term in the Taylor series expansion of the dispersion relation $\omega(k)$ will be central in understanding how the width of the pulse changes in time. We will also gain practice at looking at some complicated mathematical expressions and extracting their essential features. We will do this, in part, by defining normalized, unitless parameters that are applicable to the problem.

I. The First-Order Approximate Solution (Review)

In the last lecture we looked at a localized, propagating solution that can be described as a linear combination of traveling, normal-mode solutions of the form $e^{i[kx-\omega(k)t]}$,

$$\psi(x,t)=\frac{\psi_0\sigma}{2\sqrt{\pi}}\int_{-\infty}^{\infty}dk\,e^{-(k-k_0)^2\sigma^2/4}\;e^{i[k\,x-\omega(k)t]}. \tag{1}$$

If Eq. (1) is a solution to the SE, then the dispersion relation is $\omega(k)=\hbar k^2/2m$. In order to gain some insight into Eq. (1) we Taylor-series expanded the dispersion relation about the average wave vector k_0 associated with $\psi(x,t)$,

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

We then approximated $\omega(k)$ by the first two terms (the constant and linear-k terms) in the expansion and obtained the approximate solution

$$\psi(x,t)\approx\psi_0 e^{ik_0[x-v_{ph}(k_0)t]}e^{-[x-v_{gr}(k_0)t]^2/\sigma^2}, \tag{3}$$

where $v_{ph}(k)=\omega(k)/k$ is known as the phase velocity and $v_{gr}(k)=\omega'(k)$ is known as the group velocity. The phase velocity is the speed of the normal-mode solution $e^{ik_0[x-(\omega(k_0)/k_0)t]}$, while the group velocity is the speed of the envelope function $e^{-[x-\omega'(k_0)t]^2/\sigma^2}$. Because it is also the speed of the probability density function

$$\psi^*\psi = \psi_0^*\psi_0 \, e^{-2[x-\omega'(k_0)t]^2/\sigma^2}, \tag{4}$$

it can be though of as the average speed of the particle that the SE describes.

However, the approximate solution [Eq. (3)], does not exhibit an important property of the exact solution: the localization (or width) of the exact solution varies with time while the localization of the approximate solution is constant (and can be described by the width parameter σ.)

The three videos, *SE Wavepacket4.avi*, *SE Wavepacket5.avi*, and *SE Wavepacket6.avi* illustrate the time dependent broadening of propagation wave-packet solutions. Notice that the narrower the initial wave packet, the faster it spreads out in time. This is one result from the analysis below.

II. The Second-Order Approximate Solution

By also including the next term in Eq. (2), the Taylor's series expansion of the dispersion relation, we obtain an approximate solution that exhibits the desired feature of a width that changes as the wave packet propagates.[1] Including the first three terms in the Taylor's series expansion and substituting this into Eq. (1) produces, after a bit of algebra, the approximate solution

$$\psi(x,t) \approx \frac{\psi_0\sigma}{2\sqrt{\pi}} e^{-i[\omega(k_0)-\omega'(k_0)k_0]t} \int_{-\infty}^{\infty} dk \, e^{-(k-k_0)^2[\sigma^2/4 + i\omega''(k_0)t/2]} \, e^{ik[x-\omega'(k_0)t]} \tag{5}$$

This is exactly the same as the approximate solution that we obtained in the last lecture except for the term containing $\omega''(k_0)$. But notice where it appears – as an additive term to $\sigma^2/4$, which controls the width of the pulse. Thus we might already guess that $\omega''(k_0)$ will affect the width as the pulse propagates.

Fortunately, for purposes of further analysis Eq. (5) has an analytic solution

$$\begin{aligned} \psi(x,t) \approx {} & \frac{\psi_0\,\sigma}{\left\{\sigma^4 + [2\omega''(k_0)t]^2\right\}^{1/4}} e^{-(i/2)\arctan\left[2\omega''(k_0)t/\sigma^2\right]} \, e^{2i\omega''(k_0)t[x-\omega'(k_0)t]^2/\left\{\sigma^4+[2\omega''(k_0)t]^2\right\}} \\ & \times e^{ik_0[x-(\omega(k_0)/k_0)t]} \, e^{-[x-\omega'(k_0)t]^2/\left(\sigma^2\left\{1+[2\omega''(k_0)t/\sigma^2]^2\right\}\right)} \end{aligned} . \tag{6}$$

[1] Actually, all of the higher-order terms can contribute to the broadening of the pulse. However, if the width parameter σ is not too small, then only the contribution of the quadratic term to the time dependent broadening needs to be considered.

OK, so maybe solving the integral wasn't so fortunate. But let's see what we can do with it. First notice that, compared to our previous solution we have two new exponential-function terms, $e^{-(i/2)\arctan\left(2\omega''(k_0)t/\sigma^2\right)}$ and $e^{2i\omega''(k_0)t[x-\omega'(k_0)t]^2/\left\{\sigma^4+[2\omega''(k_0)t]^2\right\}}$ [Notice that they are both equal to 1 when $\omega''(k_0)=0$.] However, because the exponents in both of these terms are purely imaginary, they contribute nothing to the width of the wave packet (as we will see below). We will thus not worry about them. The third exponential term we are already familiar with; it is the harmonic traveling wave solution $e^{ik_0[x-(\omega(k_0)/k_0)t]}$ that propagates at the phase velocity $v_{ph}(k_0)$. (Because its exponent is also purely imaginary, it too does not contribute to the width of the wave packet.)

It is the fourth exponential-function term that has some new interest for us. Notice that it is a Gaussian function that again travels with the group velocity $\omega'(k_0)$, but with a time-dependent width

$$\bar{\sigma}(t)=\sigma\left\{1+\left[\frac{2\omega''(k_0)t}{\sigma^2}\right]^2\right\}^{1/2} \tag{7}$$

that is a minimum for $t=0$. Notice that if $\omega''(k_0)=0$, as in the case of the wave equation, then the width has no time dependence and is simply σ.[2] However, in the case of the SE, for example, $\omega''(k_0)=\hbar/m\neq 0$. Thus the SE wave packet has a time dependent width.

For large times we see from Eq. (7) that $\bar{\sigma}(t)$ is approximately linear vs time

$$\bar{\sigma}(t)\approx\frac{2\omega''(k_0)t}{\sigma}, \tag{8}$$

which tells us that

$$\frac{d\bar{\sigma}(t)}{dt}\approx\frac{2\omega''(k_0)}{\sigma}. \tag{9}$$

That is, for long times the rate of broadening is proportional to the second derivative of the dispersion relation and inversely proportional to the width parameter σ. That is, the narrower the pulse is at $t=0$, the faster it broadens with time, as the videos above illustrated.

[2] Because all derivatives of the dispersion relation for the WE higher than first order are zero, Eq. (3) is exact for the wave equation.

III. Normalized Variables

To gain some further insight into this time-dependent width let's make a graph of $\bar{\sigma}(t)$ vs t. But let's be smart about the graph; let's construct the graph so that it has *universal* applicability. To do this we will graph *unitless*, *normalized* quantities that are scaled values of $\bar{\sigma}(t)$ and t. So how do we normalize $\bar{\sigma}(t)$ and t to make them universal to the problem at hand. The answer is in Eq. (7) itself. First notice that if we divide $\bar{\sigma}(t)$ by σ then we will have a unitless width that is equal to 1 at $t=0$. So let's define a normalized width σ_N as $\bar{\sigma}(t)/\sigma$. What about the variable t? Again, the answer is in Eq. (7). Notice that the quantity $2\omega''(k_0)t/\sigma^2$ is also unitless because its value squared is added to 1 in Eq. (7). So let's define a normalized time variable $\tau = 2\omega''(k_0)t/\sigma^2$. With these two universal variables Eq. (7) can be re-expressed as

$$\sigma_N(\tau) = \left[1+\tau^2\right]^{1/2} \tag{10}$$

Ah, much simpler! The figure on the next page plots $\sigma_N(\tau)$ vs τ on two different graphs with different scales. From the graphs we can visually inspect the behavior of Eq. (10). For example, we see for $\tau << 1$ that $\sigma_N(\tau) \approx 1$. This means that for $\tau << 1$ the width is approximately constant vs time. The actual time scale (in seconds) over which this is true will, of course, depend upon the parameters that went into the definition of τ: $\omega''(k_0)$ and σ. From the graph we also see that for $\tau >> 1$, $\sigma_N(\tau) \approx |\tau|$, indicating (again) that the width changes linearly vs time for large negative or positive times.

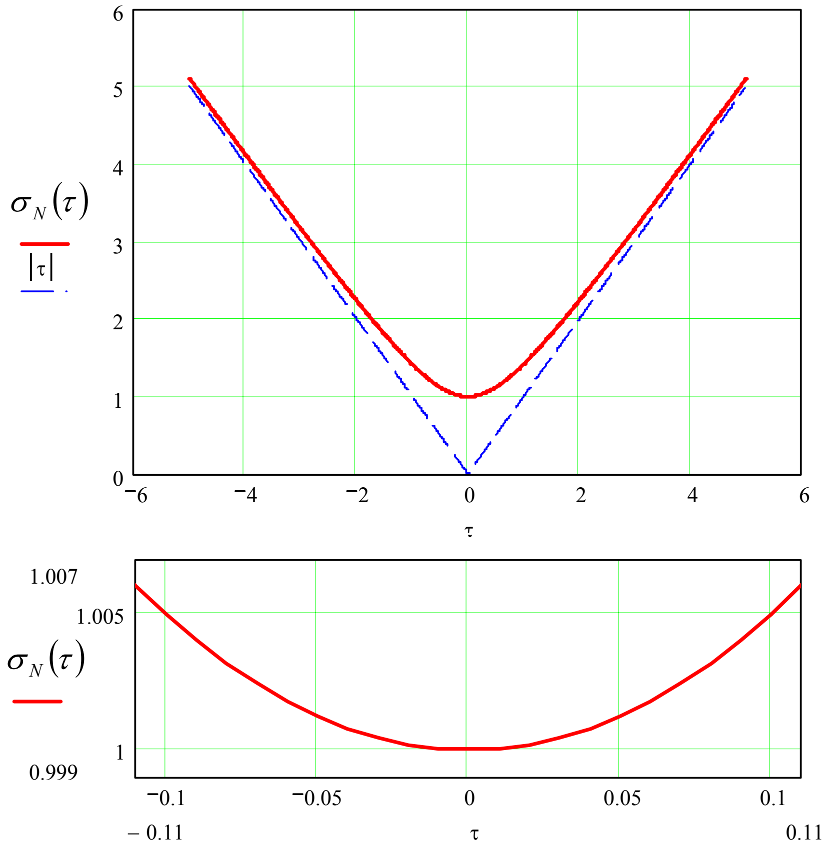
IV. Application to the Schrödinger Equation

Lastly, let's consider the probability density $\psi^*\psi$, assuming that Eq. (6) describes a solution to the SE. From Eq. (6) we calculate

$$\psi^*\psi \approx \frac{\psi_0^*\psi_0\,\sigma^2}{\left\{\sigma^4 + \left[2\omega''(k_0)t\right]^2\right\}^{1/2}}\, e^{-2[x-\omega'(k_0)t]^2 \Big/ \left(\sigma^2\left\{1+\left[2\omega''(k_0)t/\sigma^2\right]^2\right\}\right)}. \tag{11}$$

Using Eq. (7), the definition of $\bar{\sigma}(t)$, Eq. (11) can be rewritten more compactly as

$$\psi^*\psi \approx \psi_0^*\psi_0 \frac{\sigma}{\bar{\sigma}(t)}\, e^{-2[x-\omega'(k_0)t]^2/[\bar{\sigma}(t)]^2}. \tag{12}$$



Notice that the probability density retains its Gaussian shape as the wave packet propagates, but with a time-dependent width parameter equal to $\bar{\sigma}(t)/\sqrt{2}$. Notice that the amplitude $\psi_0^*\psi_0\,\sigma/\bar{\sigma}(t)$ that multiplies the Gaussian function is also time dependent; as the width $\bar{\sigma}(t)$ increases this amplitude decreases. The amplitude varies with the width such that that the total probability for finding the particle anywhere along the x axis,

$$P(t)=\int_{-\infty}^{\infty} dx\,\psi^*(x,t)\psi(x,t), \tag{13}$$

remains constant in time.

The solution given by Eq. (6) and the probability density given by Eq. (11) are illustrated for both negative and positive times in the videos *SE Wavepacket7.avi*, *SE Wavepacket8.avi*, and *SE Wavepacket9.avi*. As Eq. (10) indicates, the pulse becomes narrower as $t=0$ is approached, and the pulse becomes broader after $t=0$. Notice, especially in *SE wavepacket8.avi*, that there is a time near $t=0$ during which the pulse width is approximately constant, corresponding to $\tau << 1$. During this time the height of $\psi^*\psi$ (which is also shown in the videos) is also approximately constant.

Exercises

****28.1** Equation (2) is the Taylor's-series expansion of the dispersion relation about the point $k = k_0$. For the dispersion relation appropriate to the SE, find all terms in this expansion. Then argue why Eqs. (5) and (6) are exact solutions (as opposed to approximate solutions) to the SE.

****28.2 A SE free particle**

(**a**) Rewrite Eq. (11), the expression for the probability density, with expressions for $\omega'(k)$ and $\omega''(k)$ that are appropriate for a wave described by the Schrödinger equation.

(**b**) Make several graphs (at least 3) of the probability density $\psi_{k_0}^*(x,t)\psi_{k_0}(x,t)$ vs x for several different values of t. The graphs should clearly illustrate the change in the width of the wave packet as the wave packet propagates. For simplicity you may set $\hbar = 1$ and $m = 1$.

***28.3 The Dimensionless Time Variable τ**

(**a**) Using dimensional analysis, show that the variable $\tau = 2\omega''(k_0)t/\sigma^2$ is unitless.

(**b**) $|\tau| << 1$ and $|\tau| >> 1$ corresponds to what conditions on t?

****28.4** The figure in the notes shows that for $|\tau| < 0.1$ the width of the wave packet is nearly constant. Let's apply this result to a SE free electron with a kinetic energy of 10 eV. To do this find the value of t (in seconds) that corresponds to $\tau = 0.1$. Do this for values of σ = 10 nm and 10 μm. For these two cases how far does the electron travel in the time corresponding to $\tau = 0.1$? How does each of these distances compare with the respective initial width?

****28.5 SE probability density**.

(**a**) Substitute Eq. (12) into Eq. (13), calculate the integral, and thus show that the result does not depend upon t.

(**b**) Generally, the constant ψ_0 in Eq. (12) is chosen so that the total probability to find the particle anywhere is equal to 1. Using your result in (a), find a value for ψ_0 that satisfies this condition.

***28.6** Show that during a normalized time interval of $\tau = 1$ the normalized distance d/σ traveled is equal to k_0/σ_k (where $\sigma_k = 2/\sigma$). As the normalized width σ_N is controlled by τ, this shows that the dispersion is controlled by the ratio k_0/σ_k.