27
Quantum Wave Packets ⊙

Problem: An electron is initially confined to a 1D region of space the size of an atom. Your **problem** is to determine the behavior in time and space that results. This is different from the problem of a particle confined to a box considered in Chapter 15. There we had a time-independent situation in which we had to solve for the spatial wave function; here we have a time-dependent problem in which the state is not an eigenstate or stationary state of the Hamiltonian, and so does not have a fixed form for its time dependence.

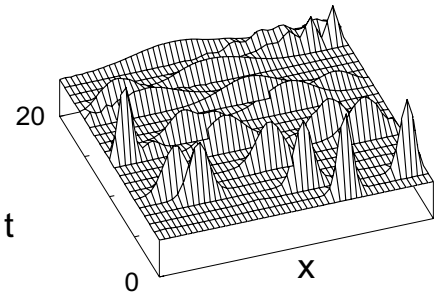

Fig. 27.1 The position as a function of time of a localized electron confined to a square well. The electron is initially on the right with a Gaussian wave packet. In time, the wave packet spreads out and collides with the walls.

27.1
Time-Dependent Schrödinger Equation (Theory)

We model an electron initially localized in space at $x = 5$ with momentum k_0 ($\hbar = 1$) by a Gaussian wave function (packet) multiplying a plane wave:

$$\psi(x, t = 0) \;=\; \exp\left[-\frac{1}{2}\left(\frac{x-5}{\sigma_0}\right)^2\right] e^{ik_0 x} \tag{27.1}$$

Your **problem** is to determine the wave function for all later times. The behavior of this wave packet when confined to a box is shown in Fig. 27.1, and when confined to an harmonic oscillator potential, in Fig. 27.2.

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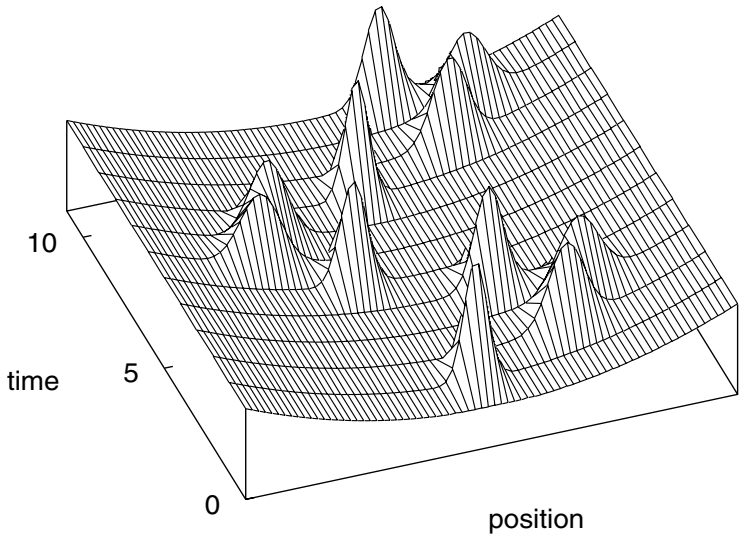

Fig. 27.2 The probability density as a function of time for an electron confined to a 1D harmonic oscillator potential well. Because the wave packet is an eigenfunction of the potential, it returns to its original form after transversing the well.

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

$$i\frac{\partial\psi(x,t)}{\partial t} \;=\; \tilde{H}\psi(x,t) \;=\; -\frac{1}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) \tag{27.2}$$

where we have set $2m = 1$ to keep the equations simple. Because the initial wave function is complex (in order to have 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

$$\psi(x,t) \;=\; R(x,t) + i\,I(x,t) \tag{27.3}$$

$$\Rightarrow \qquad \frac{\partial R(x,t)}{\partial t} \;=\; -\frac{1}{2m}\frac{\partial^2 I(x,t)}{\partial x^2} + V(x)I(x,t) \tag{27.4}$$

$$\frac{\partial I(x,t)}{\partial t} \;=\; +\frac{1}{2m}\frac{\partial^2 R(x,t)}{\partial x^2} - V(x)R(x,t) \tag{27.5}$$

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

27.1.1 Finite Difference Solution

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) for all time. For our project, we modify the *explicit* method described by [81,82], which solves the probability problem by determining the real and imaginary parts of the wave function at slightly different or "staggered" times. Explicitly, the real part R is determined at times $0, \Delta t, \ldots$, and the imaginary part I at $\frac{1}{2}\Delta t$, $\frac{3}{2}\Delta t$, and so forth. The algorithm is based on (what else) the Taylor expansions of R and I:

$$\begin{aligned} R(x,t+\tfrac{1}{2}\Delta t) &= R(x,t-\tfrac{1}{2}\Delta t) + [4\alpha + V(x)\Delta t]I(x,t) \\ &\quad - 2\alpha[I(x+\Delta x,t) + I(x-\Delta x,t)] \end{aligned} \tag{27.6}$$

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

$$R_i^{n+1} = R_i^n - 2\left\{\alpha\left[I_{i+1}^n + I_{i-1}^n\right] - 2\left[\alpha + V_i\Delta t\right] I_i^n\right\}, \tag{27.7}$$

$$I_i^{n+1} = I_i^n + 2\left\{\alpha\left[R_{i+1}^n + R_{i-1}^n\right] - 2\left[\alpha + V_i\Delta t\right] R_i^n\right\} \tag{27.8}$$

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

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

$$\rho(t) = \begin{cases} R^2(t) + I(t+\frac{\Delta t}{2})I(t-\frac{\Delta t}{2}), & \text{for integer } t, \\ I^2(t) + R(t+\frac{\Delta t}{2})R(t-\frac{\Delta t}{2}), & \text{for half-integer } t \end{cases} \tag{27.9}$$

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 ρ may seem strange, it reduces to the usual one for $\Delta t \to 0$, 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 [28,82] for details on the stability of the algorithm.

27.1.2 Wave Packet Implementation

Listing 27.1: `Harmos.java` solves the time-dependent Schrödinger equation for a particle described by a Gaussian wave packet moving within a harmonic oscillator potential.

```
//  harmos.java: Solution t-dependent Schroedinger equation for
//               Gaussian wavepacket in a harmonic oscillator potential
```

```
import java.io.*;

public class harmos {

  public static void main(String[] argv)
                    throws IOException, FileNotFoundException {

    PrintWriter w =
        new PrintWriter(new FileOutputStream("Harmos.dat"), true);
    double psr[][] = new double[751][2];
    double psi[][] = new double[751][2];
    double p2[] = new double[751];
    double v[] = new double[751];
    double dx=0.02, k0, dt, x, pi;
    int i ,n, max = 750;

    pi   = 3.14159265358979323846;
    k0   = 3.0*pi;
    dt   = dx*dx/4.0;
    x    = -7.5;
                                                  // Initial conditions
    for ( i=0; i<max; i++) {
      psr[i][0] = Math.exp(-0.5*(Math.pow((x/0.5),2.0)))
                                                 *Math.cos(k0*x);      // RePsi
      psi[i][0] = Math.exp(-0.5*(Math.pow((x/0.5),2.0)))
                                                 *Math.sin(k0*x);      // ImPsi
      v[i] = 5.0*x*x;                                              // Potential
      x    = x + dx;
    }
                                                  // Propagate in time
    for ( n=0; n<20000; n++) {
      for ( i=1; i<max-1; i++ ) {                                  // RePsi
        psr[i][1] = psr[i][0] - dt*(psi[i+1][0] + psi[i-1][0]
                    -2.0*psi[i][0])/(dx*dx)+dt*v[i]*psi[i][0];
        p2[i] = psr[i][0]*psr[i][1]+psi[i][0]*psi[i][0];
      }
      for ( i=1; i<max-1; i++ ) {                                  // ImPsi
        psi[i][1] = psi[i][0] + dt*(psr[i+1][1] + psr[i-1][1]
                    -2.0*psr[i][1])/(dx*dx)-dt*v[i]*psr[i][1];
      }
                                                 // Output every 2000 steps
      if ( (n == 0) || (n%2000 == 0) ) {
        for (i=0;i<max; i=i+10) w.println(""+(p2[i]+0.0015*v[i])+"");
           w.println("");
      }
      for ( i=0; i<max; i++ ) {                                  // New -> old
        psi[i][0] = psi[i][1];
        psr[i][0] = psr[i][1];
      }
    }
    System.out.println("data saved in Harmos.dat");
  }
}
```

On the CD you will find the program `harmon.f` that solves for the motion of the wave packet (27.1) inside harmonic oscillator potential. You should solve for the square-well potential:

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

1. Define arrays `R(751,2)` and `I(751,2)` for the real and imaginary parts of the wave function, and `Rho(751)` for the probability density. 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 Eq. (27.1) for the initial wave packet to define `R(j,1)` for all j's at $t = 0$, and `I(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 (27.7) to compute `R(j,2)` in terms of `R(j,1)`, and (27.8) to compute `I(j,2)` in terms of `I(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.

27.1.3
Wave Packet Visualization and Animation

1. Output the probability density after every 200 steps for use in animation.
2. Make a surface plot of probability versus position versus time. This should look like Fig. 27.1 or Fig. 27.2.
3. Make an animation showing the wave function as a function of time.
4. Check how well probability is conserved for early and late times by determining the integral of the probability over all of space, $\int_{-\infty}^{+\infty} dx\, \rho(x)$, and seeing by how much it changes in time (its specific value doesn't matter because that's just normalization).
5. What might be a good explanation of why collisions with the walls cause the wave packet to broaden and break up? (*Hint:* The collisions do not appear so disruptive when a Gaussian wave packet is confined within a harmonic oscillator potential well.)

27.2
Wave Packets Confined to Other Wells (Exploration)

1D Well : Consider a wave packet in the harmonic oscillator potential:

$$V(x) = \tfrac{1}{2}x^2 \qquad (-\infty \le x \le \infty)$$

Take the initial momentum of the wave packet as $k_0 = 3\pi$ and time and space steps as $\Delta x = 0.02$ and $\Delta t = \frac{1}{4}\Delta x^2$. Note that the wave packet appears to breathe, yet returns to it initial shape!

2D Well : Consider now an electron moving in 2D space (Fig. 27.3). This adds another degree of freedom to the problem, which means that we must solve the 2D time-dependent Schrödinger equation:

$$i\frac{\partial \psi(x,y,t)}{\partial t} = -\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}\right) + V(x,y)\psi \tag{27.10}$$

where we have chosen units in which $2m = \hbar = 1$. To be more specific, have the electron move in an infinitely long tube with a parabolic cross section:

$$V(x,y) = 0.9x^2 \qquad -9.0 \le x \le 9.0 \qquad 0 \le y \le 18.0.$$

Assume that the electron's initial localization is described by a Gaussian wave packet in two dimensions:

$$\psi(x,y,t=0) = e^{ik_{0x}x}\, e^{ik_{0y}y}\, \exp\left[-\frac{(x-x_0)^2}{2\sigma_0^2}\right] \exp\left[-\frac{(y-y_0)^2}{2\sigma_0^2}\right] \tag{27.11}$$

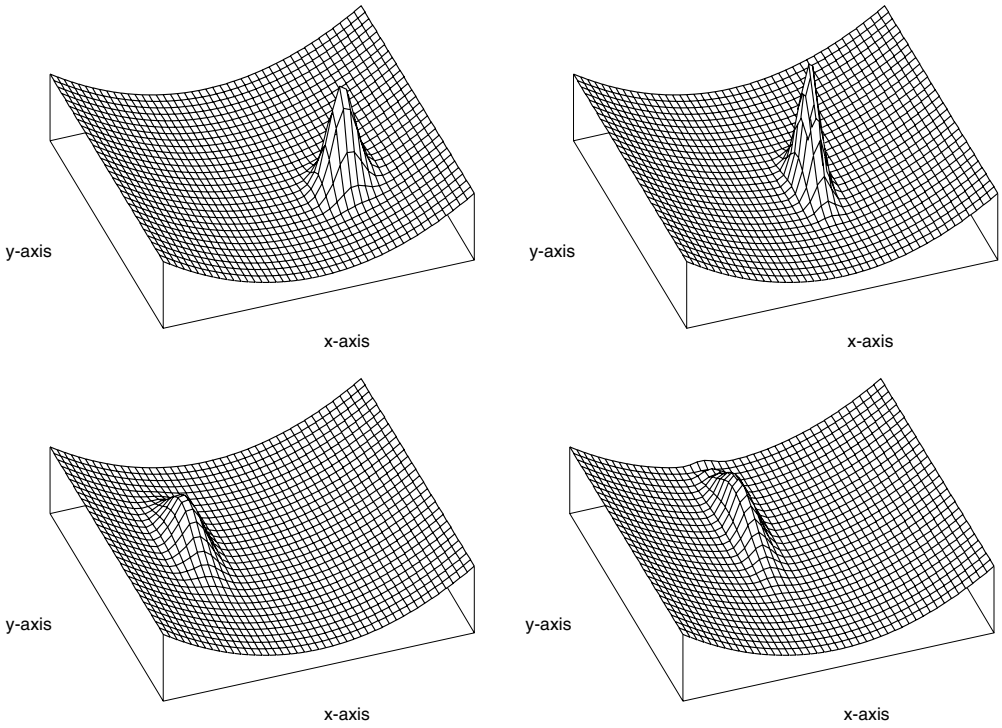

Fig. 27.3 The probability density as a function of x and y of an electron confined to a 2D parabolic "tube." The electron's initial localization is described by a Gaussian wave packet in both the x and y directions. The times are 100, 300, and 500.

27.2.1 Algorithm for 2D Schrödinger Equation

One way to develop an algorithm for solving the time-dependent Schrödinger equation in two dimensions is to extend the 1D algorithm. Rather than do that, we apply quantum theory directly to obtain a more powerful algorithm. First we note that Eq. (27.10) can be integrated in a formal sense [30, p. 4] to obtain the operator solution:

$$\psi(x,y,t) \;=\; U(t)\psi(x,y,t=0) = e^{-i\tilde{H}t}\psi(x,y,t=0) \tag{27.12}$$

$$\tilde{H} \;=\; -\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+V(x,y) \tag{27.13}$$

From this formal solution we deduce that a wave packet can be moved ahead by a time Δt with the action of the time evolution operator:

$$\psi(t+\Delta t) = U(\Delta t)\psi(t) \qquad\qquad U(\Delta t) = e^{-i\tilde{H}\Delta t} \tag{27.14}$$

If the operator U was known exactly, it would provide the exact advance of the solution by one time step:

$$\psi_{i,j}^{n+1} = U(\Delta t)\psi_{i,j}^{n} \qquad \psi_{i,j}^{n} \stackrel{\text{def}}{=} \psi(i\Delta x, j\Delta y, n\Delta t) \tag{27.15}$$

where the superscripts denote time and the subscripts denote the two spatial variables. Likewise, the inverse of the time evolution operator moves the solution back one time step:

$$\psi^{n-1} = U^{-1}(\Delta t)\psi^{n} = e^{+i\tilde{H}\Delta t}\psi^{n} \tag{27.16}$$

While it would be nice to have an algorithm based on a direct application of (27.15), the references show that the resulting algorithm is not stable. That being so, we base our algorithm on an indirect application [81], namely, the relation between the difference in ψ^{n+1} (27.15) and ψ^{n-1} (27.16):

$$\psi^{n+1} = \psi^{n-1} + [e^{-i\tilde{H}\Delta t} - e^{i\tilde{H}\Delta t}]\psi^{n} \tag{27.17}$$

where the difference in sign of the exponents is to be noted. The algorithm derives from combining the $O(\Delta x^2)$ expression for the second derivative obtained from the Taylor expansion,

$$\frac{\partial^2\psi}{\partial x^2} \simeq -\frac{1}{2}\left[\psi_{i+1,j}^{n} + \psi_{i-1,j}^{n} - 2\psi_{i,j}^{n}\right] \tag{27.18}$$

with the corresponding-order expansion of the evolution equation (27.17). When the resulting expression for the second derivative is substituted into the 2D time-dependent Schrödinger equation, there results[1]

$$\psi_{i,j}^{n+1} = \psi_{i,j}^{n-1} - 2i\left[\left(4\alpha + \tfrac{1}{2}\Delta t V_{i,j}\right)\psi_{i,j}^{n} - \alpha\left(\psi_{i+1,j}^{n} + \psi_{i-1,j}^{n} + \psi_{i,j+1}^{n} + \psi_{i,j-1}^{n}\right)\right]$$

where again $\alpha = \Delta t/2(\Delta x)^2$. We convert this complex equations into coupled real equations by substituting in the real and imaginary parts of the wave function, $\psi = R + iI$,

$$\begin{aligned} R_{i,j}^{n+1} &= R_{i,j}^{n-1} + 2\left[\left(4\alpha + \tfrac{1}{2}\Delta t V_{i,j}\right) I_{i,j}^{n} - \alpha\left(I_{i+1,j}^{n} + I_{i-1,j}^{n} + I_{i,j+1}^{n} + I_{i,j-1}^{n}\right)\right] \\ I_{i,j}^{n+1} &= I_{i,j}^{n-1} - 2\left[\left(4\alpha + \tfrac{1}{2}\Delta t V_{i,j}\right) R_{i,j}^{n} + \alpha\left(R_{i+1,j}^{n} + R_{i-1,j}^{n} + R_{i,j+1}^{n} + R_{i,j-1}^{n}\right)\right] \end{aligned} \tag{27.19}$$

This is the algorithm we use to integrate the 2D Schrödinger equation. To determine the probability, we use the same expression (27.9) as used in 1D.

[1] For reference sake, note that the constants in the equation change as the dimension of the equation change; that is, there will be different constants for the 3D equation, and therefore our constants are different from the references!

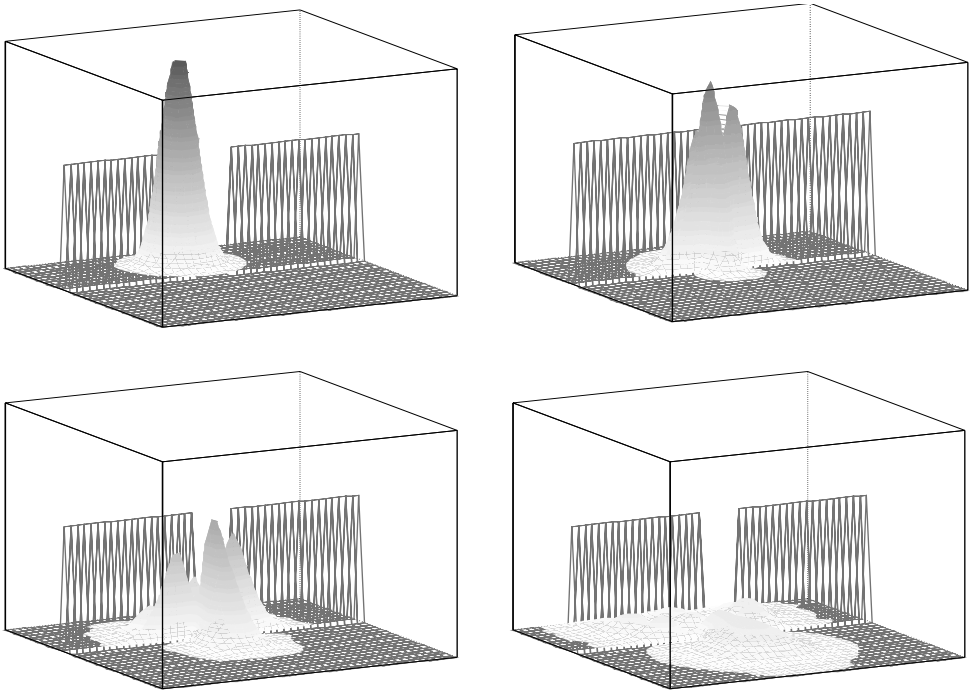

Fig. 27.4 The probability density as a function of position and time for an electron incident upon and passing through a slit.

27.2.1.1 **Exploration: Bound and Diffracted 2D Packet**

• Determine the motion of a 2D Gaussian wave packet within the 2D harmonic oscillator potential:

$$V(x,y) = 0.3(x^2+y^2) \qquad -9.0 \le x \le 9.0 \qquad -9.0 \le y \le 9.0 \quad (27.20)$$

Center the initial wave packet at $(x,y) = (3.0,-3)$, and give it momentum $(k_{0x},k_{0y}) = (3.0,1.5)$.

• Young's single-slit experiment has a wave passing through a small slit, which causes the emerging wavelets to interfere with each other. In quantum mechanics, where we represent a particle by a wave packet, this means that an interference pattern should be formed when a particle passes through a small slit. Consider a Gaussian wave packet of initial width 3 incident on a slit of width 5 (Fig. 27.4). See if you can find quantum interference effects in your solution.