ISSN: 2455-1848
International Journal of Innovative Research & Growth
A Peer Reviewed & Referred International Journal
Volume-7 Issue-1 May-2018
Impact Factor-3.0
www.ijirg.com, editor@ijirg.com

Application Of Numerical Methods In Solving Schrodinger's Equation

[1]Manisha Yadav, [2]Anchal Neha, [3]Shefali Jauhri, [4]Dr. Preetam Singh Gour
[1]Scholar of M.Sc., Department of Mathematics, Jaipur National University, Jaipur, Rajasthan, India
[2,3]Assistant Professor, Department of Mathematics, Jaipur National University, Jaipur, Rajasthan, India
[4]Assistant Professor, Department of Physics, Jaipur National University, Jaipur, Rajasthan, India
E-mail- 28.anchal@gmail.com, singhpreetamsingh@gmail.com, shefalijauhri3@gmail.com

Abstract
In this paper we work on the applications of numerical methods in quantum mechanics problem. The Schrodinger's equation has converted into polar form and the numerical solution is obtained by using Crank Nicolson's method.
***Keywords: -** Schrodinger equation, finite difference, Crank – Nicolson, implicit method.*

1- INTRODUCTION

Partial differential equations arise in physics and applied mathematics and many other fields where the number of independent variables in the problem under consideration is two or more. Those equations which involve one or more partial derivative of a function of two or more independent variable are called partial differential equation. Partial differential equations are of three types, Elliptic, Parabolic, and Hyperbolic and play an imported role in quantum mechanics. Quantum Mechanics at an advanced level addressing student of physics, mathematics, chemistry and electrical engineering. Quantum Mechanics gradually arose from theories to explain observation which not could be reconcile with classical physics, such as Max Planck's solution in 1900 to the black body radiation problem, and from the corresponding between energy and frequency in Albert Einstein 1905 which explained the photoelectric effect. Schrodinger Equation in quantum mechanics is an elliptic partial differential equation that describes changes over of time a physical system in which quantum effects, such as the first step in the development of a logically consistent theory. This equation is a mathematical formulation for studying quantum mechanical system. It was named after Erwin Schrodinger, who derived the equation in 1925 and published it in 1926, forming the basis for the work that resulted in his being awarded the Nobel Prize in physics in 1933.The use of the Schrodinger equation in quantum mechanics is analogous of Newton's law in classical mechanics.

Crank-Nicolson method is one of the most popular methods for the numerical integration of diffusion problem which introduced by J. Crank and P. Nicolson in 1947. They considered an implicit finite difference scheme to approximate the solution of a non – linear differential system of the type which arises in problem of heat flow. The search for the exact solution to many real – life problems has been an ancient quest since the time of early scientists. These real life problems are often modeled into differential equation. The mathematical formulation of most problems in science involving rates of change with respect to two or more independent variable, usually representing time, often leads to a partial differential equation. According to Smith (1965), of the numerical methods available for solving differential equation those employing finite – differences are more frequently used and more universally applicable than any other. Among these methods are the explicit and implicit finite difference methods, and their modifications. Many authors have used these methods, finding them very useful. W. Moore, Schrodinger (1989) simple explicit scheme. The first introduced by Gordon (1965), and was generalized in a series of paper by Gurley (1977) [1]. However, according to S.C. Brenner [6] and L.R. Scott, the mathematical theory of finite element method, Springer – Verlag (2002)[5]. C.F. Gerald and P.O. Wheatley used the Numerical Analysis (2003) [7]. L. Ramda Ram – Mohan used of Boundary Element Application in Quantum Mechanics (2002) [5]. Xu and L. Sun (1993) also used the finite difference scheme to solve Schrodinger equation [2].

2- MATHEMATICAL FORMULATION

1) Schrodinger's equation :

$$\nabla^2\Psi + \mathrm{k}^2\Psi = 0$$
$$\nabla^2\Psi = -k^2\Psi$$
$$\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} = -k^2\Psi \qquad (1)$$

Exact Solution: By using Bauer's formula

$$exp(ikz) = exp(ikrcos\theta) = \sum_{n=0}^{\infty}(2_{n+1})\, i^n j_n(kr)$$
$$= exp(ikr\ cos\theta) = (ikr\ cos\theta)p_n\ cos\theta$$

2) Conversion of Schrodinger's equation in Polar Form:

The Cartesian coordinates can be represented by the polar coordinates as follows:

$$x = r\cos\theta$$
$$y = r\sin\theta \qquad (2)$$

Let us first compute the partial derivative of (x, y) with respect to (r, θ) :-

$$\frac{\partial x}{\partial r} = \cos\theta, \frac{\partial x}{\partial \theta} = -r\sin\theta$$
$$\frac{\partial y}{\partial r} = \sin\theta, \frac{\partial y}{\partial \theta} = r\cos\theta \qquad (3)$$

Then we compute $\frac{\partial\Psi}{\partial r}$ in polar coordinates.

$$\frac{\partial\Psi}{\partial r} = \frac{\partial\Psi}{\partial x}\frac{\partial x}{\partial r} + \frac{\partial\Psi}{\partial y}\frac{\partial y}{\partial r}$$

$$= \frac{\partial\varphi}{\partial x}\cos\theta + \frac{\partial\Psi}{\partial y}\sin\theta \qquad using\ (3)$$
$$= \cos\theta\frac{\partial\Psi}{\partial x} + \sin\theta\frac{\partial\Psi}{\partial y} \qquad (4)$$

Now, let's compute $\frac{\partial^2\Psi}{\partial x^2}$, Noticing that both $\frac{\partial\Psi}{\partial x}$ and $\frac{\partial\Psi}{\partial y}$ are functions of (x, y) and using (3) , we have

$$\frac{\partial^2\Psi}{\partial r^2} = \cos\theta\frac{\partial}{\partial r}\frac{\partial\Psi}{\partial x} + \sin\theta\frac{\partial}{\partial r}\frac{\partial\Psi}{\partial y}$$
$$= \cos\theta\left(\frac{\partial}{\partial x}\frac{\partial\Psi}{\partial x}\frac{\partial x}{\partial r} + \frac{\partial}{\partial y}\frac{\partial\Psi}{\partial y}\frac{\partial y}{\partial r}\right) + \sin\theta\left(\frac{\partial}{\partial x}\frac{\partial\Psi}{\partial x}\frac{\partial x}{\partial r} + \frac{\partial}{\partial y}\frac{\partial\Psi}{\partial y}\frac{\partial y}{\partial r}\right)$$

$$= cos^2\theta \ \frac{\partial^2\Psi}{\partial x^2} + 2\cos\theta\sin\theta \ \frac{\partial^2\Psi}{\partial x\,\partial y} sin^2\theta \ \frac{\partial^2\Psi}{\partial y^2} \qquad (5)$$

Similarly, let's compute $\frac{\partial\Psi}{\partial\theta}$ and $\frac{\partial^2\Psi}{\partial\theta^2}$

$$\frac{\partial\Psi}{\partial\theta} = \frac{\partial\Psi}{\partial x}\frac{\partial x}{\partial\theta} + \frac{\partial\Psi}{\partial y}\frac{\partial y}{\partial\theta}$$

$$= \frac{\partial\Psi}{\partial x}(-r\sin\theta) + \frac{\partial\Psi}{\partial y}(r\cos\theta) - r\sin\theta\frac{\partial\Psi}{\partial x} + \cos\theta\frac{\partial\Psi}{\partial y}$$

$$\frac{\partial^2\Psi}{\partial\theta^2} = -r\cos\theta\frac{\partial u}{\partial x} - r\sin\theta\frac{\partial}{\partial\theta}\frac{\partial u}{\partial x} - \sin\theta\frac{\partial\Psi}{\partial y} + r\cos\theta\frac{\partial}{\partial\theta}\frac{\partial\Psi}{\partial y}$$

$$= -r\cos\theta\frac{\partial\Psi}{\partial x} - r\sin\theta\left(\frac{\partial}{\partial x}\frac{\partial\Psi}{\partial x}\frac{\partial x}{\partial\theta} + \frac{\partial}{\partial y}\frac{\partial\Psi}{\partial y}\frac{\partial y}{\partial\theta}\right) -$$

$$r\sin\theta\frac{\partial\Psi}{\partial y} + r\cos\theta\left(\frac{\partial}{\partial x}\frac{\partial\Psi}{\partial y}\frac{\partial x}{\partial\theta} + \frac{\partial}{\partial y}\frac{\partial\Psi}{\partial y}\frac{\partial y}{\partial\theta}\right)$$

$$= -r\cos\theta\frac{\partial\Psi}{\partial x} - r\sin\theta\left(\frac{\partial^2\Psi}{\partial x^2}(-r\sin\theta) + \frac{\partial^2\Psi}{\partial x\,\partial y}r\cos\theta\right)$$

$$-r\sin\theta\frac{\partial\Psi}{\partial y} + r\cos\theta\left(\frac{\partial^2\Psi}{\partial x\,\partial y}(-r\sin\theta) + \frac{\partial^2\Psi}{\partial y^2}r\cos\theta\right)$$

$$= -r\left(\cos\theta\frac{\partial\Psi}{\partial x} + \sin\theta\frac{\partial\Psi}{\partial y}\right)$$

$$+ r^2\left(sin^2\theta\frac{\partial^2\Psi}{\partial x^2} - 2\cos\theta\sin\theta\frac{\partial^2\Psi}{\partial x\,\partial y} + cos^2\theta\frac{\partial^2\Psi}{\partial y^2}\right)$$

Dividing both sides by r^2 and using (4) we have

$$\frac{1}{r}\frac{\partial^2\psi}{\partial\theta^2} = -\frac{1}{r}\frac{\partial\Psi}{\partial r} + sin^2\theta\frac{\partial^2\Psi}{\partial x^2} - 2\cos\theta\sin\theta\frac{\partial^2\Psi}{\partial x\,\partial y} + cos^2\theta\frac{\partial^2\Psi}{\partial y^2} \qquad (6)$$

Finally, adding (5) and (6) using the obvious relation $cos^2\theta + sin^2\theta = 1$ we have

$$\frac{\partial^2\Psi}{\partial r^2} + \frac{1}{r}\frac{\partial^2\Psi}{\partial\theta^2} = -\frac{1}{r}\frac{\partial\Psi}{\partial r} + \frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2}$$

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} = \frac{\partial^2\Psi}{\partial r^2} + \frac{1}{r}\frac{\partial\Psi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\Psi}{\partial\theta^2}$$

$$\frac{\partial^2\Psi}{\partial r^2} + \frac{1}{r}\frac{\partial\Psi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\Psi}{\partial\theta^2} = -k^2\Psi$$

$$\frac{\partial^2\Psi}{\partial r^2} + \frac{1}{r}\frac{\partial\Psi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\Psi}{\partial\theta^2} = -k^2\Psi \qquad (7)$$

For discretization we define the nodes by drawing radial and angular lines with $r = i\Delta r, \theta = i\Delta\theta$. Then equation (7)

$$\frac{\Psi_{i-1},j - \Psi_i,j + \Psi_{i+1},j}{(\Delta r)^2} + \frac{1}{i\Delta r}\left(\frac{\Psi_{i+1},j - \Psi_{i-1},j}{2\Delta r}\right)$$
$$+ \frac{1}{(i\Delta r)^2}\left(\frac{\Psi_i,j-1 - 2\Psi_i,j + \Psi_i,j+1}{(\Delta\theta)^2}\right)$$
$$+k^2(\Psi_{i-1},j) = 0 \qquad (8)$$

Equation (8) can be solved in the implicit form by putting

$i = 1, j = 1, 2, - - - - M$ and

$i = 2, j = 1,2, - - -M$ and so on

3- SOLUTION OF EQUATION (8) USING CRANK NICOLSON'S METHOD

Boundary Condition $\Delta r = h = .1 , r = 0, r = 0.25$

$$\frac{\Psi_{i,j+1} - \Psi_{i,j}}{k} = c^2 . \frac{1}{2}\left[\frac{\Psi_{i-1,j} - 2\Psi_{i,j} + \Psi}{h^2} + \frac{\Psi_{i-1,j+1} - 2\Psi_{i,j+1} + \Psi_{i+1,j+1}}{h^2}\right]$$

OR

$$-\alpha\Psi_{i-1,j+1} + (2 + 2\alpha)\Psi_{i,j+1} - \alpha\Psi_{i+1,j+1} = \alpha\Psi_{i-1,j} + (2 - 2\alpha)\Psi_{i,j} + \alpha\Psi_{i+1,j}$$

Where $\alpha = kc^2/h^2$

	i=1	i=2	i=3	i=4	i=5	i=6	i=7	i=8	i=9	i=10
j=1	.0895	.1590	.2085	.2380	.2475	.2370	.2065	.1563	.0892	.0355
j=2	.0890	.1580	.2070	.2360	.2450	.2340	.2032	.1536	.0969	.0569

4- CONCLUSION

This paper extends the numerical method for the computation of the solution of Schrodinger's equation. This method can also be used in other partial differential equations as diffusion equation, heat equation etc.

5- REFERENCES

[1] Ames W. A., Numerical method for partial differential equation (Academic, New York, 1977).

[2] Bickford W. B, finite element method Irwin publishing (1994).

[3] Brenner S.C and Scott L.R, The Mathematical Theory of finite Element Method, Springer- Verlag (2002).

[4] Chen R, Z. Xu and Sun L, Finite – Difference Scheme to solve Schrodinger equation phys. Rev. E47, 3799-3802 (1993)

[5] Gerald C. F. and Wheatley P. O., Applied Numerical Analysis Pearson Addison Wesley (2003).

[6] Hamzat A. Isede," Several Example of the Crank Nicleson Method for Parabolic Partial Differential Equations", Academic Journal of Sientific Research, May 2013.

[7] Liboff R. L, Introductory Quantum Mechanics, Addison – Wesley publishing company (1993).

[8] Ram L.Ramda – Mohan, Finite Element and Boundary Element Applications in Quantum Mechanics, Oxford Texts in Applied and Engineering Mathematics (2002)

[9] Strikwerda J. C, finite difference schemes and partial differential equation (SIAM 2004).

[10] Tannor D.J, Introduction to quantum mechanics: a time – dependent perspective, University Science Book, Sausalito, California pp.23-25(2007).