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 Schrödinger 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 Schrödinger 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 \( \text{LHS} = E \) and \( \text{RHS} = E \) (\( E \) is a constant)
Solving the Schrödinger 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)
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**

\[ \psi(x,t) = \phi(x)\chi(t) = \phi(x)e^{-\frac{iEt}{\hbar}} \]

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

\[ \psi(x,t) = \phi(x) \chi(t) = \phi(x)e^{\frac{-iEt}{\hbar}} \]

What is the mean and variance of the total energy?

\[ \langle H(x,p) \rangle = \int \phi^\ast(x)H(x,p)\phi(x)dx \]

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

\[ \langle H(x,p) \rangle = \int \phi^\ast(x)H(x,p)\phi(x)dx = \int \phi^\ast(x)E\phi(x)dx = E \int \phi^\ast(x)\phi(x)dx = E \]
Stationary States

Time-dependent Schrödinger equation: Separation of variables

\[ \psi(x,t) = \phi(x)\chi(t) = \phi(x)e^{-\frac{iEt}{\hbar}} \]

What is the mean and variance of the total energy?

\[ \langle H^2(x,p) \rangle = \int \phi^*(x)H^2(x,p)\phi(x)dx \]

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

So

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

Therefore

\[ \langle H^2(x,p) \rangle = \int \phi^*(x)H^2(x,p)\phi(x)dx = \int \phi^*(x)E^2\phi(x)dx = E^2 \int \phi^*(x)\phi(x)dx = E^2 \]
Stationary States

Time-dependent Schrödinger equation: Separation of variables

\[ \psi(x,t) = \phi(x) \chi(t) = \phi(x) e^{\frac{-iE_t}{\hbar}} \]

What is the mean and variance of the total energy?

\[ \langle H(x, p) \rangle = E \quad \langle H^2(x, p) \rangle = E^2 \]

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

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

\[ \psi(x,t) = \phi(x) \chi(t) = \phi(x) e^{-\frac{i E_t}{\hbar}} \]

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

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

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 $\psi(x,t)$ at time given the wave function at time $t=0$, $\psi(x,0)$, and the potential $U(x)$.

1. Solve the time independent Schrodinger equation to find the set of energy eigenstates $\phi_1(x)$, $\phi_2(x)$ ... 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

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

Thus if we can find the stationary states of a particular potential $U(x)$ (i.e, $\phi_1(x)$, $\phi_2(x)$...and $E_1$, $E_2$...), we are done!