The time-independent Schroedinger equation

A very important special case of the Schroedinger equation is the situation when the potential energy term does not depend on time. In fact, this particular case will cover most of the problems that we'll encounter in EE 439.

As the name implies, this is the situation when the potential depends only on position. (Could be a constant.)

If $U(x,t) = U(x)$, then the Schroedinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t) = i\hbar\frac{\partial \Psi(x,t)}{\partial t}$$

Separation of variables

With U independent of time, it becomes possible to use the technique of “separation of variables”, in which the wave function is written as the product of two functions, each of which is a function of only one variable.

$$\Psi(x,t) = \psi(x)\,\chi(t)$$

Inserting the product into the Schroedinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\left[\psi(x)\,\chi(t)\right]}{\partial x^2} + U(x)\left[\psi(x)\,\chi(t)\right] = i\hbar\frac{\partial\left[\psi(x)\,\chi(t)\right]}{\partial t}$$

Simplifying the derivatives:

$$-\frac{\hbar^2}{2m}\chi(t)\,\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\,\psi(x)\,\chi(t) = i\hbar\psi(x)\,\frac{\partial\left[\chi(t)\right]}{\partial t}$$

Re-arranging a bit

$$-\frac{\hbar^2}{2m}\left[\frac{1}{\psi(x)}\right]\frac{\partial^2\psi(x)}{\partial x^2}+U(x)=i\hbar\left[\frac{1}{\chi(t)}\right]\frac{\partial\chi(t)}{\partial t}$$

This is an interesting form, because we have separated the variables to opposite sides of the equation. The left-hand side is a function of position only and the right-hand side is a function of time only.

Key concept!

The only way that this can work out is if both sides are equal to a constant value.

$$-\frac{\hbar^2}{2m}\left[\frac{1}{\psi(x)}\right]\frac{\partial^2\psi(x)}{\partial x^2}+U(x)=i\hbar\left[\frac{1}{\chi(t)}\right]\frac{\partial\chi(t)}{\partial t}=E$$

The constant E has units of energy

One equation becomes two:

$$-\frac{\hbar^2}{2m}\left[\frac{1}{\psi(x)}\right]\frac{\partial^2\psi(x)}{\partial x^2}+U(x)=E \qquad i\hbar\left[\frac{1}{\chi(t)}\right]\frac{\partial\chi(t)}{\partial t}=E$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+U(x)\psi(x)=E\psi(x) \qquad i\hbar\frac{\partial\chi(t)}{\partial t}=E\chi(t)$$

Note that each of these has the form of an eigenfunction / eigenvalue equation.

$$\widehat{H}\psi(x)=E\psi(x) \qquad \widehat{E}\chi(t)=E\chi(t)$$

where

$$\widehat{H}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x)$$

Hamiltonian

the energy operator!

The separation constant, E, represents the total energy of the particle.

Working with a time-independent problem

1. Insert the time-independent potential energy function into the Hamiltonian to set up the spatial part of the problem.

$$-\frac{\hbar^2}{2m}\left[\frac{1}{\psi(x)}\right]\frac{\partial^2\psi(x)}{\partial x^2} + U(x) = E$$

2. Solve the equation to find the forms for the functions and the corresponding energies.

$$\psi_1(x), E_1 \qquad \psi_2(x), E_2 \qquad \psi_3(x), E_3 \qquad \text{etc.}$$

The functions are known as “stationary states”. The energies are the eigenenergies, one for each of the states.

3. Solve the temporal equation to find the time-dependence.

Time dependence

All time-independent problems have the same time dependence.

$$i\hbar \frac{\partial \chi(t)}{\partial t} = E\chi(t)$$

Does not depend on U.

This is easily solved by integrating.

$$\frac{d\chi}{\chi} = \frac{E}{i\hbar} dt$$

$$\ln(\chi) = -i\left(\frac{E}{\hbar}\right) t$$

$$\chi(t) = \exp\left[-i\left(\frac{E}{\hbar}\right) t\right] = e^{-i\omega t}$$

A simple harmonic oscillation in time with frequency ω, which is determined by the energy of the particular state.

Probability density

$$\Psi(x,t) = \psi(x)\exp(-i\omega t)$$

$$P(x,t) = \Psi^*(x,t)\,\Psi(x,t)$$

$$= \psi^*(x)\,e^{+i\omega t}\psi(x)\,e^{-i\omega t}$$

$$= \left[\psi^*(x)\,\psi(x)\right]\left[e^{+i\omega t}e^{-i\omega t}\right]$$

$$= \psi^*(x)\,\psi(x)$$

The probability density is independent of time, even though the wave function itself is not. Not surprising. As we said earlier, the physical properties of the particular described by the wave function will mirror the properties of the potential energy that defines the problem.

The free electron

Free electron, $U = 0$. In this case, the the time-independent Schroedinger equation (TISE) becomes

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} = E\psi(x)$$

Re-arranging

$$\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$$

$$\frac{\partial^2\psi(x)}{\partial x^2} + k^2\psi(x) = 0 \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

Solutions:

$$\psi_+(x) = Ae^{ikx} \qquad \psi_-(x) = Be^{-ikx}$$

Complete wave-functions

$$\Psi_+(x,t) = Ae^{+ikx}e^{-i\omega t} = Ae^{i(kx-\omega t)}$$ plane wave to the right ($+x$)

$$\Psi_-(x,t) = Be^{-ikx}e^{-i\omega t} = Be^{i(-kx-\omega t)}$$ plane wave to the left ($-x$)

In general

$$\Psi(x,t) = Ae^{i(kx-\omega t)} + Be^{i(-kx-\omega t)}$$

Values for A and B will be determined using boundary conditions.

Note: There is no restriction on energy. In free particle problem, we assume that we know the energy of the particle. The energy then determines k and ω.

$$E = \frac{(\hbar k)^2}{2m}$$

The parabolic *E*-*k* is indicative of a free electron. This is analogous to the classical result ($E = p^2/2m$)