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 \( \psi \) 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 simplified 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

\[ \psi(x,0) = f(x), \quad 0 < x < L. \]

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 \( f(x) \):

\[ f(x) \sim \sum_{n=1}^{\infty} b_n(f) \sin \left( \frac{n\pi x}{L} \right), \]
The solution is

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

Each of the terms

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

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

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

Then \( L = 1 \) and

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

Thus

\[ f(x) \sim b_1(f) \sin(n\pi x) + b_2(f) \sin(2n\pi x) + ... \]

\[ = \sum_{n=1}^{\infty} \frac{1}{n\pi} (-1 + 2 \cos\left(\frac{n\pi}{2}\right) - \cos(n\pi)) \cdot \sin(n\pi x). \]

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

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

Explanation:
Where does this solution come from? It comes from the method of separation of variables and the superposition 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 $X(x) = A_2 + A_3 x$, for some constants $A_2, A_3$. Therefore

$$\psi(x,t) = A_1(A_2 + A_3 x) = a + bx,$$

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

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

where $A_1 A_2$ has been renamed $a$ and $A_1 A_3$ 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:

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

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.