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Finite Integration Method for Two and Three Dimensions Linear Schrödinger Equation

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Abstract

In this paper,Finite IntegrationMethod with Ordinary Linear Approach(FIM-OLA) (uniform distribution of nodes) to find approximate analytical solution of two and three dimensional linear unsteady Schrödinger equation is presented.We use simpson1/3 rule with Trapezoidal rule for two dimensions (n is even for simpson1/3) and simpson3/8 with Trapezoidal rule for three diminution (n divided by 3 for simpson3/8) . The method was compared with the finite differences methods in the aspects accuracy and error . The results show that the finite integration method is more accurate and has more convergence than the finite differences methods in literature.

Keywords: Finite integration method (FIM), Schrödinger equation, Absolute error and Laplace transformation

1- Introduction

The relationships governing fields , stress, and strain, hydrodynamics, and thermodynamics are frequently expressed as integral or differential equations.Since the introduction of digital computer many methods have been developed for translating these experessions of integral and differential calculus into algebraic expressions The two methods most commonly applied are finite difference and finite element method , the finite difference method is based on differential calculus and the finite element methodis based on variational calculus, the finite integration method based on integral calculus.

The Schrödinger equation occurs in various areas of physics, It occurs in a broad range of application as quantum dynamic calculations [3, 4] and has received considerable attention because of its usefulness as a model that describes several important physical and chemical phenomena [6] .

Numerical solution of Schrödingerequation has been proposed by a few authors.**Dia (1999)** [12] derives the three level explicit scheme for solving Schrödinger equation with constant and with a variable coefficient which are unconditionally stable. **Subasi (2002)** [9] solves the Schrödinger equation in three methods. The first method is the fully explicit finite difference method. The second method is the Noye-Hayman implicit finite difference method. also applied the Pacemen-Rachford ADI method. **Mahdi (2008)** [10] presents a fourth order accurate finite difference scheme for solving the 2D Schrödinger equation. **Harfash(2009)** [3] introduces three finite difference schemes to solve three dimension unsteadySchrödinger equation. The first is the fully explicit scheme, the second is the Cranck-Nicolson technique and fourth order compact scheme.**Hussein(2010)** [2] solving theSchrödinger Equation by Homotopy perturbation method for two and three dimensions.

The organization of the paper is as follow: In section 2,we introduce the basic idea of finite integration method to solve the differential equation. In section 3, we apply the Finite Integration method for solving two and three dimensionsSchrödinger equation with five test problems to compare the accuracy of(FIM), finallyin section 4, we discuss the conclusions.

2- Basic concepts of finite integration method

This section showsthebasic concepts of the finite integration method (FIM) to solve one,two and threedimensiondifferential equation, integral the function U(x) can be written as [8]:

$$U(x) = \int_0^x u(\mu)\, d\mu \qquad (1)$$

By using the linear interpolation technique(OLD), equation (1) become :-

$$U(x_k) = \int_0^{x_r} u(\mu)\, d\mu = \sum_{i=1}^{k} a_{ik}\, u(x_i) \qquad (2)$$

where $x_i = h * (i-1), h = \frac{b-0}{N-1}$ $, i = 1,2,3, \dots . N$ are nodal points in the interval $[0, b]$ and

$$x_1 = 0 \quad , x_N = b$$

Applying the Simpson1/3 rule(S1/3)with Trapezoidal rule(T):

$$A = \frac{h}{6}\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 3 & 3 & 0 & 0 & 0 & 0 \\ 2 & 8 & 2 & 0 & 0 & 0 \\ 3 & 6 & 6 & 3 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 3 & 6 & 6 & 6 & 6 & 3 \end{pmatrix}_{N\times N} \begin{matrix} \\ T \\ S1/3 \\ T \\ S1/3 \\ T \end{matrix} \qquad (3)$$

where N is even

Or by using the Simpsom3/8 rule(S3/8)with Trapezoidal rule(T):

$$A=\frac{h}{8}\begin{pmatrix}0&0&0&0&0&0\\4&4&0&0&0&0\\4&8&4&0&0&0\\3&9&9&3&0&0\\\vdots&\vdots&\vdots&\vdots&\vdots&\vdots\\4&8&8&8&8&4\end{pmatrix}_{N\times N}\begin{matrix}\\T\\S3/8\\T\\S3/8\\T\end{matrix}\quad(4)$$

where N divided by 3

In matrix form Equation (2) become$U=Au$

where$U=[U_1,U_2,\dots\dots,U_N]^T$,$u=[u_1,u_2,\dots\dots,u_N]^T$ are the values of integration and integral function respectively at each nodes.

Multi-integral for one dimension problem

$$U^{(2)}(x)=\int_0^x\int_0^\mu u(\mu)\,d\mu\,d\mu\quad x\in[0,b]\qquad(5)$$

(5)

By using ordinary linear approach again for equation (5) we get

$$U^{(2)}(x_i)=\int_0^{x_k}\int_0^\mu u(\mu)\,d\mu\,d\mu\;=\sum_{i=1}^{k}\sum_{j=1}^{i}a_{ki}a_{ij}\,u(x_i)=\sum_{i=1}^{k}a_{ki}^{(2)}\,u(x_i)$$

In matrix form $U^{(2)}=A^{(2)}u=A^2u,$ where

$$A^{(2)}=A^2=\frac{h^2}{36}\begin{pmatrix}0&0&0&0&0&0\\9&9&0&0&0&0\\28&40&4&0&0&0\\39&84&30&9&0&0\\\vdots&\vdots&\vdots&\vdots&\vdots&\vdots\\66&138&84&54&36&9\end{pmatrix}_{N\times N}\quad(6)$$

For Simpson1/3 rule with Trapezoidal rule

and for S Simpson3/8 rule with Trapezoidal rule

$$A^{(2)} = A^2 = \frac{h^2}{64}\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 16 & 16 & 0 & 0 & 0 & 0 \\ 48 & 64 & 16 & 0 & 0 & 0 \\ 81 & 135 & 63 & 9 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 120 & 232 & 168 & 88 & 64 & 16 \end{pmatrix}_{N\times N} \quad (7)$$

For two dimentional problem, we difine

$$U_x(x,y) = \int_0^x u(\mu,y)d\mu \ , \quad U_x(x_k,y_k)$$

$$= \int_0^{x_k} u(\mu,y_k)\, d\mu \quad (8)$$

In matrix form Equation (8) become;

$U_x = A_x u$ where $U_x = [U_{x1}, U_{x2}, \dots \dots, U_{xM}]^T$, $u = [u_1, u_2, \dots \dots, u_M]^T$ are integral nodal values and nodal value respectively and $M = N \times N$ are grid points .

$$A_x = \begin{pmatrix} A & 0 & 0 & 0 & 0 & 0 \\ 0 & A & 0 & 0 & 0 & 0 \\ 0 & 0 & A & 0 & 0 & 0 \\ 0 & 0 & 0 & A & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & A \end{pmatrix}_{M\times M}$$

Similarly for y axis :

$$U_y(x,y) = \int_0^y u(x,\xi)d\xi \ , \quad U_y(x_k,y_k)$$

$$= \int_0^{y_k} u(x_k,y)\, dy \quad (9)$$

In matrix form Equation (9) become;

$U_y = A_y u$ where $U_y = [U_{y1}, U_{y2}, \dots \dots, U_{yM}]^T$, $u = [u_1, u_2, \dots \dots, u_M]^T$ are integral nodal values and nodal value respectively and $M = N \times N$ are grid points .

$$A_y = \begin{pmatrix} A & 0 & 0 & 0 & 0 & 0 \\ 0 & A & 0 & 0 & 0 & 0 \\ 0 & 0 & A & 0 & 0 & 0 \\ 0 & 0 & 0 & A & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & A \end{pmatrix}_{M \times M}$$

For multi-integration in two dimension problem we use the following integral w.r.t. x

$$U_x^{(2)} = \int_0^{x_k} \int_0^{\mu} u(\mu, y) d\mu \, d\mu \quad , x_k , y \in [0, b]$$

$$U_x^{(2)}(x_k , y_k) = \int_0^{x_k} \int_0^{\mu} u(\mu, y_k) d\mu \, d\mu = \sum_{i=1}^{k} \sum_{j=1}^{i} (a_{kj})_x a_{ji} u_i$$

In matrix form

$$U_x^{(2)} = A_x^2 u, \text{where} A_x^2 = A_x A_x = \begin{pmatrix} A^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & A^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & A^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & A^2 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & A^2 \end{pmatrix}_{M \times M} \quad (10)$$

Similary $U_y^{(2)}(x, y)$ w.r.t. y $U_y^{(2)} = A_y^2 \, u$

The finite integration method can be extended to the higher integrations (three , four ,…)

$$U_x^{(m)}(x_k , y_k) = \int_0^{x_k} \dots \dots \int_0^{\mu} u(\mu_1, y_k) \, d\mu_1 \, d\mu_2 \dots \dots d\mu_m \quad (11)$$

$$U_y^{(m)}(x_k\,,y_k) = \int_0^{y_k} \ldots\ldots \int_0^{\xi} u(x_k,\xi_1)\; d\xi_1\; d\xi_2 \ldots\ldots d\xi_m \qquad (12)$$

This implies

$$U_x^{(m)}(x_k\,,y_k) = \int_0^{x_k} \ldots\ldots \int_0^{\mu} u(\mu_1,y_k)\; d\mu_1\; d\mu_2 \ldots\ldots d\mu_m$$

$$= \sum_{i=1}^{M}\sum_{j=1}^{M} \left(a_{kj}\right)_x \ldots\ldots (a_{mi})_x\; u(x_i,y_i) = \sum_{i=1}^{M}\left(a_{kj}^{(m)}\right)_x u_i$$

And

$$U_y^{(m)}(x_k\,,y_k) = \int_0^{y_k} \ldots\ldots \int_0 u(x_k,\xi_1)\; d\xi_1\; d\xi_2 \ldots\ldots d\xi_m$$

$$= \sum_{i=1}^{M}\sum_{j=1}^{M} \left(a_{kj}\right)_y \ldots\ldots (a_{mi})_y\; u(x_i,y_i) = \sum_{i=1}^{M}\left(a_{kj}^{(m)}\right)_y u_i$$

In matrix form

$$U_x^{(m)} = A_x^m u \;\;,\;\; U_y^{(m)} = A_y^m u \quad (13)$$

Similary for three dimension problem, we get

$$U_x^{(m)} = A_x^m u,\; U_y^{(m)} = A_y^m u,\; U_z^{(m)} = A_z^m u \qquad (14)$$

3-Finite integration methodfor Schrödinger equation:

In this section, we present the finite integration method for solving two and three dimensional Schrodingerequation.

3.1Two dimension Schrödinger equation:

The two dimension linear unsteady Schrödinger equation with the potential w(x,y) had written as:

$$i\frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + w(x,y)u = 0, \qquad 0 \le x, y \le 1, 0 \le t \le T, \; i = \sqrt{-1} \qquad (15)$$

With the initial conditions $u(x, y, 0) = u_0(x,y)$

And boundary condition:

$u(0,y,t) = u_1(y,t)$, $u(x,0,t) = u_2(x,t)$.

$u(1,y,t) = u_3(y,t)$, $u(x,1,t) = u_4(x,t)$.

This model had derived from the vector wave equation for electric field which governs the propagation electrn-magnctic waves in a homogeneous medium.

For solving Eq. (14), according to the finite integration method, by applying Laplace transformation w.r.t. tfor (15) with initial conditions, we get :

$$i(p\bar{u} - u_0) + \frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} + w(x,y)\bar{u} = 0 \qquad (16)$$

$$\frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} + (ip + w)\bar{u} = iu_0$$

$$\frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} + \bar{E}\bar{u} = \bar{h}$$

Integration twice

$$\iint \iint \left[\frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} + \bar{E}\bar{u}\right] dxdxdydy = \iint \iint iu_0 dxdxdydy + x\varphi_y f_0 + \varphi_y f_1 + y\varphi_x g_0 + \varphi_x g_1$$

By using integration by part we have

$$\iint \bar{u}\, dydy + \iint \bar{u}\, dxdx + \iint \iint \bar{E}\bar{u}\, dxdxdydy = \iint \iint \bar{h}\, dxdxdydy + X\varphi_y f_0 + \varphi_y f_1 + Y\varphi_x g_0 + \varphi_x g_1$$

Where$\bar{u} = \int_0^{\infty} u(t)e^{-pt}\, dt$, $L\left(\frac{\partial u}{\partial t}\right) = p\bar{u} - u_0$,$\bar{E} = (ip + w)$, $\bar{h} = iu_0$

In matrix form

$$[A_x^2 + A_y^2 + \bar{E}A_x^2A_y^2]\bar{u} = A_x^2A_y^2\bar{h} + X\varphi_y f_0 + \varphi_y f_1 + Y\varphi_x g_0 + \varphi_x g_1 \qquad (17)$$

The one dimentional functions f_0, f_1 and g_0 , g_1 can be interpolated in terms of the nodal values in the following procedure [8]:

1- Determine the regions of functions $f(x)$ and $g(y)$ i.e. $[\overline{x_1}, \overline{x_r}]$, $[\overline{y_1}, \overline{y_c}]$, the number of boundary points$r$, $c$are arbitrary.
2- Distribution the points in these region uniformly .
3- Determine one-dimentional shape function matrices φ_x , φ_y by ordinary linear approximation as following :

From linear interpolation (Lagrange interpolation) we have

$$f(x) = \frac{\bar{x}_t - x}{\bar{x}_t - \bar{x}_{t-1}} f_{t-1} + \frac{x - \bar{x}_t}{\bar{x}_t - \bar{x}_{t-1}} f_t \quad if \;\; \bar{x}_{t-1} < x < \bar{x}_t \qquad and \;\; f(x) = 0 \;\; e.w.$$

(18)

$$g(y) = \frac{\bar{y}_p - y}{\bar{y}_p - \bar{y}_{p-1}} g_{p-1} + \frac{y - \bar{y}_p}{\bar{y}_p - \bar{y}_{p-1}} g_p \quad if \;\; \bar{y}_{p-1} < y < \bar{y}_p \quad and \;\; g(y) = 0 \;\; e.w.$$

Therefore the matrices of shape function are

$$\varphi_x = \begin{bmatrix} .. & .. & .. & .. & .. \\ .. & .. & .. & .. & .. \\ 0 & \frac{\bar{x}_t - x}{\bar{x}_t - \bar{x}_{t-1}} & \frac{x - \bar{x}_t}{\bar{x}_t - \bar{x}_{t-1}} & 0 & 0 \\ .. & .. & .. & .. & .. \\ .. & .. & .. & .. & .. \end{bmatrix}_{M\times r} , \quad \varphi_y = \begin{bmatrix} .. & .. & .. & .. & .. \\ .. & .. & .. & .. & .. \\ 0 & \frac{\bar{y}_p - y}{\bar{y}_p - \bar{y}_{p-1}} & \frac{y - \bar{y}_p}{\bar{y}_p - \bar{y}_{p-1}} & 0 & 0 \\ .. & .. & .. & .. & .. \\ .. & .. & .. & .. & .. \end{bmatrix}_{M\times c}$$

The transformed variables $\bar{u}(x_i, p_k)$had evaluated by the numerical procedure finite integration method .

The $u(x,t)$ in the time domain can be determined by Laplace inversion techniques [5].

In this paper, we use formula of Durbin inversion sachem which given by :

$$f(t)=\frac{2e^{aj\Delta t}}{T}\left[-\frac{1}{2}\bar{f}(a)+\sum_{k=0}^{K}Re\{\bar{f}(p_k)e^{2k\pi i/T}\}\right] \qquad (19)$$

Where $t_j=j\Delta t$ $,j=0,1,\dots .N-1$ and $p_k=a+\frac{2k\pi i}{T}$, $i=\sqrt{-1}$ is parameter of the Laplace transform,

a is free normalized parameter.

Test problem 1 [10] The exact solution of this problem is $u(x,y,t)= x^2 y^2 e^{it}$, The initial and boundary conditions are directly taken from this solution, the potential functionw(x,y)=$1-\frac{2}{x^2}-\frac{2}{y^2}$,

For simplicity, we consider $v_0(x,y)=u_0(x,y)=x^2 y^2$ as a first approximation for the solution that satisfies the initial condition.

Test problem 2 [13] The exact solution of this problem is $u(x,y,t)= e^{-it}(\sin x+\sin y)$, the initial and boundary conditions are directly taken from this solution, The potential w(x,y)=0

For simplicity, we consider $v_0(x,y)=u_0(x,y)= (\sin x+\sin y)$ as a first approximation for the

solution that satisfies the initial condition.

Test problem 3 [13] The exact solution of this problem is $u(x,y,t)=\frac{ie^{it}}{\cosh x\cosh y}$, The initial and boundary condition are directly taken from this solution, the potential w(x,y)=3-2tanh^{2}x-2tanh^{2}y, For simplicity, we consider $v_0(x,y)=u_0(x,y)=\frac{i}{\cosh x \cosh y}$

as a first approximation for the solution that satisfies the initial condition.

In three test problem we take N=10, $\Delta x = 0.1$.

The results that are obtaining fromFIM and exact solution at t=1 are listed in (Tables 1, 4, 6)(Fig. 1,2,4,5) for real and image part of u(x,y,t) respectively. To show the efficiency of the FIM for solving Schrödinger equation,we compare absolute error,L^2-error,L^∞-error for method with errors for other methodsnamely, Explicit(1,5), N-H(5,5), ADI(5,5)[9] and HOC-4 [10] (Tables 2,3)(Fig.3) and HOC-ADI[13],PR-ADI[9],SD-HOC[7] (Tables 5,7).From tables and figures.We see thatthe errors of the FIMare almost identical and are distinctly lower than those of the other method, also notice that theFIM exhibits smaller CPU times than that of the other method.

Table 1: The exact and FIM results for real and image partto 2D test problem 1

X	Y	Exact solution		FIM solution	
		Real part	Image part	Real part	Image part
0.1	0.1	0.00005403023059	0.00008414709848	0.00004403023038	0.00008414711451
0.2	0.2	0.00086448368939	0.00134635357569	0.00076448368607	0.00134635372111
0.3	0.3	0.00437644867753	0.00681591497694	0.00537644866071	0.00681591517857
0.4	0.4	0.01383173903022	0.02154165721108	0.01383173897707	0.02154165784832
0.5	0.5	0.03376889411676	0.05259193655049	0.02376889398699	0.05259193810626
0.6	0.6	0.07002317884051	0.10905463963110	0.07012317857143	0.10905464285714

Table 2: Comparison of the absolute error for real part to 2D test problem 1

X	Y	Explicit(1,5)	N-H(5,5)	ADI(5,5)	HOC-4	FIM
0.1	0.1	3.0800e-005	4.8000e-005	6.5000e-005	6.2500e-010	2.0763e-013
0.2	0.2	8.2500e-006	9.7000e-005	9.0000e-005	5.8000e-009	3.3220e-012
0.3	0.3	1.1900e-006	7.3000e-005	3.7000e-004	1.2000e-008	1.6818e-011
0.4	0.4	1.5900e-005	3.9000e-004	9.7000e-004	7.1700e-009	5.3152e-011
0.5	0.5	6.5200e-005	4.2000e-004	2.7000e-003	7.5500e-009	1.2977e-010

0.6	0.6	1.1800e-004	1.7000e-003	4.6000e-003	2.3600e-009	2.6908e-010

Table 3: Comparison of the absolute error for image part to 2D test problem 1

X	Y	Explicit(1,5)	N-H(5,5)	ADI(5,5)	HOC-4	FIM
0.1	0.1	1.0300e-005	1.3000e-005	1.3000e-005	1.9800e-011	2.4892e-012
0.2	0.2	1.8700e-006	3.1000e-005	4.4000e-005	4.5800e-011	3.9828e-011
0.3	0.3	3.2100e-006	1.1000e-004	2.9000e-004	1.5000e-009	2.0163e-010
0.4	0.4	1.2200e-005	5.4000e-004	8.0000e-004	6.9500e-009	6.3724e-010
0.5	0.5	3.4900e-007	6.3000e-005	1.6000e-003	8.8600e-009	1.5558e-009
0.6	0.6	4.1600e-005	4.4000e-004	4.0000e-003	9.1700e-009	3.2260e-009

Table4: The exact and FIM results for real and image part to 2D test problem 2

X	Y	Exact solution		FIM solution	
		Real part	Image part	Real part	Image part
0.1	0.1	0.10788045043395	-0.16801384684509	0.10788045001939	-0.16801385181525
0.2	0.2	0.21468299506770	-0.33434895487049	0.21468299424273	-0.33434896476116
0.3	0.3	0.31934049817950	-0.49734335865990	0.31934049695235	-0.49734337337224
0.4	0.4	0.42080725659342	-0.65536847200944	0.42080725497636	-0.65536849139646
0.5	0.5	0.51806944799985	-0.80684536022267	0.51806944600903	-0.80684538409066
0.6	0.6	0.61015526073285	-0.95026051630417	0.61015525838817	-0.95026054441465

Table 5: The Absolute error and (L^2, L^∞)errors comparison between the FIM and other methods to 2D test problem 2(t=1)

X	Y	Absolute error	Cpu	Reference	L^2-error	L^∞-error	Cpu

				Tim e				Time
		Real part	Image part		FIM	4.8755e-11	6.4539e-11	0.0165s
0.	0.	4.1456e-	4.9702e-	0s				
0.	0.	8.2498e-	4.9702e-	0s	HOC-ADI-I [13]	5.0842e-11	1.2615e-10	12.641s
0.	0.	1.2271e-	1.4712e-	0s				
0.	0.	1.6171e-	1.9387e-	0s	HOC-ADI-II	5.0842e-11	1.2615e-10	18.813s
0.	0.	1.9908e-	2.3868e-	0s				
0. 6	0. 6	2.3447e-009	2.8110e-008	0s	PR-ADI	2.0408e-	4.8010e-	9.094s
					SD-HOC [7]	4.9908e-11	1.2332e-10	228.094s

Table 6: The exact and FIM results for real and image part to 2D test problem 3

X	Y	Exact solution		FIM solution	
		Real part	Image part	Real part	Image part
0.1	0.1	-0.83311205678450	0.53493509990719	-0.83311208142950	0.53493509785156
0.2	0.2	-0.80868978531922	0.51925373973499	-0.80868980924177	0.51925373773962
0.3	0.3	-0.77006120050236	0.49445061066009	-0.77006122328221	0.49445060876004
0.4	0.4	-0.71999521196356	0.46230360910988	-0.71999523326236	0.46230360733335
0.5	0.5	-0.66177294835878	0.42491952356626	-0.66177296793525	0.42491952193340
0.6	0.6	-0.59877204065167	0.38446710593037	-0.59877205836446	0.38446710445295

Table 7: The Absolute error and (L^2, L^∞)errors comparison between the FIM and other methods to 2D test problem 3(t=1)

X	Y	Absolute error		Cpu Time	Reference	L^2-error	L^∞-error	Cpu Time
		Real part	Image part		FIM	3.7753e-11	4.2930e-11	0.016s
0.1	0.1	2.4645e-008	2.0556e-009	0s				
0.2	0.2	2.3923e-	1.9954e-	0s	HOC-ADI-	7.6035e-	1.7198e-9	13.703s

		008	009		I [13]	10		
0.3	0.3	2.2780e-008	1.9001e-009	0s				
0.4	0.4	2.1299e-008	1.7765e-009	0s	HOC-ADI-II [13]	1.1608e-09	4.0706e-09	20.485s
0.5	0.5	1.9576e-008	1.6329e-009	0s				
0.6	0.6	1.7713e-008	1.4774e-009	0s	PR-ADI [9]	1.4305e-06	2.9710e-06	10.047s
					SD-HOC [7]	1.4453e-10	4.0263e-10	229.094s

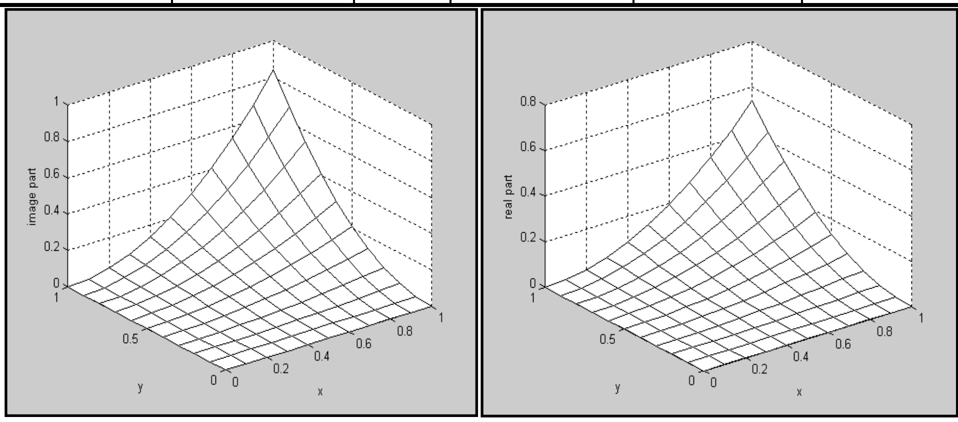

Fig. 1: The real and image part for exact solution to 2D test problem 1

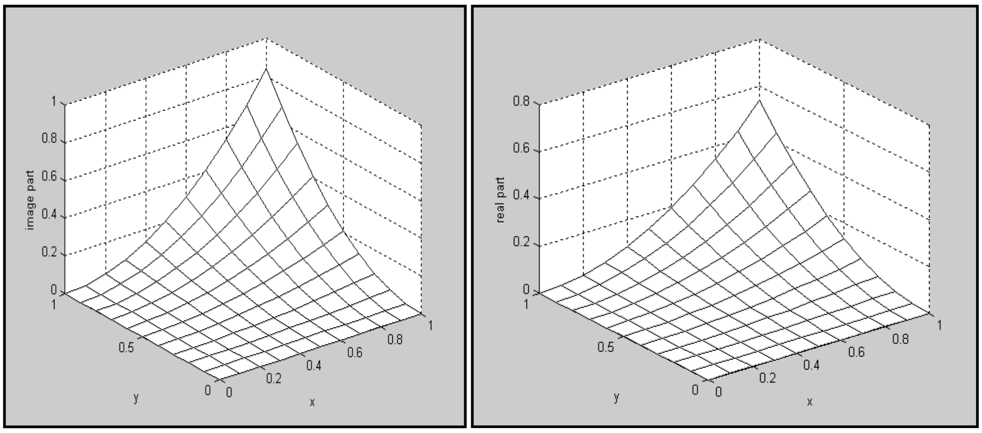

Fig. 2: The real and image part for FIM solution to 2D test problem 1

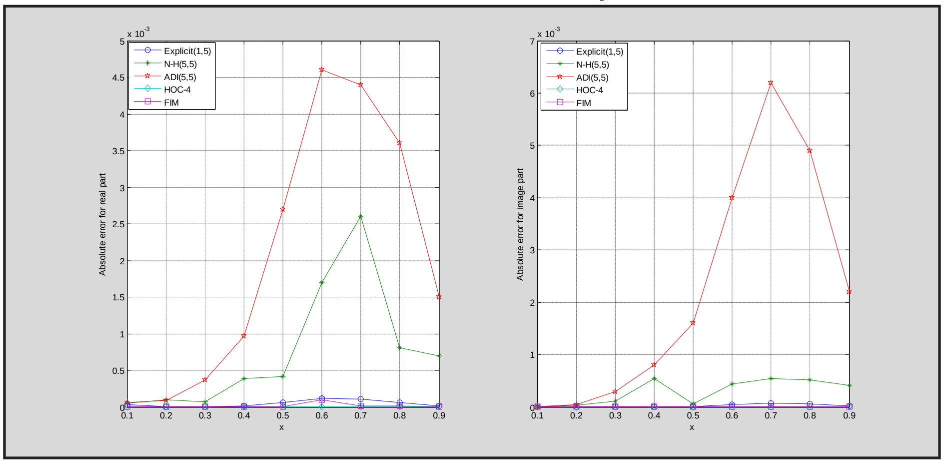

Fig. 3: Absolute error comparison between the FIM and other methods Forreal and Image part to 2D test problem 1

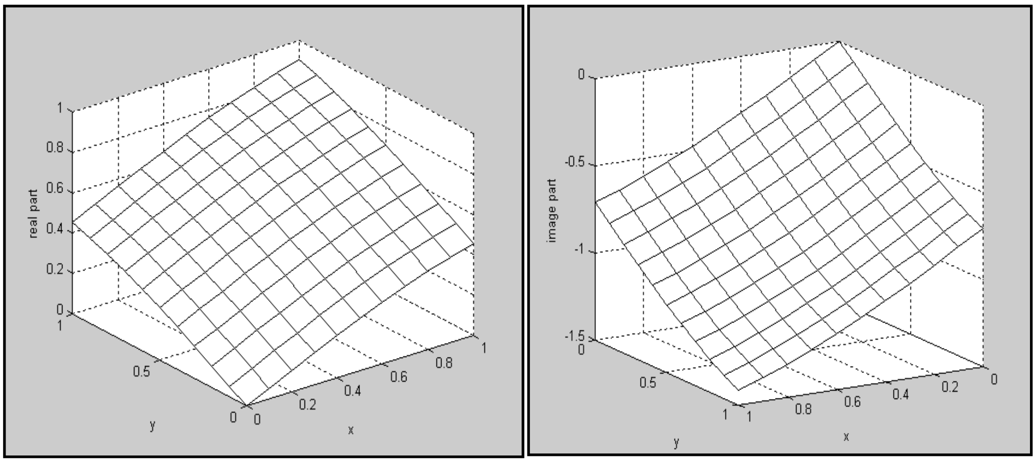

Fig.4: The real and image part for FIM solution to 2D test problem 2

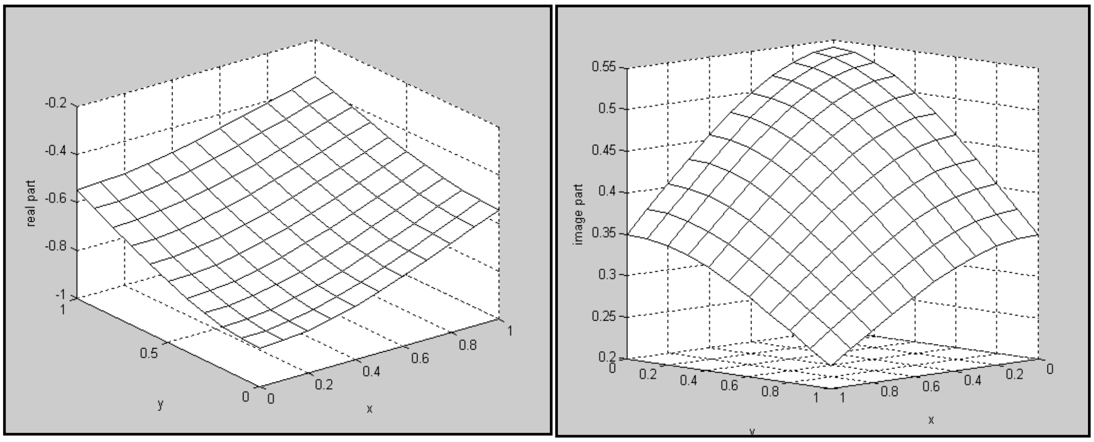

Fig.5: The real and image part for FIM solution to 2D test problem 3

3.2Three dimension Schrödinger equation:

The three dimensions unsteady Schrödinger equation with the potential w(x,y,z) had written as:

$$i\frac{\partial u}{\partial t}+\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}+\frac{\partial^2 u}{\partial z^2}+w(x,y,z)u=0, \qquad 0\le x,y,z\le 1, 0\le t\le T, i=\sqrt{-1} \quad (20)$$

With the initial condition $u(x,y,z,0) = u_0(x,y,z)$

And boundary conditions :

$u(0,y,z,t) = u_1(y,z,t)$, $u(x,0,z,t) = u_2(x,z,t)$, $u(x,y,0,t) = u_3(x,y,t)$

$u(1,y,z,t) = u_4(y,z,t)$, $u(x,1,z,t) = u_5(x,z,t)$, $u(x,y,1,t) = u_6(x,y,t)$.

For solving Eq. (20), according to the finite integration method,

$$i(p\bar{u}-u_0)+\frac{\partial^2\bar{u}}{\partial x^2}+\frac{\partial^2\bar{u}}{\partial y^2}+\frac{\partial^2\bar{u}}{\partial z^2}+w(x,y,z)\bar{u}=0 \qquad (21)$$

$$\frac{\partial^2\bar{u}}{\partial x^2}+\frac{\partial^2\bar{u}}{\partial y^2}+\frac{\partial^2\bar{u}}{\partial z^2}+(ip+w)\bar{u}=iu_0$$

$$\frac{\partial^2\bar{u}}{\partial x^2}+\frac{\partial^2\bar{u}}{\partial y^2}+\frac{\partial^2\bar{u}}{\partial z^2}+\bar{E}\bar{u}=\bar{h}$$

Where

$$\bar{u}=\int_0^\infty u(t)e^{-pt}\,dt, \qquad \bar{E}=(ip+w)\ , \quad \bar{h}=iu_0$$

Integration three times

$$\iint\iint\iint\left[\frac{\partial^2\bar{u}}{\partial x^2}+\frac{\partial^2\bar{u}}{\partial y^2}+\frac{\partial^2\bar{u}}{\partial z^2}+\bar{E}\bar{u}\right]dxdxdydydzdz$$
$$=\iint\iint\iint iu_0dxdxdydy+x\varphi_y f_0+\varphi_y f_1+y\varphi_x g_0+\varphi_x g_1$$

By using integration by part we have

$$\iint \iint \bar{u}\, dydy\, dzdz + \iint \iint \bar{u}\ dxdxdzdz + \iint \iint \bar{u}\ dxdxdydy + \iint \iint \iint \bar{E}\, \bar{u}\, dxdxdydydzdz = \iint \iint \iint \bar{h}\ dxdxdydydzdz + X\varphi_{y,z} f_0 + \varphi_{y,z} f_1 + Y\varphi_{x,z} g_0 + \varphi_{x,z}\, g_1 + Z\varphi_{x,y} h_0 + \varphi_{x,y} h_1$$

In matrix form

$$[A_y^2 A_z^2 + A_x^2 A_z^2 + A_x^2 A_y^2 + \bar{E} A_x^2 A_y^2 A_z^2]\bar{u} = A_x^2 A_y^2 A_z^2 \bar{h} + X\varphi_{y,z} f_0 + \varphi_{y,z} f_1 + Y\varphi_{x,z} g_0 + \varphi_{x,z}\, g_1 + Z\varphi_{x,y} h_0 + \varphi_{x,y} h_1$$

Where $f_i\,, g_i,\ h_i\,, i = 0{,}1$ are functions with respect to $(y, z), (x, z), (x, y)$ respectively, and are evaluated by using Lagrange polynomial in two dimension.

Now we consider two test problems to compare the accuracy of finite integration method .

Test problem 1[1] The exact solution of this problem is:

$u(x_1,x_2,x_3,t)= \sum_{k=1}^{3}\left(\sin(x_k)e^{-\frac{3}{2}it} + \cosh(x_k)e^{\frac{1}{2}it}\right)$,the initialand boundary conditions are directly taken from this solution, the potential$w(x_1,x_2,x_3,t)=-\frac{1}{2}$, for simplicity, we consider$v_0(x_1,x_2,x_3)=u_0(x_1,x_2,x_3)= \sum_{k=1}^{3}(\sin(x_k)+\cosh(x_k))$ as a first approximation for the solution that satisfies the initial condition.

Test problem 2[3] The exact solution of this problem is $u(x,y,t)= x^2\ y^2 z^2\ e^{it}$, The initial and boundary conditions are directly taken from this solution, The potential $w(x,y)=1-\frac{2}{x^2}-\frac{2}{y^2}-\frac{2}{z^2}$, for simplicity,we consider $v_0(x,y)=u_0(x,y)=x^2\ y^2 z^2$ as a first approximation for the solution that satisfies the initial condition.

The results that are obtaining fromFIM at t=1 are listed in (Tables8, 9) (Fig.8) for real and image part of u(x,y,z,t) respectively. To show the efficiency of the FIM for solving Schrödinger equation,We compare absolute error for method with absolute error for other methods namely, explicit (1, 5), C-N [9] and HOC-4 [3] (Tables 10, 11) (Figure 9, 10), from the results, we see that FIM is better than the other methods in accuracy andconvergence.

We also notice in figures 9 and 10 that the curve of absolute error with respect to FIM is more stable than the curves of absolute error of other methods.

Table 8: The exact, FIM results and absolute error for real and image part to 3D test

Problem1

X	y	z	Exact solution		FIM solution		Absolute error	
			Real part	Image part	Real part	Image part	Real part	Image part
0.1	0.1	0.1	2.6671e+00	1.1467e+000	2.6671e+00	1.1467e+000	8.0133e-008	6.3970e-007
0.2	0.2	0.2	2.7277e+00	8.7262e-001	2.7277e+00	8.7262e-001	1.5946e-007	1.2731e-006
0.3	0.3	0.3	2.8148e+00	6.1915e-001	2.8148e+00	6.1914e-001	2.3720e-007	1.8937e-006
0.4	0.4	0.4	2.9288e+00	3.8955e-001	2.9288e+00	3.8955e-001	3.1257e-007	2.4954e-006
0.5	0.5	0.5	3.0705e+00	1.8716e-001	3.0705e+00	1.8716e-001	3.8481e-007	3.0722e-006
0.6	0.6	0.6	3.2409e+00	1.5343e-002	3.2409e+00	1.5339e-002	4.5321e-007	3.6182e-006
0.7	0.7	0.7	3.4413e+00	-1.2253e001	3.4413e+00	-1.2254e-001	5.1708e-007	4.1281e-006
0.8	0.8	0.8	3.6734e+00	-2.2308e001	3.6734e+00	-2.2308e-001	5.7579e-007	4.5968e-006
0.9	0.9	0.9	3.9392e+00	-2.8292e001	3.9392e+00	-2.8292e-001	6.2874e-007	5.0196e-006

Table 9: The exact and FIM results for real and image part to 3D test problem 2

x	y	z	Exact solution		FIM solution	
			Real part	Image part	Real part	Image part
0.1	0.1	0.1	0.00000054030231	0.00000084147098	0.00000054030230	0.00000084147101
0.2	0.2	0.2	0.00003457934758	0.00005385414303	0.00003457934744	0.00005385414462
0.3	0.3	0.3	0.00039388038098	0.00061343234792	0.00039388037946	0.00061343236607
0.4	0.4	0.4	0.00221307824484	0.00344666515377	0.00221307823633	0.00344666525573
0.5	0.5	0.5	0.00844222352919	0.01314798413762	0.00844222349675	0.01314798452657
0.6	0.6	0.6	0.02520834438258	0.03925967026720	0.02520834428571	0.03925967142857
0.7	0.7	0.7	0.06356602598308	0.09899821989166	0.06356602573881	0.09899822282022
0.8	0.8	0.8	0.14163700766950	0.22058656984148	0.14163700712522	0.22058657636684
0.9	0.9	0.9	0.28713879773287	0.44719218163729	0.28713879662946	0.44719219486607

Table 10: Comparison of the absolute error for real part to 3D test problem 2

x	Y	Z	Explicit(1,7)	C-N(7,7)	HOC-4	FIM
0.1	0.1	0.1	2.14e-010	3.17e-012	5.24e-009	2.0763e-015
0.2	0.2	0.2	8.85e-011	1.37e-011	8.52e-009	1.3288e-013
0.3	0.3	0.3	3.07e-010	2.12e-011	3.53e-008	1.5136e-012
0.4	0.4	0.4	3.00e-009	3.62e-010	4.45e-008	8.5043e-012
0.5	0.5	0.5	4.95e-009	9.07e-010	9.79e-009	3.2441e-011
0.6	0.6	0.6	1.64e-008	4.84e-009	1.81e-008	9.6870e-011
0.7	0.7	0.7	1.66e-008	6.15e-009	2.71e-008	2.4427e-010
0.8	0.8	0.8	1.76e-009	1.23e-008	1.20e-007	5.4428e-010
0.9	0.9	0.9	1.26e-009	9.82e-009	5.30e-007	1.1034e-009

Table 11: Comparison of the absolute error for image part to 3D test problem 2

X	Y	Z	Explicit(1,7)	C-N(7,7)	HOC-4	FIM
0.1	0.1	0.1	2.21e-010	2.47e-011	4.89e-009	2.4892e-014
0.2	0.2	0.2	8.66e-010	1.97e-010	2.59e-009	1.5931e-012
0.3	0.3	0.3	6.01e-011	6.79e-011	5.88e-008	1.8146e-011
0.4	0.4	0.4	6.64e-010	4.82e-010	2.72e-008	1.0196e-010

0.5	0.5	0.5	5.08e-009	1.37e-009	1.75e-008	3.8894e-010
0.6	0.6	0.6	7.41e-009	4.26e-009	3.96e-009	1.1614e-009
0.7	0.7	0.7	2.26e-008	8.11e-009	6.16e-009	2.9286e-009
0.8	0.8	0.8	2.60e-008	6.57e-009	8.65e-008	6.5254e-009
0.9	0.9	0.9	2.02e-008	1.30e-008	7.83e-007	1.3229e-008

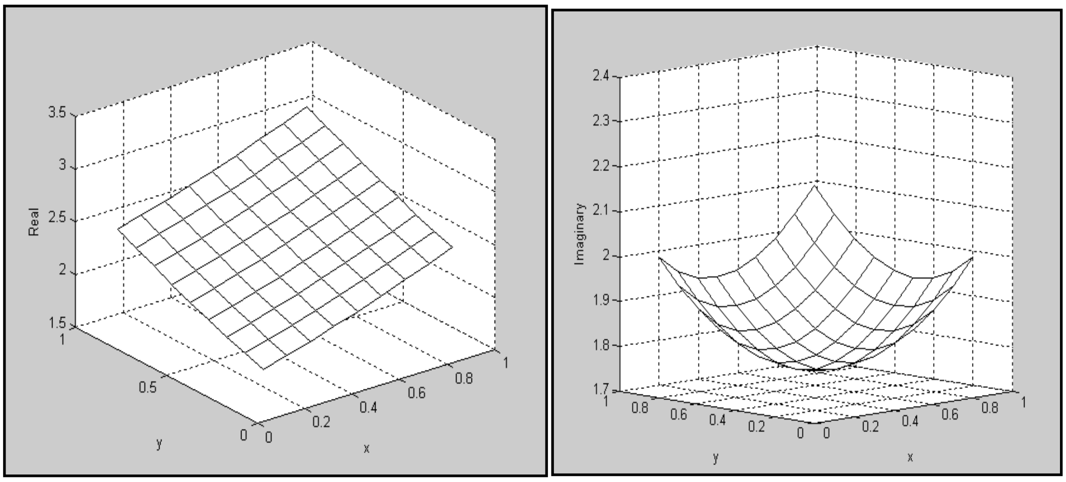

Fig. 8:FIM solution when z=0.2 and $0 \le x, y \le 1$ for real and image part to 3D test problem 1

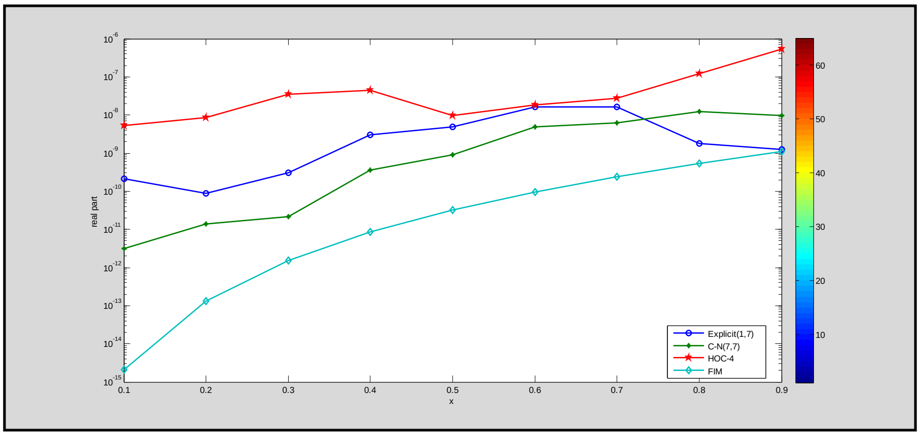

Fig.9: Absolute error comparison between the FIM and other methods Forreal part to 3D test problem 2

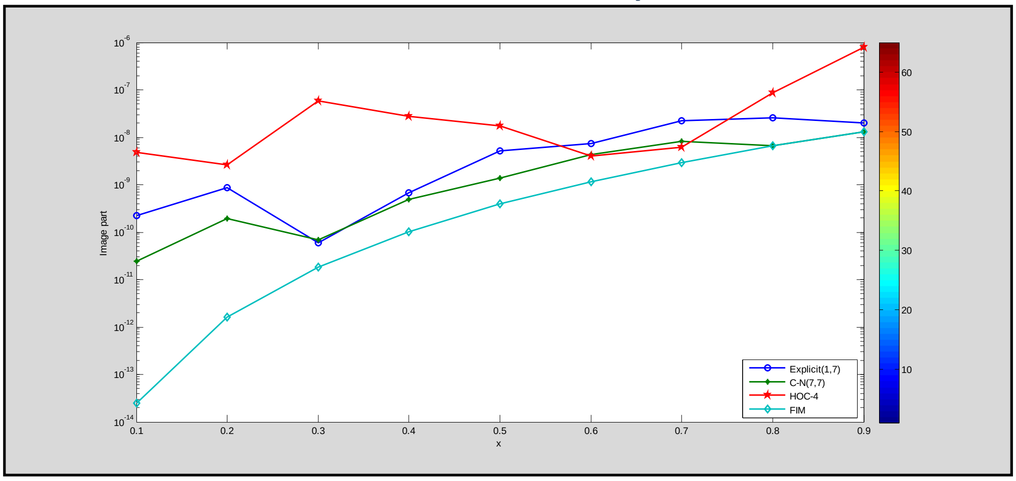

Fig.10: Absolute error comparison between the FIM and other methods For image part to 3D test problem 2

4- Conclusions

This work calculated the approximate solutions of 2D and 3D linearSchrödinger equation by using finite integration method with ordinary linear approach(FIM-OLA) (uniform distribution of nodes),the test the robustness, accuracy and efficiency of the method is applied to five examples having analytical solutions, our results exhibit good comparison with analytical solutions.

In the future work we will use the finite integration method with the Radial basis function (FIM-RBF)(uniform/random distributions of nods) that give more accurate results.

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