What is the Schrodinger Equation

The **Schrödinger equation** is a partial differential equation that describes the dynamics of quantum mechanical systems via the wave function.

All of the information for a subatomic particle is encoded within a wave function.

The solution of **Schrödinger equation is** the wavefunctionΨ(r,t)**.**

To know the trajectory, the positioning, and the energy of these systems we need to solve the Schrödinger equation.

Just for curiosity, here is the time-dependent Schrödinger equation in 3-dimensions (for a non-relativistic particle):

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t)=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\vec{r},t)\right]\Psi(\vec{r},t)$$

Why does Schrödinger equation become so necessary?

The experimental results double slit experiment and the photoelectric effectcould not be explained well with the known understanding of classical physics.

But why?

In classical physics there exists two entities, particles and waves. The features of these entities are:

Particles: localised bundles of energy and momentum with mass m.

Waves: disturbances spread over space travelling over time.

Particles and waves follow separate equation in Classical Mechanics.

The Photoelectric Emission gives us surprising results that the electron shows **both** of these properties. This was in complete contradiction with the known understanding of classical physics. Here the two entities were found mutually exclusive.

Somephysicistslike Louis de Broglie associated a momentum (for a particle) to a wavelength (for waves) given by$p = {}^{h}/_{\lambda}$

Also, from Photoelectric Emission we know that there energy absorption and emission of photons (still unsure whether particle or wave) have energy given by: E=hf=$\hbar$w
Where$\hbar = \frac{h}{2\pi}$ and $w = 2\pi f$.

Well, the electrons and photons are showing wave-like and particle-like behaviour. It hints towards the requirement of universal equation that all waves and all particles should obey.That universal equation was later deduced by Schrodinger, and hence so called.

How to derive the Schrodinger Wave Equation

$\Psi(\vec{r},t)$ is the solution of the wave equation containing all information.

We know, the electron displays wave-like behaviour and has an electromagnetic charge. So we must look at electromagnetic fields and Maxwell's equations may be applied .

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\nabla \times \vec{B} = -\mu_0 \left(\vec{J} - \epsilon_0 \frac{\partial \vec{E}}{\partial t} \right)$$

$$\nabla \cdot \vec{E} = \frac{\rho}{\epsilon_0}$$

$$\nabla \cdot \vec{B} = 0$$

Where c is the speed of light in a vacuum, $\vec{E}$ is the electric field and $\vec{B}$ is the magnetic field.

Now, let us derive the equation that any electromagnetic wave must obey by applying a curl to Maxwell equation 4($\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$) and then apply vector identity: $\nabla \times (\nabla \times T) = \nabla(\nabla \cdot T) - \nabla^2 T$ where T is some placeholder vector we get

$$\nabla^2 \vec{E} - \frac{1}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2} = 0$$

In 1-D: $\frac{\partial^2 E}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 E}{\partial t^2} = 0$

This is a second order partial differential equation and has plane wave solutions:

$$E(x,t) = E_0 e^{i(kx-wt)}$$

Where $k = \frac{2\pi}{\lambda}$ and $\omega = 2\pi f$.

Let us substitute from Einstein and Compton's work $E = \hbar\omega$ and from de-Broglie that $p = {}^{h}/_{\lambda} = \hbar k$.

$$E(x,t) = E_0 e^{\frac{i(px-Et)}{\hbar}}$$

This is the plane wave equation describing a photon.

Let's substitute this equation into our wave equation

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right) E_0 e^{\frac{i(px-Et)}{\hbar}} = 0$$

$$or, \qquad -\frac{1}{\hbar^2}\left(p^2 - \frac{E}{c^2}\right) E_0 e^{\frac{i(px-Et)}{\hbar}} = 0 \qquad (1)$$

This gives $E^2 = p^2c^2$, the energy of photon, which is massless.

This is in accordance with special relativity where the total energy for a relativistic particle with mass m is:

$$E^2 = p^2c^2 + m^2c^4$$

The wavefunction for photon: $\Psi(x,t) = \psi_0 e^{\frac{i(px-Et)}{\hbar}}, where\ E = pc$

What is the wave function of a particle with **mass**mand total relativistic energy $E^2 = p^2c^2 + m^2c^4$ (like electron)

Let $\Psi = \Psi_0 \, e^{\frac{i(px-Et)}{\hbar}}$ and $E^2 = p^2c^2 + m^2c^4$

In analogy with eq(1) $-\frac{1}{\hbar^2}\left(p^2 - \frac{E}{c^2} + m^2c^2\right) \Psi_0 \, e^{\frac{i(px-Et)}{\hbar}} = 0$

Now backsolve, and get the equation:

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\right) \Psi_0 e^{\frac{i(px-Et)}{\hbar}} = 0$$

Apply few approximations

$$E^2 = p^2c^2 - m^2c^4$$

$$E = \sqrt{(p^2c^2 - m^2c^4)}$$

$$= \sqrt{\left(c^4(\frac{p^2}{c^2} - m^2)\right)}$$

$$= \sqrt{\left(c^4m^2(\frac{p^2}{m^2c^2} - 1)\right)}$$

$$= mc^2\sqrt{\left(\frac{p^2}{m^2c^2} - 1\right)}$$

Use a Taylor Series expansion $\sqrt{1-x} \approx 1 - \frac{x}{2} - \frac{x^2}{8} - \frac{x^3}{16} - \cdots$ of this equation

x must be small, in our energy formula, $x = \frac{p^2}{m^2c^2} = \left(\frac{p}{mc}\right)^2$ is small since $p = mv \ll mc$

$$E = mc^2\sqrt{\frac{p^2}{m^2c^2} + 1}$$

$$\sim mc^2\left(1 + \frac{p^2}{2m^2c^2}\right) = mc^2 + \frac{p^2}{2m}$$

Therefore

$$\Psi = \Psi_0 \; e^{\frac{i\left(px - mc^2 t - \frac{p^2 t}{2m}\right)}{\hbar}}$$

In 3-D

$$\Psi = \Psi_0 \; e^{\frac{i\left(\vec{p}.\vec{r} - mc^2 t - \frac{p^2 t}{2m}\right)}{\hbar}} = \Psi_0 \; e^{\frac{i\left(\vec{p}.\vec{r} - \frac{p^2 t}{2m}\right)}{\hbar}} \; e^{\frac{-imc^2 t}{\hbar}} = \psi \, e^{\frac{-imc^2 t}{\hbar}}$$

Where $\psi = \Psi_0 \, e^{\frac{i\left(\vec{p}.\vec{r}-\frac{p^2 t}{2m}\right)}{\hbar}} = \Psi_0 \, e^{\frac{i(\vec{p}.\vec{r}-E_{kinetic}t)}{\hbar}}$

Let’s now take the first and second partial derivatives of $\Psi(r,t)$

$$\frac{\partial \Psi}{\partial t} = -\frac{i}{\hbar} mc^2 e^{-\frac{i}{\hbar}mc^2 t}\psi(\vec{r},t) - e^{-\frac{i}{\hbar}mc^2 t}\frac{\partial \psi(\vec{r},t)}{\partial t}$$

and the second:

$$\frac{\partial^2 \Psi}{\partial t^2} = \left(-\frac{m^2 c^4}{\hbar^2} e^{-\frac{i}{\hbar}mc^2 t}\psi - \frac{2i}{\hbar} mc^2 e^{-\frac{i}{\hbar}mc^2 t}\frac{\partial \psi}{\partial t}\right) - e^{-\frac{i}{\hbar}mc^2 t}\frac{\partial^2 \psi}{\partial t^2}$$

We should keep in mind that the last term with the second partial derivative is quite small because of the fact that there is no c^2 term carrying the order of magnitude, and therefore by approximation the actual second derivative is given by:

$$\frac{\partial^2 \Psi}{\partial t^2} \approx \left(-\frac{m^2 c^4}{\hbar^2} e^{-\frac{i}{\hbar}mc^2 t}\psi - \frac{2i}{\hbar} mc^2 e^{-\frac{i}{\hbar}mc^2 t}\frac{\partial \psi}{\partial t}\right)$$

Now put in

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\right)\Psi = 0$$

$$\Rightarrow \left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\right)\Psi_0 \; e^{\frac{i\left(\vec{p}.\vec{r} - mc^2 t - \frac{p^2 t}{2m}\right)}{\hbar}} = 0$$

$$\Rightarrow \left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\right)\Psi_0 \; e^{\frac{i\left(\vec{p}.\vec{r} - \frac{p^2 t}{2m}\right)}{\hbar}} \; e^{\frac{-imc^2 t}{\hbar}} = 0$$

$$\Rightarrow \left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\right) \Psi_0 \; e^{\frac{i(\vec{p}.\vec{r} - E_{kinetic}t)}{\hbar}} \; e^{\frac{-imc^2t}{\hbar}} = 0$$

$$\Rightarrow \left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{m^2c^2}{\hbar^2}\right)\psi \; e^{\frac{-imc^2t}{\hbar}} = 0$$

$$\Rightarrow \frac{\partial^2}{\partial x^2} \; e^{\frac{-imc^2t}{\hbar}}\psi + \frac{m^2c^2}{\hbar^2} \; e^{\frac{-imc^2t}{\hbar}}\psi + \frac{2im}{h} \; e^{\frac{-imc^2t}{\hbar}}\frac{\partial\psi}{\partial t} - \frac{m^2c^2}{\hbar^2} \; e^{\frac{-imc^2t}{\hbar}}\psi = 0$$

$$\Rightarrow \frac{\partial^2}{\partial x^2} \; e^{\frac{-imc^2t}{\hbar}}\psi + \frac{2im}{h} \; e^{\frac{-imc^2t}{\hbar}}\frac{\partial\psi}{\partial t} = 0$$

$$\Rightarrow \; e^{\frac{-imc^2t}{\hbar}}\left(\frac{\partial^2}{\partial x^2}\psi + \frac{2im}{\hbar}\frac{\partial\psi}{\partial t}\right) = 0$$

$$\Rightarrow \frac{\partial^2}{\partial x^2}\psi + \frac{2im}{\hbar}\frac{\partial\psi}{\partial t} = 0$$

$$\Rightarrow\left(-\frac{\hbar^2}{2m}\right).\frac{\partial^2}{\partial x^2}\psi+\left(-\frac{\hbar^2}{2m}\right).\frac{2im}{h}\frac{\partial\psi}{\partial t}=0$$

$$\Rightarrow\left(-\frac{\hbar^2}{2m}\right).\frac{\partial^2}{\partial x^2}\psi-i\hbar\frac{\partial\psi}{\partial t}=0$$

$$\Rightarrow\left(-\frac{\hbar^2}{2m}\right).\frac{\partial^2}{\partial x^2}\psi=i\hbar\frac{\partial\psi}{\partial t},$$ This is the Schrödinger Equation in 1D

$$\Rightarrow-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t)=i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t},$$ This is the Schrödinger Equation in 3D

Now, note the similarity of the classical Hamiltonian with the term on the right-hand side of the equation. It describes the total energy of the wave function. In our derivation, we assumed that potential energy $V(\vec{r},t)$ is 0 and that only the kinetic energy was taken into account. We know that the potential is purely additive and therefore, the full Schrödinger Equation for a non-relativistic particlein 3D with a potential is given by:

$$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t}=\left[-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t)+V(\vec{r},t)\right]$$

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