THE SCHRÖDINGER WAVE EQUATION

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + \nabla\Psi = -\frac{\hbar}{j}\frac{\partial\Psi}{\partial t} \quad \textbf{where} \quad \nabla^2\Psi = \frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}$$

This is the Scrödinger Wave Equation in three dimensions. The following concerns a one-dimensional problem where the equation is a function of *x* and *t*. Refer to pp. 38,39 in <u>Solid State Electronic Devices</u>.

THE PROBLEM

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) = -\frac{\hbar}{j}\frac{\partial\Psi(x,t)}{\partial t}$$

THE APPROACH

We are going to solve the equation by breaking it into two equations using the technique of **separation of variables**.

THE SOLUTION

Let $\Psi(x,t)$ be represented by the product $\psi(x)\phi(t)$:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}\phi(t) + V(x)\psi(x)\phi(t) = -\frac{\hbar}{j}\psi(x)\frac{\partial\phi(t)}{\partial t}$$

Now divide the equation by $\psi(x)\phi(t)$. Now the variable *x* appears only on the left and the variable *t* only on the right.

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) = -\frac{\hbar}{j}\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t}$$

Since *x* and *t* are independent variables, this equation is valid only when each side equals a constant, says our instructor. We will call the constant *E*. We lose the partial derivative symbol too.

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} + V(x) = E \qquad \text{[Eq. 1]}$$

$$-\frac{\hbar}{j}\frac{1}{\phi(t)}\frac{d\phi(t)}{dt} = E \qquad \text{[Eq. 2]}$$

Multiplying [Eq. 1] by $-\frac{2m}{\hbar^2}\psi(x)$ and [Eq. 2] by $-\frac{j}{\hbar}\phi(t)$ gives:

$$\frac{d^2\psi(x)}{dx^2} - \frac{2m}{\hbar^2}V(x)\psi(x) = -\frac{2m}{\hbar^2}E\psi(x)$$

$$\frac{d\phi(t)}{dt} = -\frac{j}{\hbar}E\phi(t)$$

Collecting terms on the left side:

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0 \qquad \text{[Eq. 3]}$$

$$\frac{d\phi(t)}{dt} + \frac{jE}{\hbar}\phi(t) = 0 \qquad \text{[Eq. 4]}$$

THE SOLUTION OF [EQ. 4]

[Eq. 4] is a **linear first order differential equation**.

$$\frac{d\phi(t)}{dt} + \frac{jE}{\hbar}\phi(t) = 0 \qquad \text{[Eq. 4]}$$

We multiply the equation by the **integrating factor** $\boxed{e^{\int \frac{jE}{\hbar} dt}}$, which is $e^{jEt/\hbar}$:

$$\frac{d\phi(t)}{dt} e^{jEt/\hbar} + \frac{jE}{\hbar}\phi(t) e^{jEt/\hbar} = 0$$

Discard the center term; this happens somehow by integrating and taking the derivative.

$$\frac{d\phi(t)}{dt} e^{jEt/\hbar} = 0$$

Integrate with respect to t.

$$\int \frac{d\phi(t)}{dt} e^{jEt/\hbar} dt = \int 0 \; dt$$

On the right side we get a **constant**, or **initial condition** ϕ_0.

$$\phi(t) e^{jEt/\hbar} = \phi_0$$

Solve for $\phi(t)$ to get:

$$\phi(t) = \phi_0 e^{-jEt/\hbar}$$

THE ANSWER

The instructor say that we put ϕ_0 into the total normalization constant and assume $\psi_n(x)$ is known corresponding to a certain E_n, and the overall wave function is:

$$\boxed{\Psi_n(x,t) = \psi_n(x) e^{-jE_n t/\hbar}}$$

ABOUT THE VARIABLES

E = the separation constant; corresponds to the energy of the particle when particular solutions are obtained, such that a wave function ψ_n corresponds to a particle energy E_n.

$V(x)$ = potential, usually resulting from an electrostatic or magnetic field. [V]

$\hbar$ = Planck's constant divided by 2π [$J - s$]

t = time [s]

m = quantum number [integer]

∇ = the nabla, del, or grad operator; not a variable