

Exploring the Origin of Schrödinger's Equations

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The purpose of this tutorial is to explore the connections between Schrödinger's equations (time-dependent and time-independent) and prior concepts in classical mechanics and quantum mechanics. For the sake of mathematical simplicity we will work in one spatial dimension.

The foundation of quantum mechanics is de Broglie's hypothesis of wave-particle duality for matter and electromagnetic radiation. Therefore, our starting point is the equation for a classical plane wave moving in the positive x direction,

$$F(x,t) = A \exp\left(i2\pi \frac{x}{\lambda}\right) \exp(-i2\pi \nu t)$$

where λ is wavelength, ν is wave frequency, and A is wave amplitude.

$F(x,t)$ can be converted to a quantum mechanical particle wave function using the relations shown below, which are succinct mathematical expressions of de Broglie's wave-particle hypothesis.

$$\lambda = \frac{h}{p} \quad \text{and} \quad E = h\nu$$

Substitution of these equations into $F(x,t)$ yields,

$$\Psi(x,t) = A \exp\left(\frac{ipx}{\hbar}\right) \exp\left(-\frac{iEt}{\hbar}\right)$$

where $\hbar = h/2\pi$.

The next step is to write the classical expression for the energy of a free particle,

$$E = \frac{p^2}{2m}$$

and ask what operations must be performed on $\Psi(x,t)$ to obtain this equation.

Clearly, with appropriate pre-multipliers, the first derivative with respect to time will yield E , and the second derivative with respect to x will give kinetic energy.

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = E \Psi(x,t)$$

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

We therefore assert that the quantum mechanical equivalent free-particle energy equation is,

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

and name it the time-dependent Schrödinger equation. For a particle subject to a time-independent potential, $V(x)$, we generalize this equation as follows,

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

An elegant expression of this equation, $i\hbar\dot{\psi} = H\psi$, can be found on Schrödinger's tombstone in Alpbach, Austria. Because $V(x)$ is independent of time, we assume $\Psi(x,t)$ is still separable in space and time,

$$\Psi(x,t) = \Psi(x) \exp\left(-\frac{iEt}{\hbar}\right)$$

Substitution of this function into the time-dependent Schrödinger equation allows us to extract the time-independent Schrödinger equation,

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

Solutions to this equation for various $V(x)$ and the appropriate boundary conditions yield, in general, a manifold of allowed energy eigenvalues and associated eigenfunctions.

Sources:

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Edward Gerjuoy, "Quantum Mechanics", in AccessScience@McGraw-Hill, <http://www.accessscience.com>, DOI 10.1036/1097-8542.562900, last modified: 9/11/2002