# The 1D Schrödinger Equation for a Free Particle

**Overview and Motivation**: Here we look at the 1D Schrödinger equation (SE), an equation that describes the quantum motion of a nonrelativistic particle. The SE can have solutions similar to those of the wave equation (WE). In fact, as we shall see, the normal-mode solutions to the SE for a free particle (one not subject to any force) are very similar to those of the wave equation: they are traveling (or standing) waves that oscillate harmonically in space and time. An importance difference, though, is that the dispersion relation $\omega(k)$ is not the same for both equations. This leads to key differences in the general solutions that are built up from the normal-mode solutions.

**Key Mathematics**: We use separation of variables to find solutions to the SE. The solution to the initial-value problem will be specified in terms of the initial conditions using the Fourier transform, as we previously did for the WE (see Lecture 17).

## I. The 1D Schrödinger Equation

The 1D SE

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V(x,t)\psi=i\hbar\frac{\partial\psi}{\partial t} \tag{1}$$

is a homogeneous and linear partial differential equation for the function $\psi=\psi(x,t)$, which is often referred to as the **wave function**. While we will not worry too much about the physical significance of this equation (that will be left to a quantum-mechanics class), we point out that $\hbar=h/(2\pi)$ (where $h$ is Planck's constant), $m$ is the mass of the particle being described by the SE, and $V(x,t)$ is the potential to which the particle is subjected. But for now simply think of $\psi(x,t)$ as the solution to Eq. (1).

## II. Separation of Variables

Let's look for separable solutions to Eq. (1). As before we start with a product function $\psi(x,t)=X(x)T(t)$ and substitute this into Eq. (1), which yields

$$-\frac{\hbar^2}{2m}\frac{X''}{X}+V(x,t)=i\hbar\frac{T'}{T} \tag{2}$$

Now $V(x,t)$ is often independent of time, in which case Eq. (2) becomes

$$-\frac{\hbar^2}{2m}\frac{X''}{X}+V(x)=i\hbar\frac{T'}{T}\,. \tag{3}$$

The variables $x$ and $t$ are now separated; both sides of the equation are thus equal to some constant, which is conventionally called $E$. This gives us two ordinary differential equations that are related via the separation constant $E$,

$$T'(t) = -i\frac{E}{\hbar}T(t), \tag{4}$$

$$-\frac{\hbar^2}{2m}X''(x) + V(x)X(x) = EX(x). \tag{5}$$

Equation (4) says that the first derivative of $T$ is proportional to $T$. The function $T$ must thus be an exponential and is given by

$$T(t) = T_0 e^{-i\frac{E}{\hbar}t}. \tag{6}$$

As with the wave equation the time dependence is harmonic, but because Eq. (4) is a first-order equation there is only one solution, not two linearly independent solutions as in the case of the wave equation. From Eq. (6) we see that the (angular) frequency of oscillation $\omega$ equals $E/\hbar$.

## III. Separable Solutions for a Free Particle

Equation (5), the differential equation for $X(x)$, has no solution until we specify the potential $V(x)$. Our interest here is in a free particle – one with no external force. Zero force implies a constant potential $V(x)$; we can thus set $V(x) = 0$.[1] Then Eq. (5) becomes

$$X''(x) + \frac{2mE}{\hbar^2}X(x) = 0, \tag{7}$$

which is our old friend, the harmonic oscillator equation! By this point you should be able to immediately write down the two independent solutions

$$X^+(x) = X_0 e^{i\sqrt{\frac{2mE}{\hbar^2}}x}, \tag{8a}$$

$$X^-(x) = X_0 e^{-i\sqrt{\frac{2mE}{\hbar^2}}x}. \tag{8b}$$

[1] As is the case in classical mechanics, making the potential some unspecified arbitrary constant (rather than zero) does not change the physics. In the case at hand it is simplest to let that constant equal zero.

As usual, we identify the wave vector $k$ as the factor that multiplies $x$ in the argument of the harmonic function (excluding the $\pm i$). Thus $k = \sqrt{2mE/\hbar^2}$. Solving this equation for $E = \hbar^2 k^2/2m$ and comparing this with the expression for the frequency $\omega = E/\hbar$ gives us the dispersion relation for the free-particle SE

$$\omega(k) = \frac{\hbar k^2}{2m}. \tag{9}$$

Notice that as a function of $k$, this is different than

$$\omega(k) = ck, \tag{10}$$

the dispersion relation for harmonic solutions to the wave equation: the wave-equation dispersion relation is a *linear* function of $k$ while the SE dispersion relation is a *quadratic* function of $k$. The significance of this difference will be discussed in a Lectures 27 and 28.

Combining the $T$ and $X$ pieces we obtain two linearly independent solutions to the free-particle SE

$$\psi_k^+(x,t) = \psi_0 e^{ikx} e^{-i\omega t} = \psi_0 e^{i(kx-\omega t)} = \psi_0 e^{ik[x-(\omega/k)t]}, \tag{11a}$$

$$\psi_k^-(x,t) = \psi_0 e^{-ikx} e^{-i\omega t} = \psi_0 e^{-i(kx+\omega t)} = \psi_0 e^{-ik[x+(\omega/k)t]}. \tag{11b}$$

These two solutions are harmonic waves that travel with speed $v_{ph} = \omega/k = \hbar k/2m$. (The subscript *ph* stands for phase – more on that later.) Unlike wave-equation solutions [which all move with the same speed ($v_{ph} = c$)], the propagation speed of these harmonic waves depends upon the wave vector $k$, with $v_{ph} \propto k$.

As defined above, the wave vector is a positive quantity. However, if we let the wave vector take on negative as well as positive values we see that $\psi_{-k}^- = \psi_k^+$. Thus we can write all the separable solutions as

$$\psi_k(x,t) = \psi_0 e^{i[kx-\omega(k)t]}. \tag{12}$$

where now $-\infty < k < \infty$, and $\omega(k)$ is still defined by Eq. (9), the dispersion relation.

## IV. The Free Particle Initial Value Problem

As it turns out (and perhaps shouldn't be too surprising) we can write any solution to the free-particle SE as a linear combination of these harmonic solutions. Because the index $k$ is continuous, the linear combination must be expressed as an integral over $k$,

$$\psi(x,t)=\int_{-\infty}^{\infty} dk\, C(k)\,\psi_k(x,t), \tag{13}$$

where $C(k)$ is the coefficient of the $k$th basis state $\psi_k(k,t)$. Using Eq. (12) we can rewrite Eq. (13) as

$$\psi(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\, C(k)\,e^{i[kx-\omega(k)t]}, \tag{14}$$

where we have set $\psi_0 = 1/\sqrt{2\pi}$.[2] As in the case of the WE, the coefficients $C(k)$ are determined by the initial conditions, but because there is only one time derivative there is only one initial condition, $\psi(x,0)$ (the value of the wave function at $t=0$). Setting $t=0$ in Eq. (14), we obtain

$$\psi(x,0)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\, C(k)\,e^{ikx}. \tag{15}$$

Now this equation tells us that $C(k)$ is simply the Fourier transform of the initial condition $\psi(x,0)$. We can thus invert Eq. (15) to write

$$C(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, \psi(x,0)\,e^{-ikx}. \tag{16}$$

Taken in tandem Eqs. (14) and (16) are the complete solution to the free-particle SE initial-value problem.

## V. An Initial-Value-Problem Example

Let's see what happens if we start with the initial condition

$$\psi(x,0)=\psi_0 e^{-x^2/\sigma^2}, \tag{17}$$

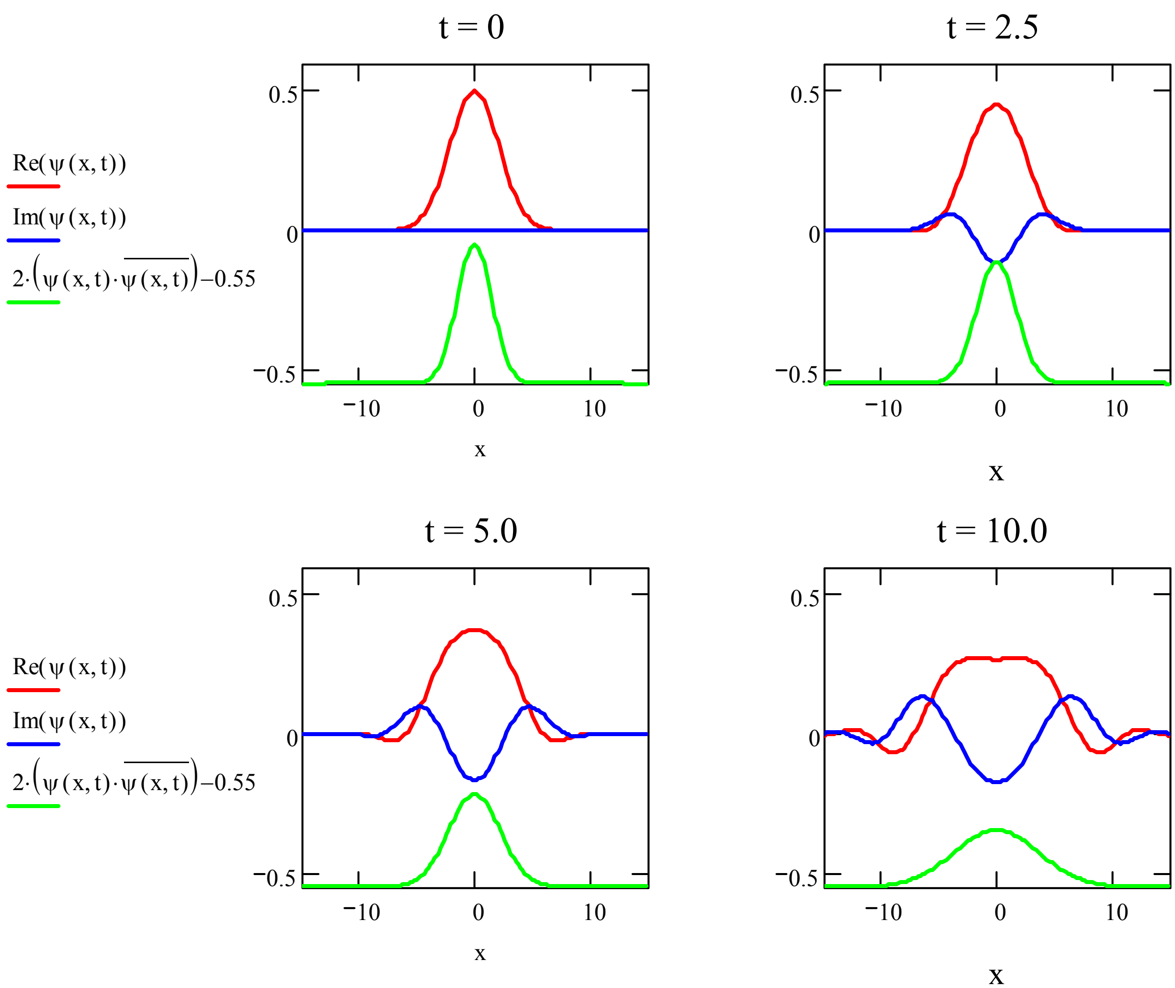
[2] The choice $\psi_0 = 1/\sqrt{2\pi}$ normalizes the harmonic basis states. See the Lecture 16 notes for details.

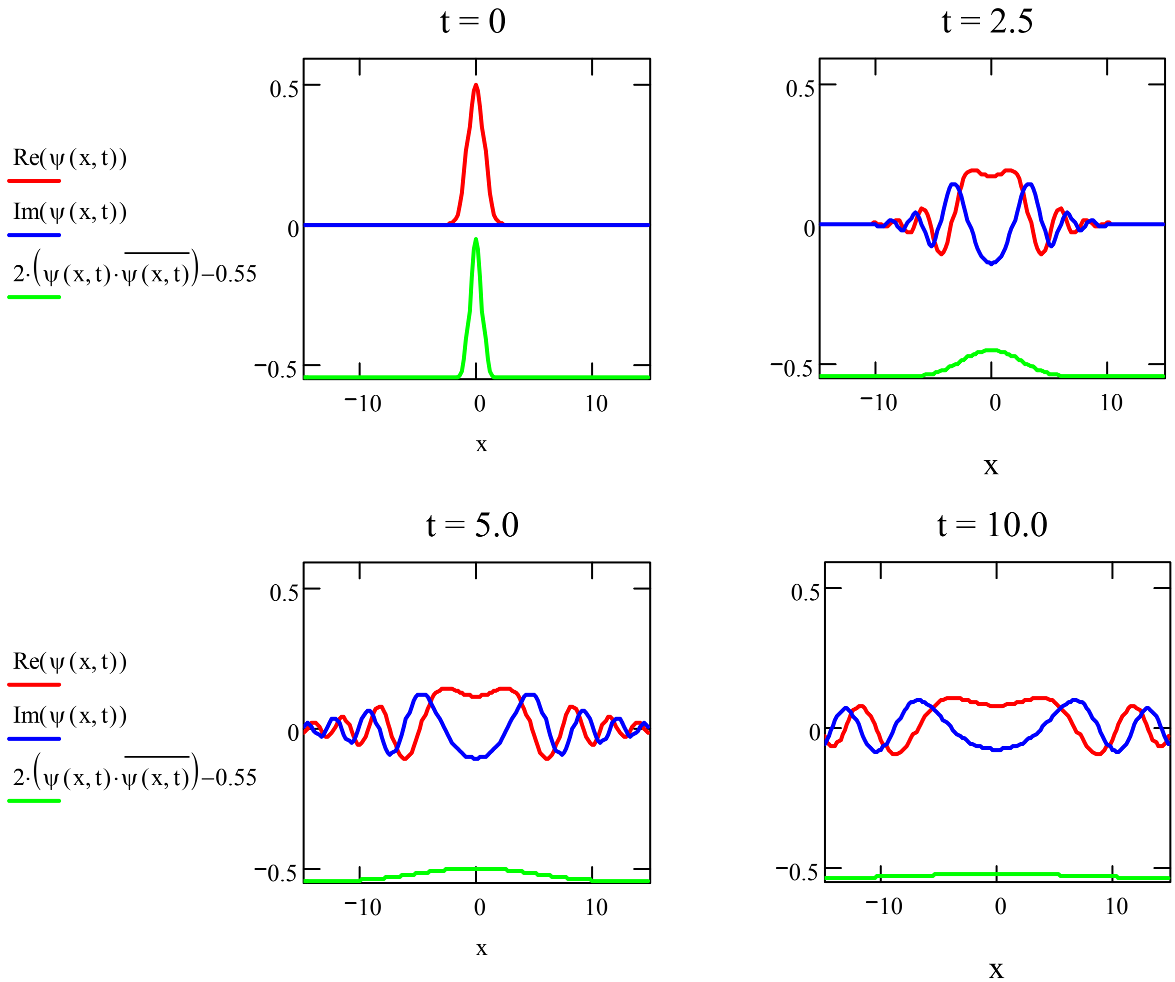
which is a Gaussian with amplitude $\psi_0$ and width parameter $\sigma$ that is centered at the origin. As will become apparent, this corresponds to a particle whose average position $\langle x\rangle$ and average momentum $\langle p\rangle$ are both zero. Furthermore, the particle has an uncertainly in position that is proportional to the width parameter $\sigma$.

Using Eq. (16) we can calculate $C(k)$,

$$C(k)=\frac{\psi_0\sigma}{\sqrt{2}}e^{-k^2\sigma^2/4}. \tag{18}$$

(For details of this calculation see the Lecture 12 notes.) This is pretty cool: the Fourier transform of the Gaussian function $\psi(x,0)$, $C(k)$, is also a Gaussian function (of $k$). Furthermore, the width parameter of $C(k)$ is $2/\sigma$, which is inversely proportional to the width parameter $\sigma$ of the original function $\psi(x,0)$. Thus the product of the two width parameters is a constant, $\sigma\cdot 2/\sigma=2$.






Using Eq. (18) in Eq. (14), we obtain the solution to this initial-value problem,

$$\psi(x,t) = \frac{\psi_0 \sigma}{2\sqrt{\pi}} \int_{-\infty}^{\infty} dk\, e^{-k^2\sigma^2/4}\; e^{i[kx-\omega(k)t]}\,, \tag{19}$$

where $\omega(k)$ is given by Eq. (9).

The previous two figures[3] show graphs of $\mathrm{Re}\psi$, $\mathrm{Im}\psi$, and $\psi^*\psi$ (the associated probability density for the particle) for various times $t$. In the first figure $\sigma = 3$, while in the second figure $\sigma = 1$. As evident from the graphs of $\psi^*\psi$, in the second case the particle is initially more localized than in the first case.

The following facts are also worth noting.

[3] These figures show snapshots of the videos *SE Wavepacket 1.avi* and *SE Wavepacket 2.avi*, which are available on the class website.

(*i*) Although $\psi(x,0)$ is real, in general $\psi(x,t)$ has both real and imaginary parts. This is due to the presence of $i$ in the Eq. (1), the SE equation.

(*ii*) Neither the real or imaginary part of $\psi(x,t)$ retains a Gaussian shape, but the probability density $\psi^*\psi$ is Gaussian for all $t$.

(*iii*) The wave function $\psi(x,t)$ spreads out along $x$ in time. This is due to something known as **group-velocity dispersion** [which depends upon the dispersion relation $\omega(k)$] We will discuss this in detail later, but for now note that the *narrower* the initial pulse, the *faster* the pulse spreads in time.

Let's think for a moment about how this solution compares to the solution to the WE that has an initial Gaussian displacement (and no initial velocity). What was the solution in that case? You should recall that the initial Gaussian pulse split into two Gaussian pulses with the same width as the original displacement, and that those pulses traveled in opposite directions away from the origin at the speed $c$. In contrast to the solution here, the traveling pulses described by the wave equation do not broaden with time.

## Exercises

*__26.1__ As illustrated, the solution $\psi(x,t)$ to the SE is in general a complex function. Write $\psi(x,t)$ as a sum of real and imaginary parts, $\psi_R(x,t)+i\psi_I(x,t)$, substitute into Eq. (1) and show that Eq. (1) can be written as two *real* coupled equations for $\psi_R$ and $\psi_I$. (Here you will need to use the fact that the real and imaginary parts of an equation are independent of each other.)

*__26.2__ The momentum $p$ of a particle in the state $\psi_k(x,t)=\psi_0 e^{i[kx-\omega(k)t]}$ is a well-defined quantity (i.e., it has no uncertainty) and is given by $p=\hbar k$. Similarly, the energy of the particle in this state is well defined and is simply the parameter $E=\hbar\omega(k)$. Using the dispersion relation $\omega(k)$, show that it is equivalent to the energy-momentum relationship for a free classical particle.

*__26.3__ The two linearly-independent solutions for the $X(x)$ equation were written as $X^+(x)=X_0 e^{i\sqrt{\frac{2mE}{\hbar^2}}x}$ and $X^-(x)=X_0 e^{-i\sqrt{\frac{2mE}{\hbar^2}}x}$. Find the appropriate linear combinations of these two solutions that give the other commonly used form of two linearly independent solutions: $X_1(x)=A_1\cos\left(\sqrt{\frac{2mE}{\hbar^2}}\,x\right)$ and $X_2(x)=A_2\sin\left(\sqrt{\frac{2mE}{\hbar^2}}\,x\right)$.

*26.4 Show for the Gaussian initial condition $\psi(x,0)=\psi_0 e^{-x^2/\sigma^2}$ that the probability density $\psi^*(x,0)\psi(x,0)$ is also a Gaussian. How is the width parameter of $\psi^*(x,0)\psi(x,0)$ related to the width parameter $\sigma$ of the wave function $\psi(x,0)$?

**26.5 A Free-Particle SE Initial Value Problem**
(**a**) Starting with the initial condition

$$\psi(x,0)=\begin{cases}1/\sqrt{2} & -1<x<1 \\ 0 & \text{otherwise}\end{cases}$$

for a free particle, find the function $C(k)$ appropriate to this initial condition.
(**b**) Then find the formal solution [the equivalent of Eq. (19)] to this initial value problem.
(**c**) Make plots of $\psi(x,t)$ for $t=0$, $t=2$, and $t=4$. For purposes of keeping things simple, set $\hbar=1$ and $m=1$ so that the dispersion relation is simply $\omega(k)=k^2/2$. Hint: when numerically evaluating the integral, set the limits only large enough so that the integrand is negligible at the endpoints of the integration.
(**d**) Discuss the time dependence of $\psi(x,t)$.

*26.6 Show that $\psi(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\, C(k)\, e^{i[kx-\omega(k)t]}$ with $\omega(k)=\frac{\hbar k^2}{2m}$ solves the 1D, free-particle Schrödinger equation for any $C(k)$.

***26.7 **Free Particle in 3D**. Consider the 3D, free-particle Schrödinger equation,

$$-\frac{\hbar^2}{2m}\nabla^2\psi = i\hbar\frac{\partial\psi}{\partial t},$$

Find separation-of-variables solutions to this equation in
(**a**) Cartesian coordinates,
(**b**) cylindrical coordinates, and
(**c**) spherical-polar coordinates.