

# Study Notes on Schrodinger Wave Equation



# Schrodinger Wave Equation

In 1926, Erwin Schrodinger gave a wave equation to describe the behavior of electron waves in atoms and molecules. In Schrodinger's wave model of an atom, the discrete energy levels or orbits proposed, by Bohr are replaced by mathematical functions,  $\Psi$ , which are generally related to the probability of finding electrons at various places around the nucleus.

Consider a simple wave motion like that of the vibration of a stretched string. Let  $y$  be the amplitude of this vibration at any point whose coordinate is  $x$  at time  $t$ . The equation for such a wave motion can be expressed as:

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{u^2} \times \frac{\partial^2 y}{\partial t^2} \quad \dots (1)$$

Here,  $u$  is the velocity with which the wave is propagating. There are two variables,  $x$  and  $t$ , in the above differential equation, i.e., the amplitude  $y$  depends upon two variables  $x$  and  $t$ .

To solve the above differential equation, it is necessary to separate the two variables. "Thus,  $y$  may be expressed as:

$$Y = f(x) g(t) \quad \dots (2)$$

Here,  $f(x)$  is a function of the coordinate  $x$  only and  $g(t)$  is a function of the time  $t$  only. For stationary waves, such as occur in a stretched string, the function  $g(t)$  can be expressed as:

$$g(t) = A \sin (2\pi vt) \quad \dots (3)$$

Here,  $v$  is the vibrational frequency and  $A$  is a constant known as the maximum amplitude. Hence, for stationary waves, the equation for  $y$  may be written as:

$$y = f(x) A \sin (2\pi vt) \quad \dots (4)$$

Hence,

$$\frac{\partial^2 y}{\partial t^2} = -f(x) 4\pi^2 v^2 A \sin(2\pi vt) \quad \dots (5)$$

$$= - 4\pi^2 v^2 f(x)g(t) \quad \dots (6)$$

Similarly,

$$\frac{\partial^2 y}{\partial x^2} = \frac{\partial^2 f(x)}{\partial x^2} g(t) \quad \dots (7)$$

Combining equations 1, 6 and 7,

$$\frac{\partial^2 f(x)}{\partial x^2} = - \frac{4\pi^2 v^2}{v^2} f(x) \quad \dots (8)$$

Also, it is known that the frequency of the vibrations  $v$  is related to the velocity  $u$  by the expression:

$$u = v\lambda$$

Here,  $\lambda$  is the corresponding wavelength. Hence, from 8, we have

$$\frac{\partial^2 f(x)}{\partial x^2} = -\frac{4\pi^2}{\lambda^2} f(x) \quad \dots (9)$$

Equation 9 is valid for the wave motion in one dimension only. The above equation can extend to three dimensions represented by the coordinates  $x$ ,  $y$  and  $z$ . Evidently,  $f(x)$  will then be replaced by the amplitude function for the three coordinates, say,  $\Psi(x, y, z)$ . So, according to this, Equation 9 takes the form:

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} = -\frac{4\pi^2}{\lambda^2} \Psi \quad \dots (10)$$

Incorporating de Broglie's relationship, viz.,  $\lambda = h/mu$ , in above equation, we have

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} = -\frac{4\pi^2 m^2 u^2}{h^2} \Psi \quad \dots (11)$$

Here,  $m$  is the mass and  $u$  is the velocity of the particle.

The kinetic energy of the particle given by  $\frac{1}{2} mu^2$ , is equal to the total energy  $E$  minus the potential energy  $V$  of the particle, i.e.,

$$KE. = \frac{1}{2} mu^2 = E - V. \quad \text{or} \quad mu^2 = 2(E - V) \quad \dots (12)$$

Combining this result with Equation 11, we get

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} + \frac{8\pi^2 m(E - V)}{h^2} \Psi = 0 \quad \dots (13)$$

The above equation is the well-known Schrodinger wave equation.

$$\left[ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V \right] = E\Psi \quad \dots (14)$$

Or 
$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V \right] \Psi = E\Psi \quad (\hbar = h/2\pi) \quad \dots (15)$$

Here,  $\nabla^2$  (read as 'del squared') is the Laplacian operator, defined as:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad \dots (16)$$

Defining the Hamiltonian operator  $\hat{H}$  as:

$$\hat{H} = \frac{-\hbar^2}{2m} \nabla^2 + V, \quad \dots (17)$$

the time independent Schrodinger equation 15 becomes:

$$\hat{H}\psi = E\psi \quad \dots (18)$$

The Schrodinger equation can have several solutions, not all of which correspond to any physical or chemical reality. Such solutions or wave functions are, therefore, not acceptable. The acceptable wave functions must satisfy the following conditions:

1. The wave function  $\Psi$  should be single-valued, i.e., for each value of the variables  $x, y, z$ , there is only one value of  $\Psi$ . Suppose one of the variables is an angle  $\theta$ , then,

$$\Psi(\theta) = \Psi(\theta + 2n\pi)$$

2. The wave function  $\Psi$  and its first derivative with respect to its variables must be continuous, i.e., there must not be any sudden change in  $\Psi$  when its variables get changed.

3. For bound states,  $\Psi$  must vanish at infinity. If  $\Psi$  is a complex function, then  $\Psi^*\Psi$  must vanish at infinity ( $\Psi^*$  is the complex conjugate of  $\Psi$ ).

Satisfying the above conditions, the Schrodinger equation yields significant solutions for certain definite values of the total energy  $E$ . These values are called eigenvalues. Hence, equation 18 is, thus, an eigenvalue equation and can be written as:

$$\hat{H}\psi_n = E_n\psi_n \quad (n = 1, 2, 3, \dots) \quad \dots (19)$$

Here,  $n$  is the quantum number. The above equation can be expressed by saying that  $\psi_n$  are the eigenfunctions and  $E_n$  are the eigenvalues. For an atom, these eigenvalues correspond to discrete sets of energy values postulated by Bohr.

4. The eigenfunctions are said to form an orthonormal set if:

$$\int \psi_n^* \psi_m \, d\tau = \begin{cases} 0, n \neq m \\ 1, n = m \end{cases} = \delta_{nm} \text{ (called the Kronecker delta)} \quad \dots (20)$$

They are orthogonal when  $\int \psi_n^* \psi_m \, d\tau = 0 \quad \dots (21)$

and normalized when  $\int \psi_n^* \psi_m \, d\tau = 1 \quad \dots (22)$

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



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