

CHAPTER II LITERATURE REVIEW

2.1 Schrödinger Equation

A wave equation which can describe the covert-like behavior of quantum particle in the theory of non-relativistic quantum mechanics is the Schrödinger Equation (Foudas, 2007; Hamdi et al., 2009; Phillips et al., 2003). The role of Schrödinger Equation in quantum mechanics is analogous to that of Newton's laws in classical mechanics. Both described motion. Newton's second law is a differential equation which describes how classical particle moves, whereas Schrödinger Equation is a partial differential which describes how wave function representing quantum particles ebbs and flows. In addition both were postulated and tested by experiment (Phillips et al., 2003; Tang 2005).

As a prelude to Schrödinger Equation, mathematics can also be used to describe waves of various shapes and sizes. We may not go into details of all waves-types, except maybe the traveling waves as an example of sinusoidal waves. The traveling wave is the most attractive wave traveling with definite wavelength λ and period τ or equivalently definite wave number, $k = \frac{2\pi}{\lambda}$, and angular frequency $\omega = \frac{2\pi}{\tau}$ (Phillips et al., 2003) can be represented by mathematical function

$$\psi(x,t) = A \cos(kx - \omega t) \quad (2.1.1)$$

Where A is constant = Amplitude

$$\tau \text{ is a period} = \frac{2\pi}{\omega}$$

t is time.

This function $\psi(x,t)$ moves with amplitude A and period $\frac{2\pi}{\omega}$.

Furthermore, these undulation move increasing x with velocity $\frac{\omega}{k}$. For example in equation (2.1.1), the maximum of $\psi(x,t)$ corresponding to $kx - \omega t = 0$, occurs when $x = \frac{\omega t}{k}$ and the minimum corresponding to $kx - \omega t = \pi$ occurs at a position $x = \frac{\lambda}{2} + \frac{\omega t}{k}$ in all the two cases, the position moves with velocity $\frac{\omega}{k}$. Also important to note in the circle of sinusoidal traveling waves is the linear superposition; this is the general traveling wave with wave number k and frequency ω given by

$$\psi(x,t) = A \cos(kx - \omega t) + B \sin(kx - \omega t) \quad (2.1.2)$$

A and B are arbitrary constant.

We will also not go into the detail of this linear superposition due to the scope constrain of this work. However, it is important to note that, in both classical and quantum Physics, traveling waves are represented by complex exponential function of the form

$$\psi(x,t) = Ae^{i(kx - \omega t)} \quad (2.1.3)$$

In classical Physics use of real part of the complex exponential is necessary, whereas in quantum Physics the use of complex number is not an option (Phillips et al., 2003; French & Tabor, 1978). In the subsequent discussion we shall see how Schrödinger equation is derived through the Hamiltonian and wave function.

2.1.1 Derivation of Hamiltonian

It has already been stated earlier that, the first person to develop a wave theory for the behavior of electron was Louis-victor, Pierre, Raymond 7th duc de Broglie, usually shortened as de Broglie (Schiesser & Griffith, 2009; Phillips et al., 2003; Tang, 2005). In his PhD thesis postulated that, the wavelength of any matter obeyed the relationship $\lambda = \frac{h}{p}$ where h is Planck's constant and p is the momentum. Though de Broglie approach has solve some simple problems, but the theory did not adequately shade light on the behavior of an electron when subjected to different types of external potential field, this led to Erwin Schrödinger to investigate alternatives and ultimately

to derive a wave function solution to describe the electron that, crucially conserved energy (Schiesser & Griffith, 2009).

The Hamiltonian of an electron with mass m , momentum p , and coordinate q acted on by a conservative force is other way called the total energy of the system usually represented by symbol H is the sum of Kinetic energy (KE) and Potential energy (PE) of the system as in Newtonian mechanics (Tang, 2005; Schiesser & Griffith, 2009) is also given by

$$H(p, q) = \frac{|p|^2}{2m} + V(q) \quad (2.1.1.1)$$

Where $\frac{|p|^2}{2m}$ is the KE, $V(q)$ is the PE and $H(p, q)$ represent the total energy

It then follows from the Hamiltonian's equation of motion that the motion of electron be given as

$$\frac{\partial H}{\partial p} = \dot{q}(t); \frac{\partial H}{\partial q} = -\dot{p}(t) \quad (2.1.1.2)$$

Where p and q are vectors, $\dot{p}(t)$ and $\dot{q}(t)$ are corresponding gradients.

Now taking the derivative from equation (2.1.1.1) we obtain

$$\dot{q}(t) = \frac{1}{m} p(t); p(t) = -\nabla V(q) \quad (2.1.1.3)$$

A consequence of Hamiltonian's equations of motion is that we obtain directly the principle of "Conservation of energy". Thus we have

$H(q(t), p(t)) = \text{constant}$ thereby having

$$\frac{d}{dt} H(q(t), p(t)) = 0, \forall t \quad (2.1.1.4)$$

2.1.2 Wave function

The solution of the Schrödinger equation can be written as

$$u(x, t) \approx u(x, t) = \sum_{l=1}^{\infty} \sum_{n=1}^{\infty} a_{ln} e^{i(k_l x - \omega_n t)} \quad (2.1.2.1)$$

Where a_{ln} is the wave function?

k_l is the wave number l

ω_n is the frequency n (r/s)

x is the position and

t is the time

The above equation (2.1.2.1) was an assumption by Schrödinger's great insight that the motion of an electron can be describe in an appropriate wave function chosen as above. But from Planck-Einstein relation, we have that, $E = h\nu = \frac{h\omega}{2\pi} = \hbar\omega$, also from de Broglie relation $k = \frac{2\pi}{\lambda} = \frac{2\pi}{(p/\hbar)}$, we will obtain (Beiser, 2003).

$$u(x, t) = \sum_{l=1}^{\infty} \sum_{n=1}^{\infty} a_{ln} e^{i(p_l x / \hbar - E_n t / \hbar)} \quad (2.1.2.2)$$

2.1.3 Derivation of Schrödinger equation.

As we stated earlier, in classical wave analysis the actual Physics solution energies as real part of complex quantity, but in quantum mechanics we do not impose this condition. If we adopt any of the two equations (2.1.3) or (2.1.2.2) as essential form of the wave function for free particle of unique momentum and energy traveling in a particular direction, (from equation 2.1.3) after differentiating twice with respect to x and differentiating once with respect to t we get

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 A e^{i(kx - \omega t)} = -\frac{p^2}{\hbar^2} \psi \quad (2.1.3.1)$$

Recall that, $p = \hbar k$, and

$$\frac{\partial \psi}{\partial t} = -\omega A e^{i(kx - \omega t)} = -\frac{iE}{\hbar} \psi \quad (2.1.3.2)$$

Recall also, $E = \hbar\omega = \frac{p^2}{2m}$, then,

Combining equation (2.1.3.1) and (2.1.3.2) we arrive at,

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{-2mE}{\hbar^2} \psi = \frac{-i2m}{\hbar} \frac{\partial \psi}{\partial t} \quad (2.1.3.3)$$

For a general case, that is, when the total energy includes a potential energy term, we put

$$p^2 = 2m(E - V) = \hbar^2 k^2 \quad (2.1.3.4)$$

This embodies the fact that (familiar from classical mechanics) a particle of some definite total energy E has momentum P that changes from one place to another as a result of spatial variation of PE, V (French & Tabor, 1978). For quantum case, we have therefore;

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{-2mE}{\hbar^2} (E - V)\psi = \frac{i2m}{\hbar} \frac{\partial \psi}{\partial t} + \frac{2m}{\hbar^2} V\psi$$

These can be written in to two different forms of equations,

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = E\psi \quad (2.1.3.5)$$

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = i\hbar \frac{\partial \psi}{\partial t} \quad (2.1.3.6)$$

The two immediate equations above represent alternative forms of Schrödinger equation in one dimension. Equation (2.1.3.5) does not include time explicitly, is known as *Time independent Schrödinger equation* it provide basis for analyzing the stationary state of atomic system (French & Tabor, 1978). Equation (2.1.3.5) is not our concern either, but equation (2.1.3.6) must be used when dealing with problems such as actual motion of particles from one form to another, and it is our main subject of discussion in this work.

The Schrödinger equation, Schwabl (2007) and French & Tabor (1978) have properties that cause them to be more preferred over all other possibilities:

- They have properties of linearity, so that if ψ_1 and ψ_2 are specific solutions to one of these equations, then, any linear combination of them is a solutions to one of the same equation. This property of superposition is one of the basic properties of waves.

- The solutions are perfectly suited to the interpretation of ψ as a probability amplitude
- Finally there is all the accumulated evidence that the Schrödinger equation's work; they provide the basis for correct analysis of all kinds of molecular, atomic and nuclear systems. What ever questionable features there may be in the manner of their formulation are swept away in evidence of their manifest success.

To set this discussion in order and clear, for mathematical convenience equation (2.1.3.6) can also be written as,

$$i\hbar \frac{\partial u(x,t)}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 u(x,t)}{\partial x^2} + u(x,t)V(x) \quad (2.1.3.7)$$

Let $V(x) = -q|u|^2$ and let also normalize $\hbar$ and $2m$ to unity, when we do this we obtain the preceding normalized nonlinear or *cubic Schrödinger equation* (Schiesser & Griffith, 2009) that is

$$i \frac{\partial u}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 u}{\partial x^2} + qu|u|^2 = 0 \quad (2.1.3.8)$$

In equation (2.1.3.8), the term $|u|^2$ represents the probability density of the wave function. This means that the probability of electron being in a state defined by $u(x,t)$ is given by $p(x,t) = u^*(x,t)u(x,t) = |u|^2$ where u^* represent the complex conjugate of u ($p(x,t)$ should not be confused with p in the Hamiltonian) (Schiesser & Griffith, 2009). The normalization condition implies that the probability is given by;

$$P(t) = \int_{\zeta} p(x,t) dx = \int_{\zeta} |u(x,t)|^2 dx = 1$$

That is the probability of electron being located some where within the domain under consideration ζ is one.

2.1.4 Solution of Schrödinger equation by Computer Approach

We have seen in the presiding section how analytical mathematical methods can leads to solution of Schrödinger equation. However, in the current or contemporary research, almost all the manipulation of Schrödinger equation is done numerically

using computer but not analytically. This is because, the solution of differential equations constitutes an entire discipline of mathematics.

In contrast to analytical methods, the computer solution procedure for one-dimensional potentials can be standardized. Therefore some professionals will use computer methods for all problems where accurate wave function or numerical values of energy are required, even for those special cases for which analytical solutions exist (French & Taylor, 1978). Now, we shall discuss some relevant literatures that solve this Schrödinger equation using numerous computational approaches of their choices.

As far back as 1970, the numerical analysis has been used to find the solution of Schrödinger equation by Canosa & Oliva (1970). Basically, Canosa & Oliva approximated the potential in the one-dimensional Schrödinger equation by a step function with a finite number of steps. They then integrated exactly in terms of circular hyperbolic functions. The resulting differential equation has constant coefficient. They then matched the solutions at the interface of each layer in order to construct the eigenfunctions in the whole domain. They found out that the unique features of the numerical method were that; (a) All the eigenfunctions and eigenvalues are obtained with the same absolute accuracy for the same number of steps in the potential; (b) any desired number of eigenvalues and eigenfunctions are obtained in one single pass without any need to supply initial guesses for the eigenvalues (c) for any number of steps in the potential, they obtained in the principle the whole infinite spectrum of eigenvalues and eigenfunctions. Though, they stated the simplicity of its application as one of the greatest advantage of the method, but also admitted that, there is need for improvement in the area of error analysis, which according to them, is a question they could not yet explore fully.

Stern (1977) gave a brief analysis on the various methods for computing radial wave functions and scattering phase shift of short-range local interactions and presented a numerical result for a static electron-hydrogen potential. He then found that, a quadrature solution of integral equation is highly competitive in terms of accuracy

especially at very low energies where it has superior numerical stability over differential equation methods and is also less demanding in computing time.

Using Fourier method Kosloff, D. & Kosloff, R. (1982) found a solution for time-dependent Schrödinger equation. They discretized the space and time on grid and produced both special derivatives and second order differencing for time derivatives. They added that, the method conserved norm and energy and preserves quantum mechanical commutation relations.

Then in 1994, Simos and Mitsou (1994) proposed another approach to the numerical solution of Schrödinger equation called "Expert system". Using computer package they called ODEXPERT designed for numerical solution of phase shift problem of the one-dimensional Schrödinger equation. Finally, they tested the package on calculation of the phase shifts of some potential.

Based on Galerkin-finite element formulation in space and use of time stepping techniques (a modification of Runge-Kutta methods), Lee (1994) constructed and analyzed a fully discrete method for the nonlinear Schrödinger equation. Lee approach consisted of an extrapolation technique and (according to him) has two advantages over the usual implementation. First, the scheme is implicit in the linear term and explicit in the nonlinear term; as a result, the linear system that has to be solved at every time level involved fixed matrices. Second, by choosing the extrapolated values appropriately, the temporal rates of convergence can be shown to be those of classical ones.

Due to the higher demand of numerical solution of time-dependent Schrödinger equation since two hundred years ago (Iitaka et al., 1995) the quest for it remained constantly in progress with multiple number of researchers (in Physics and Chemistry) using various approaches and techniques to see to the actualization of their dreams. Again in 1995, Iitaka et al. (1995) study the stability of the Multistep scheme (ESM) as a numerical method of solving time-dependent Schrödinger equation. Iitaka used

the most general set of ESM and found a set of coefficients that gives the widest range of stability (i.e the coefficients that work stable with larger time step at cost of round off error).

Ramos & Villatoro (1994) did their research in this area of Schrödinger equation on the nonlinear Schrödinger equation in the finite line. Their work was based on the numerical study of the nonlinear Schrödinger (NLS) equation subject to homogeneous Dirichlet, Neumann and Robin boundary conditions in the finite line. They compared the result with both the exact analytical ones for the initial-value problem (IVP) of the NLS equation and the numerical ones for periodic boundary conditions. They shows that the initial solutions obtained by truncating the exact N-soliton solution of the IVP of the NLS equation into a finite interval develop solitary waves that behave as solitons, even after collisions with the boundaries. Ramos & Villatoro further added that for periodic and homogeneous Dirichlet and Neumann boundary conditions, it is observed that the interaction between solitons and boundaries is equivalent to the collision between solitons in IVP or quarterplane problems. It is shown that for homogeneous Robin boundary conditions, boundary layers that trap and delay the soliton are formed at the boundaries. Phase diagrams for the soliton amplitude at the boundary points and for the soliton's maximum amplitude show a recurrent phenomenon, and are similar to those of the cubic Duffing equation. Finally they also showed that, the phase diagrams were strong functions of the parameter that defines the Robin boundary conditions. As part of their achievement, a method of images, similar to the one used in potential theory, was developed for the NLS equation in the quarterplane with homogeneous Dirichlet and Neumann boundary conditions at the finite boundary.

Ramos (2002) studied numerically, the nonlinear Schrödinger equation in one-dimensional Cartesian coordinates by three linear implicit finite difference methods that resulted in block triangular matrices at each time level as a function of the damping, pumping changes in refractive index. As part of his procedure, Ramos performed the numerical experiments to determine the effects of time step, spatial step

size and implicitness parameters of the dispersion and nonlinear term shows that the most accurate result are obtained when both the dispersion and nonlinear terms are treated by means of second-order- accurate trapezoidal Discretization and full linearization of the nonlinear terms. Ramos further showed that if either the dispersion or the nonlinear terms are treated with first-order-accurate approximation, substantial errors are found and these errors became very large when the nonlinear terms by means of first-order difference and don't decrease substantially as number of grid points is increased. As regards to the nature and formation of the solitons, Ramos observed that when they move from a medium to another, one characterized by a higher refraction index, the amplitude and speed increases whereas its width decreases. That, upon approaching the interface, the amplitude of the soliton was found to increase down stream while some radiation was found upstream.

As mentioned earlier, even in the aspect of chemistry, the numerical solution of Schrödinger equation has find a place to stay. Nakanishi & Sugawara (2000) presented a new approach for solving the Schrödinger equation based on a magnetic algorithm ($\mu - GA$). They used what they called "feed forward neural work" to represent the solution, while random point evaluation method (RPEM) was also introduced to define the fitness score to be maximized in the $\mu - GA$ breeding procedure. And finally Nakanishi & Sugawara found out that, the convergence of final stage of searching was accelerated by invoking the domestic optimizer.

Jimenez et al. (2003) developed another new adaptive multigrid finite difference scheme useful for the analysis of wave collapse process. As a test of validity of the ideas beyond their scheme, they applied it to the simulation of collapse in the critical nonlinear Schrödinger equation. They verified the width evaluation which satisfies the viral identities and rate of self-similar collapse near singularity. The scheme as Jimenez et al., highlighted was able to follow numerically the collapse process up to amplification of 10^{13} and to determine the collapse time with high precision. As part of its application as Jimenez et al., pointed out was that, their scheme may be used to approximate many other collapse phenomena related to recent problems, example non

local collapse in Bose-Einstein condensation, collapse in saturable media ectra. They also stated that their scheme is linearly implicit, which allows fast implementation and conservative, which is a desirable property of any numerical scheme which is to be use in the simulation of the Hamiltonian wave equation. However, it is not clear to me whether the fastness of its implementation may not cause the results to have large errors when compared to the other explicit methods used by other researchers.

Van de vyver (2005) introduced yet another new way for constructing efficient Runge-Kutta (RK) method for the numerical integration of one-dimensional Schrödinger equation. Van de vyver modified Runge-Kutta methods in order to integrate exactly the test problem with his theoretical investigation of the asymptotic expressions of local errors for large energies and the numerical results, he became convinced that his proposed new Runge-Kutta approach is more fruitful procedure for integration of the Schrödinger equation than other RK procedures known in the literature.

Han et al. (2005) had another contribution in this problem under study. In their finite difference method for one-dimensional time-dependent Schrödinger equation on the unbounded domain, they introduced artificial conditions to reduce the original problem in a finite computational domain. By the use of method of reduction of order, they constructed this finite-difference scheme to solve the reduced problem. Han et al., also maintained that their scheme was proved to be uniquely solvable, unconditionally stable and convergent.

Inui (2007) found the numerical errors resulting from finite difference approximation in computations of one-dimensional Schrödinger equation with Trotter formula. In his research, Inui used parallel algorithm for solving time-dependent Schrödinger equations devised by De Raedt and based on the Trotter formula. He also added that is not only simple but also unconditionally stable, explicit, and local. Inui then consider the numerical errors resulting from the finite-difference approximation of De Raedt's

algorithm by comparing an exact solution of a free particle with the approximate solution calculated by using the Trotter formula which depends on the size of the spatial-temporal lattice. He then further noted that his algorithm can be applied to even high dimensional quantum system but he was only able to use one-dimensional equation given as

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \hat{H} \psi(x,t) \quad (2.1.4.1)$$

Where $\hat{H}$ is a self-ad joint Hamiltonian and $\psi(x, t)$ is the wave function of the system. If the wave function at the initial time t_0 is given by $\psi_0(x)$, then the formal solution at times $t > t_0$ is given by

$$\psi(x,t) = e^{-\frac{i(t-t_0)\hat{H}}{\hbar}} \psi_0(x) \quad (2.1.4.2)$$

Inui further introduced the Trotter formula by postulating that the Hamiltonian consists of the kinetic operator $\hat{T}$ and the potential $\hat{V}$, the time-evolution operator is expressed by $e^{-\frac{i(t-t_0)(\hat{T}+\hat{V})}{\hbar}}$, therefore Trotter formula is given by

$$e^{-i(A+B)} = \lim_{n \rightarrow \infty} [e^{-iA/n} e^{-iB/n}]^n \quad (2.1.4.3)$$

After solving the problem, Inui compared the result with the analytical once. Finally he admitted that there was one total error that is the norm of wave function diverges fairly quickly.

Samrout (2007) did a very interesting work in his new second-and fourth-order accurate numerical schemes for nonlinear cubic Schrödinger equation. Samrout's problem was quite similar to our problem only that he used two different algorithms and tackled his problem. Samrout (2007) combined Method of lines (MOL) and Lancozos's Tau Method. According to him, the methods are self-starting and prove to be stable, accurate and energy conservative for long-time integration periods. Approximate were sought on segmented sets of parallel lines finite expansions in terms of a given orthogonal polynomial basis. In the same work, Samrout carried out

numerical application concerning several cases of the propagation, collision and bound states of N solitons, $2 \leq N \leq 5$. Accurate results were then obtained using both shifted Chebyshev and Legendre polynomials. Samrout then said his results were found to be competitively compared with some other published results obtained using different methods. These was the equation he used;

$$\begin{aligned} iu_t + u_{xx} + qu|u|^2 &= 0 & -\infty < x < \infty, t > 0 \\ u(x, 0) &= g(x) & -\infty < x < \infty \end{aligned} \quad (2.1.4.4)$$

Where $u(x, t)$ is a complex-value function defined over the whole real line, i is the imaginary complex number and q is a real parameter. Samrout (2007) further gave some convincing reasons as to why he chose the technique. First he said, the Lanczos Tau method has been proved to be highly accurate spectral technique. The method has been discussed analytically and applied numerically on various nonlinear systems of ordinary and partial differential equations. Second, the Method of Lines (MOL) is a well known powerful method. It was proved to have numerous advantages over fully discrete methods in several contexts. Third, the combination of the Tau method and MOL yielded the so called TLM, and its results were favorably compared with other well-established schemes. Fourth, he presented automatically segmented, self adaptive and simple-to-implement numerical procedures for the approximate solutions in terms of finite orthogonal expansions, namely Legendre and Chebyshev polynomials. This choice, Samrout added, is of interest, regarding the stability, algebraic manipulations, differentiation, integration and evaluation of solution. Finally, Samrout noted that, the time-integration step size, the spatial spacing between the parallel lines and order of approximations can automatically be controlled and error can be checked simultaneously throughout the numerical process in order to ensure that it is kept within the requirement of problem and then maintaining the stability in the numerical solution.

Another numerical analysis done in this area of Schrödinger equation were by Koch et al. (2006). In their work titled "Approximation of time-dependent-electronic Schrödinger equation by multi-configuration time-dependent Hartree-fock method (MCTDHF) where they discussed numerical approximation of the solution of the

time-dependent Schrödinger equation arising in ultrafast laser dynamics. Koch et al. reduced the linear electronic Schrödinger equation to a computationally tractable, lower dimensional system of nonlinear partial differential equations by the multi-configuration time-dependent Hartree–Fock method (MCTDHF). The method – they added, uses an ansatz for the wave function on a nonlinear manifold, taking into account the antisymmetry inherent in the model to reduce the dimension of the solution space. Koch et al, also showed that the ansatz is consistent with the original equation and the solution can be represented exactly in principle using the solutions of the nonlinear PDEs associated with MCTDHF. For the practical solution of the MCTDHF equations, several numerical techniques are discussed, and it is demonstrated that physically relevant problems can be solved satisfactorily. Koch et al. also employed the use of MOL for spatial discretization of what they called “working equation”. Some of the advantages of using this method they added that, the approach reduces a lower dimensional, nonlinear system of coupled Schrödinger equation for those who are interested in making the original Schrödinger equation tractable for numerical computation, the method excels in its favorable computational complexity in relation to the number of particles feasible.

The nonlinear Schrödinger equation has been subject of many studies aimed at building and comparing numerical methods that preserve or not its invariant quantities (mass, energy and momentum) (Moebs, 1998). Even in the optical fibers, Moebs (1998) considered a stochastic nonlinear Schrödinger equation as a model for its propagation. In his work, Moebs described the modeling of the problem and described the objectives. He presented a new multilevel method for its solution. The method he said gives better quality results with significantly shorter computing time than other numerical methods used in the literature.

Fibich et al. (2005) also tried their own method in solving the numerical solution of Schrödinger equation. In their work – New singular solutions of the nonlinear Schrödinger equation – they presented numerical simulations of a new type of singular solutions of the critical nonlinear Schrödinger equation (NLS), that collapse with a

quasi self-similar ring profile at a square root blowup rate. They then found and analyzed the equation of the ring profile. They observed that the self-similar ring profile is an attractor for a large class of radially-symmetric initial conditions, but is unstable under symmetry-breaking perturbations. The equation for the ring profile admits also multi-ring solutions that give rise to collapsing self-similar multi-ring solutions, but these solutions (Fibich et al. added) were unstable even in the radially-symmetric case, and eventually collapse with a single ring profile. They eventually observed that, the collapsing ring solutions were also observed in the supercritical nonlinear Schrödinger equation.

Coupled nonlinear Schrödinger equation can also be solved and their solution can be found, as it has been proven by Aydin & Karasozen (2007). In the titled of their work “symplectic and multi-symplectic methods for coupled nonlinear Schrödinger equation with period solutions” tried their effort to see the behavior of the periodic plane wave solutions of the coupled nonlinear Schrödinger equation (CNLS) system. After a semi discretization in space variables, they obtained a system of Hamiltonian ordinary differential equations for which various symplectic integrators can be applied. Next they gave a symplectic integrator based on the splitting of the semi-discretized Hamiltonian system in linear and nonlinear parts. At their findings, they admitted in the method that due to splitting of the Hamiltonian in linear and nonlinear parts and using composition of two equations in time, the symplectic method requires more computing time than multi-symplectic integrator.

Another similar breakthrough in a coupled Schrödinger equation is the work of Wang et al. (2008), in their numerical simulation of nonlinearity coupled Schrödinger equation. The work described a finite difference scheme which is linearly uncoupled in computation for a nonlinearly coupled Schrödinger system. According to them the numerical scheme has been proved to preserve the original conservative properties. Using the discrete energy analysis method, they also proved that the scheme is unconditionally stable and second-order convergent in discrete L_2 -norm based on

some preliminary estimation. Finally, they added that their results showed that the new scheme is very efficient.

Utsumi et al. (2006) also proposed another solution for one-dimensional coupled nonlinear Schrödinger equation (CNLS) by the constrained interpolation Profile-Basic set (CIP-BS) method by introducing matrix representations clarifying the relation with differential algebra to adapt it to nonlinear partial differential equations. They reduced the linear and nonlinear partial differential equations (PDEs) to ordinary differential equations (ODEs) for values and spatial derivatives at grid points. They also proved that the method gives stable low diffusion and accurate results.

Also, Chang et al. (2007) provided a novel algorithm for computing the ground state and excited state solutions of M-coupled nonlinear Schrödinger equations (MCNLS). They first transformed the MCNLS to the stationary state ones by using separation of variables. They then used the energy level of a quantum particle governed by Schrödinger eigen value problem (SEP) as an initial guess to computing their counter part of nonlinear Schrödinger equation (NLS). They also discretized the system via centered difference approximation. A predictor-correction continuation method was then exploited as an alternative method to trace solution curves and surfaces of MCNLS, where the chemical potentials are treated as continuation parameters. Chang et al further found that the wave function can be easily obtained whenever the solution manifolds are numerically traced.

Mazzone & Morandi (2006) had in their research examined the possible solutions for many particles time-dependent Schrödinger equations. They focused on the use of Monte Carlo methods and on numerical integration. And in all the two cases, they observed that a real space formulation can be adopted. Apart, they added that it avoids the increase in the computing time with the system size.

In 2005, Muslu & Erbay (2005) did almost the same work as done by Aydin and Karasozen, only that, the former used higher-order split-step Fourier schemes for the

generalized nonlinear Schrödinger equation. As mentioned in Aydin & Karasozen (2007). The basic idea in the split-step method is to decompose the original problem into subproblems which are simpler than the original problem and then to compose the approximate solution of the original problem by using the exact or approximate solutions of the subproblems in a given sequential order. Muslu & Erbay added that the choice of operator splitting one should use depends solely on a particular application, and no general method is known. However, for nonlinear dispersive wave equations that are derived by balancing the effects of dispersion and nonlinearity, such as the GNLS equation that we will be solving, an appropriate approach is to split the original problem into linear and nonlinear subproblems that take into account purely dispersive and purely nonlinear effects, respectively.

Zisowsky & Ehrhardt (2008) did well in trying to explore more methods on the numerical solutions of Schrödinger equations. In their work; Discrete artificial boundary conditions for nonlinear Schrödinger equations, the duo proposed, constructed and analyzed discrete artificial boundary conditions (ABCs) for different finite difference schemes to solve nonlinear Schrödinger equations. These new discrete boundary conditions were motivated by the continuous ABCs recently obtained by the potential strategy of Szeftel. Since these new nonlinear ABCs are based on the discrete ABCs for the linear problem. They therefore first reviewed the well-known results for the linear Schrödinger equation. Zisowsky & Ehrhardt further presented their approach for a couple of finite difference schemes, including the Crank–Nicholson scheme, the Duran–Sanz–Serna scheme, the DuFort–Frankel method and several split-step (fractional-step) methods such as the Lie splitting, the Strang splitting and the relaxation scheme of Besse. Finally, they added, several numerical tests illustrated the accuracy and stability of their new discrete approach for the considered finite difference schemes.

Chang & Kang (2008) described a new accurate discretization technique for integro-differential Schrödinger equations whose kernel of integral part can be discontinuous along main diagonal. The new method according to Chang and Kang was based on

Clenshaw-curtis quadrature for the numerical solution of the integro-differential Schrödinger equation. They also added that, the method showed it converges quickly and that, the truncation decreases faster than any power of inverse number of Chebyshev support points.

In the area of Nano-physics, Shao et al. (2006) found the accurate calculation of Green's function of the Schrödinger equation in the presence of block layered potentials. In their paper, they proposed a method for calculating the Green's function of the two-dimensional Schrödinger equation in the presence of block layered potentials. The Schrödinger operator is assumed to be separable in the presence of such potentials. Their overall procedure occurred in two steps. Firstly, they represented the Green's function by means of separating the Schrödinger operator into vertical and horizontal components. An infinite sequence of eigenfunctions is generated from the vertical equation while the coefficients for the corresponding infinite series expansion are obtained by solving the horizontal equation. Shao et al also noted that, the eigenfunctions can be pre-calculated using one-dimensional Sturm–Liouville eigenvalue-problem solvers for piecewise constant coefficients. Secondly, the continuity condition of the Green's function along the potential block boundaries via a collocation method was used to determine the coefficients in the eigenfunction expansions of the first step. They also found that, such Green's functions have various and practical applications in quantum modeling of electron transport within nano-MOSFET transistors. Summarily, they added their proposed method was based on expansions of the eigenfunctions of the subordinate Sturm–Liouville problems and a collocation matching procedure along possibly curved interfaces of the potential blocks. They mentioned accuracy in their numerical results was provided to validate the proposed algorithm.

Nash (2007) proposed another method for the solutions of extended nonlinear Schrödinger equation. Nash used Fourier-Based method and showed to be capable of at least qualitatively resolving pulse filamentation. With no certainty, Nash admitted that the method could be adopted to provide numerical solutions of pulse propagation

problems for other system that are governed by linear and nonlinear, local and nonlocal, Schrödinger types of equations and that, those effects may have important implications and application in practical fields such as laser-initiated fusion and optical communications.

Moreover, in the area of nuclear physics – deformed nuclear field Rizea et al. (2008) presented a grid-based procedure to solve the eigenvalue problem for the two-dimensional Schrödinger equation in cylindrical coordinates. The Hamiltonian, after a variable transformation which removes the first derivative from the Laplacean, is discretized by using finite difference approximations of the derivatives and they arrived to an algebraic eigenvalue problem with large (sparse) matrix, which was solved by the package ARPACK, based on Implicitly Restarted Method of Arnoldi. Rizea et al then introduced new special finite difference formulae adapted to the behavior of the solution near the origin. They contain variable coefficients deduced from fitting conditions. Their advantages according to them were demonstrated on a one-dimensional equation. The formulae were then extended to two dimensions. The potential was then assumed to be axially symmetric (without other constraints on the shape) and the Hamiltonian includes a spin-orbit coupling and, for charged particles, the Coulomb potential. The nuclear shape was described by Cassini Ovaloids. By this method, Rizea et al added, the single particle eigenstates of nuclear systems with arbitrary deformations can be obtained and used in different investigations. Additionally again, as an application they considered the emission of scission neutrons from fissioning nuclei. To study this process, they used the sudden approximation, in which the scission is seen as a sudden transition between two very different nuclear configurations. The scission neutrons are characterized by their wave functions just-before-scission and immediately-after-scission. Numerically, these wave functions were the bound states of the bidimensional Schrödinger equation with different deformation parameters and, consequently, with different potentials. They have illustrated the formalism in the case of the nucleus ^{236}U . The approach allows the evaluation of important physical quantities: the number of emitted neutrons per fission event, the excitation energy of primary fission fragments and the spatial distribution of

the emission points. Calculations of this type for a large series of isotopes would open new perspectives for improved description and evaluation of neutrons emitted during nuclear fission. Also, the quasi-stationary eigenfunctions provided in this way were appropriate as initial wave functions for the solution of the time-dependent Schrödinger equation in two spatial dimensions, a very attractive dynamical approach to be used in processes with temporal evolution as the quantum tunneling through time-dependent potential barriers.

One of the latest literatures that contributed immensely in the computation of eigenvalues of Schrödinger equation is the work of Kalogiratos et al. (2009). In their research titled “computation of eigenvalues of Schrödinger equation by exponentially fitted Runge-Kutta-Nystrom method”, they produced RKN methods with exponentially fitted property and applied these methods (Trig5 and Trig6) to the computation of the eigenvalues of the Schrödinger equation. From their tabulated result they concluded that their new methods has superior performance in comparison to the classical RKN methods for low state eigenvalues. For higher state eigenvalues the new methods produced much more accurate results.

In 2001, another similar breakthrough was witnessed when Lambert (2001) used an integration approach to solve the eigenfunctions and eigenvalues of Schrödinger equation in a one-dimensional quantum well. Lambert made use of *Shooting method* and *Runge-Kutta method* to integrate across the specific well and the calculated eigenvalues. They also added that, the finite barrier provided with a tool to investigate the use of structures in semi-conductors, and even gave them a glimpse of yet another future in the form of quantum computing. The idea of quantum ‘binding’ between the two ways of quantum tunneling through an intervention potential and the energy level-splitting that ensues, forms the foundation of the concept of ‘qubits’ or quantum bits. Lambert also admitted that they investigated the limitation of their method via the propagation of errors in the potentials with corresponding analytical solutions, and loss of accuracy with the Landau-Lifshitz potential. While we can be fairly certain that, this won’t occur with our finite barrier potential, it could be a problem if we

wanted to apply shooting method to an application which involves similar ‘high-frequency’ errors as Landau’s Cosh potential – Lambert highlighted.

A perfectly match layer technique was also presented by Zheng (2007) used for absorbing boundary conditions (ABCs) which are generally required for simulating waves in unbounded domains. Zheng applied this method to nonlinear Schrödinger equation. In this paper we apply PML to the nonlinear Schrödinger wave equations. The idea (Zheng highlighted) involved is stimulated by the good performance of PML for the linear Schrödinger equation with constant potentials, together with the time-transverse invariant property held by the nonlinear Schrödinger wave equations. He also did the numerical test to demonstrate the effectiveness of his PML approach for both nonlinear Schrödinger equations and some Schrödinger-coupled systems in each spatial dimension. As one of those approaches for designing ABCs, Zheng said, perfectly matched layer (PML) has achieved great success for both linear and nonlinear wave equations. Though he admitted that using the numerical test, it is not applicable to all Schrödinger wave equations. This could be one of the set back of Zheng method.

Last but not the least among the literature we found very interesting and relevant in the numerical solution of Schrödinger equations is the research conducted by de la Hoz & Vadillo (2008) whom proposed an exponential time differencing fourth-order Runge–Kutta (ETDRK4) method – a scheme that was derived by Cox and Matthews in [S.M. Cox, P.C. Matthews, Exponential time differencing for stiff systems, *J. Comp. Phys.* 176 (2002) 430–455] and was modified by Kassam and Trefethen in [A. Kassam, L.N. Trefethen, Fourth-order time stepping for stiff PDEs, *SIAM J. Sci. Comp.* 26 (2005) 1214–1233]. La Hoz and Vadillo then computed its amplification factor and plotted its stability region, which gave them an explanation of its good behavior for dissipative and dispersive problems. They applied this method to the Schrödinger equation, obtaining excellent results for the cubic equation and the critical exponent case and, later, as an experimental approach to describe the various possible asymptotic behaviors with two space variables. The proposers of the ETDRK schemes

also argued and concluded that they are more accurate than other methods (standard integrating factor techniques or linearly implicit schemes); they have good stability properties and are widely applicable to nonlinear wave equations. However, they said, Cox and Matthews were aware of the numerical instability for the ETDRK4 method when computing the coefficients. Later, Kassan and Trefethen modified the ETDRK4 method with very good results. The authors opined that, the modified ETDRK4 is the best by a clear margin compared with other methods.

2.2 Method of lines:

The method of lines (MOL, NMOL, NUMOL)(Schiesser, 1991; Hamdi et al., 2007) is a technique for solving partial differential equations (PDEs) in which all but one dimension is discretized (Sadiku & Obiozor, 2000; Lee et al., 2003; Wikipedia, free encyclopedia, 04 November 2009; Cutlip and Schacham, 2001; Pregla, 2008; Shakeri & Dehghan, 2008; Wouwer, 2009; Schiesser, 1991). The MOL must often refers to the construction or analysis of numerical PDEs that proceeds by first discretizing the spatial derivatives only and leaving the time variable continuous. This will lead to ordinary differential equation (ODE) to which numerical method for initial value ordinary equation can be applied (Wikipedia, free encyclopedia, 04 November 2009). The MOL also has been applied to the theoretical physics (Pregla, 2008; Lee et al., 2003; Shakeri & Dehghan, 2008; Demirkaya et al., 2005). The idea was first applied by German mathematician – Erich Rothe in 1930 to equation of parabolic type. But it can be used much more widely (Pregla, 2008).

By differential equation (Susan, 2004; Ranvile et al., 1997) we mean, an equation of a function of one or more variable that includes derivative of f with respect to one or more of those variables. Susan also added that, when we have a function of more than one variable such as $y(x, t)$ and equation involve partial derivatives with respect to x and t , is referred to Partial differential equation (PDE).

Furthermore, MOL according to Sadiku and Obiozor (2000) is a well established numerical technique (or rather a semi analytical method) for analysis of transmission lines, wave guide structures and scattering problems. It was also used by Schiesser & Griffith (2009) when they solve Schrödinger equation for one dimension. The method originally developed by mathematicians and used for boundary value problems in physics was introduced into electromagnetic (EM) community (Sadiku & Obiozor, 2000). The method involves reducing initial boundary value problem to a system of ODE in time through the use of discretization in space. The resulting ODE system can be solve through standard initial value software, which may used variable time step/variable order approach with time local error control (Pregla, 2008). MOL has therefore advantage of finite difference method and analytical method: it does not yield spurious modes nor the problem of relative convergence – Sadiku & Obiozor added. MOL has the following properties that justify its usage.

- a. *Computational accuracy*:- the semi analytical character of the formulation leads to a simple and compact algorithm which yields accurate results with less computational effort than other techniques.
- b. *Numerical stability*:- by separating discretization of space and time, it is easy to establish stability and convergence for wide range of the problems.
- c. *Reduced programming effort*:- by making use of state-of-the-art well reduced. When compared with other methods (for example Monte Carlo), Demirkaya et al. (2005) found that the Monte Carlo requires more processing effort than MOL.
- d. *Reduced Computational time*:- since only a small amount of discretization are necessary in the computation, there is no need to solve large system of equations; hence computing time is small. In what follows, we shall discuss some basics about the PDEs, the types of solutions, system of PDE and element and origin of MOL.

2.2.1 Some Basics about Partial Differential Equations (PDE)

Spacetime is an abbreviation for the three-dimensional (3D) space and time Science and engineering to describe the physical world. PDEs provide a mathematical description of physical *Spacetime*, and they are therefore among the most widely used forms of mathematics. As a consequence, methods for the solution of PDEs, such as the MOL, are of broad interest in science and engineering (Hamdi et al., 2007; Schiesser & Griffith, 2009). As a basic illustrative example of a PDE, we consider the equation

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \quad (2.2.1.1)$$

Where

u is a dependent variable (dependent on x and t)

t is an independent variable representing time

x is independent variable representing one dimension of 3-dimensional space

α is Constant

Equation (2.2.1.1) (if we can observe) has x and t as independent variables – which is the reason it is classified as a PDE (any differential equation with *more than one independent variable is a PDE*) (Hamdi et al., 2007; Schiesser & Griffith, 2009). A differential equation with only one independent variable is generally termed an (ODE). Equation (2.2.1.1) is a *diffusion equation*, u is the temperature in Kelvin (K), t is the time in seconds (s) and α is the thermal diffusivity in metre square per second (m^2/s) given by $k/\rho C_p$. In this treatment, the thermal conductivity k in W/m.K, the density ρ in kg/m^3 and heat capacity C_p in J/kg.K are all considered to be constant. $\frac{\partial u}{\partial t}$ is the partial derivative of u with respect to t (x is held constant when taking this partial derivative, which is why partial is used to describe this derivative). Eq.(2.2.1.1) is *first order in t* since the highest order partial derivative in t is first order; it is *second order in x* since the highest order partial derivative in x is second order. Eq. (2.2.1.1) is *linear or first degree* since all of the terms are to the first power (note that order and degree can be easily confused) (Hamdi et al., 2007; Schiesser & Griffith, 2009).

2.2.2 Initial and Boundary Conditions

Before finding the solution of any PDE, one must specify some auxiliary conditions. The number of required auxiliary conditions is determined by the *highest order derivative in each independent variable*.

Now taking equation (2.2.1.1) as an example, since it is first order in t and second order in x , then, therefore it requires one auxiliary condition in t and two auxiliary conditions in x .

t is termed an *initial value variable* and therefore requires *one initial condition (IC)*. It is an initial value variable since it starts at an initial value, t_0 , and moves forward over a *finite interval* $t_0 \leq t \leq t_f$ or a *semi-infinite interval* $t_0 \leq t \leq \infty$ without any additional conditions being imposed. Typically in a PDE application, the initial value variable is time, as in the case of equation (2.2.1.1).

x on the other hand is termed a *boundary value variable* and therefore requires *two boundary conditions (BCs)*. It is a boundary value variable since it varies over a *finite interval* $x_0 \leq x \leq x_f$, a *semi-infinite interval* $x_0 \leq x \leq \infty$ or a *fully infinite interval* $-\infty \leq x \leq \infty$, and at *two different values* of x , conditions are imposed on x in equation (2.2.2.1). Typically, the two values of x correspond to boundaries of a physical system, and hence the name *boundary conditions*.

As examples of auxiliary conditions for equation (2.2.2.1) (there are other possibilities),

- An IC could be

$$u(x, t = 0) = u_0 \quad (2.2.2.1)$$

where u_0 is a given function of x .

- Two BCs could be

$$u(x = x_0, t) = u_b \quad (2.2.2.2a)$$

$$\frac{\partial u(x = x_f, t)}{\partial x} = 0 \quad (2.2.2.2b)$$

where u_b is a given boundary (constant) value of u for all t . Another common possibility is where the initial condition (IC) is given as above and the boundary conditions are $u_0(x = x_0, t) = f_0(t)$ and $u(x = x_f) = f_b(t)$. An important consideration is the possibility of discontinuities at the boundaries, produced for example, by differences in initial and boundary conditions at the boundaries; which can cause computational difficulties, particularly for hyperbolic problems (such as classic linear wave equation $\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}$) (Hamdi et al., 2007; Schiesser & Griffith, 2009). They also added that BCs can be of three types:

1. If the dependent variable is specified, as in BC (2.2.2.2a), the BC is termed *Dirichlet*.
2. If the derivative of the dependent variable is specified, as in BC (2.2.2.2b), the BC is termed *Neumann*.
3. If both the dependent variable and its derivative appear in the BC, it is termed a *BC of the third type* or a *Robin BC*.

2.2.3 Types of PDE Solutions

Equations (2.2.1.1), (2.2.2.1), (2.2.2.2a) and (2.2.2.2b) constitute a complete PDE problem and we can now consider what we mean by a solution to this problem (Hamdi et al., 2007; Schiesser & Griffith, 2009). Briefly, the solution of a PDE problem is a *function that defines the dependent variable as a function of the independent variables*, in this case $u(x, t)$. In other words, we seek a function that when substituted

in the PDE and all of its auxiliary conditions, satisfies simultaneously all of these equations.

The solution can be of two types:

1. If the solution is an actual mathematical function, it is termed an *analytical solution*. While analytical solutions are the *gold standard* for PDE solutions in the sense that they are exact, they are also generally difficult to derive mathematically for all but the simplest PDE problems (in much the same way those solutions to nonlinear algebraic equations generally cannot be derived mathematically except for certain classes of nonlinear equations).
2. If the solution is in numerical form, for example $u(x,t)$, tabulated numerically as a function of x and t , it is termed a *numerical solution*. Ideally, the numerical solution is simply a numerical evaluation of the analytical solution. But since an analytical solution is generally unavailable for realistic PDE problems in science and engineering, the *numerical solution is an approximation to the analytical solution*, and our expectation is that it represents the analytical solution with good accuracy. However, numerical solutions can be computed with modern-day computers for very complex problems, and they will generally have good accuracy (even though this cannot be established directly by comparison with the analytical solution since the latter is usually unknown).

The focus of the MOL is the calculation of accurate numerical solutions.

Vital information probably we need to highlight on the “PDE solution is the *subscript notation*. That is an alternative way of representing the PDEs such that, it will be easier to state and bears a closer resemblance to the associated computer coding. For example, we can write equation (2.2.1.1) as

$$u_t = \alpha u_{xx} \quad (2.2.2.3)$$

where, for example, u_t is subscript notation for $\frac{\partial u}{\partial t}$. In other words, a partial derivative is represented as the dependent variable with a subscript that defines the independent variable. For a derivative that is of order n , the independent variable is repeated n times, e.g., for eq. (2.2.1.1), u_{xx} represents $\frac{\partial^2 u}{\partial x^2}$.

2.2.4 A System of Partial Differential equation

Let us consider some general PDEs. For example, a general PDE first order in t can be considered

$$\bar{u}_t = \tilde{f}(\bar{x}, t, \bar{u}, \bar{u}_{\bar{x}}, \bar{u}_{\bar{x}\bar{x}}, \dots) \quad (2.2.4.1)$$

where an overbar (overline) denotes a vector. For example, $\bar{u}$ denotes a vector of n dependent variables

$$\bar{u} = (u_1, u_2, \dots, u_n)^T$$

That is, a system of n simultaneous PDEs. Similarly, $\tilde{f}$ denotes an n vector of derivative functions

$$\tilde{f} = (f_1, f_2, \dots, f_n)^T$$

where T denotes a *transpose* (here a row vector is transposed to a column vector). Note also that $\bar{x}$ is a vector of spatial coordinates, so that, for example, in *Cartesian coordinates* $\bar{x} = (x, y, z)^T$ while in *cylindrical coordinates* $\bar{x} = (r, \theta, z)^T$. Thus, equation (2.2.4.1) can represent PDEs in one, two and three spatial dimensions.

Since equation (2.2.4.1) is first order in t , it requires one initial condition (IC)

$$\bar{u}(\bar{x}, t = 0) = \bar{u}_0 = (\bar{x}, \bar{u}, \bar{u}_{\bar{x}}, \bar{u}_{\bar{x}\bar{x}}, \dots) \quad (2.2.4.2)$$

where $\bar{u}_0$ is an n vector of initial condition functions

$$\bar{u}_0 = (u_{10}, u_{20}, \dots, u_{n0})^T$$

The derivative vector $\bar{f}$ of equation (2.2.4.1) includes functions of various spatial derivatives, $\bar{u} = (\bar{u}, \bar{u}_x, \bar{u}_{xx}, \dots)$, and therefore we cannot state a priori the required number of BCs. For example, if the highest order derivative in $\bar{x}$ in all of the derivative functions is second order, then we require $2 \times d \times n$ BCs where d is the number of spatial dimensions. For each of the spatial independent variables, e.g., $2 \times 2 \times n$ for a 2D PDE system, $2 \times 3 \times n$ BCs for a 3D PDE system. Thus for equation (2.2.2.3), the number of BC is 2 (second order) $\times$ (one dimension) $\times$ (PDE) $= 2$.

We can now state the general BC requirement of equation (2.2.4.1) as

$$\bar{f}_b(\bar{x}_b, \bar{u}, \bar{u}_{xx}, \dots, t) = 0 \quad (2.2.4.3)$$

the subscript b denotes *boundary*. The vector of boundary condition functions, $\bar{f}_b$ has a length (number of functions) determined by the highest order derivative in $\bar{x}$ in each PDE (in equation (2.2.4.1)) as discussed previously.

2.2.5 The Geometric classification of PDE

Before we go into dealing with the basic idea of MOL and its origin, let us shade some light on the classification of PDE geometrically as pointed out by Hamdi et al. (2007) and Schiesser & Griffith (2009). Here we go!

If the derivative functions in eq. (2.2.4.1) contain *only first order* derivatives in $\bar{x}$, the PDEs are classified as *first order hyperbolic*. As an example, the equation

$$u_t + \nu u_x = 0 \quad (2.2.5.1)$$

is generally called the *linear advection equation*; in physical applications, ν is a linear or flow velocity. Although equation (2.2.5.1) is possibly the simplest PDE, this

simplicity is deceptive in the sense that it can be very difficult to integrate numerically since it *propagates discontinuities*, a distinctive feature of first order hyperbolic PDEs.

Equation (2.2.5.1) is termed a *conservation law* since it expresses conservation of *mass, energy or momentum* under the conditions for which it is derived, i.e., the *assumptions on which the equation is based*. Conservation laws are bedrock of PDE mathematical models in science and engineering, and an extensive literature pertaining to their solution, both analytical and numerical, has evolved over many years.

An example of a first order hyperbolic system (using the notation $u_1 \Rightarrow u, u_2 \Rightarrow v$) is

$$u_t = v_x \quad (2.2.5.2a)$$

$$v_t = u_x \quad (2.2.5.2b)$$

Equations (2.2.5.2a) and (2.2.5.2b) constitute a system of *two linear, constant coefficients, first order hyperbolic PDEs*.

Differentiation and algebraic substitution can occasionally be used to eliminate some dependent variables in systems of PDEs. For example, if equation (2.2.5.2a) is differentiated with respect to t and equation (2.2.5.2b) is differentiated with respect to x we then have

$$u_{tt} = v_{xt}$$

$$v_{tx} = u_{xx}$$

we can then eliminate the mixed partial derivative between these two equations (assuming v_{xt} in the first equation equals v_{tx} in the second equation) to obtain

$$u_{tt} = u_{xx} \quad (2.2.5.3)$$

This equation is the *second order hyperbolic wave equation*.

If the derivative functions in equation (2.2.4.1) contain *only* second order derivatives in $\bar{x}$, the PDEs are classified as *parabolic*. Equation (2.2.1.1) is an example of a parabolic PDE.

Finally, if a PDE contains *no derivatives in t* (e.g., the LHS of equation (2.2.4.1) is zero) it is classified as *elliptic*. As an example,

$$u_{xx} + u_{yy} = 0 \quad (2.2.5.4)$$

is *Laplace's equation* where x and y are spatial independent variables in Cartesian coordinates. Note that with no derivatives in t , *elliptic PDEs require no ICs*, i.e., they are entirely boundary value PDEs.

PDEs with *mixed geometric characteristics* are possible, and in fact, are quite common in applications. For example, the PDE

$$u_t = -u_x + u_{xx} \quad (2.2.5.5)$$

is *hyperbolic-parabolic*. Since it frequently models convection (hyperbolic) through the term u_x and diffusion (parabolic) through the term u_{xx} , it is generally termed a *convection-diffusion equation*. If additionally, it includes a function of the dependent variable u such as

$$u_t = -u_x + u_{xx} + f(u) \quad (2.2.5.6)$$

then it might be termed a *convection-diffusion-reaction equation* since $f(u)$ typically models the rate of a chemical reaction. If the function depends only the independent variables, i.e.,

$$u_t = -u_x + u_{xx} + g(x, t) \quad (2.2.5.7)$$

the equation could be labeled an *inhomogeneous PDE*.

With this long discussion given by Hamdi et al. (2007) and Schiesser & Griffith (2009) clearly indicates that PDE problems come in an infinite variety, depending, for example, on linearity, types of coefficients (constant, variable), coordinate system, geometric classification (hyperbolic, elliptic, parabolic), number of dependent variables (number of simultaneous PDEs), number of independent variables (number of dimensions), type of BCs, smoothness of the IC, etc., so it might seem impossible to formulate numerical procedures with any generality that can address a relatively broad spectrum of PDEs. But in fact, the MOL provides a surprising degree of generality, although the success in applying it to a new PDE problem depends to some extent on the experience and inventiveness of the analyst, i.e., MOL is not a single, straightforward, clearly defined approach to PDE problems, but rather, is a general concept (or philosophy) that requires specification of details for each new PDE problem. We now proceed to illustrate the formulation of a MOL numerical algorithm with the caveat that this will not be a general discussion of MOL as it might be applied to any conceivable PDE problem. In the next chapter, we are going to discuss the methodology to be involved when solving our problem.