Lecture 5.4: The Schrödinger equation

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Some history

Newton's second law of motion, $m\frac{d^2x}{dt^2} = F(x)$, 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 goverened 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 $\hbar = h/(2\pi)$, where $h \approx 6.625 \cdot 10^{-34}$ kg m^2/s is Planck's constant.

The special case, when $V = 0$ (free particle subject to no forces), and $m = 1$, and $\hbar = 1$ ("atomic units") is the free Schrödinger equation

$$\Psi_t = \frac{i}{2}\Psi_{xx}.$$

Solving the Schrödinger equation by separating variables

To solve

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

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

A boundary value problem for the free Schrödinger equation

Example

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

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