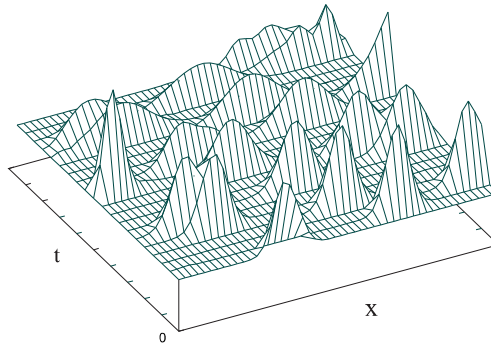


Figure 18.7 The position as a function of time of a localized electron confined to a square well (computed with the code `SqWell.py` available in the instructor's manual). The electron is initially on the right with a Gaussian wave packet. In time, the wave packet spreads out and collides with the walls.



to make the approximation

$$c(x)^2 \simeq \frac{T(x)}{\rho} = \frac{T_0 \cosh(x/d)}{\rho}.$$

See if you get a better representation of the first two normal modes if you include some  $x$  dependence in  $k$ .

## 18.5 UNIT II. QUANTUM WAVE PACKETS

**Problem:** An experiment places an electron with a definite momentum and position in a 1-D region of space the size of an atom. It is confined to that region by some kind of attractive potential. Your **problem** is to determine the resultant electron behavior in time and space.

### 18.6 TIME-DEPENDENT SCHRÖDINGER EQUATION (THEORY)

Because the region of confinement is the size of an atom, we must solve this problem quantum mechanically. Nevertheless, it is different from the problem of a particle confined to a box considered in Chapter 9, “Differential Equation Applications”, because now we are starting with a particle of definite momentum and position. In Chapter 9 we had a time-independent situation in which we had to solve the eigenvalue problem. Now the definite momentum and position of the electron imply that the solution is a wave packet, which is not an eigenstate with a uniform time dependence of  $\exp(-i\omega t)$ . Consequently, we must now solve the time-dependent Schrödinger equation.

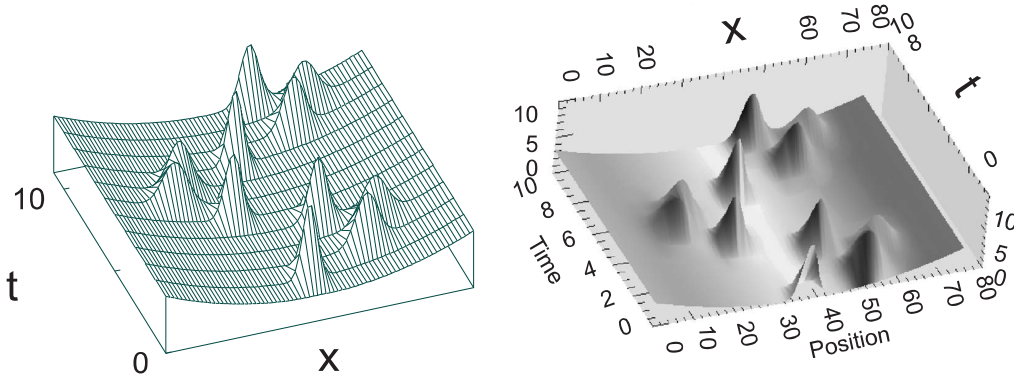
**Applet** We model an electron initially localized in space at  $x = 5$  with momentum  $k_0$  ( $\hbar = 1$  in our units) by a wave function that is a wave packet consisting of a Gaussian multiplying a plane wave:

$$\psi(x, t = 0) = \exp \left[ -\frac{1}{2} \left( \frac{x - 5}{\sigma_0} \right)^2 \right] e^{ik_0 x}. \quad (18.39)$$

To solve the **problem** we must determine the wave function for all later times. If (18.39) were an eigenstate of the Hamiltonian, its  $\exp(-i\omega t)$  time dependence can be factored out of the Schrödinger equation (as is usually done in textbooks). However,  $\tilde{H}\psi \neq E\psi$  for this  $\psi$ , and so we must solve the full time-dependent Schrödinger equation. To show you where we are going, the resulting wave packet behavior is shown in Figures 18.7 and 18.8.

The time and space evolution of a quantum particle is described by the 1-D time-

Figure 18.8 The probability density as a function of time for an electron confined to a 1-D harmonic oscillator potential well. On the left is a conventional surface plot from Gnuplot, while on the right is a color visualization from OpenDX of the same output.



dependent Schrödinger equation,

$$i \frac{\partial \psi(x, t)}{\partial t} = \tilde{H} \psi(x, t) \quad (18.40)$$

$$i \frac{\partial \psi(x, t)}{\partial t} = -\frac{1}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2} + V(x) \psi(x, t), \quad (18.41)$$

where we have set  $2m = 1$  to keep the equations simple. Because the initial wave function is complex (in order to have a definite momentum associated with it), the wave function will be complex for all times. Accordingly, we decompose the wave function into its real and imaginary parts:

$$\psi(x, t) = R(x, t) + i I(x, t), \quad (18.42)$$

$$\psi(x, t) = R(x, t) + i I(x, t), \quad (18.43)$$

$$\Rightarrow \frac{\partial R(x, t)}{\partial t} = -\frac{1}{2m} \frac{\partial^2 I(x, t)}{\partial x^2} + V(x) I(x, t), \quad (18.44)$$

$$\frac{\partial I(x, t)}{\partial t} = +\frac{1}{2m} \frac{\partial^2 R(x, t)}{\partial x^2} - V(x) R(x, t), \quad (18.45)$$

where  $V(x)$  is the potential acting on the particle.

### 18.6.1 Finite-Difference Algorithm

The time-dependent Schrödinger equation can be solved with both implicit (large-matrix) and explicit (leapfrog) methods. The extra challenge with the Schrödinger equation is to ensure that the integral of the probability density  $\int_{-\infty}^{+\infty} dx \rho(x, t)$  remains constant (conserved) to a high level of precision for all time. For our project we use an *explicit* method that improves the numerical conservation of probability by solving for the real and imaginary parts of the wave function at slightly different or “staggered” times [Ask 77, Viss 91, MLP 00]. Explicitly, the real part  $R$  is determined at times  $0, \Delta t, \dots$ , and the imaginary part  $I$  at  $\frac{1}{2}\Delta t, \frac{3}{2}\Delta t, \dots$ . The algorithm is based on (what else?) the Taylor expansions of  $R$  and  $I$ :

$$\begin{aligned} R\left(x, t + \frac{1}{2}\Delta t\right) &= R\left(x, t - \frac{1}{2}\Delta t\right) + [4\alpha + V(x) \Delta t] I(x, t) \\ &\quad - 2\alpha [I(x + \Delta x, t) + I(x - \Delta x, t)], \end{aligned} \quad (18.46)$$

where  $\alpha = \Delta t/2(\Delta x)^2$ . In discrete form with  $R_{x=i\Delta x}^{t=n\Delta t}$ , we have

$$R_i^{n+1} = R_i^n - 2 \{ \alpha [I_{i+1}^n + I_{i-1}^n] - 2 [\alpha + V_i \Delta t] I_i^n \}, \quad (18.47)$$

$$I_i^{n+1} = I_i^n + 2 \{ \alpha [R_{i+1}^n + R_{i-1}^n] - 2 [\alpha + V_i \Delta t] R_i^n \}, \quad (18.48)$$

where the superscript  $n$  indicates the time and the subscript  $i$  the position.

The probability density  $\rho$  is defined in terms of the wave function evaluated at three different times:

$$\rho(t) = \begin{cases} R^2(t) + I(t + \frac{\Delta t}{2})I(t - \frac{\Delta t}{2}), & \text{for integer } t, \\ I^2(t) + R(t + \frac{\Delta t}{2})R(t - \frac{\Delta t}{2}), & \text{for half-integer } t. \end{cases} \quad (18.49)$$

Although probability is not conserved exactly with this algorithm, the error is two orders higher than that in the wave function, and this is usually quite satisfactory. If it is not, then we need to use smaller steps. While this definition of  $\rho$  may seem strange, it reduces to the usual one for  $\Delta t \rightarrow 0$  and so can be viewed as part of the art of numerical analysis. You will investigate just how well probability is conserved. We refer the reader to [Koon 86, Viss 91] for details on the stability of the algorithm.

## 18.6.2 Wave Packet Implementation, Animation

In Listing 18.2 you will find the program `HarmosAnimate.py` that solves for the motion of the wave packet (18.39) inside a harmonic oscillator potential. The program `slit.py` in the instructor's manual solves for the motion of a Gaussian wave packet as it passes through a slit (Figure 18.10). You should solve for a wave packet confined to the square well:

$$V(x) = \begin{cases} \infty, & x < 0, \text{ or } x > 15, \\ 0, & 0 \leq x \leq 15. \end{cases}$$

1. Define arrays `psr[751][2]` and `psi[751][2]` for the real and imaginary parts of  $\psi$ , and `Rho[751]` for the probability. The first subscript refers to the  $x$  position on the grid, and the second to the present and future times.
2. Use the values  $\sigma_0 = 0.5$ ,  $\Delta x = 0.02$ ,  $k_0 = 17\pi$ , and  $\Delta t = \frac{1}{2}\Delta x^2$ .
3. Use equation (18.39) for the initial wave packet to define `psr[j][1]` for all  $j$  at  $t = 0$  and to define `psi[j][1]` at  $t = \frac{1}{2}\Delta t$ .
4. Set `Rho[1] = Rho[751] = 0.0` because the wave function must vanish at the infinitely high well walls.
5. Increment time by  $\frac{1}{2}\Delta t$ . Use (18.47) to compute `psr[j][2]` in terms of `psr[j][1]`, and (18.48) to compute `psi[j][2]` in terms of `psi[j][1]`.
6. Repeat the steps through all of space, that is, for  $i = 2-750$ .
7. Throughout all of space, replace the present wave packet (second index equal to 1) by the future wave packet (second index 2).
8. After you are sure that the program is running properly, repeat the time-stepping for  $\sim 5000$  steps.

Listing 18.2 `HarmosAnimate.py` solves the time-dependent Schrödinger equation for a particle described by a Gaussian wave packet moving within a harmonic oscillator potential.

```
# HarmosAnimate: Soltn of t-dependent Sch Eqt fro HO with animation
```