2.2 The Schrödinger Equation

In 1926 and 1927, Schrödinger and Heisenberg published papers on wave mechanics, descriptions of the wwave properties of electrons in atoms, that used very different mathematical techniques. In spite of the different approaches, it was soon shown that their theories were equivalent. Schrödinger's differential equations are more commonly used to introduce the theory, and we will follow that practice.

The Schrödinger equation describes the wave properties of an electron in terms of its position, mass, total energy, and potential energy. The equation is based on the **wave function**, Ψ, which describes an electron wave in space; in other words, it describes an atomic orbital. In its simplest notation, the equation is

$$H\Psi = E\Psi$$

$$H = Hamiltonian\ operator \tag{1}$$

$$E = energy\ of\ the\ electron \tag{2}$$

$$\Psi = wave\ function \tag{3}$$

The **Hamiltonian operator**, frequently called simply the *Hamiltonian*, includes derivatives that **operate** on the wave function.[1] When the Hamiltonian is carried out, the result is a constant(the energy)times Ψ. The operation can be performed on any wave function describing an atomic orbital. Different orbitals have different wave functions and different values of E. This is another way of describing quantization in that each orbital, characterized by its own function Ψ, has a characteristic energy.

In the form used for calculating energy levels, the Hamiltonian operator for oneelectron systems is

$$H = \frac{-h^2}{8\pi^2 m}\left(\frac{\partial^2}{\partial x^2}\frac{\partial^2}{\partial y^2}\frac{\partial^2}{\partial z^2}\right) - \frac{Ze^2}{4\pi\varepsilon_0\sqrt{x^2+y^2+z^2}}$$

This part of the operator describes the *kinetic energy* of the electron, its energy of motion.

This part of the operator describes the *potential energy* of the electron, the result of electrostatic attraction between the electron and the nucleus. It is commonly designated as V.

[1] An *operator* is an instruction or set of instructions that states what to do with the function that follows it. It mmay be a simple instruction such as multiply the following function by 6, or it may be much more complicated than the Hamiltonian.

where

$$
\begin{aligned}
h &= \text{Planck constant} \\
m &= \text{mass of the electron} \\
e &= \text{charge of the electron} \\
\sqrt{x^2+y^2+z^2} \;=\; r &= \text{distance from the nucleus} \\
Z &= \text{charge of the nucleus} \\
4\pi\varepsilon_0 &= \text{permittivity of a vacuum}
\end{aligned}
$$

This operator can be applied to a wave function Ψ,

$$\left[\frac{-h^2}{8\pi^2 m}\left(\frac{\partial^2}{\partial x^2}\frac{\partial^2}{\partial y^2}\frac{\partial^2}{\partial z^2}\right) + V(x,y,z)\right]\Psi(x,y,z) = E\Psi(x,y,z)5$$

where

$$V \;=\; \frac{-Ze^2}{4\pi\varepsilon_0 r} \;=\; \frac{-Ze^2}{4\pi\varepsilon_0\sqrt{x^2+y^2+z^2}}$$

The potential energy V is a result of electrostatic attraction between the electron and the nucleus. Attractive forces, such as those between a positivee nucleus and a negative electron, are defined by convention to have a negative potential energy. An electron near the nucleus (small r) is strongly attracted to the nucleus and has a large negative potential energy. Electrons farther from the nucleus have potential energies that are small and negative. For an electron at infinite distance from the nucleus ($r = \infty$), the attraction between the nucleus and the electron is zero, and the potential energy is zero. The hydrogen atom energy level diagram in Figure 2.2 illustrates these concepts.