Solving the Schrodinger Equation

Time-dependent Schrödinger equation

The wave function of a particle undergoing a force **F(x)** is the solution to the Schrödinger equation:

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

U(x) is the **potential energy** associated with the force:

$$F = -\frac{\partial U}{\partial x}$$

Solving the Schrodinger Equation

Time-dependent Schrödinger equation: Separation of variables

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

Since U(x) does not depend on time, solutions can be written in **separable** form as a part that is only position dependent and a part that is only time dependent:

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

Inserting this into the above equation, we get

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

Solving the Schrodinger Equation

Time-dependent Schrödinger equation: Separation of variables

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

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

Dividing by $\psi(x,t)$,

$$\frac{i\hbar}{\chi(t)}\frac{\partial}{\partial t}\chi(t) = -\frac{1}{\phi(x)}\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi(x) + U(x)$$

Left hand side (LHS) is a function of t alone
Right hand side (RHS) is a function of x alone

LHS=RHS only if **LHS = E** and **RHS = E** (E is a constant)

Solving the Schrodinger Equation

Time-dependent Schrödinger equation: Separation of variables

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

$$\frac{i\hbar}{\chi(t)}\frac{\partial}{\partial t}\chi(t) = -\frac{1}{\phi(x)}\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi(x) + U(x)$$

LHS=RHS only if LHS = E and RHS = E (E is a constant)

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

$$-\frac{1}{\phi(x)}\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) + U(x) = E$$

Solving the Schrodinger Equation

Time-dependent Schrödinger equation: Separation of variables

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

Solutions for the time-dependent equation:

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

$$\chi(t) = e^{-i\omega t}, \quad \omega = \frac{E}{\hbar}$$

Check:

$$\frac{d}{dt}\chi(t) = -\frac{iE}{\hbar}e^{-\frac{i}{\hbar}Et} \Rightarrow i\hbar\frac{d}{dt}\chi(t) = Ee^{-\frac{i}{\hbar}Et} = E\chi(t)$$

Stationary States

Time-dependent Schrödinger equation: Separation of variables

$$\psi(x,t) = \phi(x)\chi(t) = \phi(x)e^{-\frac{i}{\hbar}Et}$$

Notice that

$$P(x,t) = |\psi(x,t)|^2 = |\phi(x)\chi(t)|^2 = |\phi(x)|^2 = |\psi(x,0)|^2$$

Notice also that for any operator,

$$\langle O(x,p)\rangle = \int \psi^*(x,t)O(x,p)\psi(x,t)dx = \int \phi^*(x)O(x,p)\phi(x)dx$$

These separable solutions are called **stationary states** because the corresponding probability function is stationary in time, and hence no observable quantity changes in time.

Stationary States

Time-dependent Schrödinger equation: Separation of variables

$$\psi(x,t) = \phi(x)\chi(t) = \phi(x)e^{-\frac{i}{\hbar}Et}$$

What is the mean and variance of the total energy?

$$\langle H(x,p)\rangle = \int \phi^*(x)H(x,p)\phi(x)dx$$

But

$$H(x,p)\phi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi(x) + U(x)\phi(x) = E\phi(x)$$

Therefore

$$\langle H(x,p)\rangle = \int \phi^*(x)H(x,p)\phi(x)dx = \int \phi^*(x)E\phi(x)dx = E\int \phi^*(x)\phi(x)dx = E$$

Stationary States

Time-dependent Schrödinger equation: Separation of variables

$$\psi(x,t) = \phi(x)\chi(t) = \phi(x)e^{-\frac{i}{\hbar}Et}$$

What is the mean and variance of the total energy?

$$\left\langle H^2(x,p)\right\rangle = \int \phi^*(x)H^2(x,p)\phi(x)dx$$

But $H(x,p)\phi(x) = E\phi(x)$

So

$$H^2(x,p)\phi(x) = H(x,p)\left[H(x,p)\phi(x)\right] = H(x,p)E\phi(x) = EH(x,p)\phi(x) = E^2\phi(x)$$

Therefore

$$\left\langle H^2(x,p)\right\rangle = \int \phi^*(x)H^2(x,p)\phi(x)dx = \int \phi^*(x)E^2\phi(x)dx = E^2\int \phi^*(x)\phi(x)dx = E^2$$

Stationary States

Time-dependent Schrödinger equation: Separation of variables

$$\psi(x,t) = \phi(x)\chi(t) = \phi(x)e^{-\frac{i}{\hbar}Et}$$

What is the mean and variance of the total energy?

$$\langle H(x,p)\rangle = E \qquad \langle H^2(x,p)\rangle = E^2$$

$$\sigma_H = \sqrt{\langle H^2(x,p)\rangle - \langle H(x,p)\rangle^2} = 0$$

There is no spread of energies in a stationary (separable) state.
Every measurement of energy gives exactly the same value.
Stationary states are called energy eigenstates. (more on this later).

Stationary States

Time-dependent Schrödinger equation: Separation of variables

$$\psi(x,t) = \phi(x)\chi(t) = \phi(x)e^{-\frac{i}{\hbar}Et}$$

Any linear combination of stationary states (each with a different allowed energy of the system) is also a valid solution of the Schrodinger equation

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n \phi_n(x) e^{-\frac{i}{\hbar}E_n t}$$

In fact all possible solutions to the Schrodinger equation can be written in this way.

This gives us a recipe for finding the wave function $\psi(x,t)$ at time given the wave function at time t=0 , $\psi(x,0)$ and the potential U(x)….

Stationary States

Recipe for finding the wave function ψ(x,t) at time given the wave function at time t=0 , ψ(x,0), and the potential U(x)….

1. Solve the time independent Schrodinger equation to find the set of energy eigenstates $\varphi_1(x)$, $\varphi_2(x)$ ….each with corresponding energy eigenvalues E_1, E_2…
2. Rewrite the initial wave function in terms of these solutions:

$$\psi(x,0) = \sum_{n=1}^{\infty} c_n \phi_n(x)$$

3. Then the wave function at later times is simply

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n \phi_n(x) e^{-\frac{i}{\hbar}E_n t}$$

Thus if we can find the stationary states of a particular potential U(x) (i.e, $\varphi_1(x)$, $\varphi_2(x)$…and E_1, E_2…), we are done!