Journal of Physical Science and Application 12 (1) (2022) 12-18
doi: 10.17265/2159-5348/2022.01.003

Numerical Solutions of Finite Well in Two Dimensions Using the Finite Difference Time Domain Method

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Abstract: The higher excited states for two dimensional finite rectangular well potential are calculated numerically, by solving the Schrödinger equation using the finite difference time domain method. Although, this method is suitable to calculate the ground state of the quantum systems, it has been improved to calculate the higher excited states directly. The improvement is based on modifying the iterative process involved in this method to include two procedures. The first is known as cooling steps and the second is known as a heating step. By determining the required length of the cooling iteration steps using suitable excitation energy estimate, and repeating these two procedures using suitable initial guess function for sufficient times. This modified iteration will lead automatically to the desired excited state. In the two dimensional finite rectangular well potential problem both of the suitable excitation energy and the suitable initial guess wave function are calculated analytically using the separation of variables technique.

Keywords: Finite difference time domain method, diffusion equation, separation of variables method, finite well potential, Schrödinger equation.

1. Introduction

The main goal of this work is to calculate the eigenfunctions and their corresponding eigenvalues for the higher excited states for two dimensional finite rectangular well potential, since there are no solutions exist for this problem. These calculations are performed using the finite difference time domain method (FDTD). In general, the (FDTD) method is used to solve the Schrödinger equation in the diffusion form iteratively, by starting with an initial random wave function that contains a mixture of all the wave functions of the system and applying the iterative procedure for enough simulation time, the wave function converges to the ground state wave function of the quantum system [1, 2]. Beside this, the (FDTD) method is employed to calculate the lowest angular excited states of the quantum system by considering symmetric arguments [3, 4]. Moreover, the (FDTD) method has been modified recently to calculate any higher excited state directly by improving the iterative procedure [5], the improved iteration involves essentially two steps, first in order to reach the desired excited state we apply the iterative procedure for a certain time steps which depends on the energy eigenvalue of this desired excited state, this procedure is viewed physically as cooling of the system and lowering its energy toward this desired state. Second applying the iterative procedure using the derivative of the last wave function with respect to the imaginary time domain as a new initial guess wave function in order to raise the system to this excited state, this second step is viewed physically as sudden heating of the system, and one has to repeat these two steps which are the cooling and the heating of the system using suitable initial guess wave function until getting acceptable results. It is clear shown that calculating the higher excited states using the modified (FDTD) method requires an expected energy eigenvalue to determine the number of cooling steps and an appropriate eigenfunction to be the initial guess wave function. In general, the appropriate initial guess wave

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function is arbitrary function which has the same symmetric properties of the desired eigenfunction, while for the two dimensional rectangular finite well potential both of the expected energy eigenvalue and the appropriate eigenfunction can be obtained analytically using the separation of variables technique, since solving the Schrödinger equation for two dimensional finite rectangular well potential analytically by dividing it to two one dimensional finite well potentials with depths that depend on the lengths of the rectangular produces energy eigenvalues and eigenfunctions close to the exact ones. Therefore, we can consider the solutions of the separation of variables technique as a semi-analytical approximation used as initial guess values to help driving the (FDTD) method to get any desired excited state directly if it exists. It is worth mentioning, that introducing semi-analytical wave function prevents the numerical calculations from numerical frustration.

In addition to this introduction, this paper is organized in three other sections as follows; The general theory section which includes two subsections, the former presents a brief description of the (FDTD) method and how we can extend it to calculate the higher excited states, and the later presents the separation of variables technique that is used to calculate the semi-analytical solutions. The calculation section also includes two subsections, in the former the applicability of the separation of variables technique is illustrated by comparing the ground state calculated using this technique with the exact numerical ground state, and in the later we take advantage of this approach to use these semi-analytical solutions to calculate the exact numerical solutions of the higher excited states which is the main goal of our paper. The last section is devoted to the conclusion.

2. General Theory

2.1 The Modified Finite Difference Time Domain Method

In this section, we briefly present the modified iteration that is used to calculate the higher excited states, a detailed explanation about this method and its numerical scheme in two dimensions can be found in [1, 3-5].

The diffusion form of the Schrödinger equation is given by

$$\hat{H}\psi(\vec{r},\tau) = -\frac{\partial\psi(\vec{r},\tau)}{\partial\tau} \quad (1)$$

Where $\hat{H}$ is the Hamiltonian of the system which is given in the dimensionless form by,

$$\hat{H} = -\nabla^2 + V(\vec{r}) \quad (2)$$

and τ is the imaginary time domain given by $\tau = \frac{i}{h}t$.

The formal solution of Eq. (1) can be written as,

$$\psi(\vec{r},\tau) = \sum_{i=0}^{\infty} c_i\varphi_i(\vec{r})\exp\left(-E_i\tau\right) \quad (3)$$

where φ_i, E_i are a complete set of eigenfunctions and their corresponding energy eigenvalues for the time-independent Schrödinger equation and c_i are expansion coefficients.

This formal solution can be rewritten in an iterative form as

$$\psi(\vec{r},n\Delta\tau) = \psi(\vec{r},(n-1)\Delta\tau)\exp(-E(n-1)\Delta\tau) \quad (4)$$

where n is an integer representing the number of iterations and $\Delta\tau$ is the temporal spacing.

The iterative process of Eq. (4) increases the value of $n\Delta\tau$ for each iteration by value of $\Delta\tau$ [6, 7]. Hence the iterative process can be viewed physically as cooling the system and lowering its energy, thereby all the excited states will condense to the ground state,

$$\lim_{n\to\infty} ?\,\psi(\vec{r},n\Delta\tau) \approx c_0\varphi_0(\vec{r})\exp(-E_0 n\Delta\tau) \quad (5)$$

Where E_0 is the smallest energy eigenvalue and in this case it corresponds to the ground state.

The higher excited states can be calculated directly using the (FDTD) method by modifying the iterative procedure as follows; first in order to drive the system to the desired excited state we apply the iterative procedure using appropriate initial guess wave

function which subjected to the symmetric properties of the desired excited state and iterate it for a certain number of imaginary time steps given by [5]

$$n = \frac{1}{E'\Delta\tau} \tag{6}$$

where E' is the expected energy eigenvalue of the desired excited state.

Second introducing a new initial guess wave function $\chi(\vec{r}, n\Delta\tau)$ which is given by,

$$\chi(\vec{r}, n\Delta\tau) = -\frac{\partial\psi(\vec{r},n\Delta\tau)}{\partial\Delta\tau} \equiv \frac{\psi(\vec{r},(n-1)\Delta\tau)-\psi(\vec{r},n\Delta\tau)}{\Delta\tau} \tag{7}$$

where $\psi(\vec{r}, n\Delta\tau)$ is the result of the last iterative step wave function that obtained from the first iterative step. This last replacement of the wave function is viewed physically as sudden heating of the system to arise it to the excited state, then repeating these two steps for *M*-times to reach to the acceptable resulted eigenfunction and eigenvalue. Numerically, both the even excited states and the odd excited states are calculated separately using the suitable boundary conditions which are subjected to the symmetric properties of the desired wave function [3-5].

The energy eigenvalues are calculated using their corresponding eigenfunctions by [7, 8]

$$E = -\frac{1}{2\Delta\tau} ln \iint_{-\infty}^{\infty} \psi^*(\vec{r}, n\Delta\tau)\, \psi(\vec{r}, n\Delta\tau)\, dx\, dy \tag{8}$$

2.2 The Separation of Variables Technique

The separation of variables technique is the most widely used to solve the partial differential equations, by splitting the partial differential equation of n-variables to n-ordinary differential equation [9-11]. The required condition to apply this technique to solve the Schrödinger equation successfully is that the potential governs the problem is separable potential, while the rectangular finite well potential is not separable. In this paper we propose for the first time a unique way to arrive at a separable potential for the two dimensional finite well, this can be achieved by approximately expressing this potential as a sum of two independent one dimensional potentials given by,

$$V_x = \frac{L_y}{L_x+L_y} V_0 \tag{9}$$

$$V_y = \frac{L_x}{L_x+L_y} V_0 \tag{10}$$

where V_0 is the potential depth, $2L_x$ and $2L_y$ are the lengths of the rectangular potential. That is the finite rectangular potential in two dimensions is given by,

$$V(x,y) = \begin{cases} -V_0 & |x| \le L_x, |y| \le L_y \\ 0 & \text{Otherwise} \end{cases} \tag{11}$$

Here after we present a short overview of the separation of variables technique. Using ρ as a distance unit and $\frac{h^2}{2m\rho^2}$ as an energy unit, the dimensionless form of the time independent Schrödinger equation for this potential is given by,

$$-\nabla^2\psi(x,y) + v(x,y)\psi(x,y) = \varepsilon\psi(x,y) \tag{12}$$

where $v = \frac{2m\rho^2}{h^2}V$ and $\varepsilon = \frac{2m\rho^2}{h^2}|E|$.

within this technique the two dimensions wave function is written as a product of two independent one dimension components as

$$\psi(x,y) = X(x)Y(y) \tag{13}$$

By plugging Eq. (13) into Eq. (12) we get the following two independent ordinary differential equations,

$$\frac{d^2X}{dx^2} + (v_x - \varepsilon_x)X = 0 \tag{14}$$

$$\frac{d^2Y}{dy^2} + (v_y - \varepsilon_y)Y = 0 \tag{15}$$

The total energy of the two dimensional system is the sum of the energies from each one dimensional equation,

$$\varepsilon = \varepsilon_x + \varepsilon_y \tag{16}$$

The general solution of the second order differential equation Eq. (14) is given by the two following equations,

$$X(x) = \begin{cases} A\cos\sqrt{v_x - \varepsilon_{xe}}x & |x| \le L_x \\ Be^{-\sqrt{\varepsilon_{xe}}x} & \text{Otherwise} \end{cases} \tag{17}$$

for the even parity wave functions, while

$$X(x) = \begin{cases} C\sin?\sqrt{v_x - \varepsilon_{xo}}x & |x| \le L_x \\ De^{-\sqrt{\varepsilon_{xo}}x} & \text{Otherwise} \end{cases} \tag{18}$$

for the odd parity wave functions.

By applying the continuous conditions at the well boundary in both even parity wave function and odd parity wave function, one can get two sets of energy eigenvalues of ε_x, one is ε_{xe} which is corresponding to the even parity wave functions and the other is ε_{xo} which is corresponding to the odd parity wave functions. The eigenfunctions are calculated by plugging their corresponding energy eigenvalues into suitable equation which is Eq. (17) for even parity wave functions and Eq. (18) for odd parity wave functions. Similar argument is used to solve Eq. (15) and getting the energy eigenvalues of ε_y and their corresponding eigenfunctions. The eigenfunctions and the eigenvalues of the two dimensional system are calculated using Eq. (13) and Eq. (16) respectively.

3. Applications

3.1 The Applicability of the Separation of Variables Technique

In this section we compare the ground state eigenvalues for several lengths of the rectangular well potential obtained using the semi-analytical solutions with their corresponding exact numerical solutions calculated using (FDTD) method, in order to confirm our proposed approximation for separating the rectangular potential into two one dimensional wells. This comparison is shown in Fig. 1, which organized as follows; in Fig. 1a, the ground state eigenvalues with our proposed one dimensional well $\varepsilon_x(1)$ and $\varepsilon_y(1)$ for finite rectangular well potential with depth $v_0 = 25$ are presented as a function of the ratio L_y/L_x. The blue curve corresponds to the energy eigenvalues $\varepsilon_x(1)$, while the red curve corresponds to the energy eigenvalues $\varepsilon_y(1)$. In Fig. 1b, the two dimensional eigenvalues calculated using the separation of variables technique by applying Eq. (16) (the black curve) and those calculated using the (FDTD) method (the green curve) are presented as a function of the ratio L_y/L_x, it is clear obvious from the figure that they are in a good agreement which allows us to

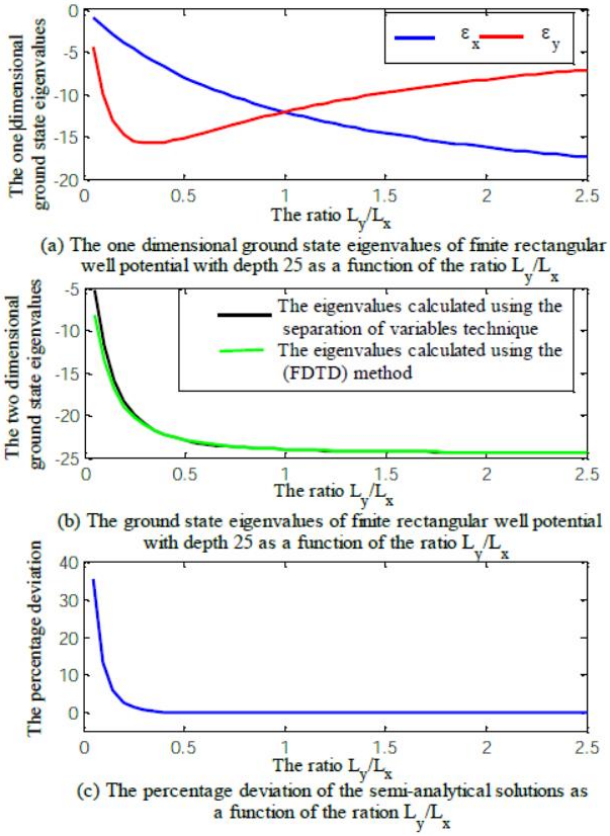


Fig. 1 Illustrates the applicability of the separation of variables technique.

consider the separation of variables solutions as a semi-analytical solutions. Numerically, the results of (FDTD) method are obtained using the following parameters the temporal spacing $\Delta\tau = 0.001$, the spatial spacing separation $\Delta x = \Delta y = 0.1$ and 1400 cooling steps. Furthermore, in Fig. 1c, we present the percentage deviation of the semi-analytical solutions as a function of the ratio L_y/L_x, as shown from the figure, that is at the ratio $L_y/L_x < 0.25$ the value of the percentage deviation is nearly 40% because at these lengths the two dimensional well potential approaches to be as one dimensional well potential, while the percentage deviation is decreased rapidly as the ratio increases.

In Table 1, the semi-analytical solutions for finite rectangular well potential with depth 25 and lengths $L_x = 3$, $L_y = 2$ are listed in details in order to use them as initial guess values to calculate the exact numerical solutions in the next subsection.

Table 1 The semi-analytical solutions for finite rectangular well potentials with depth 25 and lengths 6X4.

ε_x		ε_y	
ε_{xe}	ε_{xo}	ε_{ye}	ε_{yo}
$\varepsilon_x(1) = -9.7758$	$\varepsilon_x(2) = -9.1052$	$\varepsilon_y(1) = -14.5167$	$\varepsilon_y(2) = -13.0746$
$\varepsilon_x(3) = -7.9949$	$\varepsilon_x(4) = -6.4584$	$\varepsilon_y(3) = -10.6998$	$\varepsilon_y(4) = -7.4523$
$\varepsilon_x(5) = -4.5231$	$\varepsilon_x(6) = -2.2552$	$\varepsilon_y(5) = -3.4867$	

3.2 The Higher Excited States

Armed with the semi-analytical solutions presented in Table 1, we calculate the exact numerical solutions for the allowable excited states of the finite rectangular well potential with depth 25 and lengths $L_x = 3$, $L_y = 2$ using the modified (FDTD) method. The number of the required cooling steps for each state is determined using the semi-analytical eigenvalue in according to Eq. (6), and introducing the semi-analytical eigenfunctions as initial guess wave functions. These results are listed in the following tables which organized as follows: The even parity states that include no zero lines are listed in Table 2 in addition to the ground state energy eigenvalue $\varepsilon(1,1)$ which is calculated using the only cooling steps. The odd parity states that include one zero line lays on $x\text{-}axis$ are listed in Table 3. The odd parity states that include one zero line lays on $y\text{-}axis$ are listed in Table 4. The even parity states that include two zero lines lay on the both axes are listed in Table 5. The suitable parameters for each state are listed in the same tables as well. In these calculations only one heating step is sufficient to get acceptable results, this reducing in the number of the heating steps is due to introducing the semi-analytical eigenfunction instead of general initial guess wave function which is a significant advantage. The deviation of the semi-analytical solutions from the exact numerical solutions are listed in the last column for each table, the maximum value of the deviation is nearly 5% which reflects the high accuracy of the separation of variables technique.

In Fig. 2 the semi-analytical eigenfunction $\psi_{3,3}(x,y)$ and its corresponding numerical eigenfunctions are

Table 2 The allowable even excited states energy eigenvalues of finite rectangular well potential with depth 25 and dimensions 6×4 calculated numerically, in these cases there aren't zero lines included.

The state	$\Delta\tau$	No. of cooling steps	Exact numerical eigenvalue	% Deviation
$\varepsilon(1,1)$	0.001	1400	-24.2923	0.0007
$\varepsilon(1,3)$	0.0005	442	-20.4417	0.3130
$\varepsilon(1,5)$	0.0003	251	-13.1780	0.6416
$\varepsilon(3,1)$	0.001	402	-22.4666	0.2004
$\varepsilon(3,3)$	0.0005	317	-18.5045	1.0279
$\varepsilon(3,5)$	0.0002	369	-11.3108	1.5102
$\varepsilon(5,1)$	0.0005	335	-19.1356	0.5009
$\varepsilon(5,3)$	0.0003	340	-14.8379	2.5941
$\varepsilon(5,5)$	0.00015	392	-7.5988	5.4088

Table 3 The allowable odd excited states energy eigenvalues of finite rectangular well potential with depth 25 and dimensions 6×4 calculated numerically, in these cases there is *x*- zero axis.

The state	$\Delta\tau$	No. of cooling steps	Exact numerical eigenvalue	% Deviation
$\varepsilon(1,2)$	0.001	465	-22.8592	0.0385
$\varepsilon(1,4)$	0.0004	322	-17. 1789	0.2862
$\varepsilon(3,2)$	0.0005	509	-20.9228	0.7009
$\varepsilon(3,4)$	0.0003	349	-15.1194	2.1678
$\varepsilon(5,2)$	0.0004	338	-17.4541	0.8229
$\varepsilon(5,4)$	0.0003	256	-11.4372	4.7059

presented respectively, the figure shows that although applying the separation of variables technique products energy eigenvalues close to the exact ones, the results of eigenfunctions are not. It should be noted that for fast reliable estimates of energy eigenvalues for the two dimensional rectangular potential our proposed scheme for separating the

Table 4 The allowable odd excited states energy eigenvalues of finite rectangular well potential with depth 25 and dimensions 6×4 calculated numerically, in these cases there is *y*- zero axis.

The state	$\Delta\tau$	No. of cooling steps	Exact numerical eigenvalue	% Deviation
$\varepsilon(2,1)$	0.001	726	-23.6029	0.0804
$\varepsilon(2,3)$	0.0005	385	-19.6921	0.5734
$\varepsilon(2,5)$	0.0001	806	-12.6741	0.6489
$\varepsilon(4,1)$	0.001	248	-20.9071	0.3253
$\varepsilon(4,3)$	0.0005	255	-16.8809	1.6428
$\varepsilon(4,5)$	0.0001	664	-9.6493	3.0652
$\varepsilon(6,1)$	0.0003	405	-17.2231	2.6195
$\varepsilon(6,3)$	0.0003	277	-12.7406	1.6827
$\varepsilon(6,5)$	0.0001	519	-5.5558	3.0374

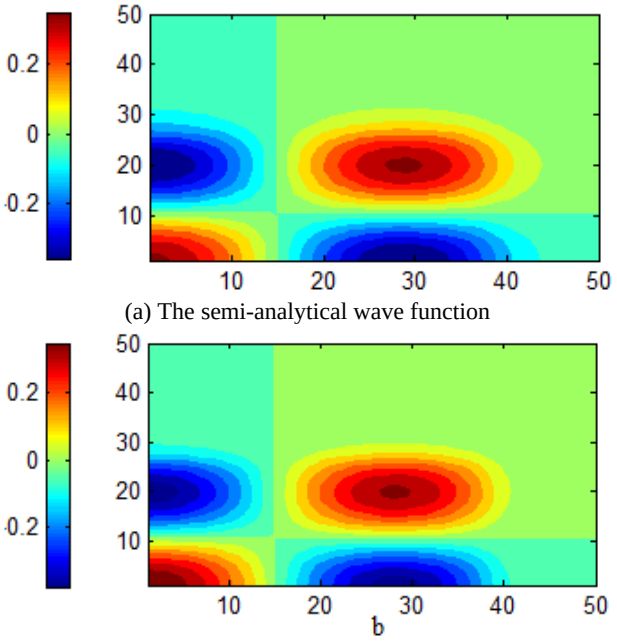
Table 5 The allowable even excited states energy eigenvalues of finite rectangular well potential with depth 25 and dimensions 6×4 calculated numerically, in these cases there are *x*-zero axis and *y*- zero axis.

The state	$\Delta\tau$	No. of cooling steps	Exact numerical eigenvalue	% Deviation
$\varepsilon(2,2)$	0.001	355	-22.1691	0.0481
$\varepsilon(2,4)$	0.0003	395	-16.3251	1.4238
$\varepsilon(4,2)$	0.0004	457	-19.2312	1.5693
$\varepsilon(4,4)$	0.0003	300	-13.4705	3.268
$\varepsilon(6,2)$	0.0003	345	-15.4323	0.6641
$\varepsilon(6,4)$	0.0002	327	- 9.2496	4.9500

potential into equivalent two one dimensional potentials is more than sufficient. If, however the need arises to get accurate wave functions then the full implementation of the modified (FDTD) method is recommended as we showed in this paper.

4. Conclusion

In the present work the separation of variables technique is employed to solve the two dimensional finite rectangular well potential problem to get the semi-analytical solutions which play an important role to calculate the exact numerical solutions. This employment based on splitting the two dimensional finite well potential to two one dimensional finite well



(a) The semi-analytical wave function

(b) The exact numerical wave function

Fig. 2 The eigenfunction $\psi_{3,3}(x,y)$.

with depths depend inversely on the lengths of the well as shown in Eq. (9) and Eq. (10). Then by using the semi-analytical solutions as initial guess values in the modified (FDTD) method one can get the exact numerical solutions, that is, for each state the semi-analytical eigenvalue is used to calculate the cooling steps that required to reach this state using Eq. (6), and the semi-analytical wave function is used as initial guess wave function. Numerically, by using symmetry arguments, both of the even excited states and the odd excited states are calculated separately, also the parameters included in the (FDTD) method, namely the spatial spacing separation and the temporal spacing, must be subjected to the stability condition [8, 12, 13]. As example, we present the numerical eigenvalues for rectangular well potential with depth 25 and lengths L_x = 3, L_y = 2 accompanied by the percentage deviation of the semi-analytical solutions which are listed in the last column in each table. It is notable that according to these results that if one only interested in the eigenvalues of a system, the separation of variables technique is simple and sufficient, which is the advantage of this work.

Another advantage of the separation of variables technique is that introducing the semi-analytical wave function as initial guess wave function reduces the numerical cost of the modified (FDTD) method comparing with using initial guess wave function depending only to the symmetric property of the desired state.

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