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Alternative Approach for the Time Domain Solution of the Schrödinger Equation

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Abstract: In this work, we propose to solve an equivalent real-valued second order differential equation instead of solving the complex-valued Schrödinger equation itself using the finite difference time domain method (FDTD). This reduces the number of variables involved and hence memory space requirements and code amount. This allows obtaining also a more relaxed stability relation which reduces time requirements. Some examples are given at the end to validate the proposed formulation.

Keywords: FDTD, Quantum Tunneling, Schrodinger Equation, Time Domain.

1 Introduction

The Finite Difference Time Domain (FDTD) Method is a numerical method developed to solve the problems of electromagnetism [1]. It has been extended later to include other domains of science and engineering [2]. The Quantum FDTD (Q-FDTD) is a variant of the FDTD method developed to solve quantum physics problems. Since the Schrödinger equation is the fundamental equation in quantum physics, it has gained most of developers' interest.

Because it is a complex valued equation and can not be implemented directly using a time domain method, different approaches were introduced to allow the integration of the Schrödinger equation in the FDTD code.

Soriano and his co-workers [3] divided the complex wave function into two parts: real part and imaginary part. After inserting this complex wave function in the Schrödinger equation, they obtained two coupled real-valued equations to be solved following a leapfrog scheme.

The main drawback of this approach is its memory space and CPU time consumption. To reduce these computational costs, different schemes were introduced later: for instance, a parallel algorithm in [4], a non-linear grid mapping in [5] and a generalized algorithm in [6, 7].

Sudartha and Geldart [8] transformed the Schrödinger equation into a diffusion equation with imaginarytimeand applied it for the calculation of the ground state and excited states' eigenvalues and eigenfunctions of electrons in a potential well.

The use of imaginary time nevertheless, leads to decaying solutions, notably for higher order modes, which complicates the extraction of the eigenvalues of those modes [5].

In this work, a new approach for the solution of the Schrödinger equation is presented. It consists of solving a real-valued second order differential equation equivalent to the Schrödinger equation, instead of solving the Schrödinger equation itself. Details of the implementation of the obtained wave equation will be given and the stability relation presented. Some numerical examples will be presented also to show the validity and efficiency of the proposed approach.

2 Derivation

Schrödinger equation in its simple form is written as

$$E\Psi(r,t) = H\Psi(r,t) \tag{1}$$

,where: E and H are the energy and the Hamiltonian operators respectively; $\Psi(r,t)$ is the wave function (state function), having the expression

$$\Psi(r,t) = \Psi(r)e^{\frac{-jEt}{\hbar}} \tag{2}$$

where $\hbar = 1.0504\times10^{-34}$.

The left term of (1) can be obtained by multiplication of the time derivative of (2) with the quantity $j\hbar$

$$j\hbar.\frac{\partial\Psi}{\partial t} = j\hbar.\left(-j\frac{E}{\hbar}\Psi\right) = E\Psi(r,t) \tag{3}$$

Consequently, we can rewrite (1) as follows

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$$j\hbar\frac{\partial\Psi}{\partial t}=\hat{H}\Psi=\left(-\frac{\hbar^2\nabla^2}{2m}+V\right)\Psi \tag{4}$$

$$\hat{H}=-\frac{\hbar^2\nabla^2}{2m}+V \tag{5}$$

where m is the mass of the particle and V is the time-independant potential energy.

The equation (4) is the time dependent Schrödinger equation; It contains a complex number and can not be implemented directly using the FDTD method. For this reason, two main different approaches were presented for its implementation.

In the first approach [3], the complex wavefunction (2) is assumed to have the form

$$\psi=\psi_r+j\psi_i \tag{6}$$

, where 'r' and 'i' refer to the real and the imaginary parts respectively. Inserting (6) in (4), we obtain two coupled real-valued equations

$$\hbar\frac{\partial\Psi_r}{\partial t}=\hat{H}\Psi_i \tag{7}$$

$$-\hbar\frac{\partial\Psi_i}{\partial t}=\hat{H}\Psi_r \tag{8}$$

that can be updated following a leapfrog scheme. The details of the discretization as well as the stability criteria are presented in [3].

This algorithm was used later in many applications, for instance, for the solution of the coupled Maxwell-Schrödinger equations [9, 10] and for the simulation of electrons in quantum dots [3] [11].

This algorithm nevertheless requires large memory space. At least, we need two arrays for each component (Ψ_r and Ψ_i), one for the storage of the old variables ($n-\frac{1}{2}$), and the other for the new ones ($n+\frac{1}{2}$). For the sake of reducing these requirements, different schemes were proposed [4, 5, 6, and 7].

In the second approach [8], the expression of the wavefunction (2) is written using the concept of imaginary time $\tau=jt$

$$\Psi(r,t)=\Psi(r)e^{\frac{-E\tau}{\hbar}} \tag{9}$$

Consequently (4) transforms to a diffusion-like equation

$$\hbar\frac{\partial\Psi}{\partial\tau}=-\hat{H}\Psi \tag{10}$$

to be solved in the imaginary time domain.

This approach leads to decaying solutions notably for higher order modes, which complicates the post processing and the extraction of numerical results. This approach has gained little interest and was used in very few papers.

In the following, an alternative approach is proposed. Multiplying the second time derivative of (2) with the quantity $-\hbar^2$, we get

$$-\hbar^2\frac{\partial^2\Psi}{\partial t^2}=-\hbar^2\left(-\frac{E^2}{\hbar^2}\Psi\right)=E^2\Psi(r,t) \tag{11}$$

From (11), (1) and (5), we obtain

$$-\hbar^2\frac{\partial^2\Psi}{\partial t^2}=H^2\Psi \tag{12}$$

This is a real-valued second order differential equation that we propose to solve instead of solving the complex-valued Schrödinger equation (4) itself.

Actually, we can obtain (12) from the couple of equationss (7) and (8). Derivating both of them with respect to time, we obtain

$$\hbar\frac{\partial^2\Psi_r}{\partial t^2}=\hat{H}\frac{\partial\Psi_i}{\partial t} \tag{13}$$

$$-\hbar\frac{\partial^2\Psi_i}{\partial t^2}=\hat{H}\frac{\partial\Psi_r}{\partial t} \tag{14}$$

From (13) and (8), we obtain

$$-\hbar^2\frac{\partial^2\Psi_r}{\partial t^2}=\hat{H}^2\Psi_r \tag{15}$$

Similarly, from (14) and (7), we obtain

$$-\hbar^2\frac{\partial^2\Psi_i}{\partial t^2}=\hat{H}^2\Psi_i \tag{16}$$

Note that the two equtions (15) and (16) are identical and can be written

$$-\hbar^2\frac{\partial^2\Psi_p}{\partial t^2}=\hat{H}^2\Psi_p \tag{17}$$

with $p=r, i$. If we omit the indice p, we will get the equation (12).

3 Discretization

From (12) and (5), we obtain

$$\frac{\partial^2\Psi}{\partial t^2}=\left(-\frac{\hbar^2}{4m^2}\nabla^4+\frac{V}{m}\nabla^2-\frac{V^2}{\hbar^2}\right)\Psi \tag{18}$$

Using the approximating formula for the time derivative

$$\frac{\partial^2\Psi}{\partial t^2}\approx\frac{\delta^2\Psi}{\Delta t^2}=\frac{\Psi^{n+\frac{1}{2}}-2\Psi^{n-\frac{1}{2}}+\Psi^{n-\frac{3}{2}}}{\Delta t^2} \tag{19}$$

$$\psi \approx \psi^{n-1/2} \tag{20}$$

and similar formulas for the special derivatives

$$\nabla^4\Psi = \frac{\partial^4\Psi}{\partial x^4} = \frac{\Psi(i+2)-4\psi(i+1)+6\psi(i)-4\psi(i-1)+\psi(i-2)}{\Delta x^4} \tag{21}$$

$$\nabla^2\Psi = \frac{\partial^2\Psi}{\partial x^2} = \frac{\psi(i+1)-2\psi(i)+\psi(i-1)}{\Delta x^2} \tag{22}$$

we obtain finally

$$\begin{aligned}\Psi^{n+1/2} &= 2\Psi^{n-1/2} - \Psi^{n-3/2} \\ &- \Delta t^2 \frac{\hbar^2}{4m^2\Delta x^4}\begin{pmatrix}\Psi^{n-1/2}(i+2)-4\psi^{n-1/2}(i+1)+6\psi^{n-1/2}(i)\\ -4\psi^{n-1/2}(i-1)+\psi^{n-1/2}(i-2)\end{pmatrix} \\ &+ \frac{\Delta t^2}{m\Delta x^2}\begin{pmatrix}V(i+1)\psi^{n-1/2}(i+1)-2V(i)\psi^{n-1/2}(i)\\ +V(i-1)\psi^{n-1/2}(i-1)\end{pmatrix} \\ &- \Delta t^2 \frac{V(i)^2}{\hbar^2}\psi(i)^{n-1/2}\end{aligned} \tag{23}$$

Note that the potential as well as the mass of the particle are denser in this equation than they are in the Schrödinger equation – this would allow a better treatment of complex problems where different regions with different values of the potential are involved.

4 Stability Analysis

To obtain the stability condition of the proposed algorithm, we follow a similar approach to that used in [3].

4.1 Temporal Eigenvalue

Expressing the left-hand side of (12) in terms of the temporel eigenvalue λ_t , we obtain

$$-\hbar^2\frac{\partial^2\Psi}{\partial t^2} \approx -\hbar^2\frac{\delta^2\Psi}{\Delta t^2} = -\hbar^2\frac{\Psi^{n+1/2}-2\Psi^{n-1/2}+\Psi^{n-3/2}}{\Delta t^2} = \lambda_t\Psi^{n-1/2} \tag{24}$$

Introducing the groth factor

$$q = \frac{\Psi^{n+1/2}}{\Psi^{n-1/2}} = \frac{\Psi^{n-1/2}}{\Psi^{n-3/2}} \tag{25}$$

we obtain from (24)

$$-\hbar^2\frac{q-2+\frac{1}{q}}{\Delta t^2} = \lambda_t \tag{26}$$

, or

$$q^2 - \left(2-\lambda_t\frac{\Delta t^2}{\hbar^2}\right)q+1=0 \tag{27}$$

The stability requires that

$$|q| \le 1 \tag{28}$$

, or

$$-1 \le q \le 1 \tag{29}$$

From (27), we can see that this condition is verified when

$$2-\lambda_t\frac{\Delta t^2}{\hbar^2} \ge -2 \tag{30}$$

, or

$$\lambda_t \le \frac{4\hbar^2}{\Delta t^2} \tag{31}$$

4.2 Special Eigenvalue

Similarly, expressing the right-hand side of (12) in terms of the spacial eigenvalue λ_s , we obtain

$$H^2\Psi = \left(\frac{\hbar^4\hbar^2}{4m^2}\nabla^4 - \frac{\hbar^2 V}{m}\nabla^2 + V^2\right)\Psi = \lambda_s\Psi \tag{32}$$

or

$$\left(\frac{16\hbar^4}{4m^2}\frac{\sin^4\left(\frac{K_x\Delta x}{2}\right)}{\Delta x^4} + \frac{4\hbar^2 V}{m}\frac{\sin^2\left(\frac{K_x\Delta x}{2}\right)}{\Delta x^2} + V^2\right)\Psi = \lambda_s\Psi \tag{33}$$

or

$$\lambda_s = \frac{4\hbar^4}{m^2}\frac{\sin^4\left(\frac{K_x\Delta x}{2}\right)}{\Delta x^4} + \frac{4\hbar^2 V}{m}\frac{\sin^2\left(\frac{K_x\Delta x}{2}\right)}{\Delta x^2} + V^2 \tag{34}$$

4.3 Stability Relation

The stability requires that

$$\lambda_s \le \lambda_t \tag{35}$$

From (31) and (34), we obtain

$$\frac{4\hbar^2}{\Delta t^2} \geq \frac{4\hbar^4}{m^2}\frac{\sin^4\left(\frac{K_x\Delta x}{2}\right)}{\Delta x^4} + \frac{4\hbar^2 V}{m}\frac{\sin^2\left(\frac{K_x\Delta x}{2}\right)}{\Delta x^2} + V^2 \quad (37)$$

, or

$$\Delta t^2 \leq \frac{\hbar^2}{\frac{\hbar^4}{m^2}\frac{\sin^4\left(\frac{K_x\Delta x}{2}\right)}{\Delta x^4} + \frac{\hbar^2 V}{m}\frac{\sin^2\left(\frac{K_x\Delta x}{2}\right)}{\Delta x^2} + \frac{V^2}{4}} \quad (38)$$

When $\Delta x \to 0$, we obtain

$$\Delta t^2 \leq \frac{\hbar^2}{\frac{\hbar^4}{m^2}\frac{1}{\Delta x^4} + \frac{\hbar^2 V}{m}\frac{1}{\Delta x^2} + \frac{V^2}{4}} \quad (39)$$

, or

$$\Delta t \leq \frac{\hbar}{\sqrt{\frac{\hbar^4}{m^2}\frac{1}{\Delta x^4} + \frac{\hbar^2 V}{m}\frac{1}{\Delta x^2} + \frac{V^2}{4}}} \quad (40)$$

This stability relation (40) is more relaxed than that of [3], and the maximum value allowed for the time step is larger. The two relations are identical only when $V = 0$.

5 Numerical Results and Discussion

In the first example, we alalyse the quantum tunneling phenomena of an electron through a potential barier.

Figure 1 shows the obtained results for the transmission coefficientg of an electron with enegy $E = 500eV$ through a barrier of potential $V_0 = 600eV$. The width of the barrier W varies from 0 to $5dx$, where $dx = 0.054\ pm$ is the space step.

Figure 2 shows the results obtained for the transmission coefficient of the electron through a potential barrier of width $W = 1dx$.

The magnitude of the potential varies from $500eV$ to $750eV$.

The maximum value allowed for the time step $\Delta t_{\max}$ is obtained from (13). For instance, for $V = 750eV$, we get $\Delta t_{\max} = 2.26\times10^{-19}$, whereas the obtained value from the relation of [3] is $\Delta t_{\max} = 2.00\times10^{-19}$, which means an increment of 13%.

In both figures, the obtained results are compared with other results obtained using the formulation of [3] and the exact results obtained from the relation

$$T = \frac{1}{\left(1 + \frac{V_0^2 \sinh(kW)^2}{4E(V_0 - E)}\right)} \quad (41)$$

$$k = \sqrt{2m(V_0 - E)/\hbar^2} \quad (42)$$

Good agreement was obtained.

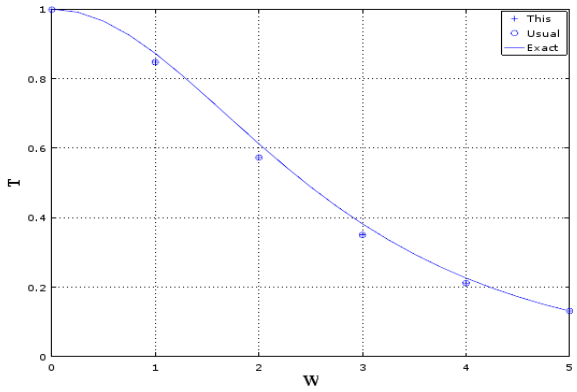

Figure 1: variation of the transmission coefficient in function of the width of the potential barriar.

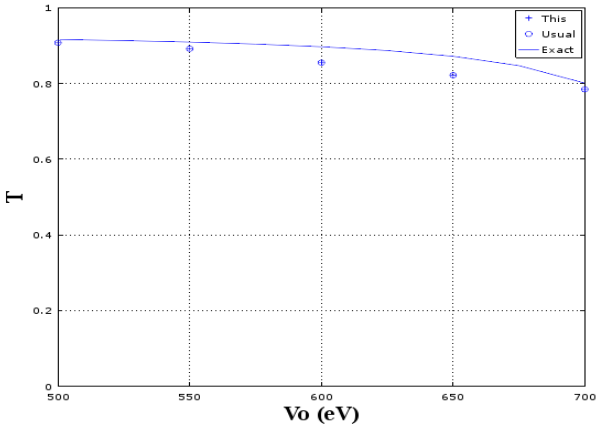

Figure 2: variation of the transmission coefficient in function of the potential of the barriar.

Table 1 shows a comparison between this method and the usual one in terms of time and memory-space required for the simulation.

Table 1. Comparison of Efficiency.

	This	*Usual*
Memory Space (bytes)	19400	38600
Processing Time (steps)	541	611

The simulation was performed using a 1D scheme; in the 3D scheme, the difference between the two methods will be much more significant.

6 Conclusion

In this paper, we derived a second-order differential equation from the Schrodinger equation. This equation involves only real entities and can be implemented directly using the finite-difference time-domain method. The derivation of the discretized form of the obtained equation as well as its stability relation was presented. It was applied later for the calculation of the transmission coefficient of an electron through a potential barier for different values of the potential and the width of the barrier and the obtained results were in agreement with the exact results and with other results obtained using the usual FDTD algorithm, which proves the accuracy of the present approach. A significant reduction in memory-space and time requirements was also observed, which proves the efficiency of the present approach.

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