11.6: Schrödinger's Equation

Quantum mechanics is the study of microscopic systems such as electrons or atoms. Calculus of variations and the idea of a Hamiltonian are fundamental ideas of quantum mechanics [136]. In Chapter 13, we apply the ideas of calculus of variations to an individual atom in a semiclassical way.

We can never say with certainty where an electron or other microscopic particle is located or its energy. However, we can discuss the probability of finding it with a specific energy. The probability of finding an electron, for example, in a particular energy state is specified by \(|\psi|^2\) where \(|\psi\rangle\) is called the wave function [136]. As with any probability \(0 \leq |\psi|^2 \leq 1\).

For example, suppose that as an electron moves, kinetic energy is converted to potential energy. The quantum mechanical Hamiltonian \(H_{QM}\) is then the sum of the kinetic energy \(E_{\text{kinetic}}\) and potential energy \(E_{\text{potential}}\).

\[
H_{QM} = E_{\text{kinetic}} + E_{\text{potential}}
\]

Kinetic energy is expressed as

\[
E_{\text{kinetic}} = \frac{1}{2m} (M_{QM})^2
\]

where \(m\) is the mass of an electron. In the expression above, \((M_{QM})\) is the quantum mechanical momentum operator, and

\[
(M_{QM})^2 = (M_{QM}) \cdot (M_{QM})
\]

The quantum mechanical momentum operator is defined by
where the quantity \( \hbar \) is the Planck constant divided by \( 2\pi \). The del operator, \( \nabla \), was introduced in Sec. 1.6.1, and it represents the spatial derivative of a function. The quantities \( H_{QM} \), \( M_{QM} \), and \( \nabla \) are all operators, not just values. An operator, such as the derivative operator \( \frac{d}{dt} \), acts on a function. It itself is not a function or value.

Using the of momentum definition of Equation \ref{11.6.4} and the vector identity of Equation 1.6.8, we can rewrite the Hamiltonian.

\[
[H_{QM} = \frac{-\hbar^2}{2m} \nabla^2 + E_{\text{potential\, energy}}]
\]

In quantum mechanics, the Hamiltonian is related to the total energy.

\[
[H_{QM}] \psi = E_{\text{total}} \psi
\]

The above two equations can be combined algebraically.

\[
\left( \frac{-\hbar^2}{2m} \nabla^2 + E_{\text{potential\, energy}} \right) \psi = E_{\text{total}} \psi \label{11.6.7}
\]

With some more algebra, Equation \ref{11.6.7} can be rewritten.

\[
\nabla^2 \psi + \frac{2m}{\hbar^2} \left( E_{\text{total}} - E_{\text{potential\, energy}} \right) \psi = 0 \label{11.6.8}
\]

Equation \ref{11.6.8} is the time independent Schrödinger equation, and it is one of the most fundamental equations in quantum mechanics. Energy level diagrams were introduced in Section 6.2. Allowed energies illustrated by energy level diagrams satisfy the Schrödinger equation. At least for simple atoms and ground state energies, energy level diagrams can be derived by solving Schrödinger equation.