

7.8: Schrödinger's Equation

If the behaviour of an electron can be described as if it were a wave, then it can presumably be described by the wave Equation:

$$v^2 \nabla^2 \Psi = \ddot{\Psi}. \quad (7.8.1)$$

Here v is the speed of the electron, or, rather, the group velocity of its wave manifestation.

Periodic solutions for Ψ are given by $\ddot{\Psi} = -\omega^2 \Psi$, and, since $\omega = kv$, Equation 7.8.1 can be written in the form

$$\nabla^2 \Psi + k^2 \Psi = 0. \quad (7.8.2)$$

The total energy E is the sum of the kinetic and potential energies $T + V$, and the kinetic energy is $p^2/(2m)$. This, of course, is the nonrelativistic form for the kinetic energy, and you can judge for yourself from the calculation you did just before we arrived at Equation 7.4.5 to what extent this is or is not justified. If, instead of p you substitute the de Broglie expression in the form of Equation 7.7.3, you arrive at Schrödinger's Equation:

$$\nabla^2 \Psi + \frac{2m}{\hbar^2} (E - V) \Psi = 0 \quad (7.8.3)$$

To describe the behaviour of a particle in any particular situation in which it finds itself -e.g. if it found itself confined to the interior of a box, or attached to the end of a spring, or circling around a proton - we have to put in the Equation how V depends on the coordinates. The stationary states of an atom, i.e. its energy levels, are described by standing, rather than progressive, waves, and we have seen that standing waves are described as a product of a function of space and a function of time:

$$\Psi(x, y, z; t) = \psi(x, y, z) \cdot \chi(t). \quad (7.8.4)$$

If you put this into Equation 7.8.3 (all you have to do is to note that $\nabla^2 \Psi = \chi \nabla^2 \psi$ and that $\Psi = \psi \chi$), you find that the time-independent part of Schrödinger's Equation satisfies

$$\nabla^2 \psi + \frac{2m}{\hbar^2} (E - V) \psi = 0. \quad (7.8.5)$$

When we are dealing with time-varying situations - for example, when an atom is interacting with an electromagnetic wave (light), we must use the full Schrödinger Equation 7.8.3. When dealing with stationary states (i.e. energy levels), we deal with the time-independent Equation 7.8.5.

Let's suppose for a moment that we are discussing not something complicated like a hydrogen atom, but just a particle moving steadily along the x -axis with momentum p_x . We'll try and describe it as a progressive wave function of the form

$$\Psi = \text{constant} \times e^{i(kx - \omega t)}. \quad (7.8.6)$$

(That's just a compressed way of writing $a \cos(kx - \omega t) + b \sin(kx - \omega t)$.) This means that

$$\frac{\partial \Psi}{\partial t} = -i\omega \Psi \quad \text{and} \quad \frac{\partial^2 \Psi}{\partial x^2} = -k^2 \Psi. \quad (7.8.7)$$

Now let us use $E = h\nu = \hbar\omega$ and $p = h/\lambda = \hbar k$ as well as the (nonrelativistic, note) relation between kinetic energy and momentum $E = p^2/(2m)$, and we arrive at

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x, t) \Psi. \quad (7.8.8)$$

In three dimensions (i.e. if the particle were not restricted to the x axis but were moving in some arbitrary direction in space), this appears as:

$$i\hbar \dot{\Psi} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(x, y, z; t) \Psi. \quad (7.8.9)$$

This is referred to as Schrödinger's *Time-dependent Equation*.

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