



Non-standard finite-difference time-domain method for solving the Schrödinger equation

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Abstract. In this paper, an improvement of the finite-difference time-domain (FDTD) method using a non-standard finite-difference scheme for solving the Schrödinger equation is presented. The standard numerical scheme for a second derivative in the spatial domain is replaced by a non-standard numerical scheme. In order to apply the non-standard FDTD (NSFDTD), first, the estimates of eigenenergies of a system are needed and computed by the standard FDTD method. These first eigenenergies are then used by the NSFDTD method to obtain improved eigenenergies. The NSFDTD method can be employed iteratively using the resulting eigenenergies to obtain more accurate results. In this paper, the NSFDTD method is validated using infinite square well, harmonic oscillator and Morse potentials. Significant improvements are found when using the NSFDTD method.

Keywords. Time-dependent Schrödinger equations; non-standard finite difference method; finite-difference time-domain method; eigenvalues; eigenfunctions.

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1. Introduction

The finite-difference time-domain (FDTD) method has been used extensively to simulate various electromagnetic wave radiations and interactions [1,2]. Because of its usefulness, ease in programming, good accuracy and flexibility, the FDTD method has been applied to other fields such as sound wave propagations [3] and simulations of quantum systems [4,5].

To simulate a quantum system in real time using the FDTD method, one can use the split method where the time-dependent Schrödinger equation (TDSE) is split into two equations for real and imaginary parts [6] or one can also directly use complex computation without splitting the TDSE [7]. Eigenvalues and eigenfunctions cannot be directly obtained from the real-time FDTD method. It requires a Fourier transformation procedure to obtain eigenvalues and an additional FDTD simulation to compute the eigenfunctions. Besides that, for an infinite spatial domain, the FDTD method requires also an absorbing boundary condition (ABC) to remove unwanted reflection from the computational boundary [8,9].

Sudiarta and Geldart [5] showed that the Fourier transformation procedure and ABC are not needed when the TDSE in imaginary time is used to compute eigenenergies and eigenfunctions. The TDSE in real time is transformed into the TDSE in imaginary time (or a diffusion equation) by replacing a real-time variable with an imaginary time variable. The diffusion equation is then used to simulate decay of a wave function to the ground-state wave function. The ground-state energy and ground-state wave function can be computed directly in a single simulation run. Besides that, another advantage of the FDTD method in imaginary time is that it uses only real values of the wave function, and therefore, it requires less computer memory.

The FDTD method in imaginary time (called simply the FDTD method for the rest of this paper) has been applied to various quantum systems. Sudiarta and Geldart [10] have used the FDTD method for an electron in a quantum dot and in a magnetic field. Dumitru *et al* [11] have studied quarkonium states in QCD plasma. Strickland and Yager-Elorriaga [12] have used the FDTD method with a parallel algorithm for a computer cluster to simulate a large quantum system.

Margotta *et al* [13] have used the FDTD method to study quarkonium binding energies using a realistic complex-valued potential. The FDTD method has also been used by Alford and Strickland [14] to study quarkonium states in an external magnetic field. Sudiarta and Geldart [15] have applied the FDTD method to compute single-particle density matrices. Sudiarta and Angraini [16] have also applied the FDTD method with the supersymmetry technique to obtain the ground and excited states of a particle in one-dimensional (1D) potentials.

For a quite small spatial grid spacing, the FDTD method has been found to give accurate results for 1D to 3D quantum systems [5]. For larger systems, the FDTD method with small spacing is not possible due to the limited computer memory. One can overcome this problem by using a cluster of computers and doing computation in parallel which can be easily done for the FDTD method as presented by Strickland and Yager-Elorriaga [12].

Another method to overcome this limitation is to increase its accuracy by using a non-standard finite-difference (NSFD) scheme that was found to be successfully applied to various differential equations [17–19]. The NSFD scheme for the Schrödinger equation was applied by Mickens and Ramadhani [19]. It is shown by Mickens and Ramadhani [19] and Chen *et al* [20] that the NSFD scheme performs better than the standard method and it is also found to be exact for a constant potential. Application of the FDTD method with the NSFD scheme has not been done previously. In this paper, the NSFD scheme is used to modify the standard FDTD method such that the non-standard FDTD (or NSFDTD) method can be used for large spatial grid spacing.

The NSFD scheme is generally applied to a system with one spatial dimension. Extension to two or more spatial dimensions is currently in progress and it will be published in our future publication. One possible extension is given by Cole [21,22] for electromagnetic waves. In this paper, only the theory and numerical method of the NSFDTD method for one spatial dimension are presented.

This paper is organised as follows: the theory of the NSFDTD method is introduced in the next section, numerical results of energies and wave functions for three potential wells are given in §3 and the conclusion is given in §4.

2. Theory

The TDSE in imaginary time for a system of one particle in a 1D potential $V(x)$ using atomic units ($\hbar = m = 1$) is given by [5]

$$\begin{aligned} \frac{\partial \psi(x, t)}{\partial t} &= -\hat{H} \psi(x, t) \\ &= -\left[-\frac{1}{2} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x, t). \end{aligned} \quad (1)$$

The corresponding time-independent Schrödinger equation (TISE), which is an eigenvalue equation, is given by

$$\frac{\partial^2 \psi(x, t)}{\partial x^2} + W(x) \psi(x, t) = 0, \quad (2)$$

where $W(x) = 2[E - V(x)]$. It is noted that E is the eigenenergy.

A solution of the TISE can be obtained iteratively by using eq. (1). Using an arbitrary initial wave function $\psi(x, 0)$ and a suitable discretisation scheme, a simulation with the discretised eq. (1) can be done to evolve the initial wave function. After a long enough simulation time, the wave function converges to the ground state of the system. Excited states of the system can be obtained in turn by evolving the initial wave function with the component of lower energy wave functions removed from the wave function [5]. For computational purpose, the computational domain is limited and the boundary of the computational domain is terminated by a Dirichlet boundary condition, $\psi(\text{boundary}) = 0$. This boundary condition is equivalent to the infinite potential wall. After the wave function is obtained, the corresponding energy is computed with

$$E = \frac{\int \psi^*(x) \hat{H} \psi(x) dx}{\int |\psi(x)|^2 dx}. \quad (3)$$

In the FDTD method [5], the standard discretisation for the second derivative of eq. (1) is the central finite difference scheme [23] in the form of

$$\frac{\partial^2 \psi(x)}{\partial x^2} \approx \frac{\psi(i+1) - 2\psi(i) + \psi(i-1)}{(\Delta x)^2}, \quad (4)$$

where we have used the notation $\psi(i) \equiv \psi(i \Delta x)$ and Δx is the spatial grid spacing.

For certain applications, the NSFD scheme developed by Mickens [24,25] has been shown to give exact numerical results. A non-standard scheme for the Schrödinger equation given by Mickens and Ramadhani [19] can be found by using a Taylor series for finite difference of the second derivative as follows:

$$\begin{aligned} &\psi(i+1) - 2\psi(i) + \psi(i-1) \\ &= 2 \left[\frac{(\Delta x)^2}{2!} \psi'' + \frac{(\Delta x)^4}{4!} \psi^{(4)} + \frac{(\Delta x)^6}{6!} \psi^{(6)} + \dots \right], \end{aligned} \quad (5)$$

where $\psi'' = \partial^2 \psi / \partial x^2$, $\psi^{(4)} = \partial^4 \psi / \partial x^4$ and $\psi^{(6)} = \partial^6 \psi / \partial x^6$. Equation (2) with a constant potential,

$W(x) = W$, can be used to simplify eq. (5). It can be shown that

$$\begin{aligned} &\psi(i + 1) - 2\psi(i) + \psi(i - 1) \\ &= 2 \frac{\psi''}{W} \left[\frac{(\Delta x \sqrt{W})^2}{2!} - \frac{(\Delta x \sqrt{W})^4}{4!} \right. \\ &\quad \left. + \frac{(\Delta x \sqrt{W})^6}{6!} - \dots \right]. \end{aligned} \tag{6}$$

Equation (6) can be simplified further using the Maclaurin series of $2 \sin^2(\theta/2)$, and we obtain

$$\begin{aligned} &\psi(i + 1) - 2\psi(i) + \psi(i - 1) \\ &= \psi'' \left[\frac{4}{W} \sin^2(\sqrt{W}\Delta x/2) \right]. \end{aligned} \tag{7}$$

Therefore, the second derivative can be accurately approximated by

$$\frac{\partial^2 \psi(x)}{\partial x^2} \approx \frac{\psi(i + 1) - 2\psi(i) + \psi(i - 1)}{g(i)}, \tag{8}$$

where the denominator function $g(i) \equiv g(i \Delta x) = g(x)$ is given by

$$g(x) = \begin{cases} (\Delta x)^2 & \text{for } W(x) = 0, \\ \frac{4}{W(x)} \sin^2(\sqrt{W(x)}\Delta x/2) & \text{for } W(x) > 0, \\ -\frac{4}{-W(x)} \sinh^2(\sqrt{-W(x)}\Delta x/2) & \text{for } W(x) < 0, \end{cases} \tag{9}$$

$g(x)$ can be rewritten in a simpler form using a Taylor series as

$$g(x) \approx (\Delta x)^2 - \frac{W(x)}{12}(\Delta x)^4 + \frac{[W(x)]^2}{360}(\Delta x)^6. \tag{10}$$

It is noted in eq. (10) that the NSFD scheme reduces to the standard scheme when the value of $W(x)$ is close to zero or the spatial interval Δx is small. The NSFD scheme of eq. (8) is found to give exact results for eq. (2) when $W(x)$ has no spatial dependence or a constant as indicated by eq. (7). This is in agreement with Mickens and Ramadani [19] and Chen *et al* [20]. When $W(x)$ is not a constant, the non-standard scheme has an accuracy of the order $(\Delta x)^2$ and known to perform better than other methods such as the standard finite-difference method and the Numerov method for large values of Δx [20].

In order to apply the NSFDTD scheme, the initial values of eigenenergies E are required as input parameters. The first estimates of energies can be obtained by using the standard FDTD method or by using $E = 0$. The

values of eigenenergies are then improved by using the NSFDTD method. Further improvement can be done by reapplying the NSFDTD method. This process can be iterated until the converged energies are obtained.

3. Numerical methods

An explicit iterative procedure given by Sudiarta and Geldart [5] is used for the NSFDTD method. The temporal derivative in eq. (1) is approximated by the forward difference equation and spatial second derivative is approximated using eq. (8). For better numerical stability and accuracy, $\psi(x, t)$ in eq. (1) should be equal to an average value $(\psi^{n+1}(i) + \psi^n(i))/2$. After some manipulations, it is found that an explicit equation is given by

$$\begin{aligned} \psi^{n+1}(i) &= \alpha(i)\psi^n(i) + \frac{\beta(i)\Delta t}{2g(i)} [\psi^n(i + 1) \\ &\quad - 2\psi^n(i) + \psi^n(i - 1)], \end{aligned} \tag{11}$$

where $\alpha(i) = [1 - \Delta t V(i)]/[1 + \Delta t V(i)]$ and $\beta(i) = 1/[1 + \Delta t V(i)]$.

Using initial random values of an initial wave function $\psi(i)$, we then iterate with eq. (11) and after sufficient number of iterations, the wave function converges to the ground-state wave function. Excited states are obtained by redoing the iteration with lower states removed from the wave function (see [5] for details).

The energy is computed numerically by

$$E = \frac{1}{\sum_i \psi(i)^2} \sum_i \left\{ V(i)\psi(i)^2 - \frac{\psi(i)[\psi(i + 1) - 2\psi(i) + \psi(i - 1)]}{g(i)} \right\}. \tag{12}$$

As previously mentioned, in order to use the NSFDTD method, initial eigenenergies are needed and in this paper we obtain them by performing iteration with $g(i) = (\Delta x)^2$ or setting $W(x) = 0$ in eq. (9). The resulting energies and wave functions for this case are the same as the numerical results found using the standard FDTD method. Alternatively, we can also use $E_n = 0$ as the initial eigenenergies and it is found that the same final results of the NSFDTD method are obtained regardless of the values of the initial eigenenergies. In this paper, only numerical results using $W(x) = 0$ are given.

4. Results and discussion

4.1 Infinite square well potential

To demonstrate significant improvements when using the NSFDTD in particular for a constant potential

$V(x) = V_0$ or simply $V(x) = 0$, we first consider a free particle in an infinite square well given by $V(x) = 0$ for $0 < x < 1$ and $V(x) = \infty$ for $x < 0$ and $x > 1$. The eigenenergies are known to be $E_n = n^2\pi^2/2$ and the eigenstates are given by $\psi_n(x) = \sqrt{2} \sin(n\pi x)$. The computational domain is terminated using $\psi(x) = 0$ at $x = 0$ and 1 , which corresponds to an infinite potential wall.

The numerical parameters used for computation are $\Delta x = 0.1$ and $\Delta t = (\Delta x)^2/10$. The numerical results for eigenenergies and state functions are shown in table 1 and figure 1.

It is noted that after the first iteration, the NSFDTD results have shown better accuracy than the standard FDTD method. Further reapplication of the NSFDTD method produces even better eigenenergies. After about 10 iterations, the final eigenenergies converge to the exact values. These results confirm that the NSFDTD method is the exact method when the potential is constant. Furthermore, the resulting wave functions are in good agreement with the analytical wave functions and the same as the standard FDTD results. This is a consequence of the fact that the values of $g(i)$ are constant. The discretisation of the TISE using the standard and non-standard schemes yields difference equations that differ only in energy scaling factor.

4.2 Harmonic oscillator potential

The second application of the NSFDTD method is for a particle in a harmonic oscillator potential $V(x) = \frac{1}{2}\omega x^2$. The eigenenergies are $E_n = (n + \frac{1}{2})\omega$. The wave functions are products of $\exp(-\omega x^2/2)$ and Hermite polynomials (details can be found in [26,27]). Numerical results of eigenenergies for angular frequency $\omega = 1$, grid spacing $\Delta x = 0.8$ and 0.5 with computational lengths of 16 and 10 are given in table 2. Numerical wave functions for the first five states are shown

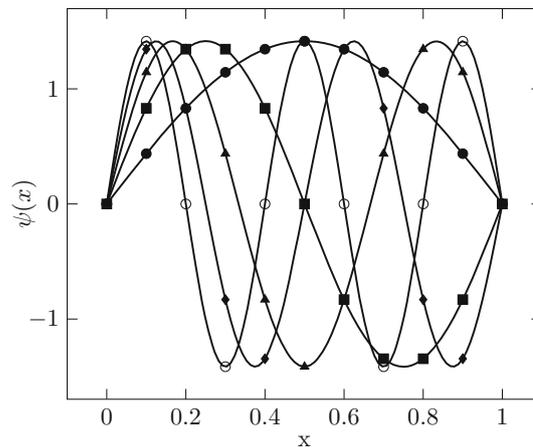


Figure 1. Comparison of ground and excited state wave functions (symbols: for state $n = 1$ (●), $n = 2$ (■), $n = 3$ (▲), $n = 4$ (◆), $n = 5$ (○)) with analytical wave functions (lines) for a particle in an infinite square well.

in figure 2. To compare the accuracy of the FDTD and NSFDTD results, the absolute errors of numerical wave functions for states $n = 3$ and 4 are shown in figure 3.

In this application, the potential $V(x)$ and consequently $W(x)$ are dependent on x . It is clearly shown, especially for excited states, that the first iteration of the NSFDTD method is also found to significantly improve the standard FDTD method. Although the NSFDTD method is not exact in this case, its accuracy is still higher than the standard FDTD results. It is obviously shown that the numerical results become more accurate when the spacing is reduced. Because the wave function of the harmonic oscillator has exponential dependence, in order to get accurate results using the NSFDTD method, we need to verify that the wave function has decayed approximately to zero near the computational boundary. This is to ensure that the boundary does not affect wave functions.

Table 1. Numerical eigenenergies of a particle in an infinite square well potential computed by the FDTD method (standard scheme), the NSFDTD method after first (1st), second (2nd), third (3rd) and final iterations are compared with exact values. The NSFDTD parameters used are $\Delta x = 0.1$ and the length of the square well or the computational domain is 1. The correct numbers are in bold.

n	FDTD	NSFDTD				Exact
		1st	2nd	3rd	Final	
1	4.894348	4.934469	4.934799	4.934802	4.934802	4.934802
2	19.098301	19.717997	19.738506	19.739186	19.739209	19.739209
3	41.221475	44.174164	44.395261	44.411870	44.413220	44.413220
4	69.098301	77.637465	78.778707	78.932758	78.956835	78.956835
5	100.000000	118.475509	122.325053	123.146042	123.370050	123.370055

Table 2. Numerical eigenenergies of a particle in a harmonic oscillator potential computed by the FDTD method (standard scheme), the NSFDTD after first (1st), second (2nd), third (3rd) and final iterations are compared with the exact values. The lengths of the computational domains are 16 and 10 for $\Delta x = 0.8$ and 0.5, respectively.

No.	FDTD	NSFDTD				Exact
		1st	2nd	3rd	Final	
<i>Spatial interval $\Delta x = 0.8$</i>						
1	0.479077	0.497481	0.498004	0.498019	0.498019	0.5
2	1.391838	1.483898	1.491834	1.492521	1.492586	1.5
3	2.188108	2.435512	2.471583	2.476871	2.477781	2.5
4	2.954963	3.357062	3.439530	3.456553	3.460975	3.5
5	3.236360	4.050845	4.306467	4.384808	4.418670	4.5
<i>Spatial interval $\Delta x = 0.5$</i>						
1	0.492062	0.499624	0.499705	0.499706	0.499706	0.5
2	1.459805	1.497690	1.498910	1.498949	1.498951	1.5
3	2.393936	2.491568	2.496825	2.497108	2.497125	2.5
4	3.292528	3.479435	3.493647	3.494727	3.494816	3.5
5	4.153118	4.459088	4.489421	4.492424	4.492753	4.5

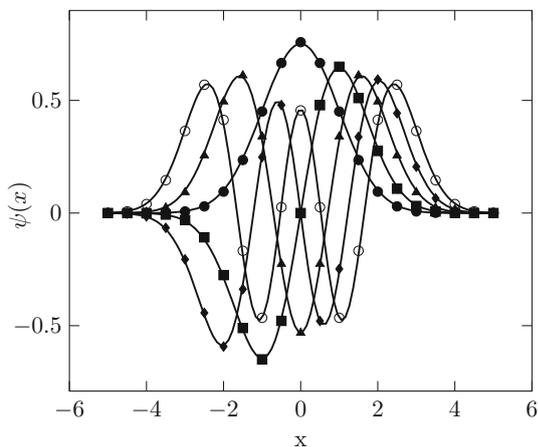


Figure 2. Comparison of ground and excited state wave functions (symbols: state $n = 1$ (●), $n = 2$ (■), $n = 3$ (▲), $n = 4$ (◆), $n = 5$ (○)) with analytical wave functions (lines) for a particle in a harmonic oscillator potential.

A comparison of numerical and analytical wave functions is shown in figure 2 and the sum of squared errors (SSE) of the wave functions is given in table 3. The numerical wave functions are shown to be in agreement with the analytical wave functions. It is noted that the SSE of the wave functions decrease as we increase the number of iterations. It is also shown that the wave functions are very small near the computational boundaries. The numerical wave functions obtained by the NSFDTD method are more accurate than that by the FDTD method which is clearly shown by smaller absolute errors in figure 3.

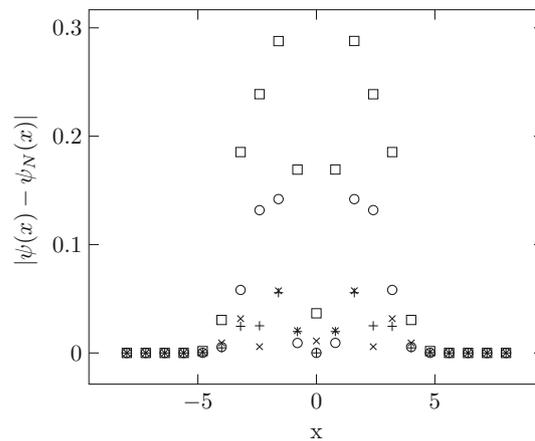


Figure 3. Absolute errors of numerical wave functions $\psi_N(x)$ for states $n = 3$ (○) and $n = 4$ (□) obtained by the FDTD method, and for states $n = 3$ (+) and $n = 4$ (*) obtained by the NSFDTD method.

4.3 Morse potential

For application in atomic vibrations, the Morse potential well is usually chosen as the model potential. The Morse potential as an example for this paper is in the form of $V(x) = D[1 - \exp(-(x - x_0))]^2$. (13)

The analytical eigenenergies are given by $E_n = \omega(n + \frac{1}{2})[1 - \omega(n + \frac{1}{2})/4D]$ with $\omega^2 = 2D$.

For numerical computations, the NSFDTD parameters are $x_0 = 2$, $\Delta x = 0.2$, the computational domain is $[0, 8]$ and the Morse parameter $D = 50$ is used

Table 3. Same as table 2 except that this is for the SSE of wave functions.

No.	FDTD	NSFDTD			
		1st	2nd	3rd	Final
<i>Spatial interval $\Delta x = 0.8$</i>					
1	0.002640	0.001655	0.001631	0.001630	0.001630
2	0.015449	0.004473	0.003858	0.003807	0.003802
3	0.071309	0.011986	0.008113	0.007629	0.007548
4	0.134618	0.022206	0.011478	0.009849	0.009463
5	0.662104	0.118040	0.031514	0.017526	0.013284
<i>Spatial interval $\Delta x = 0.5$</i>					
1	0.000611	0.000381	0.000379	0.000379	0.000379
2	0.003254	0.000878	0.000827	0.000826	0.000826
3	0.011101	0.001747	0.001501	0.001489	0.001488
4	0.029720	0.002703	0.001972	0.001925	0.001921
5	0.068005	0.003694	0.002016	0.001898	0.001886

Table 4. Numerical eigenenergies of a particle in a Morse potential computed by the FDTD method (standard scheme), the NSFDTD after first (1st), second (2nd), third (3rd) and final iterations are compared with the exact values. The parameters used are $\Delta x = 0.2$, $x_0 = 2$ and the computational domain is at an interval [0,8].

No.	FDTD	NSFDTD				Exact
		1st	2nd	3rd	Final	
1	4.754956	4.865394	4.867215	4.867245	4.867246	4.875
2	13.365245	13.830904	13.851604	13.852525	13.852568	13.875
3	20.758056	21.762245	21.828617	21.832999	21.833308	21.875
4	27.087090	28.686514	28.818009	28.828801	28.829763	28.875
5	32.484206	34.633288	34.831976	34.850315	34.852177	34.875

for simplicity. The resulting numerical eigenvalues are given in table 4. In this case, it is also found that the NSFDTD method is more accurate than the standard FDTD method.

5. Conclusion

A numerical method known as the NSFDTD method has been presented and validated using three potential wells. The numerical results of eigenenergies and wave functions are compared with the standard FDTD and analytical results. It has been shown that the NSFDTD method is an exact method for the case of a constant potential. The NSFDTD method has also been shown to perform better than the standard FDTD method for all cases.

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References

- [1] A Taflove and S C Hagness, *Computational electrodynamics: The finite-difference time-domain method* (Artech House, Boston, 2000)
- [2] A Taflove, A Oskooi and S G Johnson, *Advances in FDTD computational electrodynamics: Photonics and nanotechnology* (Artech House, Boston, 2013)
- [3] D Botteldooren, *J. Acoust. Soc. Am.* **98**, 3302 (1995)
- [4] D Sullivan and D S Citrin, *J. Appl. Phys.* **89**, 3841 (2001)
- [5] I W Sudiarta and D J W Geldart, *J. Phys. A Math. Theor.* **40**, 1885 (2007)
- [6] P B Visscher, *Comput. Phys.* **5**, 596 (1991)
- [7] A Askar and A S Cakmak, *J. Chem. Phys.* **68**, 2794 (1978)
- [8] D M Sullivan and D S Citrin, *J. Appl. Phys.* **91**, 3219 (2002)
- [9] D M Sullivan and D S Citrin, *J. Appl. Phys.* **97**, 104305 (2005)

- [10] I W Sudiarta and D J W Geldart, *Phys. Lett. A* **372**, 3145 (2008)
- [11] A Dumitru, Y Guo, A Mocsy and M Strickland, *Phys. Rev. D* **79**, 054019 (2009)
- [12] M Strickland and D Yager-Elorriaga, *J. Comput. Phys.* **229**, 6015 (2010)
- [13] M Margotta, K McCarty, C McGahan, M Strickland and D Yager-Elorriaga, *Phys. Rev. D* **83**, 105019 (2011)
- [14] J Alford and M Strickland, *Phys. Rev. D* **88**, 105017 (2013)
- [15] I W Sudiarta and D J W Geldart, *J. Phys. A Math. Theor.* **42**, 285002 (2009)
- [16] I W Sudiarta and L M Angraini, *AIP Conf. Proc.* **1729**, 020030 (2016)
- [17] R E Mickens, *Applications of nonstandard finite difference schemes* (World Scientific, Singapore, 2000)
- [18] A Aydin and C Koroglu, *Pramana – J. Phys.* **89**: 72 (2017)
- [19] R E Mickens and I Ramadhani, *Phys. Rev. A* **45**, 2074 (1992)
- [20] R Chen, Z Xu and L Sun, *Phys. Rev. E* **47**, 3799 (1993)
- [21] J B Cole, *IEEE Trans. Microw. Theory Tech.* **45**, 991 (1997)
- [22] J B Cole, *IEEE Trans. Antennas Propag.* **50**, 1185 (2002)
- [23] S C Chapra and R P Canale, *Numerical methods for engineers*, 5th edn (McGraw-Hill, New York, 2006)
- [24] R E Mickens, *J. Comput. Acoust.* **7**, 39 (1999)
- [25] R E Mickens, *J. Differ. Equ. Appl.* **8**, 823 (2002)
- [26] B H Bransden and C J Joachain, *Introduction to quantum mechanics* (Longman Scientific & Technical, Essex, 1989)
- [27] P W Atkins and R S Friedman, *Molecular quantum mechanics* (Oxford University Press, Oxford, 2011)