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Numerical Solution of two-dimensional time-dependent Schrödinger equations using Haar wavelet

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Abstract—An algorithm based on collocation points and two-dimensional Haar wavelet basis functions is developed for numerical solutions of two-dimensional time-dependent Schrödinger equations. Error analysis of a proposed algorithm confirm the convergence of the present method. Numerical examples are performed to illustrate the accuracy of the proposed method.

Keywords—Haar wavelet method; 2D time-dependent Schrödinger equations; Operational matrices; Error analysis.

I. Introduction

In the past few decades, wavelet analysis has been a recently developed mathematical tool for solving linear and nonlinear differential and integral equations. Greater attempts have been done to find wavelet based solutions of differential equations. There are many similarities between Fourier analysis and wavelet theory. The first wavelet was introduced by Haar in 1909. In mathematics, the Haar wavelet is a sequence of rescaled square shaped functions which together form a wavelet family or basis. The Haar wavelet is also the simplest possible wavelet. The technical disadvantage of the Haar wavelet is that it is not continuous and therefore not differentiable. But, due to integration of such functions, Haar wavelet method is one of the simplest and easiest method for solving linear and nonlinear partial differential equations. Chen & Hsiao [4] introduced the concept of operational matrices of integrations based on Haar wavelet for analyzing the lumped and distributed-parameter dynamical system. Haar wavelet based collocation methods are developed for solving differential equations in [1], [3], [7], [10], [11], [13], [14], [15].Some useful numerical techniques for the study of partial differential equations are discussed in [17], [18].

This paper is devoted to the numerical computation of two-dimensional time dependent Schrodinger equation:

$$-i\hbar\frac{\partial u}{\partial t} = \frac{\hbar^2}{2m}\left[\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2}\right](x,y,t)V(x,y)\Psi(x,y,t), \quad (1)$$

where i is the imaginary unit, Ψ is the time dependent wave function and V is the potential function. This equation has many applications in science and engineering such as in quantum mechanics for modeling of quantum devices [2], in various quantum calculators [6, 9], in design of certain opto-electronic devices [8], in electromagnetic wave propagation [12] and in underwater acoustics [16].

This paper is organized as: In Section II, concept of Haar wavelet is discussed. The proposed method is presented for solving two- dimensional time dependent Schrodinger equations in Section III. In Section IV, error analysis is described to confirm the convergence of the proposed method. In Section V, some numerical examples are presented to illustrate the accuracy of the propose method.

II. Haar wavelet

Haar functions are an orthogonal family of switched rectangular waveforms where amplitudes can differ from one function to another. These functions are defined as:

$$H_f(x) = \begin{cases} 1, & x \in [\alpha,\beta) \\ -1, & x \in [\beta,\gamma) \\ 0, & Otherwise, \end{cases} \quad (2)$$

where $\alpha = \frac{k}{m},\ \beta = \frac{k+0.5}{m},\ \gamma = \frac{k+1}{m}$.

Integer $\boldsymbol{m = 2^j}$, $\boldsymbol{j = 0,1,2,3,\dots\dots J}$ and $\boldsymbol{J}$ denotes the level of resolution. The integer $\boldsymbol{k = 0,1,2,3,\dots\dots m-1}$ is the translation parameter. The wavelet number $\boldsymbol{f}$ can be calculated as $\boldsymbol{f = m + k + 1}$. The minimum value of the number $\boldsymbol{f = 2}$ and the maximum value of $\boldsymbol{f = 2M = 2^{J+1}}$. The collocation points are defined as:

$$\boldsymbol{x_l = \frac{l - 0.5}{2M}}, \quad \boldsymbol{l = 1, 2, 3, \dots\dots\dots, 2M}$$

The operational matrices are obtained by using the relation

$$P_{1,f}(x) = \int_0^x H_f(t)dt, \qquad (3)$$

$$P_{n,f}(x) = \int_0^x P_{n-1,f}(t)dt, \;\; n = 1,2,3, \dots \qquad (4)$$

III. PROPOSED METHOD FOR SOLVING TWO-DIMENSIONAL SCHRODINGER EQUATION

Consider the wavelet approximation

$$\dot{\Psi}_{xxyy}(x,y,t) = \sum_{f,g=1}^{2M}[A_{fg} + iB_{fg}]H_f(x)H_g(y), \qquad (5)$$

where $(\cdot)$ denotes the differentiation with respect to t. The constants A_{fg} and B_{fg} are real and imaginary components of wavelet coefficients respectively. Integrating (5) one time with respect to t, from 0 to t_s, we obtain

$$\Psi_{xxyy}(x,y,t) = \Psi_{xxyy}(x,y,t_s) + (t - t_s) \sum_{f,g=1}^{2M}[A_{fg} + iB_{fg}]H_f(x)H_g(y). \qquad (6)$$

Integrating (6) twice with respect to y, from 0 to y, we obtain

$$\Psi_{xx}(x,y,t) = \Psi_{xx}(x,0,t) + \Psi_{xx}(x,y,t_s) - \Psi_{xx}(x,0,t_s) + y[\Psi_{xxy}(x,0,t) - \Psi_{xxy}(x,0,t_s)] + (t - t_s)\sum_{f,g=1}^{2M}[A_{fg} + iB_{fg}]H_f(x)P_{2,g}(y). \qquad (7)$$

Substituting $y = 1$ in (7), we obtain

$$\left[\Psi_{xxy}(x,0,t) - \Psi_{xxy}(x,0,t_s)\right] = \Psi_{xx}(x,1,t) - \Psi_{xx}(x,0,t) - \Psi_{xx}(x,1,t_s) + \Psi_{xx}(x,0,t_s) - (t - t_s)\sum_{f,g=1}^{2M}[A_{fg} + iB_{fg}]H_f(x)P_{2,g}(1). \qquad (8)$$

From (7) and (8), we obtain

$$\Psi_{xx}(x,y,t) = \Psi_{xx}(x,0,t) + \Psi_{xx}(x,y,t_s) - \Psi_{xx}(x,0,t_s) + y[\Psi_{xx}(x,1,t) - \Psi_{xx}(x,0,t) - \Psi_{xx}(x,1,t_s) + \Psi_{xx}(x,0,t_s)] + (t - t_s)\sum_{f,g=1}^{2M}[A_{fg} + iB_{fg}]H_f(x)[P_{2,g}(y) - yP_{2,g}(1)]. \qquad (9)$$

Integrating (6) twice with respect to x, from 0 to x, we obtain

$$\Psi_{yy}(x,y,t) = \Psi_{yy}(0,y,t) + \Psi_{yy}(x,y,t_s) - \Psi_{yy}(0,y,t_s) + x[\Psi_{xyy}(0,y,t) - \Psi_{xyy}(0,y,t_s)] + (t - t_s)\sum_{f,g=1}^{2M}[A_{fg} + iB_{fg}]P_{2,f}(x)H_g(y). \qquad (10)$$

Substituting $x = 1$ in (10), we obtain

$$\left[\Psi_{xyy}(0,y,t) - \Psi_{xyy}(0,y,t_s)\right] = \Psi_{yy}(1,y,t) - \Psi_{yy}(0,y,t) - \Psi_{yy}(1,y,t_s) + \Psi_{yy}(0,y,t_s) - (t - t_s)\sum_{f,g=1}^{2M}[A_{fg} + iB_{fg}]P_{2,f}(1)H_g(y). \qquad (11)$$

From (10) and (11), we obtain

$$\Psi_{yy}(x,y,t) = \Psi_{yy}(0,y,t) + \Psi_{yy}(x,y,t_s) - \Psi_{yy}(0,y,t_s) + x[\Psi_{yy}(1,y,t) - \Psi_{yy}(0,y,t) - \Psi_{yy}(1,y,t_s) + \Psi_{yy}(0,y,t_s)] + (t - t_s) \sum_{f,g=1}^{2M}[A_{fg} + iB_{fg}][P_{2,f}(x) - xP_{2,f}(1)]H_g(y), \qquad (12)$$

Integrating (10) twice with respect to x, from 0 to x, we obtain

$$\Psi(x,y,t) = U1(x,y,t) + yU2(x,t) + xU3(x,y,t) + (t - t_s)\sum_{f,g=1}^{2M}[A_{fg} + iB_{fg}]P_{2,f}(x)[P_{2,g}(y) - yP_{2,g}(1)], \qquad (13)$$

where

$$U1(x,y,t) = \Psi(0,y,t) + \Psi(x,0,t) - \Psi(0,0,t) + \Psi(x,y,t_s) - \Psi(0,y,t_s) - \Psi(x,0,t_s) + \Psi(0,0,t_s),$$

$$U2(x,t) = [\Psi(x,1,t) - \Psi(0,1,t) - \Psi(x,0,t) + \Psi(0,0,t) - \Psi(x,1,t_s) + \Psi(0,1,t_s) + \Psi(x,0,t_s) - \Psi(0,0,t_s)],$$

$$U3(x,y,t) = \begin{bmatrix}\Psi_x(0,y,t) - \Psi_x(0,0,t) - \Psi_x(0,y,t_s) \\ +\Psi_x(0,0,t_s)\end{bmatrix} + y[\Psi_x(0,0,t) - \Psi_x(0,1,t) + \Psi_x(0,1,t_s) - \Psi_x(0,0,t_s)]$$

Substituting $x = 1$ in (13), we obtain

$$U3(x,y,t) = \Psi(1,y,t) - U1(1,y,t) - yU2(1,t)$$

$$-(t-t_s)\sum_{f,g=1}^{2M}[A_{fg}+iB_{fg}]P_{2,f}(1)[P_{2,g}(y)-yP_{2,g}(1)]. \quad (14)$$

From (13) and (14), we obtain

$$\Psi(x,y,t)=U1(x,y,t)+yU2(x,t)$$
$$+x[\Psi(1,y,t)-U1(1,y,t)-yU2(1,t)]+(t-t_s)$$
$$\sum_{f,g=1}^{2M}[A_{fg}+iB_{fg}][P_{2,f}(x)-xP_{2,f}(1)][P_{2,g}(y)-yP_{2,g}(1)]. \quad (15)$$

Differentiating (15) one time with respect to t, we obtain

$$\dot{\Psi}(x,y,t)=[\dot{U}1](x,y,t)+y[\dot{U}2](x,t)$$
$$+x\left[\dot{\Psi}(1,y,t)-[\dot{U}1](1,y,t)-y[\dot{U}2](1,t)\right]$$
$$+\sum_{f,g=1}^{2M}[A_{fg}+iB_{fg}][P_{2,f}(x)-xP_{2,f}(1)][P_{2,g}(y)-yP_{2,g}(1)]. \quad (16)$$

Discretizing (9), (12), (15) and (16) by using $x\to x_l$, $y\to y_l$ and $t\to t_{s+1}$, we obtain

$$\Psi_{xx}(x_l,y_l,t_{s+1})=\Psi_{xx}(x_l,0,t_{s+1})+\Psi_{xx}(x_l,y_l,t_s)$$
$$-\Psi_{xx}(x_l,0,t_s)+y_l[\Psi_{xx}(x_l,1,t_{s+1})$$
$$-\Psi_{xx}(x_l,0,t_{s+1})-\Psi_{xx}(x_l,1,t_s)+\Psi_{xx}(x_l,0,t_s)]$$
$$+(t_{s+1}-t_s)\sum_{f,g=1}^{2M}[A_{fg}+iB_{fg}]H_f(x_l)[P_{2,g}(y_l)-y_lP_{2,g}(1)], \quad (17)$$

$$\Psi_{yy}(x_l,y_l,t_{s+1})=\Psi_{yy}(0,y_l,t_{s+1})+\Psi_{yy}(x_l,y_l,t_s)$$
$$-\Psi_{yy}(0,y_l,t_s)+x_l[\Psi_{yy}(1,y_l,t_{s+1})-\Psi_{yy}(0,y_l,t_{s+1})$$
$$-\Psi_{yy}(1,y_l,t_s)+\Psi_{yy}(0,y_l,t_s)]+(t_{s+1}-t_s)$$
$$\sum_{f,g=1}^{2M}[A_{fg}+iB_{fg}][P_{2,f}(x_l)-x_lP_{2,f}(1)]\,H_g(y_l), \quad (18)$$

$$\Psi(x_l,y_l,t_{s+1})=U1(x_l,y_l,t_{s+1})+y_lU2(x_l,t_{s+1})+$$
$$x_l[\Psi(1,y_l,t_{s+1})-U1(1,y_l,t_{s+1})-yU2(1,t_{s+1})]$$
$$+(t_{s+1}-t_s)\sum_{f,g=1}^{2M}[A_{fg}+iB_{fg}][P_{2,f}(x_l)-x_lP_{2,f}(1)][P_{2,g}(y_l)-y_lP_{2,g}(1)], \quad (19)$$

$$\dot{\Psi}(x_l,y_l,t_{s+1})=[\dot{U}1](x_l,y_l,t_{s+1})+y_l[\dot{U}2](x_l,t_{s+1})$$
$$+x_l\begin{bmatrix}\dot{\Psi}(1,y_l,t_{s+1})-[\dot{U}1](1,y_l,t_{s+1})\\ -y_l[\dot{U}2](1,t_{s+1})\end{bmatrix}+$$
$$\sum_{f,g=1}^{2M}[A_{fg}+iB_{fg}][P_{2,f}(x_l)-x_lP_{2,f}(1)]\,[P_{2,g}(y_l)-y_lP_{2,g}(1)]. \quad (20)$$

In the given scheme

$$-i\hbar\frac{\partial\Psi}{\partial t}(x_l,y_l,t_{s+1})=\frac{\hbar^2}{2m}\left[\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}\right](x_l,y_l,t_{s+1})+V(x_l,y_l)\Psi(x_l,y_l,t_{s+1}). \quad (21)$$

Substituting the values from (17)-(20) in (21), we obtain the system of algebraic equations

$$\sum_{f,g=1}^{2M}\boldsymbol{a_{fg}}[\boldsymbol{R}+\boldsymbol{S}+\boldsymbol{iT}](\boldsymbol{x_l},\boldsymbol{y_l},\boldsymbol{t_{s+1}})=\boldsymbol{F}(\boldsymbol{x_l},\boldsymbol{y_l},\boldsymbol{t_{s+1}}), \quad (22)$$

where

$$\boldsymbol{R}=(\boldsymbol{t_{s+1}}-\boldsymbol{t_s})\boldsymbol{H_f}(\boldsymbol{x_l})[\boldsymbol{P_{2,g}}(\boldsymbol{y_l})-\boldsymbol{y_lP_{2,g}}(\boldsymbol{1})],$$

$$\boldsymbol{S}=(\boldsymbol{t_{s+1}}-\boldsymbol{t_s})[\boldsymbol{P_{2,f}}(\boldsymbol{x_l})-\boldsymbol{x_lP_{2,f}}(\boldsymbol{1})]\boldsymbol{H_g}(\boldsymbol{y_l}),$$

$$\boldsymbol{T}=[\boldsymbol{P_{2,f}}(\boldsymbol{x_l})-\boldsymbol{x_lP_{2,f}}(\boldsymbol{1})][\boldsymbol{P_{2,g}}(\boldsymbol{y_l})-\boldsymbol{y_lP_{2,g}}(\boldsymbol{1})].$$

In (22), $\boldsymbol{F}$ consists of the remaining terms from (17)-(20) and $\boldsymbol{V}$. In matrix form, from (22), we obtain

$$[\boldsymbol{A}][\boldsymbol{W}]=[\boldsymbol{G}]. \quad (23)$$

The dimension of matrix $\boldsymbol{A}$is $\boldsymbol{1}\times(\boldsymbol{2M})^{\boldsymbol{2}}$, the dimension of matrix $\boldsymbol{W}$ is $(\boldsymbol{2M})^{\boldsymbol{2}}\times(\boldsymbol{2M})^{\boldsymbol{2}}$ and the dimension of the matrix $\boldsymbol{G}$ is $\boldsymbol{1}\times(\boldsymbol{2M})^{\boldsymbol{2}}$. From (23), real and imaginary components of Haar wavelet coefficients are obtained. The numerical solution of (1) is obtained by substituting the real and imaginary components of wavelet coefficients into (19).

IV. ERROR ANALYSIS OF PROPOSED METHOD

In order to analyze the convergence of our method, we state the following convergence theorem:

Theorem: Suppose that $\boldsymbol{f}(\boldsymbol{x},\boldsymbol{y})$ satisfies a Lipschitz condition on $[\boldsymbol{0},\boldsymbol{1}]\times[\boldsymbol{0},\boldsymbol{1}]$, that is, there exists a positive constant$\boldsymbol{L}$such that for all $(\boldsymbol{x_1},\boldsymbol{y})$, $(\boldsymbol{x_2},\boldsymbol{y})\in[\boldsymbol{0},\boldsymbol{1}]\times[\boldsymbol{0},\boldsymbol{1}]$, we have

$$|\boldsymbol{f}(\boldsymbol{x_1},\boldsymbol{y})-\boldsymbol{f}(\boldsymbol{x_2},\boldsymbol{y})|\le\boldsymbol{L}|\boldsymbol{x_1}-\boldsymbol{x_2}|.$$

Then, the error bound for $\|\boldsymbol{e_m}(\boldsymbol{x},\boldsymbol{y})\|_{\boldsymbol{2}}$ is obtained as

$$\|\boldsymbol{e_m}(\boldsymbol{x},\boldsymbol{y})\|_{\boldsymbol{2}}\le\frac{\boldsymbol{L}}{\sqrt{\boldsymbol{3}}}\left(\frac{\boldsymbol{1}}{\boldsymbol{m}}\right)^{\boldsymbol{3}},$$

where $e_m(x,y) = \Psi(x,y,t) - \Psi_m(x,y,t)$ *in which* $\Psi(x,y,t)$ *is the exact solution and* $\Psi_m(x,y,t)$ *is the Haar wavelet solution. The Haar wavelet method will be convergent, if* $e_m(x,y)$ *converge to zero when* m *goes to infinity. The order of convergence of the proposed method is 3. That is*

$$\|e_m(x,y)\|_2 = \left(\frac{1}{m}\right)^3 \text{ (see [16]).}$$

V. NUMERICAL EXAMPLES AND DISCUSSION

To illustrate the accuracy of the proposed method, some numerical examples are solvedusing proposed method. The obtained numerical results are compared with exact solutions. We alsoreport $L_\infty(\Psi)$ and $L_2(\Psi)$ errors of the computed solutions which are defined as

$$L_\infty(\Psi) = \max_{1 \le i,j \le 2M} \left|\Psi_{Ex}(x_i,y_j,t_l) - \Psi_{App.}(x_i,y_j,t_l)\right|,$$

and

$$L_2(\Psi) = \left[\sum_{i,j=1}^{2M} [\{\left|\Psi_{Exact}(x_i,y_j,t_l) - \Psi(x_i,y_j,t_l)\right|\}^2]\right]^{1/2}.$$

Example 1: Consider the two-dimensional Schrodinger equation (1) with $V(x,y) = (2\pi^2+1)$. The exact solution of the problem is

$$\Psi(x,y,t) = e^{it}\sin(\pi x)\sin(\pi y).$$

Table 1 show the comparison of different modes of errors of Example 1 at different time with $\Delta t = 0.001$ and $J = 2$. Table 2 show the comparison of different modes of errors of Example 1 at different time with $\Delta t = 0.01$ and $J = 2$.

Table 1: Comparison of errors at different time

	$L_\infty(\Psi)$ $(\Delta t = 0.001)$		$L_2(\Psi)$ $(\Delta t = 0.001)$	
T	Real part	Imaginary part	Real part	Imaginary part
0.005	5.916e-07	5.697e-09	2.460e-06	2.369e-08
0.01	1.838e-06	1.458e-09	7.645e-06	6.063e-09
0.015	7.290e-06	4.103e-08	3.031e-05	1.706e-07
0.02	1.289e-05	3.009e-07	5.362e-05	1.251e-06

Table 2: Comparison of errors at different time

	$L_\infty(\Psi)$ $(\Delta t = 0.01)$		$L_2(\Psi)$ $(\Delta t = 0.01)$	
t	Real part	Imaginary part	Real part	Imaginary part
0.05	5.896e-05	5.693e-06	2.452e-04	2.367e-05
0.1	1.844e-04	1.426e-06	7.670e-04	5.930e-06
0.15	7.284e-04	4.108e-05	3.029e-03	1.708e-04
0.2	1.259e-03	2.989e-04	5.237e-03	1.243e-03

Example 2: Consider the two-dimensional Schrodinger equation (1) with

$$V(x,y) = 1 - \frac{6(1-2x)}{x^2(1-x)} - \frac{6(1-2y)}{y^2(1-y)}$$

The exact solution of the problem is

$$\Psi(x,y,t) = e^{it}x^3y^3(1-x)(1-y).$$

Table 3 show the comparison of different modes of errors of Example 2 at different time with $\Delta t = 0.001$ and $J = 2$. Table 4 show the comparison of different modes of errors of Example 2 at different time with $\Delta t = 0.01$ and $J = 2$.

Table 3: Comparison of errors at different time

	$L_\infty(\Psi)$ $(\Delta t = 0.001)$		$L_2(\Psi)$ $(\Delta t = 0.001)$	
T	Real part	Imaginary part	Real part	Imaginary part
0.005	7.455e-08	1.026e-08	2.690e-07	2.756e-08
0.01	2.342e-07	4.215e-08	8.508e-07	1.216e-07
0.015	4.750e-07	8.533e-08	1.737e-06	2.836e-07
0.02	1.817e-06	3.254e-07	5.366e-06	7.904e-07

Table 4: Comparison of errors at different time

	$L_\infty(\Psi)$ $(\Delta t = 0.01)$		$L_2(\Psi)$ $(\Delta t = 0.01)$	
T	Real part	Imaginary part	Real part	Imaginary part
0.05	8.211e-06	1.159e-06	2.593e-05	3.422e-06
0.1	2.613e-05	4.608e-06	8.126e-05	1.120e-05
0.15	5.338e-05	1.009e-05	1.655e-04	2.546e-05
0.2	1.845e-04	4.678e-05	4.964e-04	1.311e-04

Example 3: Consider the two-dimensional Schrodinger equation (1) with

$$V(x,y) = \pi^2 + 1 - \frac{6(1-2x)}{x^2(1-x)}$$

The exact solution of the problem is

$$\Psi(x,y,t) = e^{it}x^3(1-x)\sin(\pi y).$$

Table 5 show the comparison of different modes of errors of Example 3 at different time with $\Delta t = 0.001$ and $J = 2$. Table 6 show the comparison of different modes of errors of Example 3 at different time with $\Delta t = 0.01$ and $J = 2$.

Table 5: Comparison of errors at different time

	$L_\infty(\Psi)$ $(\Delta t = 0.001)$		$L_2(\Psi)$ $(\Delta t = 0.001)$	
t	Real part	Imaginary part	Real part	Imaginary part
0.005	3.938e-07	9.961e-08	1.665e-06	2.187e-07

0.01	1.036e-06	4.103e-07	4.640e-06	9.657e-07
0.015	1.972e-06	8.333e-07	8.841e-06	2.250e-06
0.02	6.013e-06	1.318e-06	2.427e-05	4.073e-06

Table 6: Comparison of errors at different time

	$L_\infty(\Psi)$ $(\Delta t = 0.01)$		$L_2(\Psi)$ $(\Delta t = 0.01)$	
t	Real part	Imaginary part	Real part	Imaginary part
0.05	4.274e-05	6.989e-06	1.567e-04	2.606e-05
0.1	1.168e-04	2.119e-05	4.219e-04	7.423e-05
0.15	2.208e-04	4.300e-05	7.952e-04	1.373e-04
0.2	6.439e-04	1.376e-04	2.313e-03	4.473e-04

VI. CONCLUSION

In the view of above numerical examples, it is concluded that two-dimensional Haar wavelet basis functions are more reliable and accurate mathematical tool for solving two-dimensional time-dependent Schr***ö***dinger equations. For getting the necessary accuracy, the number of calculation points may be increased.

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