Appendix B: The Schrödinger Wave Equation

According to wave mechanics, the behavior of a corpuscle is described by the Schrödinger wave equation in the form

$$\frac{h}{2\pi i}\frac{\partial \psi}{\partial t} = \frac{h^2}{8\pi^2 m}\nabla^2\psi - E_p\psi, \tag{B.1}$$

where ψ denotes the wave function, m is the mass, E_p is the potential energy of the corpuscle, which is a function of position only, and $\nabla^2 = \partial^2/\partial^2 x + \partial^2/\partial^2 y + \partial^2/\partial^2 z$. The quantum-mechanical Hamiltonian operator is defined as

$$H = -\frac{h^2}{8\pi^2 m}\nabla^2 + E_p. \tag{B.2}$$

Thus, we have

$$\frac{h}{2\pi i}\frac{\partial \psi}{\partial t} = -H\psi. \tag{B.3}$$

We may express the wave function as the product of two variables such that

$$\psi(q, t) = \varphi(q)\phi(t), \tag{B.4}$$

where q represents the particle position or coordinate. It follows that

$$\frac{h}{2\pi i}\varphi(q)\frac{d\phi(t)}{dt} = -\phi(t)H\varphi(q). \tag{B.5a}$$

Dividing both sides by $\varphi(q)\,\phi(t)$ yields

$$\frac{h}{2\pi i}\frac{1}{\phi(t)}\frac{d\phi(t)}{dt} = -\frac{1}{\varphi(q)}H\varphi(q) = -E. \tag{B.5b}$$

The left-hand side is a function of t only, but the right-hand side is a function of position q only. It follows that each must be equal to the same constant, which has the dimension of energy. This constant is identified with the total energy of the

particle and is denoted by $-E$. Thus, we obtain two equations from Eq. (B.5b) as follows:

$$\frac{h^2}{8\pi^2 m}\nabla^2\varphi + (E - E_p)\varphi = 0, \tag{B.6}$$

$$\frac{d\phi}{dt} = -\frac{2\pi i}{h}E\phi. \tag{B.7}$$

The solution of the time-dependent equation upon ignoring a constant of integration is

$$\phi = \exp(-2\pi i Et/h). \tag{B.8}$$

Thus, the wave function from Eq. (B.4) is given by

$$\psi(q,t) = \varphi(q)\exp(-2\pi i Et/h), \tag{B.9}$$

where the amplitude of the wave function φ is soluble from Eq. (B.6) only for certain specific values of E, referred to as the eigenvalues. A particular function that satisfies Eq. (B.6) is called the eigenfunction of the problem. The eigenfunctions and eigenvalues depend on the form of the potential energy function E_p of the corpuscle.

For a hydrogen atom in which one electron moves under the Coulomb attraction of the nucleus, the potential energy is given by

$$E_p = -e^2/r, \tag{B.10}$$

where e is the charge of the electron and r is the distance between the electron and the nucleus. Equation (B.6) can then be solved and the eigenvalues of this case are defined by

$$E_n = -R_H hc/n^2, \tag{B.11}$$

where $R_H = 1.097 \times 10^5$ cm^{-1} is the Rydberg constant. See also Eq. (1.3.3).