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Review of Mathematical Modelling of the Time Dependent Schrodinger Wave Equation using Different methods

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Abstract: This paper focuses on the principle of time dependent Schrödinger equation (TDSE) which simplified so many reviewed ideas, class room teaching, research ideologies and personal study meant for advanced knowledge. In this research work, the enlightenment of the basic concept of Schrödinger wave equation to improve knowledge about simple ways for mathematical understanding in deriving TDSE using different technique in more comprehensive approach. The research shows clearly that TDSE can be derived using time independent equation, wave mechanics, classical & Hamilton-Jacobi's equations. Different methods and ways by different researchers/scholars have been used in the past. In this paper, we review the quantum field theoretic route to the Schrodinger wave equation which treats time and space as parameters, not operators. Furthermore, we recall that a classical (nonlinear) wave equation can be derived from the classical action via Hamiltonian-Jacobi theory. By requiring the wave equation to be linear we again arrive at the Schrodinger equation, without postulating operator relations. The underlying philosophy is operational. Surely, a particle is what a particle detector detects. This leads us to a useful physical picture combining the wave (field) and particle paradigms which points the way to the time-dependent Schrodinger equation. However, the result provides a comprehensive well derived derivation, derived using various approaches, which would make this research a unique one from different areas of specializations.

Keywords: *Time Independent Equation, Hamilton-Jacobi's equations and Wave Mechanics.*

INTRODUCTION

In the theoretical approach, when solving scientific problems, Quantum Mechanics is an important part of Physics, Engineering and other Science discipline. This physics area clearly talk about the sub-atomic particles, specifically where the Newtonian laws are not valid. Thousands of terms in quantum mechanics principles differ with classical mechanics. This clearly shows the importance and need of a clearer approach towards the new principles of scientific symbols. Interestingly, quantum mechanics becomes great as a researcher result to Schrödinger's equations (SE). Effort are not taken to derive them from "known to unknown" path clearly and reach where derivations of these equations are giving physical meaningful significance. Many researchers of knowledge, have attempted to derive SE beginning from simple principles to complex equations, although this attempts have not been satisfactory. This article provide the derivation of SE giving detailed description of related principles and theorems with simpler step in deriving it. It is therefore intended that the reader/researcher should get introduced with a variety of methods to derive the SE, using quantum mechanics. This research provides clearer derivation of Time Dependent Schrödinger's Equation starting from wave mechanics, Schrödinger Time Independent Equation, classical and Hamilton-Jacobi equations, Nilesh et. al. (2015), Pranab (2011), Bodurov (2005), Ogborn et. al. (2005).

De-Broglie in 1924, stressed that, particle in motion are associated with a wave within it, and is called matter wave. Moreover, Erwin Schrödinger in continuing de Broglie's view, came up with a differential wave equation of second order to clearly define the wave nature of matter and particle related to wave, Piece (1996). Although, this equation is analogous to the equation for waves in optics, clearly relate that, the particle replicate wave and gives rise to result in terms of a function called the wave function, Ogiba (2011). In solving the equation, it produces the wave function Ψ and the energy E of that particle under study. Immediately the wave function Ψ is determine, then everything about the particle is known or can be deduced from the wave function, Heisenberg (1925), Field (2004), Nilesh et. al. (2015).

The wave function Ψ is physically not significance, but happen to be the most important thing. That means, the absolute square of Ψ (i.e. $|\Psi|^2$) gives the probability in a particular region of space at giving time. The energy E in the equation represent the energy of the particle at the potential V and boundary conditions which is constraints on the particle which can be continuous or quantized. In physics, Quantization of energy is very important and related to quantum mechanics. A particle cannot have any energy or continuous energy, but can have only that permitted energy described by Schrödinger equation which is inclusive with the potential V and the boundary conditions, Schrödinger (1926), Jackson (1999), Nilesh et. al. (2015).

Schrödinger's equation was very much popular, though initially it was questioned by scientific community which was due to its limitation regarding a non-relativistic particles. Heisenberg derived a matrix mechanics in which physical quantities are explained in terms of Eigen values of the matrix, Feyman (1948), Vic (2006). The mathematical equations shown by Schrödinger was consequently called as wave mechanics. Heisenberg's matrix mechanics and Schrödinger's wave mechanics were known to be two different descriptions of quantum mechanics Schrödinger (1926), Dirac (1958), Lajos (2012), Putnam (2005). Basically Schrödinger equations have two forms: one consisting of time termed as time dependent equation and the other in which time factor is eliminated and hence named as time independent equation, Dubeibe (2010), Nilesh et. al. (2015).

Physical Model and Mathematical Formulations

Different methods are used to derive TDSE. Briggs & Rost (2001), Hall & Reginatto (2002) & Nilesh et. al. (2015) pointed out that, using wave mechanics, Propagation of a wave makes particles of the medium to oscillate about their mean position. These oscillations are 'to and fro, along the same path' and the motion is referred as Simple Harmonic Motion (S.H.M.). Displacement of a particle from its mean position is given by a simple equation from wave mechanics, as

$$y = A \sin t = (\omega - \delta) \tag{2.1}$$

Which can be modified as

$$y = A\, sin \frac{2\pi v}{\lambda}\left(t - \frac{x}{v}\right) \tag{2.2}$$

Xavier (2008), stressed that S.H.M. in relation with equation (2.1), (2.2), described a wave represented by a wave function ψ(x, t), which function is not a directly measurable quantity and may be complex in nature. The wave function related with a particle moving along +x direction is given by the equation below;

$$\psi = A.e^{-i\omega\left(t-\frac{x}{v}\right)} \tag{2.3}$$

Where:
A is the amplitude of oscillations,
ω is angular frequency,
t is the time,
x is position and
v is its velocity.
As $\omega = 2\pi\nu$, $v = \nu.\lambda$,

Equation (2.3) is simplified to;

$$\psi = A.e^{-i2\pi\nu\left(t-\frac{x}{\nu\lambda}\right)} \tag{2.4}$$

$$\psi = A.e^{-i2\pi\left(\nu t-\frac{x}{\lambda}\right)} \tag{2.5}$$

When
ν = the frequency of oscillations,

The total energy is given by

$$E = h\nu = 2\pi\hbar\nu \tag{2.6}$$

Where
h = Planck's constant and

$$\hbar = \frac{h}{2\pi} \tag{2.7}$$

Thus,

$$\nu = \frac{E}{2\pi\hbar} \tag{2.8}$$

Also, $\lambda = \frac{h}{p} = \frac{2\pi\hbar}{p}$ (2.9)

Considering de-Broglie's hypothesis
Equation (2.5) becomes

$$\psi = A.e^{-i2\pi\left(\frac{Et}{2\pi\hbar}-\frac{xp}{2\pi\hbar}\right)} \tag{2.10}$$

$$\psi = A.e^{-\frac{i2\pi}{2\pi\hbar}(Et-xp)} \tag{2.11}$$

$$\psi = A.e^{-\frac{i}{\hbar}(Et-xp)} \tag{2.12}$$

Equation (2.12) is a mathematical representation of an unrestricted particle of total energy E and momentum p moving along x- direction.
Then, the total energy (E) of the particle can be written as

T. E. = E = K.E. + P.E

$$E = \frac{1}{2}mv^2 + V = \frac{m^2v^2}{2m} + V = \frac{p^2}{2m} \tag{2.13}$$

$$E\Psi = \frac{p^2\Psi}{2m} + V\Psi \tag{2.14}$$

Where
V is potential energy of the particle which is a function of x.
Differentiating equation (2.13), (2.14) with respect to x, which result to;

$$\frac{\partial \Psi}{\partial x} = A.e^{\frac{i}{\hbar}(Et-xp)}.\frac{ip}{\hbar} \tag{2.15}$$

Again differentiating with respect to x,

$$\frac{\partial \Psi}{\partial x^2} = -\frac{p^2}{\hbar^2}.A.e^{\frac{i}{\hbar}(Et-xp)} \tag{2.16}$$

Using equation (2.14),

$$\frac{\partial^2 \Psi}{\partial x^2} = -\frac{p^2}{\hbar^2} \tag{2.17}$$

Which then becomes

$$P^2\psi = -\hbar^2\frac{\partial^2 \Psi}{\partial x^2} \tag{2.18}$$

Again differentiating equation (2.14) with respect to t,

$$\frac{\partial \Psi}{\partial x} = A.e^{\frac{i}{\hbar}(Et-xp).}.\frac{iE}{\hbar} \tag{2.19}$$

Using equation (2.14), the evaluation will then be

$$\frac{\partial \Psi}{\partial x} = \frac{-iE}{\hbar^2}\psi \tag{2.20}$$

Making $E\psi$ the subject of the formular,

$$E\psi = -\frac{\hbar\partial\psi}{i\,\partial t} \tag{2.21}$$

And as such, Equation (2.15) becomes, which is expressed in terms of $\frac{h\partial\psi}{i\,\partial t}$

$$-\frac{\hbar\partial\psi}{i\,\partial t} = -\frac{\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi \tag{2.22}$$

Substituting equations (2.17) and (2.18) into equation (1.15), Equation (2.22) is the one dimensional TDSE. The same can be written in three dimensions as

$$-\frac{\hbar\partial\psi}{i\;\partial t}=-\frac{\hbar^2}{2m}\nabla^2\psi-V\psi \qquad (2.23)$$

Where $\nabla^2=-\frac{\partial^2}{\partial x^2}+=\frac{\partial^2}{\partial y^2}\frac{\partial^2}{\partial z^2}$ is a laplacian operator

Which means that, the time Dependent Schrodinger Equation, TDSE, can be easily derived from the wave mechanics considering the equations for a particle which is describing S.H.M. The derivation has its own importance as it paves the way from the physics of classical mechanics to the physics of quantum mechanics, Nilesh et. al. (2015).

Methods / Solution and Discussion of Results

Using the techniques of Schrodinger's time independent equation in solving problems

In quantum mechanics, the Schrödinger equation is a mathematical equation that describes the changes over time of a physical system in which quantum effects, such as wave–particle duality are significant. These systems are referred to as quantum (mechanical) systems. The equation is considered a central result in the study of quantum systems, and its derivation was a significant landmark in the development of the theory of quantum mechanics. It was named after Erwin Schrödinger, who derived the equation in 1925, and published it in 1926, forming the basis for his work that resulted in him being awarded the Nobel Prize in Physics in 1933, Nilesh et. al. (2015), Ogiba (2011), Piece (1996).

In classical mechanics, Newton's second law (F = *m*a) is used to make a mathematical prediction as to what path a given physical system will take over time following a set of known initial conditions. Solving this equation gives the position, and the momentum of the physical system as a function of the external force F on the system. Those two parameters are sufficient to describe its state at each time instant. In quantum mechanics, the analogue of Newton's law is Schrödinger's equation for a quantum system (usually atoms, molecules, and subatomic particles whether free, bound, or localized). The equation is mathematically described as a linear partial differential equation, which describes the time-evolution of the system's wave function (also called a "state function"), Pranab (2011), Putnam (2005).

The concept of a wave function is a fundamental postulate of quantum mechanics, which defines the state of the system at each spatial position, and time. Using these postulates, Schrödinger's equation can be derived from the fact that the time-evolution operator must be unitary, and must therefore be generated by the exponential of a self-adjoint operator, which is the quantum Hamiltonian. This derivation is explained below, Nilesh et. al. (2015), Xavier (2008).

In the Copenhagen interpretation of quantum mechanics, the wave function is the most complete description that can be given of a physical system. Solutions to Schrödinger's equation describe not only molecular, atomic, and subatomic systems, but also macroscopic systems, possibly even the whole universe. Schrödinger's equation is central to all applications of quantum mechanics including quantum field theory which combines special relativity with quantum mechanics. Theories of quantum gravity, such as string theory, also do not modify Schrödinger's equation, Pranab (2011), Putnam (2005), Xavier (2008).

The Schrödinger equation is not the only way to study quantum mechanical systems and make predictions, as there are other quantum mechanical formulations such as matrix mechanics, introduced by Werner Heisenberg, and path integral formulation, developed chiefly by Richard Feynman. Paul Dirac incorporated matrix mechanics and the Schrödinger equation into a single formulation, Piece (1996), Nilesh et. al. (2015), Xavier (2008).

The time-dependent Schrödinger equation (TDSE) which gives a description of a system evolving with time. Where i is the imaginary unit, $\hbar$ is the reduced Planck constant, H is the Hamiltonian operator (which

characterizes the total energy of the system under consideration). The position-space wave function of the quantum system is nothing but the components in the expansion of the state vector in terms of the position eigenvector, Ogiba (2011), Putnam (2005), Nilesh et. al. (2015).
The Schrodinger's time independent equation in 3-D is presented as;

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0 \tag{3.1}$$

Considering a wave function written as:

$$\psi = A.e^{-iwt} \tag{3.2}$$

Where
A is amplitude of the wave.
ω is an angular frequency and
t is the time period.

If you differentiate equation (3.2) with respect to t, making $\frac{\partial\psi}{\partial t}$ the subject of the formula;

$$\frac{\partial\psi}{\partial t} = -i\omega A.e-^{i\omega t} = -i(2\pi v)A.e^{-i\omega t} \tag{3.3}$$

Then, if E = hv , $\frac{\partial\psi}{\partial t}$ will becomes;

$$-\frac{\partial\psi}{\partial t} = -i\left(\frac{2\pi E}{h}\right)A.e - i\omega t = -i\frac{2\pi E}{h}\psi \tag{3.4}$$

$$E\psi = -\frac{h}{i2\pi}\frac{\partial\psi}{\partial t} = -\frac{i^2 h\partial\psi}{2\pi\,\partial t} = \frac{ih}{2\pi}\frac{\partial\psi}{\partial t} = ih\frac{\partial\psi}{\partial t} \tag{3.5}$$

Which means that equation (3.1) becomes will automatically become;
(3.4)

$$\nabla^2\psi + = -\frac{2mE}{h^2}\psi - \frac{2mv}{h^2}\psi = 0 \tag{3.6}$$

$$\nabla^2\psi - \frac{2mV}{h^2}\psi = -\frac{2mv}{h^2}ih\frac{\partial\psi}{\partial\psi} \tag{3.7}$$

$$-\frac{h^2}{2m^2}\nabla^2 + V = H \tag{3.8}$$

Equation (3.8) is the Hamiltonian operator
The two legendary equations have a connection to each other and are like statics and dynamics in classical mechanics, where derivability of the time dependent equation from the time independent equation form is much significant and meaningful.

When using the technique of classical wave equation in solving Problems

According to Nilesh et. al. (2015), in classical physics, the **wave equation** is the name given to a certain real partial differential equation in which the second derivative with respect to position *x* is proportional to the second derivative with respect to time *t*. The **wave equation** is an important second-order linear partial differential equation for the description of waves as they occur in classical physics such as mechanical waves (e.g. water waves, sound waves and seismic waves) or light waves. It arises in fields like acoustics, electromagnetics, and fluid dynamics.

The equation for an electromagnetic wave is expressed in 1-D form as

$$\frac{\partial^2 E}{\partial x^2} = -\frac{1}{c^2}\frac{\partial^2 E}{\partial t^2} = 0 \qquad (3.9)$$

Where
E is the energy of the wave,
c is the velocity of light and
t is the time, for a wave progragting in x- direction.

Equation (3.9) is derived from Maxwell's equations which governs EM waves in electrodynamics above. And the solution is a plane wave solution which satisfies equation (3.8) written as;

$$E(x, t) = E_0 e^{i(kx-\omega t)} \qquad (3.10)$$

Where
k is propagation constant is an angular frequency.

Considering differentiating equation (3.10) with respect to x, the equation becomes

$$\frac{\partial E}{\partial x} = E_0 ik.e^{i(kx-\omega t)} \qquad (3.11)$$

Repeating the differentiation with respect to x, making $\frac{\partial^2 E}{\partial x^2}$ the subject of the formula

$$\frac{\partial^2 E}{\partial x^2} = -E_0 K^2 e^{i(kx-\omega t)} \qquad (3.12)$$

Now, differentiating (3.12) with respect to t, instead of x, we will have;

$$\frac{\partial E}{\partial t} = E_o(-\omega i).e^{i(kx-\omega t)} \qquad (3.13)$$

Repeating the differentiation of equation (3.13) with respect to t, making $\frac{\partial^2 E}{\partial t^2}$ the subject of the formula;

$$\frac{\partial^2 E}{dt^2} = -E_o\omega^2.e^{i(kx-\omega t)} \qquad (3.14)$$

Then, Equation (3.14) will then become;

$$\left(-E_o k^2 + \frac{1}{c^2}E_o\omega^2\right).e^{i(kx-\omega t)} = 0 \qquad (3.15)$$

$$\left(-k^2 + \frac{\omega^2}{c^2}\right) E_o . e^{i(kx-\omega t)} = 0 \tag{3.16}$$

$$-k^2 = \frac{\omega^2}{c^2}, k = \frac{\omega}{c} \tag{3.17}$$

If c $=v\lambda$, then, the above solutions will becomes;
E = hv = $2\pi\hbar v$ (3.18)

Recall that E = $\hbar\omega$, then simplifying the equation result to;

$$p = \frac{\hbar}{\lambda} = \frac{2\pi\hbar}{(c/v)} = \frac{2\pi\hbar v}{c} = \hbar k \tag{3.19}$$

Then, Equation (3.19) will be represented as,

$$E(x,t) = E_o . e^{i(\frac{p}{\hbar}\times - \frac{E}{\hbar}t)} = E_o . e^{\frac{i}{\hbar}(px-Et)} \tag{3.20}$$

Differentiating equation (3.20) with respect to t, result to;

$$\frac{\partial E}{\partial x} E_o . e^{\frac{i}{\hbar}(px-Et)} . \frac{ip}{\hbar} \tag{3.21}$$

Repeating the differentiation with x, will result to;

$$\frac{\partial^2 E}{dx^2} = -\frac{p^2}{\hbar^2} E_o . e^{\frac{i}{\hbar}(px-Et)} \tag{3.22}$$

Differentiating equation (3.20) with respect to t, will result to;

$$\frac{\partial E}{\partial x} E_o . e^{\frac{i}{\hbar}(px-Et)} \tag{3.23}$$

Differentiating again with respect to t, making $\frac{\partial^2 E}{dx^2}$ the subject

$$\frac{\partial^2 E}{dt^2} = -\frac{E^2}{\hbar^2} E_o . e^{\frac{i}{\hbar}(px-Et)} \tag{3.24}$$

Comparing equation (3.23) and (3.24), it will eventually become;

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right) E_0 . e^{\frac{i}{h}(px-Et)} = 0 \tag{3.25}$$

$$-\left(\frac{p^2}{h^2} + \frac{E^2}{h^2 c^2}\right) E_0 . e^{\frac{i}{h}(px-Et)} = 0 \tag{3.26}$$

$$-\frac{1}{h^2}\left(p^2 - \frac{E^2}{c^2}\right)E_0.e^{\frac{i}{h}(px-Et)} = 0 \qquad (3.27)$$

$$p^2 - \frac{E^2}{c^2} = 0 \qquad (3.28)$$

$$E^2 = p^2c^2 \qquad (3.29)$$

Based on equation (3.25) to (3.29), the relativistic mass of a particle at rest with mass m_0 , is generated as;

$$m = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}} \qquad (3.30)$$

Where
m = Relativistic mass
m_0 = Mass of particle at rest
Applying simple simplification to clear the square roots; equation (3.30) become

$$m^2 = \frac{m^2}{1-\frac{v^2}{c^2}} \qquad (3.31)$$

If you multiply equation (3.30) by c^4 , the solution will eventually become;

$$m^2c^4\left(1-\frac{v^2}{c^2}\right) = m_0^2c^4 \qquad (3.32)$$

$$m^2c^4\left(c^2 - v^2\right) = m_0^2c^4 \qquad (3.33)$$

$$m^2c^4 \;\; p^2 - v^2 = m_0^2c^4 \qquad (3.34)$$

$$m^2c^4 \;\; p^2 - v^2 = m_0^2c^4 \qquad (3.35)$$

Considering E mc² for an EM wave equation will become

$$E^2 = \;\; p^2c^2 = + m_0^2c^4 \qquad (3.36)$$

Assuming $m = m_0$, then equation (3.36) will result to;

$$\frac{E^2}{c^2} = \quad p^2 + m^2c^2 \tag{3.37}$$

Making E the subject of the formula, equation (3.37) become

$$E = \sqrt{p^2c^2 + m^2c^4} \ = \sqrt{m^2c^4\left(1 + \frac{p^2}{m^2c^2}\right)} \tag{3.38}$$

Therefore the value for E will be represented as;

$$E = mc^2\sqrt{1 + \frac{p^2}{2m^2c^2}} \tag{3.39}$$

From equation (3.39), if the higher order terms are neglected, the value of E become;

$$E = mc^2 \ + \frac{p^2}{2m}\ mc \ + \ \frac{(mv)^2}{2m} \ = mc^2 \ \ + T \tag{3.40}$$

Where
T is the classical kinetic energy.

Since we are not considering the electric field, the total energy in equation (3.40) is replaced by any wave function which is presented in the form;

$$\psi(x,t) = \psi_0 . e^{\frac{1}{\hbar}(px - Et)} \tag{3.41}$$

Where
ψ_0 is amplitude of the wave.
Then, the total energy from equation (3.40) can be substituted in equation (3.41) which leads to the wave equation shown below;

$$\psi\,(x,t) = \psi_0 . e^{\frac{i}{\hbar}\left[px - (mc^2 + T)t\right]} \tag{3.42}$$

Opening the brackets by simple simplification, equation (3.42) turn to be;

$$\psi(x,t) = \psi_0 . e^{\frac{i}{h}\left[px - (mc^2 + T)t\right]} \tag{3.43}$$

$$\psi(x,t) = \psi_0 . e^{\frac{-imc^2t}{h}}\ e^{\frac{i}{h}(px - Pt)} \tag{3.44}$$

Equation (3.44) shows that the first term $e^{\frac{-imc^2t}{h}}$ is related to the velocity of light (c), and the second power $e^{\frac{i}{h}(px-Pt)}$ is related to the velocity of the particle. Which the particle velocity can never be greater than that of the light. From the principles of physics, it is very clear that the first term will oscillate faster than the second term. That means that, equation (3.38) can be expressed as;

$$\psi(x,t) = \Phi . e^{\frac{-imc^2 t}{h}} \tag{3.45}$$

So that

$$\Phi = \psi_0 . e^{\frac{i}{h}(px - Pt)} \tag{3.46}$$

Which is a non-relativistic function.

Considering differentiating equation (3.45) twice with respect to t, the result turn to;

$$\frac{\partial^2 \psi}{dt^2} = -\frac{m^2 c^4}{h^2} e^{\frac{-imc^2 t}{h}} \frac{\partial \Phi}{\partial t} + e^{\frac{-mc^2 t}{h}} \frac{\partial^2 \Phi}{\partial t^2} \tag{3.47}$$

Equation (3.47) shows that, the second term is much smaller than the first term.

Using equation (3.37) above,

$$-\frac{1}{h^2}\left(p^2 - \frac{E^2}{c^2} + m^2 c^2\right)\psi . e^{\frac{1}{h}(pxxEt)} = 0 \tag{3.48}$$

The energy and momentum operators can be written as;

$$p^2 \to -h \frac{\partial^2}{\partial x^2} \quad \text{and} \quad E \to \frac{h}{i}\frac{\partial}{\partial t}$$

The representation above becomes,

$$-\frac{1}{h^2}\left(-h^2 \frac{\partial^2}{\partial x^2} - \frac{1}{c^2} + \left(\frac{-h}{i}\frac{\partial}{\partial t}\right)^2 + m^2 c^2\right)\psi . e^{\frac{i}{h}(px - Et)} = 0 \tag{3.49}$$

$$-\frac{1}{h^2}\left(-h^2 \frac{\partial^2}{\partial x^2} + \frac{h^2}{c^2}\frac{\partial^2}{c^2} + m^2 c^2\right)\psi . e^{\frac{i}{h}(px - Et)} = 0 \tag{3.50}$$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{1}{c^2}\frac{\partial^2}{\partial^2} + \frac{m^2 c^2}{h^2}\right)\psi . e^{\frac{i}{h}(px - Et)} = 0 \tag{3.51}$$

Neglecting small terms from equation (3.49) and using large terms in equation (3.50) and (3.51) above,

$$\left\{\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\left[-\frac{m^2 c^2}{h^2} e^{\frac{-imc^2}{h}}\right] - \frac{2i}{h} mc^2 e^{\frac{-imc^2}{h}}\right\}\Phi = 0 \tag{3.52}$$

By expanding equation (3.52)

$$\left\{\frac{\partial^2}{\partial x^2}\ x\ \frac{m}{h^2} e^{\frac{-imc^2}{h}} + \frac{2i}{h} me^{\frac{-imc^2}{h}} \frac{\partial}{\partial t} - \frac{m^2c^2}{h^2}\right\}\Phi = 0 \qquad (3.53)$$

Equation (3.53) reduces to;

$$\frac{\partial^2\Phi}{\partial x^2} + \frac{2i}{h} m \frac{\partial\Phi}{\partial t} = 0 \qquad (3.54)$$

By neglecting two terms equation (3.54) become;

$$\frac{\partial^2\Phi}{\partial x^2} = -\frac{2i}{h} m \frac{\partial\Phi}{\partial t} \qquad (3.55)$$

$$\frac{\partial^2\Phi}{\partial x^2} = -\frac{2i}{h^2} mh \frac{\partial\Phi}{\partial t} \qquad (3.56)$$

$$-\frac{h^2}{2m}\frac{\partial^2\Phi}{\partial x^2} = ih\frac{\partial\Phi}{\partial t} \qquad (3.57)$$

Equation (3.57) is the TDSE in 1-D without potential energy term.

In 3-D form, equation (3.57) become;

$$-\frac{h}{2m}\nabla^2\Phi = ih\frac{\partial\Phi}{\partial t} \qquad (3.58)$$

Where:

$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is a Laplacian operator (3.59)

It is important to derive TDSE from classical wave equation, as this helps the researcher to understand the interlinkage between the physics of classical theory of electrodynamics and the physics of modem quantum mechanics.

Using Hamilton-Jacobi equation

In physics, the Hamilton-Jacobi equation (HJE) is an alternative formulation of classical mechanics, equivalent to other formulations such as Newton's laws of motion, Lagrangian mechanics and Hamiltonian mechanics. The Hamilton–Jacobi equation is particularly useful in identifying conserved quantities for mechanical systems, which may be possible even when the mechanical problem itself cannot be solved completely, Hamilton, (1833); Goldstein & Herbert (2002); Fetter & Walecka (2003); Nakane et al (2002).

The HJE is also the only formulation of mechanics in which the motion of a particle can be represented as a wave. In this sense, the HJE fulfilled a long-held goal of theoretical physics of finding an analogy between the propagation of light and the motion of a particle. The wave equation followed by mechanical systems is similar to, but not identical with, Schrödinger's equation, as described below; for this reason, the HJE is

considered the "closest approach" of classical mechanics to quantum mechanics, Hamilton, (1834); Fetter & Walecka (2003); Jacobi (1884).
Landau & Lifshitz (1975) and Sakurai (1985) stress that the Hamilton equations can be obtained by applying Canonical transformation equations to the spatial coordinates qi and canonical momenta pi for n-dimensional classical mechanical system. The Hamilton-Jacobi equation is basically related to classical mechanics and is particularly used where conserved quantities mechanical systems are to be identified and is represented as;

$$\frac{dqi}{dt} = \frac{\partial H}{\partial pi} \tag{3.60}$$

$$\frac{dpi}{dt} = -\frac{\partial H}{\partial qi} \tag{3.61}$$

Where
H is the Hamilton of the system at any instant.

The canonical transformed coordinates Qi and momenta Pi for n-dimensional system satisfies the Hamilton equation as;

$$\frac{dQ_i}{dt} = \frac{\partial k}{\partial P_i} \tag{3.62}$$

$$\frac{\partial P_i}{\partial t} = -\frac{\partial k}{\partial Q_i} \tag{3.63}$$

Where
k is the transformed Hamiltonian related to the original H as;

$$k(Q_i, P_i, t) = H(q_i, p_i, t) + \frac{dF}{dt} \tag{3.64}$$

Where
F is a generating function of the canonical transformation, Such that F (q_i, Q_i, t).

The generating function (S) is called as Hamilton's principle function represented as;

$$S = F(q_i, p_i, t) \tag{3.65}$$

With this, the transformed Hamiltonian k vanishes

$$H(q_{i,} p_i t) + \frac{DS}{dt} = 0 \tag{3.66}$$

The transformed equations for spatial coordinate q_i and momenta p_i are

$$Qi, = \frac{\partial S}{\partial Pi} \tag{3.67}$$

$$Pi \ \frac{\partial S}{\partial qi} \tag{3.68}$$

Substituting equation (3.67) and (3.68) in equation (3.66);

$$H\left(qi, \frac{\partial S}{\partial qi}, t \right) + \frac{ds}{dt} = 0 \tag{3.69}$$

Equation (3.69) usually is called the Hamilton-Jacobi equation.

A particle with Newtonian mass m and potential V. The Hamilton-Jacobi equation is represented as;

$$\frac{1}{2m}\left[\left(\frac{\partial S}{\partial x} \right)^2 + \left(\frac{\partial S}{\partial y} \right)^2 + \left(\frac{\partial S}{\partial z} \right)^2 \right] + V + \frac{\partial S}{\partial t} = 0 \tag{3.70}$$

Then, the quantum wave function in terms of coordinate x is represented by;

$$\psi(X,t) = e^{\frac{1}{\hbar}S(X,t)} \tag{3.71}$$

In taking logarithm on both sides, equation (3.71) turns to;

$$\log \psi(X, t) = \log e^{\frac{1}{\hbar}S(x,t)} \tag{3.72}$$

By simplifying the equation;

$$\log \psi(X,t) = \frac{1}{\hbar} S(X,t) \ \log e \tag{3.73}$$

$$\log (X, t) = \frac{1}{\hbar} \ln \psi \ \text{(natural log)} \tag{3.74}$$

$$S = -i\hbar \ 1n\psi \tag{3.75}$$

Where
X = (x, y, z) is the space coordinate.

Differentiating equation (3.73), (3.74) and (3.75) with respect to x, y, z, and t;

$$\frac{\partial S}{\partial x} = -\frac{ih}{\psi}\frac{\partial \psi}{\partial x} \quad (3.76)$$

$$\frac{\partial S}{\partial y} = -\frac{ih}{\psi}\frac{\partial \psi}{\partial y} \quad (3.77)$$

$$\frac{\partial S}{\partial x} = -\frac{ih}{\psi}\frac{\partial \psi}{\partial t} \quad (3.78)$$

Differentiating first equation only from above equation with respect to x.

$$\frac{\partial \psi}{\partial x} = -\frac{\partial \psi}{ih}\frac{\partial S}{\partial x} \quad (3.79)$$

$$\frac{\partial \psi}{\partial x} = \frac{i\psi}{h}\frac{\partial S}{\partial x} \quad (3.80)$$

$$\frac{\partial^2 S}{\partial x^2} = \frac{i}{h}\frac{\partial S}{\partial x}\frac{\partial \psi}{\partial x} + \frac{i}{h}\psi\frac{\partial^2 S}{\partial x^2} \quad (3.81)$$

Differentiating momentum coordinate equation from equation with respect to x
By taking I $\rightarrow$ q $\rightarrow$ x, then;

$$\frac{\partial^2 S}{\partial x^2} = \frac{\partial p_x}{\partial x} = \frac{\partial (mix)}{\partial x} = \frac{\partial\left(m\frac{\partial x}{\partial t}\right)}{\partial x} = m\frac{\partial^2 x}{\partial x \partial t} = 0 \quad (3.82)$$

The schrodinger equation is used to determine the allowed or permissible energy levels of quantum mechanical systems like atoms, electrons, protons, neutrons etc. The associated wave function gives the probability of finding the particle at a certain position. The allowed energy levels of a particle constrained to a rigid box can also be determined using SE.The best example can be an electron in a thin conducting wire. Here, the electron can be considered to move freely back and forth along the length of the wire but cannot escape from it. Then, using SE, one can derive the expression for the allowed energies of the electron, as given below

$$\frac{\partial S}{\partial x} = -\frac{ih}{\psi}\frac{\partial \psi}{\partial x} \quad (3.83)$$

$$\frac{\partial \psi}{\partial x} = -\frac{\psi}{ih}\frac{\partial S}{\partial x} \quad (3.84)$$

By simple substitution

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{i}{h}\frac{\partial S}{\partial x}\left(\frac{\psi S}{\partial x}\right)^2 + \frac{i}{h}\ \psi\ \ x\ \ 0 \tag{3.85}$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{\psi}{h^2}\left(\frac{\partial S}{\partial x}\right)^2 \tag{3.86}$$

$$\left(\frac{\partial S}{\partial x}\right)^2 = -\frac{h^2}{\psi}\frac{\partial^2 \psi}{\partial x^2} \tag{3.87}$$

Similarly,

$$\left(\frac{\partial S}{\partial y}\right)^2 = -\frac{h^2}{\psi}\frac{\partial^2 \psi}{\partial y^2} \tag{3.88}$$

$$\left(\frac{\partial S}{\partial z}\right)^2 = -\frac{h^2}{\psi}\frac{\partial^2 \psi}{\partial z^2} \tag{3.89}$$

Considering equation (3.76), (3.77) and (3.78) for t, by putting equation (3.86), (3.88) and (3.89) into equation (3.70) will result to;

$$\frac{1}{2m}\left[-\frac{h^2}{\psi}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi\right] + V - \frac{ih}{\psi}\frac{\partial \psi}{\partial t} = 0 \tag{3.90}$$

$$-\frac{h^2}{2m}\nabla^2\psi + V\psi - \frac{ih}{\psi}\frac{\partial \psi}{\partial t} = 0 \tag{3.91}$$

$$-\frac{h^2}{2m}\nabla^2\psi + V\psi = \frac{ih}{\psi}\frac{\partial \psi}{\partial t} \tag{3.92}$$

$$-\frac{h}{i}\frac{\partial \psi}{\partial t} = -\frac{h^2}{2m}\nabla^2\psi + V\psi \tag{3.93}$$

The equation above represent the Time Dependent Schrodinger Equation in 3-D form. Deriving it with this methodology helps to have similar treatment in the physics of quantum mechanics.

Conclusions

The Schrödinger equation and its solutions introduced a breakthrough in thinking about physics. The solutions led to consequences that were very unusual and unexpected for the time. Discussion on Schrödinger's equation, in particular, its derivation, is dealt with much complexity in books as well as during class room teaching. Present article is been an attempt to bridge this gap and to give a clear illustration of the concept along with its derivation, starting from many simpler concepts in classical mechanics. These 'starting points' included the equations from wave mechanics, Schrödinger Time Independent Equation, classical and Hamilton-Jacobi equations. The Schrödinger equation provides a way to calculate the wave function of a system and how it changes dynamically in time. However, the Schrödinger equation does not directly say *what*, exactly, the wave function is. Interpretations of quantum mechanics address questions such as what the relation is between the wave function, the underlying reality, and the results of experimental measurements It can be concluded that the article provides a stepping stone for the beginners or researchers in quantum mechanics to have an insight into SE and a varieties of way to derive it.

Nomenclature

A = Amplitude of Oscillation
ω = Angular Frequency,
t = Time
x = Position coordinates
v = velocity
T = Classical Kinetic Energy
Ψ = Amplitude of the wave [The Greek letter psi is the state vector of the quantum system]
k = Propagation Constant
ħ = The reduced Planck constant
H = Hamiltonian Operator
E = Energy of the wave
M = Mass
P.E= Potential Energy
K.E = Kinetic Energy
h = Plank's constant
∇^2 = Laplace Operator
F = Generating function of the canonical transformation
X = (x,y,z) = Space coordinate
V = Potential energy of the particle
I = The imaginary unit
d/d*t* = indicates a derivative with respect to time *t*

Reference

1. Bodurov T., (2005). Derivation of the Nonlinear Schrödinger Equation from First Principles, *Annales de la Fondation Louis de Broglie, 30*(3-4), 343-352.
2. Briggs, J. S., & Rost, J. M. (2001). On the derivation of the time-dependent equation of Schrödinger. *Foundations of Physics*, *31*(4), 693-712.
3. Dirac P. A. M., (1958). The Lagrangian in Quantum Mechanics, Reprinted in 'Selected Papers on Quantum Electrodynamics, Ed. Schwinger J., (New York: Dover), 312-320.
4. Dubeibe F. L., (2010). Solving the Time Independent Schrödinger Equation with Absorbing Boundary Conditions and Source Terms in Mathematical 6.0", International Journal of Modern Physics C
5. Fetter, A., Walecka, J. (2003). Theoretical Mechanics of Particles and Continua. Dover Books. ISBN 0-486-43261-0.
6. Feynman, R. P. (1948). Space-Time Approach to Non-Relativistic Quantum Mechanics, Rev. Mod. Phys. 20, 367.
7. Field J. H., (2004). Relationship of Quantum Mechanics to Classical Electromagnetism and Classical Relativistic Mechanics, Eur. J. Phys., 25, 385-397.
8. Goldstein, H. (2002). Classical Mechanics (3rd ed.). Addison Wesley. ISBN 0-201-65702-3.

9. Hall M. J. W., & Reginatto M. (2002). Schrodinger Equation from an Exact Uncertainty Principle, J. Phys. A, 35, 3289-3303.
10. Hamilton, W. (1833). On a General Method of Expressing the Paths of Light, and of the Planets, by the Coefficients of a Characteristic Function, (PDF). Dublin University Review: 795–826.
11. Hamilton, W. (1834). On the Application to Dynamics of a General Mathematical Method previously Applied to Optics, (PDF). British Association Report: 513–518.
12. Heisenberg W., (1925). Über Quantentheoretische Umdeutung Kinematischer und Mechanischer Beziehungen, Zeitschrift f¨ur Physik, 33, 879.
13. Jackson J. D., (1999). Classical Electrodynamics, Wiley, New York, 3rd ed.
14. Jacobi, C. G. J. (1884), Vorlesungen über Dynamik, C. G. J. Jacobi's Gesammelte Werke (in German), Berlin: G. Reimer
15. Lajos Diosi, (2012). Classical-Quantum Coexistence: a 'Free Will' test, IOP Publishing, Journal of Physics: Conference Series, 361, 012028.
16. Landau, L. D.; Lifshitz, E. M. (1975). Mechanics. Amsterdam: Elsevier.
17. Nakane, Michiyo; Fraser, Craig G. (2002). The Early History of Hamilton-Jacobi Dynamics. Centaurus. Wiley. 44 (3–4): 161. doi:10.1111/j.1600-0498.2002.tb00613.x. PMID 17357243
18. Nilesh P Barde, Sandeep D. Patil, Pravin M. Kokne, Pranav P. & Bardapurkar (2015) Deriving Time Dependent Schrödinger Equation from wave Mechanics, Schrödinger Time Independent Equation, Classical and Hamilton-Jacobi Equations. Leonardo Electronic Journal of Practics and Technologies. Issue 26,ISSN 1583-1078, 31-48.
19. Ogborn J., Taylor E. F., (2005). Quantum Physics Explains Newton's Laws of Motion, *Phys. Educ.*, *40*(1), 26-34.
20. Ogiba F., (2011). Phenomenological Derivation of the Schrödinger Equation, *Progress in Physics*, 4, 25-28.
21. Piece P., (1996). Another Schrodinger Derivation of the Equation, *Eur. J. Phys*. 17, 116117.
22. Pranab R. S. (2011). Direct Derivation of Schrödinger Equation from Hamilton-Jacobi Equation Using Uncertainty Principle, *Romanian Journal of Physics, 56*(9-10), 1053-1056.
23. Putnam H., (2005). A Philosopher Looks at Quantum Mechanics (Again), Brit. J. Phil. Sci., 56, 615-634.
24. Sakurai, J. J. (1985). Modern Quantum Mechanics. Benjamin/Cummings Publishing. ISBN 0-8053-7501-5.
25. Schrödinger E., (1926). On the Relationship of the Heisenberg-Born-Jordan Quantum Mechanics to Mine, Annalen der Physik, 79, 734. [English translation in Gunter Ludwig Wave Mechanics 127-150 (Pergamon Press, 1968) ISBN 0-08-203204-1]
26. Schrödinger E., (1926). Quantization as an Eigenvalue Problem (First Communication), Annalen der Physik, 79, 361-376.
27. Schrödinger E., (1926). Quantization as an Eigenvalue Problem, (Fourth Communication) Annalen der Physik, 81, 109-139. [English translation in Gunter Ludwig Wave Mechanics 151-167 (Pergamon Press, 1968) ISBN 0-08-203204-1]
28. Schrödinger E., (1926). Quantization as an Eigenvalue Problem, (Second Communication) Annalen der Physik, 79, 489-527. [English translation in Gunter Ludwig Wave Mechanics 106-126 (Pergamon Press, 1968) ISBN 0-08-203204-1]
29. Vic Dannon H. (2006). Wave Particle Duality: de Broglie Waves and Incertainity, *Gauge Institute Journal, 2*(4), 1-19.
30. Xavier A., et al, (2008). A Review of Transparent and Artificial Boundary Conditions Techniques for Linear and Nonlinear Schrödinger Equations, *Communications in Computational physics, 4*(4), p. 729-796.