International Journal of Mathematical Research 2017 Vol. 6, No. 1, 1-12. ISSN(e): 2306-2223 ISSN(p): 2311-7427 DOI: 10.18488/journal.24.2017.61.1.12 © 2017 Conscientia Beam. All Rights Reserved. © CrossMark

ON THE NUMERICAL SOLUTION OF TWO DIMENSIONAL SCHRÖDİNGER EQUATION

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ABSTRACT

This paper includes a MAPLE[®] code giving numerical solution of two dimensional Schrödinger equation in a functional space. The Galerkin method has been used to get the approximate solution. The results have been examined with numerical examples.

Keywords: Time dependent schrödinger equation, Weak solution, Numerical approximation, Galerkin method, Maple.

JEL Classification: 35Q41, 34L16, 65N30.

Received: 22 November 2016/ Revised: 17 December 2016/ Accepted: 28 December 2016/ Published: 9 January 2017

Contribution/ Originality

This study is one of very few studies which have investigated to obtain an efficient computation tool for numerical examinations of two dimensional Schrödinger Equation.

1. INTRODUCTION

As it is known the Schrödinger equation appears in underwater acoustics, in electromagnetic wave propagation, in optics and in optoelectronic devices [1-4]. The analytical and numerical solutions have been a subject of considerable interest [5-8].

The numerical investigations on two dimensional Schrödinger equation have drawn considerable interest in different aspects [9-13].

We consider one single electron of an atomic system that could be extended for several electron problems and assume that external potential is time dependent only. Besides, we assume that the system has a perturbing term. Depending on the nature of perturbation the system can set out quite complicated features.

The purpose of this study is to obtain an operable and efficient code for the solution of a general two dimensional Schrödinger equation in the form of;

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + v(t)\psi + f(\mathbf{x},t), \ (\mathbf{x},t) \in \Omega$$
⁽¹⁾

$$\psi(\mathbf{x}, \mathbf{0}) = \varphi(\mathbf{x}), \ \mathbf{x} \in D \tag{2}$$

$$\psi(\mathbf{x},t)\Big|_{\Gamma} = 0, \ t \in (0,T]$$
⁽³⁾

where $D := (0, l_1) \times (0, l_2) \subset \square^2$, $\Omega = D \times (0, T]$ and Γ is the boundary of D.

+ Corresponding author © 2017 Conscientia Beam. All Rights Reserved. For the sake of simplicity, we take $\hbar = m = 1$ (unit Planck constant and reduced mass) in the rest of the paper.

The potential function v(t) is dependent only time variable on the interval [0,T] and $f(\mathbf{x},t)$ is the perturbing term.

By the concept of solution of the problem (1)-(3), we mean the function $\psi \in C([0,T], H^2(D))$ satisfying the following integral equation

$$\int_{D} \left(i \frac{\partial \psi}{\partial t} + \Delta \psi - v(t) \psi \right) \overline{\eta} d\mathbf{x} = \int_{D} f(\mathbf{x}, t) \overline{\eta} d\mathbf{x} \quad \forall t \in [0, T]$$
for $\eta(\mathbf{x}, t) \in C([0, T], L_2(D)).$
(4)

The space $L_2(D)$ is the set of square integrable functions on the domain D.

The space $C([0,T], L_2(D))$ is the set of functions which are continuously defined on [0,T] and take their values from the space $L_2(D)$.

The space $H^2(D)$ is the set of functions whose derivatives up to order two are in the space $L_2(D)$.

The space $C([0,T], H^2(D))$ is the set of functions which are continuously defined on [0,T] and take their values from the space $H^2(D)$.

The space $L_{\infty}([0,T])$ is the set of functions which are essentially bounded on the interval $L_{\infty}([0,T])$.

As a result of Theorem 1 in the study [14] the problem (1)-(3) is uniquely solvable in the sense of (4), if the given functions belong to the following spaces

$$v(t) \in L_{\infty}([0,T]), f(\mathbf{x},t) \in L_{2}(\Omega), \quad \varphi(\mathbf{x}) \in L_{2}(D).$$
⁽⁵⁾

The paper is organized as follows. In section 2, we apply the Galerkin method to the problem (1)-(3) and obtain a system of ordinary differential equations. Also, we prove a theorem giving the stability of approximate solution to the given data. In section 3, we illustrate three numerical examples belonging to different types of given data. Moreover the examples include both zero and nonzero $f(\mathbf{x},t)$ functions. In section 4, we give results and discussion. In the Appendix, we give the MAPLE[®] code used to get the approximate solutions for numerical examples.

2. THE APPLICATION OF GALERKIN METHOD

It is known that, in numerical analysis, Galerkin method is a kind of method for converting a continuous operator problem to a discrete problem. Actually, it is the equivalent of applying the method of variation of parameters to a function space, by converting the equation to a weak formulation. So, some constraints can be applied on the function space to characterize the space with a finite set of basis functions.

According to the Faedo-Galerkin Method or mostly briefly as Galerkin Method, the approximations for the solution of the problem (1)-(3) are such as

$$\psi^{N}(\mathbf{x},t) = \sum_{k=1}^{N} \sum_{m=1}^{N} c_{km}^{N}(t) u_{km}(\mathbf{x}) \ddot{\mathbf{o}}$$
(6)

where the functions $c_{km}^{N}(t)$ are defined by $c_{km}^{N}(t) = \langle \psi^{N}(\mathbf{x},t), u_{km}(\mathbf{x}) \rangle_{L_{2}(D)}$ and the functions $u_{km}(\mathbf{x})$ for k, m = 1, 2, ..., N produce an orthonormal set in the space $L_{2}(D)$. Namely, $\langle u_{km}(\mathbf{x}), u_{rs}(\mathbf{x}) \rangle_{L_{2}(D)} = \delta_{rs}^{km}$ where δ_{rs}^{km} is Kronecker delta.

In order to get the functions $c_{km}^{N}(t)$, we write the equation (1) for the approximations $\psi^{N}(\mathbf{x},t)$

$$i\sum_{k=1}^{N}\sum_{m=1}^{N}\frac{dc_{km}^{N}}{dt}(t)u_{km}(\mathbf{x}) + \sum_{k=1}^{N}\sum_{m=1}^{N}c_{km}^{N}(t)\Delta u_{km} - v(t)\sum_{k=1}^{N}\sum_{m=1}^{N}c_{km}^{N}(t)u_{km}(\mathbf{x}) = f(\mathbf{x},t)$$

Then, we multiply both sides with $u_{rs}(\mathbf{x})$ for r, s = 1, 2, ..., N and integrate over the domain D.

$$\int_{D} \left[i \sum_{k=1}^{N} \sum_{m=1}^{N} \frac{dc_{km}^{N}}{dt}(t) u_{km}(\mathbf{x}) + \sum_{k=1}^{N} \sum_{m=1}^{N} c_{km}^{N}(t) \Delta u_{km} - v(t) \sum_{k=1}^{N} \sum_{m=1}^{N} c_{km}^{N}(t) u_{km}(\mathbf{x}) \right] u_{rs}(\mathbf{x}) d\mathbf{x}$$

$$= \int_{D} f(\mathbf{x}, t) u_{rs}(\mathbf{x}) d\mathbf{x}$$
(7)

In this system $\langle u_{km}(\mathbf{x}), u_{rs}(\mathbf{x}) \rangle_{L_2(D)} = 0$ and $\langle \Delta u_{km}(\mathbf{x}), u_{rs}(\mathbf{x}) \rangle_{L_2(D)} = 0$ for $\{k, m\} \neq \{r, s\}$.

So we can state this system in the matrix form of

$$i\frac{d}{dt}C^{N}(t) + A(t)C^{N}(t) = F(t)$$

$$C^{N}(0) = B$$
(8)

In the system (7),

$$C^{N}(t) = \begin{bmatrix} c_{11}^{N}(t) & c_{12}^{N}(t) & \cdots & c_{1N}^{N}(t) \\ c_{21}^{N}(t) & c_{22}^{N}(t) & \cdots & c_{2N}^{N}(t) \\ \vdots & \vdots & \ddots & \vdots \\ c_{N1}^{N}(t) & c_{N2}^{N}(t) & \cdots & c_{NN}^{N}(t) \end{bmatrix}$$

is the matrix of unknown functions and

$$B = \begin{bmatrix} c_{11}^{N}(0) & c_{12}^{N}(0) & \cdots & c_{1N}^{N}(0) \\ c_{21}^{N}(0) & c_{22}^{N}(0) & \cdots & c_{2N}^{N}(0) \\ \vdots & \vdots & \ddots & \vdots \\ c_{N1}^{N}(0) & c_{N2}^{N}(0) & \cdots & c_{NN}^{N}(0) \end{bmatrix}$$

is the matrix of initial data given by $c_{km}^{N}(0) = \langle \varphi(\mathbf{x}), u_{km}(\mathbf{x}) \rangle_{L_{2}(D)}$ for k, m = 1, 2, ..., N.

The coefficient matrix A(t) has the form of

$$A(t) = \begin{bmatrix} \left\langle \Delta u_{11}(\mathbf{x}) - v(t)u_{11}(\mathbf{x}), u_{11}(\mathbf{x})\right\rangle_{L_{2}(D)} & \left\langle \Delta u_{12}(\mathbf{x}) - v(t)u_{12}(\mathbf{x}), u_{12}(\mathbf{x})\right\rangle_{L_{2}(D)} & \cdots & \left\langle \Delta u_{1N}(\mathbf{x}) - v(t)u_{1N}(\mathbf{x}), u_{1N}(\mathbf{x})\right\rangle_{L_{2}(D)} \\ \left\langle \Delta u_{21}(\mathbf{x}) - v(t)u_{21}(\mathbf{x}), u_{21}(\mathbf{x})\right\rangle_{L_{2}(D)} & \left\langle \Delta u_{22}(\mathbf{x}) - v(t)u_{22}(\mathbf{x}), u_{22}(\mathbf{x})\right\rangle_{L_{2}(D)} & \cdots & \left\langle \Delta u_{2N}(\mathbf{x}) - v(t)u_{2N}(\mathbf{x}), u_{2N}(\mathbf{x})\right\rangle_{L_{2}(D)} \\ \vdots & \vdots & \ddots & \vdots \\ \left\langle \Delta u_{N1}(\mathbf{x}) - v(t)u_{N1}(\mathbf{x}), u_{N1}(\mathbf{x})\right\rangle_{L_{2}(D)} & \left\langle \Delta u_{N2}(\mathbf{x}) - v(t)u_{N2}(\mathbf{x}), u_{N2}(\mathbf{x})\right\rangle_{L_{2}(D)} & \cdots & \left\langle \Delta u_{NN}(\mathbf{x}) - v(t)u_{NN}(\mathbf{x}), u_{NN}(\mathbf{x})\right\rangle_{L_{2}(D)} \end{bmatrix} \\ & = \begin{bmatrix} f_{11}(t) & f_{12}(t) & \cdots & f_{1N}(t) \\ f_{21}(t) & f_{22}(t) & \cdots & f_{2N}(t) \end{bmatrix} \end{bmatrix}$$

Also, the right hand side matrix is
$$F(t) = \begin{bmatrix} f_{21}(t) & f_{22}(t) & \cdots & f_{1N}(t) \\ \vdots & \vdots & \ddots & \vdots \\ f_{N1}(t) & f_{N2}(t) & \cdots & f_{NN}(t) \end{bmatrix}$$
 defined by

$$f_{km}(t) = \left\langle f(\mathbf{x},t), u_{km}(\mathbf{x}) \right\rangle_{L_2(D)} \text{ for } k, m = 1, 2, \dots, N.$$

Obtaining the solution of the system (8) is a Cauchy problem for the system of first order ordinary differential equations. Since the coefficients and right hand side of the equations are square integrable functions, this system is uniquely solvable.

The problem of obtaining the approximate solutions from given data φ and f is well-posed. So the approximate solution $\psi^N(\mathbf{x},t)$ is uniquely obtainable. Also, we state the following theorem indicating the dependence of this approximate solution to the functions φ and f.

Theorem: The approximate solutions given by (6) of the problem (1)-(3) hold the following inequality on the domain $\Omega_t := D \times (0, t]$;

$$\left\| \psi^{N} \left(\mathbf{x}, t \right) \right\|_{L_{2}(D)}^{2} \leq c \left(\left\| \varphi \right\|_{L_{2}(D)}^{2} + \left\| f \right\|_{L_{2}(\Omega_{t})}^{2} \right)$$
(9)

for $\forall t \in [0,T]$. Here c is independent from N , φ and f .

Proof: Considering the equality given by (7), it can be written that

$$\left\langle i\frac{\partial\psi^{N}}{\partial t}, u_{km}\right\rangle_{L_{2}(D)} = \left\langle \nabla\psi^{N}, \nabla u_{km}\right\rangle_{L_{2}(D)} + \left\langle v(t)\psi^{N}, u_{km}\right\rangle_{L_{2}(D)} + f_{km}(t)$$

$$c_{km}^{N}(0) = \left\langle \varphi, u_{km}\right\rangle_{L_{2}(D)} = \varphi_{km}$$
(10)

for k, m = 1, 2, ..., N.

In this system, after multiplying the $\{k, m\}$. equation with $\overline{c}_{km}^{N}(t)$ (complex conjugate of the $c_{km}^{N}(t)$ functions), summing from 1 to N both for k and m then integrating over (0, t), we get the equality;

$$\int_{\Omega_{t}} \left[-i \frac{\partial \overline{\psi}^{N}}{\partial t} \psi^{N} - \left| \nabla \psi^{N} \right|^{2} - v(\mathbf{x}, t) \left| \psi^{N} \right|^{2} \right] d\mathbf{x} d\tau = \int_{\Omega_{t}} f \psi^{N} d\mathbf{x} d\tau .$$
⁽¹¹⁾

Its complex conjugate is

$$\int_{\Omega_{t}} \left[-i \frac{\partial \overline{\psi}^{N}}{\partial t} \psi^{N} - \left| \nabla \psi^{N} \right|^{2} - v(\mathbf{x}, t) \left| \psi^{N} \right|^{2} \right] d\mathbf{x} d\tau = \int_{\Omega_{t}} f \psi^{N} d\mathbf{x} d\tau .$$
⁽¹²⁾

Subtracting (12) from (11), we have

$$\int_{\Omega_{t}} i \left(\frac{\partial \psi^{N}}{\partial t} \overline{\psi}^{N} + \frac{\partial \overline{\psi}^{N}}{\partial t} \psi^{N} \right) d\mathbf{x} d\tau = \int_{\Omega_{t}} \left(f \overline{\psi}^{N} - f \psi^{N} \right) d\mathbf{x} d\tau$$

and

$$\int_{\Omega_{\tau}} i \left(\frac{\partial \psi^{N}}{\partial t} \overline{\psi}^{N} + \frac{\partial \overline{\psi}^{N}}{\partial t} \psi^{N} \right) dx d\tau = 2i \int_{\Omega_{\tau}} \operatorname{Im} \left(f \overline{\psi}^{N} \right) dx d\tau$$

$$\int_{\Omega_{\tau}} \frac{\partial}{\partial t} \left| \psi^{N} \right|^{2} dx d\tau = 2 \int_{\Omega_{\tau}} \operatorname{Im} \left(f \overline{\psi}^{N} \right) dx d\tau.$$
(13)

By Cauchy-Schwartz inequality, this equality gives the inequality of

$$\left\|\boldsymbol{\psi}^{N}\left(.,t\right)\right\|_{L_{2}(D)}^{2} \leq \left\|\boldsymbol{\psi}^{N}\left(.,0\right)\right\|_{L_{2}(D)}^{2} + 2\int_{\Omega_{t}} \left|f\left(\mathbf{x},t\right)\right| \left|\boldsymbol{\psi}^{N}\left(\mathbf{x},t\right)\right| d\mathbf{x}d\tau .$$

$$\tag{14}$$

On the other hand we know that

$$\left\|\psi^{N}\left(.,0\right)\right\|_{L_{2}(D)}^{2} = \sum_{k=1}^{N} \sum_{m=1}^{N} \left|c_{km}^{N}\left(0\right)\right|^{2} = \sum_{k=1}^{N} \sum_{m=1}^{N} \left|\varphi_{km}\right|^{2} \le \sum_{k=1}^{\infty} \sum_{m=1}^{\infty} \left|\varphi_{km}\right|^{2} = \left\|\varphi\left(\mathbf{x}\right)\right\|_{L_{2}(D)}^{2}.$$
(15)

So, we get

$$\left\|\psi^{N}\left(.,t\right)\right\|_{L_{2}(D)}^{2} \leq \left\|\varphi\left(\mathbf{x}\right)\right\|_{L_{2}(D)}^{2} + \left\|f\right\|_{L_{2}(\Omega_{t})}^{2} + \int_{0}^{t} \left\|\psi^{N}\left(.,\tau\right)\right\|_{L_{2}(D)}^{2} d\tau.$$
(16)

Applying Gronwall's lemma to this inequality, we write

$$\left\|\psi^{N}(.,t)\right\|_{L_{2}(D)}^{2} \leq e^{t}\left(\left\|\varphi(\mathbf{x})\right\|_{L_{2}(D)}^{2} + \left\|f\right\|_{L_{2}(\Omega_{t})}^{2}\right), \ \forall t \in [0,T].$$
⁽¹⁷⁾

Hence, taking $c = e^{T}$ the theorem is proven.

3. NUMERICAL ILLUSTRATIONS

In this section we have generated three test problems and obtained numerical examples reflecting the results of the method. These examples are produced by using the code given in the Appendix.

Example 1. On the domain $D = (0, \pi) \times (0, \pi)$ and $\Omega_t := \overline{D} \times [0, t]$, let us consider the problem

$$i\frac{\partial\psi}{\partial t} + \Delta\psi - 117\psi = 0 \tag{18}$$

$$\psi(\mathbf{x},\mathbf{0}) = \sin 10x \sin 4y \tag{19}$$

$$\psi(\mathbf{x},t)\big|_{\Gamma} = \mathbf{0}, \ t \in [0,t].$$
⁽²⁰⁾

The exact solution to this problem is the function $\psi(\mathbf{x},t) = e^{it} \sin 10x \sin 4y$. The function ψ and its

spatial derivatives up to order two are continuous. Hence it is in the space $C([0,T], H^2(D))$ also. Also, v(t)

and $f(\mathbf{x},t)$ are continuous, hence they are in the spaces $L_{\infty}(0,T)$ and $L_{2}(\Omega_{t})$, respectively.

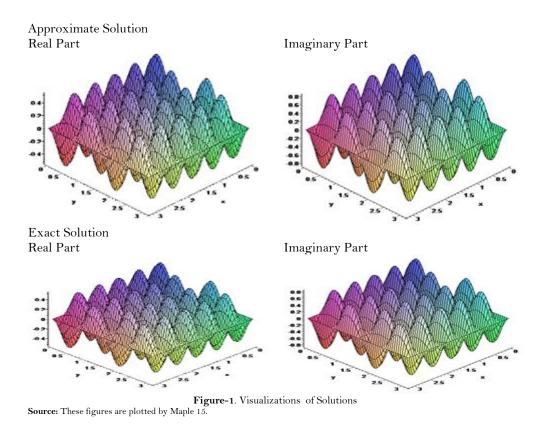
If we use the code given in the Appendix for the following entry;

> TDSE(Pi,Pi,10, -117, $\sin(10x)\sin(4y)$,0);

then we get the approximate solution for N = 10 such as;

 $\frac{1570796327}{500000000} \frac{e^{it} \sin(10x) \sin(4y)}{\pi}$

The graphs of approximate and exact solutions for T = 1 are given in the following;



The errors for some T values are given in Table 1.

Т	$\left\ \psi^{N}-\psi\right\ _{L_{2}(D)}$
0.5	0.19×10^{-19}
1	0.18×10^{-19}
2	0.20×10^{-19}
10	0.19×10^{-19}

Table-1. Some error calculations

Source: These calculations are executed by Maple 15.

Example 2. On the domain $D = (0,1) \times (0,2)$ and $\Omega_t := \overline{D} \times [0,t]$, let us consider the problem

$$i\frac{\partial\psi}{\partial t} + \Delta\psi - t\psi = f(\mathbf{x}, t) \tag{21}$$

where

$$f(\mathbf{x},t) = \begin{cases} -\frac{1}{8}e^{-it} \Big[(8t+18\pi^2-8)x^2 - (4t+9\pi^2-4)x - 16 \Big] \sin \frac{3\pi}{2}y & \left[0,\frac{1}{2} \right] \times [0,2] \times [0,t] \\ \frac{1}{8}e^{-it} \Big[(8t+18\pi^2-8)x^2 - (12t+27\pi^2-12)x + 4t + 9\pi^2 - 20 \Big] \sin \frac{3\pi}{2}y & \left[\frac{1}{2},1 \right] \times [0,2] \times [0,t] \end{cases}$$

$$\psi(\mathbf{x},0) = \begin{cases} \left(x^2 - \frac{x}{2}\right) \sin \frac{3\pi}{2} y & \left[0, \frac{1}{2}\right] \times [0, 2] \\ \left(-x^2 + \frac{3x}{2} - \frac{1}{2}\right) \sin \frac{3\pi}{2} y & \left[\frac{1}{2}, 1\right] \times [0, 2] \end{cases}$$
(22)

$$\psi(\mathbf{x},t)\Big|_{\Gamma} = 0, \ t \in [0,t].$$
 (23)

The exact solution to this problem is the function;

$$\psi(\mathbf{x},t) = e^{-it} \begin{cases} \left(x^2 - \frac{x}{2}\right) \sin \frac{3\pi}{2} y & \left[0, \frac{1}{2}\right] \times [0, 2] \times [0, t] \\ \left(-x^2 + \frac{3x}{2} - \frac{1}{2}\right) \sin \frac{3\pi}{2} y & \left[\frac{1}{2}, 1\right] \times [0, 2] \times [0, t] \end{cases}$$

The function $\frac{\partial^2 \psi}{\partial x^2}(\mathbf{x},t)$ is not continuous on the interval $x \in [0,1]$. Nevertheless, the function ψ is in the space

 $C([0,T], H^2(D))$. Also v(t) is continuous, hence it is in the space $L_{\infty}(0,T)$. $f(\mathbf{x},t)$ is not continuous on

the interval $x \in [0,1]$ but it is in the space $L_2(\Omega_t)$.

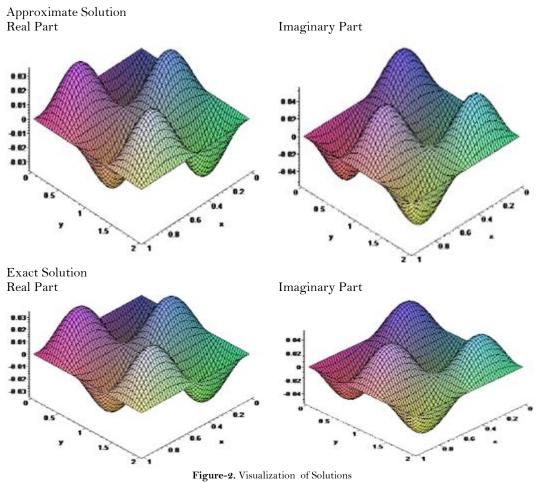
If we use the code given in the Appendix for the following entry;

 $> TDSE(1,2,4,t,PIECEWISE([(x^2-1/2*x)*sin(3/2*Pi*y), 0 <= x and x < 1/2],[(-x^2+3/2*x-1/2)*sin(3/2*Pi*y), 1/2 <= x and x <= 1]),PIECEWISE([-1/8*exp(-I*t)*(18*Pi^2*x^2-9*Pi^2*x+8*t*x^2-4*t*x-8*x^2+4*x-16)*sin(3/2*Pi*y), x < 1/2],[1/8*exp(-I*t)*(18*Pi^2*x^2-27*Pi^2*x+8*t*x^2+9*Pi^2-12*t*x-8*x^2+4*t+12*x-20)*sin(3/2*Pi*y), x < 1]));$

then we get the approximate solution for N = 4 such as;

$$-0.282 \times 10^{-18} \left(\left(0.99 \times 10^9 - 0.10 \times 10^{10} i \right) e^{\left(-0.512 \times 10^{-13} i \left(0.97 \times 10^{13} t^2 - 0.12 \times 10^{16} t + 0.36 \times 10^{17} \right) \right)} + 0.10 \times 10^{10} i \text{erf} \left(0.5t - 0.5it + 30.24 - 30.24i \right) e^{\left(-0.512 \times 10^{-13} i \left(0.97 \times 10^{13} t^2 - 0.12 \times 10^{16} t + 0.36 \times 10^{17} \right) \right)} - 0.10 \times 10^{10} \text{erf} \left(0.5t - 0.5it + 30.24 - 30.24i \right) e^{\left(-0.512 \times 10^{-13} i \left(0.97 \times 10^{13} t^2 - 0.12 \times 10^{16} t + 0.36 \times 10^{17} \right) \right)} + 0.228 \times 10^{18} e^{-it} + 0.1 \times 10^9 \left(e^{-0.32 \times 10^{-6} it \left(0.15 \times 10^7 t + 0.19 \times 10^9 \right)} \right) \sin \left(2\pi x \right) \sin \left(\frac{3\pi}{2} y \right)$$

The figures of approximate and exact solutions for T = 1 are given in the following;



Source: These figures are plotted by Maple 15.

The errors for some T values are given in Table 2.

Т	$\left\ \psi^{\scriptscriptstyle N} - \psi \right\ _{_{L_2(D)}}$
0.5	0.24×10^{-5}
1	0.23×10^{-5}
2	0.25×10^{-5}
10	0.23×10 ⁻⁵

Table-2. Some error calculations

Source: These calculations are executed by Maple 15.

Example 3. On the domain $D = (0, \pi/2) \times (0, \pi)$ and $\Omega_t := \overline{D} \times [0, t]$, let us consider the problem

$$i\frac{\partial\psi}{\partial t} + \Delta\psi - v(t)\psi = f(\mathbf{x}, t)$$
⁽²⁴⁾

where

$$v(t) = \begin{cases} -2, & [0,1] \\ \frac{1}{\sqrt{t}}, & [1,t] \end{cases}$$

and

$$f(\mathbf{x},t) = -e^{-it} \begin{cases} 77\cos(8x)\cos(4y) - 61\cos(8x) - 13\cos(4y) - 3 & [0,\pi/2] \times [0,\pi] \times [0,1) \\ \frac{(79\sqrt{t}+1)\cos(8x)\cos(4y) - (63\sqrt{t}+1)\cos(8x) - (15\sqrt{t}+1)\cos(4y) - \sqrt{t}+1}{\sqrt{t}} & [0,\pi/2] \times [0,\pi] \times [1,t] \end{cases}$$

$$\psi(\mathbf{x}, 0) = (1 - \cos(8x))(1 - \cos(4y))$$

$$\psi(\mathbf{x}, t)|_{\Gamma} = 0, \ t \in [0, t].$$
(25)
(25)

The exact solution to this problem is the function $\psi(\mathbf{x},t) = e^{-it} (1 - \cos(8x))(1 - \cos(4y))$. The function ψ

and its spatial derivatives up to order two are continuous. Hence it is in the space $C([0,T], H^2(D))$. Besides

v(t) is discontinuous but it is in the space $L_{\infty}(0,T)$. Also $f(\mathbf{x},t) \in L_{2}(\Omega_{t})$.

If we use the code given in the Appendix for the following entry;

 $> \text{TDSE}(\text{Pi}/2,\text{Pi},10,\text{PIECEWISE}([-2, t < 1],[1/(t^{(1/2)}), \text{ otherwise}]),(1-\cos(8^*x))^*(1-\cos(4^*y)),\text{PIECEWISE}([-\exp(-I^*t)^*(77^*\cos(8^*x)^*\cos(4^*y)-61^*\cos(8^*x)-13^*\cos(4^*y)-3), t < 1],[-\exp(-I^*t)^*(79^*\cos(8^*x)^*\cos(4^*y)^*t^{(1/2)}+\cos(8^*x)^*\cos(4^*y)-63^*\cos(8^*x)^*t^{(1/2)}-15^*\cos(4^*y)^*t^{(1/2)}-\cos(8^*x)-\cos(4^*y)^*t^{(1/2)}+1)/t^{(1/2)}, 1 <= t])); then we get the approximate solution for <math>N = 10$.

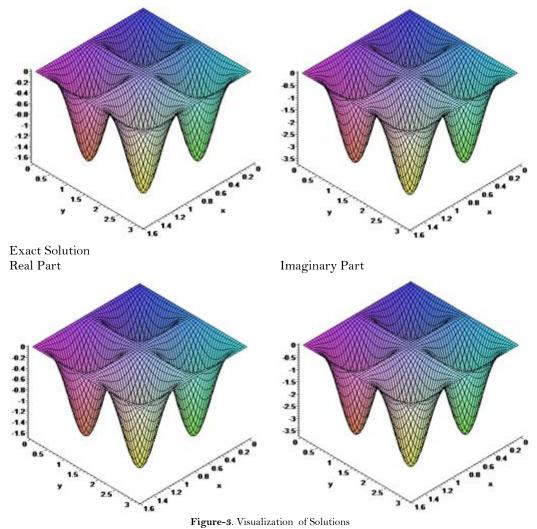
The output of approximate solution is too long, we don't give here.

The figures of approximate and exact solutions for T = 2 are given in the following;

Approximate Solution Real Part

Imaginary Part

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Source: These figures are plotted by Maple 15.

The errors for some T values are given in Table 3.

Т	$\left\ \psi^{\scriptscriptstyle N} - \psi \right\ _{L_2(D)}$
0.5	0.0029
1	0.0028
2	0.0031
10	0.0028

Table-3. Some error calculations

Source: These calculations are executed by Maple 15.

4. RESULT AND DISCUSSION

The better results are obtained with continuous v(t) and $f(\mathbf{x},t)$ functions compared with discontinuous

ones. The errors do not increase as final T values increase.

The code in the appendix is very easy to use and these results show that the approximations are very efficient because of reasonable error values and can be applied to a large class of related problems.

So, instead of long and complicated numerical processes this given code can be operated in an effective and applicative way.

5.1. Appendix (A Code for Approximate Solution)

The following code TDSE(Two-Dimensional-Schrödinger-Equation) has been written in MAPLE® and gives

the approximate solution $\psi^{N}(\mathbf{x},t) = \sum_{k=1}^{N} \sum_{m=1}^{N} c_{km}^{N}(t) u_{km}(\mathbf{x})$ for the two dimensional Schrödinger equation given

in (1)-(3). The code operates the given data $l_1,~l_2,~N,~v,~arphi,f~$ and produces ψ^N .

> TDSE:=proc(l1,l2,N,v,phi,f) > u:=array(1..N,1..N):du:=array(1..N,1..N):A:=array(1..N,1..N):C:=array(1..N,1..N): > F:=array(1..N,1..N):IC:=array(1..N,1..N):S:=array(1..N,1..N): > for k from 1 to N do > for m from 1 to N do > u[k,m]:=2/sqrt(l1*l2)*sin(k*Pi/l1*x)*sin(m*Pi/l2*y):> du [k,m] := simplify(diff(u[k,m],x\$2)+diff(u[k,m],y\$2)):> od;>od; > for i from 1 to N do > for j from 1 to N do $> C[\underline{i},\underline{j}] := c[\underline{i},\underline{j}](t):$ > A[i,j]:=evalf(int((du[i,j]-v*u[i,j])*u[i,j],x=0..l1,y=0..l2)); > F[i,j]:=evalf(int(f*u[i,j],x=0..l1,y=0..l2));> IC[i,j]:=evalf(int(phi*u[i,j],x=0..l1,y=0..l2));> od; > od;> for i from 1 to N do > for j from 1 to N do > d[i,j]:=I*diff(C[i,j],t)+A[i,j]*C[i,j]=F[i,j];> S[i,j]:=rhs(dsolve({d[i,j],c[i,j](0)=IC[i,j}],C[i,j])); > od: > od: > psi:=sum(sum(S[r,s]*u[r,s],s=1..N),r=1..N);> end:

Funding: This study received no specific financial support.

Competing Interests: The authors declare that they have no competing interests.

Contributors/Acknowledgement: We are very grateful to the referee for his/her appropriate and constructive suggestions and for his/her proposed corrections to improve the paper

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