The Schrödinger equation

The one-dimensional Schrödinger equation for a free particle is

$$ik\frac{\partial^2\psi(x,t)}{\partial x^2} = \frac{\partial\psi(x,t)}{\partial t},$$

where $k > 0$ is a constant (involving Planck's constant and the mass of the particle) and $i = \sqrt{-1}$ as usual. The solution ψ is called the *wave function* describing instantaneous "state" of the particle. For the analog in 3 dimensions (which is the one actually used by physicists - the one-dimensional version we are dealing with is a simplified mathematical model), one can interpret the square of the absolute value of the wave function as the probability density function for the particle to be found at a point in space. In other words, $|\psi(x,t)|^2 \, dx$ is the probability of finding the particle in the "volume dx" surrounding the position x, at time t.

If we restrict the particle to a "box" then (for our simplied one-dimensional quantum-mechanical model) we can impose a boundary condition of the form

$$\psi(0,t) = \psi(L,t) = 0,$$

and an initial condition of the form

$$\psi(x,0) = f(x), \qquad 0 < x < L.$$

Here f is a function (sometimes simply denoted $\psi(x)$) which is normalized so that

$$\int_0^L |f(x)|^2 \, dx = 1.$$

If $|\psi(x,t)|^2$ represents a pdf of finding a particle "at x" at time t then $\int_0^L |f(x)|^2 \, dx$ represents the probability of finding the particle somewhere in the "box" initially, which is of course 1.

Method:

- Find the sine series of $f(x)$:

$$f(x) \sim \sum_{n=1}^{\infty} b_n(f) \sin(\frac{n\pi x}{L}),$$

- The solution is

$$\psi(x,t) = \sum_{n=1}^{\infty} b_n(f)\sin(\frac{n\pi x}{L})\exp(-ik(\frac{n\pi}{L})^2 t).$$

Each of the terms

$$\psi_n(x,t) = b_n \sin(\frac{n\pi x}{L})\exp(-ik(\frac{n\pi}{L})^2 t).$$

is called a *standing wave* (though in this case sometimes b_n is chosen so that $\int_0^L |\psi_n(x,t)|^2\,dx = 1$).

Example:
Let

$$f(x) = \begin{cases} -1, & 0 \le x \le 1/2, \\ 1, & 1/2 < x < 1. \end{cases}$$

Then $L = 1$ and

$$b_n(f) = \frac{2}{1}\int_0^1 f(x)\sin(\frac{n\pi x}{1})dx = \frac{1}{n\pi}(-1 + 2\cos(\frac{n\pi}{2}) - \cos(n\pi)).$$

Thus

$$\begin{aligned} f(x) &\sim b_1(f)\sin(\pi x) + b_2(f)\sin(2\pi x) + ... \\ &= \textstyle\sum_n \frac{1}{n\pi}(-1 + 2\cos(\frac{n\pi}{2}) - \cos(n\pi)) \cdot \sin(n\pi x)\ . \end{aligned}$$

Taking more and more terms gives functions which better and better approximate $f(x)$. The solution to Schrödinger's equation, therefore, is

$$\psi(x,t) = \sum_{n=1}^{\infty} \frac{1}{n\pi}(-1 + 2\cos(\frac{n\pi}{2}) - \cos(n\pi)) \cdot \sin(n\pi x) \cdot \exp(-ik(n\pi)^2 t).$$

Explanation:
Where does this solution come from? It comes from the method of separation of variables and the superposution principle. Here is a short explanation.

First, assume the solution to the PDE $ik\frac{\partial^2\psi(x,t)}{\partial x^2} = \frac{\partial\psi(x,t)}{\partial t}$ has the "factored" form

$$\psi(x,t) = X(x)T(t),$$

for some (unknown) functions X, T. If this function solves the PDE then it must satisfy $kX''(x)T(t) = X(x)T'(t)$, or

$$\frac{X''(x)}{X(x)} = \frac{1}{ik}\frac{T'(t)}{T(t)}.$$

Since x, t are independent variables, these quotients must be constant. In other words, there must be a constant C such that

$$\frac{T'(t)}{T(t)} = ikC, \quad X''(x) - CX(x) = 0.$$

Now we have reduced the problem of solving the one PDE to two ODEs (which is good), but with the price that we have introduced a constant which we don't know, namely C (which maybe isn't so good). The first ODE is easy to solve:

$$T(t) = A_1 e^{ikCt},$$

for some constant A_1. It remains to "determine" C.

Case $C > 0$: Write (for convenience) $C = r^2$, for some $r > 0$. The ODE for X implies $X(x) = A_2 \exp(rx) + A_3 \exp(-rx)$, for some constants A_2, A_3. Therefore

$$\psi(x,t) = A_1 e^{-ikr^2t}(A_2 \exp(rx) + A_3 \exp(-rx)) = (a \exp(rx) + b \exp(-rx))e^{-ikr^2t},$$

where A_1A_2 has been renamed a and A_1A_3 has been renamed b. This will not match the boundary conditions unless a and b are both 0.

Case $C = 0$: This implies $X(x) = A_2 + A_3x$, for some constants A_2, A_3. Therefore

$$\psi(x,t) = A_1(A_2 + A_3x) = a + bx,$$

where A_1A_2 has been renamed a and A_1A_3 has been renamed b. This will not match the boundary conditions unless a and b are both 0.

Case $C < 0$: Write (for convenience) $C = -r^2$, for some $r > 0$. The ODE for X implies $X(x) = A_2 \cos(rx) + A_3 \sin(rx)$, for some constants A_2, A_3. Therefore

$$\psi(x,t) = A_1 e^{-ikr^2 t}(A_2 \cos(rx) + A_3 \sin(rx)) = (a \cos(rx) + b \sin(rx)) e^{-ikr^2 t},$$

where A_1A_2 has been renamed a and A_1A_3 has been renamed b. This will not match the boundary conditions unless $a = 0$ and $r = \frac{n\pi}{L}$

These are the solutions of the heat equation which can be written in factored form. By superposition, "the general solution" is a sum of these:

$$\begin{aligned} \psi(x,t) &= \sum_{n=1}^{\infty}(a_n \cos(r_n x) + b_n \sin(r_n x)) e^{-ikr_n^2 t} \\ &= b_1 \sin(r_1 x) e^{-ikr_1^2 t} + b_2 \sin(r_2 x) e^{-ikr_2^2 t} + ..., \end{aligned} \quad (1)$$

for some b_n, where $r_n = \frac{n\pi}{L}$. Note the similarity with Fourier's solution to the heat equation.

There is one remaining condition which our solution $\psi(x,t)$ must satisfy. We have not yet used the IC $\psi(x,0) = f(x)$. We do that next.

Plugging $t = 0$ into (1) gives

$$f(x) = \psi(x,0) = \sum_{n=1}^{\infty} b_n \sin(\frac{n\pi}{L}x) = b_1 \sin(\frac{\pi}{L}x)) + b_2 \sin(\frac{2\pi}{L}x)) + ... \ .$$

In other words, if $f(x)$ is given as a sum of these sine functions, or if we can somehow express $f(x)$ as a sum of sine functions, then we can solve Schrödinger's equation. In fact there is a formula for these coefficients b_n:

$$b_n = \frac{2}{L}\int_0^L f(x) \cos(\frac{n\pi}{L}x) dx.$$

It is this formula which is used in the solutions above.

Written by wdj, last updated 3-9-2007.