Lecture 5.4: The Schrödinger equation

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Some history

Newton's second law of motion, $mx''(t) = F(x)$, fails on the atomic scale.

According to quantum mechanics, particles have no definite position or velocity. Instead, their states are described probabilistically by a wave function $\Psi(x, t)$, where

$$\int_a^b |\Psi(x,t)|^2 \, dx = \text{Probability of the particle being in } [a, b] \text{ at time } t.$$

Motivation

The wave function is governed by the following PDE, called Schrödinger's equation:

$$i\hbar\Psi_t = -\frac{\hbar^2}{2m}\Psi_{xx} + V(x)\Psi,$$

where $V(x) =$ potential energy, $m =$ mass, and $\hbar = \frac{h}{2\pi}$, where $h \approx 6.625 \cdot 10^{-34}$ kg m^2/s is Planck's constant. The linear operator $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$ is the Hamiltonian.

The special case of $V = 0$ (free particle subject to no forces) is the free Schrödinger equation

$$i\hbar\Psi_t = -\frac{\hbar^2}{2m}\Psi_{xx}.$$

Solving the Schrödinger equation

To solve $i\hbar\Psi_t = H\Psi$, i.e.,

$$i\hbar\Psi_t = -\frac{\hbar^2}{2m}\Psi_{xx} + V(x)\Psi,$$

assume that $\Psi(x,t) = f(x)g(t)$.

The infinite potential well

Example

The wave function of a free particle of mass m confined to $0 < x < L$ is described by the boundary value problem

$$i\hbar\Psi_t = -\frac{\hbar^2}{2m}\Psi_{xx}, \qquad \Psi(0,t) = \Psi(L,t) = 0.$$

Summary

Consider the Schrödinger equation on a bounded domain,

$$i\hbar\Psi_t = -\frac{\hbar^2}{2m}\Psi_{xx} + V(x)\Psi, \qquad 0 < x < L.$$

For each $n = 1, 2, \dots,$ we have a solution of the form

$$\Psi_n(x,t) = f_n(x)e^{-iE_n t/\hbar}, \qquad E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2}$$

where $f_n(x)$ solves the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{f_n''}{f_n} + V(x) = E.$$

The solution is the superposition and time-evolution given by

$$\Psi(x,t) = \sum_{n=1}^{\infty} f_n(x)e^{-iE_n t/\hbar}, \qquad \text{and} \qquad \int_0^L |\Psi(x,t)|^2\,dx = 1.$$

In the special case of the free Schrödinger equation ($V(x) = 0$) and the infinite potential well, this becomes

$$\Psi(x,t) = \sum_{n=1}^{\infty} b_n \sin\left(\tfrac{n\pi x}{L}\right) e^{-iE_n t/\hbar}.$$