Time-Domain Simulation of Three Dimensional Quantum Wires

Dennis M. Sullivan¹ *, Sean Mossman², Mark G. Kuzyk²

¹ Department of Electrical and Computer Engineering, University of Idaho, Moscow, Idaho, United States of America, ² Department of Physics and Astronomy, Washington State University, Pullman, Washington, United States of America

* dennis@ee.uidaho.edu

Abstract

A method is presented to calculate the eigenenergies and eigenfunctions of quantum wires. This is a true three-dimensional method based on a direct implementation of the time-dependent Schrödinger equation. It makes no approximations to the Schrödinger equation other than the finite-difference approximation of the space and time derivatives. The accuracy of our method is tested by comparing it to analytical results in a cylindrical wire.

Introduction

Quantum wires have become extremely important structures in the field of quantum nanodevices. They have found applications in such diverse fields as quantum electronics [1–5] and nonlinear optics [6–10]. This paper describes the use of the finite-difference time-domain (FDTD) method to determine the eigenenergies and eigenfunctions of quantum wires from the potential function [11–15]. Specifically, a method is described to accurately model long, thin wires without using excessive computer resources. Furthermore, a Bessel function method is presented that can be used to verify the calculations of the FDTD method.

An important application of this method is to nonlinear optics, where nonlinear susceptibilities are calculated from the quantum properties of the material. For example, transition moments, which are calculated from wave functions, and energies are used in a sum-over-states expression to get nonlinear susceptibilities. This approach was used to find optimized potentials [16, 17] as well as to analyze the character of a potential that gives the largest nonlinearity by analyzing ones made of a finite number for straight line segments, as demonstrated by Burke [18–20].

FDTD can be used to quickly calculate nonlinear susceptibilities, which can be used to optimize the nonlinear response by varying the shapes of arbitrary structures. In this work, we consider structures made of fused conducting cylinders because these are the types of structures that can be made using common fabrication techniques found in nanotechnology labs. As such, this work can be seen as providing the computational building blocks with applications to nonlinear optics, electronics, and related fields.

In the next section of this paper, we describe the implementation of the FDTD method and its use to calculate eigenenergies and eigenfunctions. This includes a description of a method to
increase the resolution of the FDTD simulation by averaging the potential in cells bordering two different materials. We then present the results of determining the eigenenergies of a quantum wire at various radii along with the Bessel function results to confirm the accuracy. The flexibility of the method is demonstrated by modeling potentials that do not otherwise easily lend themselves to analysis. We end by summarizing the results of the paper and discussing future directions. S1 Appendix describes the Bessel function method.

The Finite-Difference Time-Domain Method

We begin describing the FDTD implementation of the time-dependent Schrödinger equation [13, 14], which is written in the following form

\[
\frac{\partial \psi(x, y, z, t)}{\partial t} = i \frac{\hbar}{2m} \left[ \frac{\partial^2 \psi(x, y, z, t)}{\partial x^2} + \frac{\partial^2 \psi(x, y, z, t)}{\partial y^2} + \frac{\partial^2 \psi(x, y, z, t)}{\partial z^2} \right] - \frac{i}{\hbar} V(x, y, z) \psi(x, y, z, t).
\]  

(1)

We separate \( \psi(x, y, z, t) \) into real and imaginary components:

\[
\psi(x, y, z, t) = \psi_{\text{real}}(x, y, z, t) + i \cdot \psi_{\text{imag}}(x, y, z, t).
\]  

(2)

Inserting Eq 2 into Eq 1 leads to two coupled equations:

\[
\frac{\partial \psi_{\text{real}}(x, y, z, t)}{\partial t} = - \frac{\hbar}{2m} \nabla^2 \psi_{\text{imag}}(x, y, z, t) + \frac{1}{\hbar} V(x, y, z) \psi_{\text{imag}}(x, y, z, t),
\]  

(3a)

\[
\frac{\partial \psi_{\text{imag}}(x, y, z, t)}{\partial t} = \frac{\hbar}{2m} \nabla^2 \psi_{\text{real}}(x, y, z, t) - \frac{1}{\hbar} V(x, y, z) \psi_{\text{real}}(x, y, z, t).
\]  

(3b)

To code these equations, we take the finite-difference approximations in space and time which results in the following two coupled equations:

\[
\psi_{\text{real}}^{k+1}(m, n, l) = \psi_{\text{real}}^k(m, n, l) + \frac{\Delta t}{\hbar} V(m, n, l) \psi_{\text{imag}}^{k+1/2}(m, n, l)
\]

\[
- \frac{\hbar}{2m} \frac{\Delta t}{(\Delta x)^2} \left[ \psi_{\text{imag}}^{k+1/2}(m + 1, n, l) + \psi_{\text{imag}}^{k+1/2}(m - 1, n, l) + \psi_{\text{imag}}^{k+1/2}(m, n + 1, l) + \psi_{\text{imag}}^{k+1/2}(m, n - 1, l) + \psi_{\text{imag}}^{k+1/2}(m, n, l + 1) + \psi_{\text{imag}}^{k+1/2}(m, n, l - 1) - 6 \psi_{\text{imag}}^{k+1/2}(m, n, l) \right],
\]  

(4a)

\[
\psi_{\text{imag}}^{k+1/2}(m, n, l) = \psi_{\text{imag}}^{k+1/2}(m, n, l) - \frac{\Delta t}{\hbar} V(m, n, l) \psi_{\text{real}}^{k+1}(m, n, l)
\]

\[
+ \frac{\hbar}{2m} \frac{\Delta t}{(\Delta x)^2} \left[ \psi_{\text{real}}^{k+1}(m + 1, n, l) + \psi_{\text{real}}^{k+1}(m - 1, n, l) + \psi_{\text{real}}^{k+1}(m, n + 1, l) + \psi_{\text{real}}^{k+1}(m, n - 1, l) + \psi_{\text{real}}^{k+1}(m, n, l + 1) + \psi_{\text{real}}^{k+1}(m, n, l - 1) - 6 \psi_{\text{real}}^{k+1}(m, n, l) \right].
\]  

(4b)

In Eq 4 integer indices \( m, n, l \) representing the positions in a matrix have replaced the Cartesian coordinates \( x, y, z \), respectively, in Eq 3. Similarly, the time step \( k \) has replaced \( t \). Once the cell size \( \Delta x \) is chosen, the time step \( \Delta t \) must also be chosen so the constants preceding the spatial Laplacian are small enough to maintain stability [21]. The alternate iteration of the real and

PLOS ONE | DOI:10.1371/journal.pone.0153802 April 28, 2016 2/11
imaginary Eq (4a) and (4b) simulates the behavior of the waveform propagating in time. Details are available in the literature [11–15]. It is also necessary to be able to absorb outgoing waveforms to prevent them from being reflected back into the problem space and interfering with the simulation. This is accomplished with a perfectly matched layer (PML) [22]. The PML effectively adds artificial impedance between the real and imaginary parts of the waveform. The PML being used is based on Zheng [23] as described in a previous paper [24], so details will not be repeated here.

Fig 1 illustrates the quantum wires to be simulated. The aspect ratio is at least ten to one, so we will use a length of 100 Angstroms, and a diameter of 10 Angstroms or less. We assume that the inside of the wire is at zero potential and the background medium is 4.6 eV corresponding to the work function of silver. Fig 2 illustrates the problem space being used to simulate quantum wires. Normally, the potential of a quantum structure is specified by setting the $V$ parameter in Eq 4a and 4b) to the potential corresponding to the location in the structure being simulated. As an example, the cross-section of a quantum wire of radius 5 Angstroms using cells of one Angstrom might appear as shown in Fig 3A. The red indicates the inside of the wire which is at zero potential, while the green indicates the surrounding potential at $V = 4.6$ eV. Grey represents the PML. Borrowing from a method developed for electromagnetic simulation [25], a more accurate representation of the boundaries can be achieved by averaging the fraction of each material that is in a cell and assigning the value of potential accordingly. The results are shown in Fig 3B.
Determining the Eigenenergies and Eigenfunctions

The FDTD method can be used to determine the eigenenergies and eigenstates of a potential that does not otherwise lend itself to an analytic solution. Any quantum wave function in a given quantum system can be written in the following manner,

$$\psi(r, t) = \sum_{n=0}^{N} \phi_n(r) e^{-i\epsilon_n t / \hbar}, \quad (5)$$

where the $\phi_n(r)$ are the eigenfunctions of the system and the $\epsilon_n$ are the corresponding eigenenergies [11]. We can write the state variable in this fashion even if we do not know the eigenfunctions and eigenenergies.

The eigenenergies can be determined by monitoring the time-domain data at one point in the problems space, say $r_0$, and then taking the Fourier transform,

$$\mathcal{F}\{\psi(r_0, t)\} = \int_{-\infty}^{\infty} dt \left[ \sum_{n=0}^{N} \phi_n(r_0) e^{-i\epsilon_n t / \hbar} \right] e^{i\omega t} = \sum_{n=0}^{N} \phi_n(r_0) \delta \left( \omega - \frac{\epsilon_n}{\hbar} \right). \quad (6)$$

The last step results from the following Equations:

$$\int_{-\infty}^{\infty} e^{-i(\epsilon_n - \epsilon_m) t} dt = \begin{cases} 1 & n = m \\ 0 & n \neq m \end{cases} \quad (7)$$

**Fig 3. Illustration of the difference between the two methods of specifying the potential.** Green represents a potential of 4.6 eV while red represents zero potential. The shades of orange represent weighted averages between the two. (a) The “in or out” method; (b) Averaging method.

doi:10.1371/journal.pone.0153802.g003
The above transform produces a series of delta functions in the frequency domain corresponding to the eigenenergies.

The simulation starts by initializing a test function in the potential, as shown in Fig 4. The test function is a narrow Gaussian pulse. It chosen to ensure that it contains all the eigenfunctions of the structure being analysed. As the time-domain simulation proceeds, the pulse spreads out, some of it being absorbed by the PML. However, most of the waveform remains in the wire. During the simulation, the time-domain data at the original source point is saved. All the waveform simulations in this paper are in three dimensions. Since only two dimensions are displayed, we show the middle of the problems space in the $y$ direction.

After 100,000 iterations, the program is halted. The stored time-domain data is shown in Fig 5(A), and the Fourier transform of this data is shown in Fig 5(B). The first two eigenenergies appear at 0.6378 and 0.6488.

Fig 4. A test function is initialized in the problems space. As the FDTD simulation proceeds, the waveform spreads out.

doi:10.1371/journal.pone.0153802.g004
In order to verify the accuracy of the FDTD technique, an analytic method based on Bessel functions has been developed and is described in S1 Appendix of this paper. Table 1 shows a comparison of the FDTD determination of the ground state energies of the quantum wire of Fig 1 for various radii versus the Bessel function method. The results are also graphed in Fig 6.

To determine the eigenfunction $\phi_m(r)$ corresponding to an eigenenergy $\epsilon_m$, we take the discrete Fourier transform of the state variable at the frequency $\omega_m = \epsilon_m / \hbar$ at every point in the problems space:

$$DFT\{\psi(r, t)\}_{\omega=\epsilon_m/\hbar} = \int_{-\infty}^{\infty} dt \left[ \sum_{n=0}^{N} \phi_n(r) e^{-i(\epsilon_n/\hbar)t} \right] e^{i(\epsilon_m/\hbar)t}$$

$$= \int_{-\infty}^{\infty} dt \left[ \sum_{n=0}^{N} \phi_n(r) e^{-i(\epsilon_n-\epsilon_m)/\hbar t} \right] = \phi_m(r).$$

Table 1. Ground state energies for the cylindrical wire illustrated in Fig 1 for various radii as determined by the FDTD method and the Bessel function method.

| Radius (A) | FDTD (eV) | Bessel (eV) | Difference (%) |
|------------|-----------|------------|----------------|
| 5.0        | 0.6378    | 0.6297     | 1.3            |
| 4.5        | 0.7504    | 0.7489     | 0.8            |
| 4.0        | 0.9207    | 0.9051     | 1.7            |
| 3.5        | 1.1135    | 1.1148     | -1.2           |
| 3.0        | 1.4315    | 1.4041     | 1.9            |
| 2.5        | 1.7983    | 1.8151     | -0.9           |
| 2.0        | 2.4590    | 2.4131     | 1.9            |
| 1.5        | 3.2131    | 3.2734     | -1.8           |
| 1.0        | 4.3439    | 4.2797     | 1.5            |

doi:10.1371/journal.pone.0153802.t001

doi:10.1371/journal.pone.0153802.g005

doi:10.1371/journal.pone.0153802.g006

Fig 5. (a) The stored time-domain data; (b) the Fourier transform. Frequency has been converted to energy.
To construct the ground state eigenfunction at \( \varepsilon_0 = 0.6378 \text{ eV} \) the original test function is initialized in the problem space as in Fig 4. However, as the simulation proceeds, the discrete Fourier transform at the frequency corresponding to 0.6378 eV is taken at every cell in the problem space. The process is repeated for the second eigenstate at 0.6488 eV. The results are shown in Fig 7.

![Fig 6. Comparison of the FDTD method vs. Bessel function in calculating ground state energies of the 100 Angstrom cylinder as a function of the radius of the cylinder.](doi:10.1371/journal.pone.0153802.g006)

![Fig 7. The first two eigenfunctions corresponding to the first two eigenenergies for the cylinder of Fig 1 with a radius of 5 Angstroms. (a) 1st eigenstate at 0.6378 eV; 2nd eigenstate at 0.6488 eV.](doi:10.1371/journal.pone.0153802.g007)
Other Wire Configurations

In the previous section the simulation examples used simple cylinders to establish the accuracy by comparison with an analytic solution. The true strength of the FDTD method is that it can be used on a potential that is not necessarily a simple, regular structure. Two examples are given in this section.

By adding short cylinders perpendicular to the main cylinder, it may be possible to substantially increase the hyperpolarization of the system [6]. One possible configuration is illustrated in Fig 8(A), where a small cylinder seven Angstroms long was added to the main cylinder. Fig 8(B) shows the corresponding problem space. Fig 8C illustrates the corresponding ground state eigenfunction.

Another example is shown in Fig 9(A) where the cylinder is tapered slightly in the middle. The tapering has been proposed as a method of controlling transport in nanowire MOSFETs (metal oxide semiconductor, field effect transistors.) [2].

Conclusion

We have shown that the FDTD method can be used to determine the eigenenergies and eigenfunctions of quantum wires on size scales that are of interest to nanotechnologists. We have applied the FDTD method to solve the simple cylinder, which has analytic solutions in the
form of Bessel functions. The two methods give eigenenergies that are accurate to better than two percent. Comparisons with other methods were not made. The more complex structures that we have calculated here cannot be tested against analytic solutions. However, given that they are made of merged cylinders, we expect that the accuracy will be comparable.

The simulations described in this paper were done on an HP DL140 with eight cores, a high end workstation, and does not represent extraordinary computational resources. A typical simulation to determine the eigenenergy and eigenfunction requires about 40 seconds. Note that these simulations require no assumptions about the shape of the object, so computational speeds are not affected by the shape.

Future projects include simulating multiple particles in a quantum wire. The FDTD method has already been shown to be capable of simulating two particles in a quantum dot [26].

**Supporting Information**

S1 Appendix. Bessel Function Determination of Eigenenergies of a Cylindrical Wire. (DOC)

**Acknowledgments**

SM and MGK acknowledge the generous support of the National Science Foundation, Grant ECCS-1128076.
Author Contributions
Analyzed the data: DMS SM MGK. Wrote the paper: DMS SM MGK.

References
1. Neophytou N, Paul A, Lundstrom MS, Klimeck G. Bandstructure effects in silicon nanowire electron transport. IEEE Trans. Electron Devices 2008; 55: 1286–1297. doi: 10.1109/TED.2008.920233
2. Kim R, Ludstrom M. Characteristic features of 1-D ballistic transport in nanowire MOSFETs. IEEE Trans. Nanotech. 2008; 7: 787–794. doi: 10.1109/TNANO.2008.920196
3. Afzalian A, Lee C, Akhavan ND, Yan R, Ferain I, Colinge J. Quantum confinement effects in capacitance behavior of multigate silicon nanowire MOSFETs. IEEE Trans. Nanotech, 2011; 10: 2. doi: 10.1109/TNANO/2009.2039800
4. Yin Z, Wu J, Zang J, Kong D, Qiu J, Shi J, et al. All-optical Logic gate for XOR operation between 40-Gbaud QPSK tributaries in an ultra-short silicon nanowire. IEEE Photonics J. 2014; 6: 3. doi: 10.1109/JPHOT.2014.2319101
5. Belkin A, Belkin M, Vakaryuk V, Khlebnikov A, Bezrydin A. Formation of quantum phase slip pairs in superconducting nanowires. Phys. Rev. X 2015; 5: 021023. doi: 10.1103/PhysRevX.5.021023
6. Lytel R, Mossman SM, Kuzyk MG. Phase disruption as a new design paradigm for optimizing the non-linear-optical response. Optics Letters 2015; 40: 20. doi: 10.1364/OL.40.004735
7. Yu Y, Zhu S, Guo XX. Electron-phonon interaction effect on optical absorption in cylindrical quantum wires. Solid State Communication 2006; 139: 76–79. doi: 10.1016/j.ssc.2006.04.009
8. Wang G, Guo G. Third-harmonic generation in cylindrical parabolic quantum wires with static magnetic fields. Physica B 2008; 403: 37–43. doi: 10.1016/j.physb.2007.08.003
9. Wang G. Third-harmonic generation in cylindrical parabolic quantum wires with an applied electric field. Phys. Rev. B 2008; 72: 15532. doi: 10.1103/PhysRevB.72.155323
10. Sercel PC, Vahala KJ. Polarization dependence of optical absorption and emission in quantum wires. Phys. Rev. B 1991; 44: 5681. doi: 10.1103/PhysRevB.44.5681
11. Sullivan DM, Citrin DS. Determination of the eigenfunctions of arbitrary nanostructures using time domain simulation. J. Applied Physics 2002; 91: 3219–3226. doi: 10.1063/1.1445277
12. Sullivan DM, Citrin DS. Determining quantum eigenfunctions in three-dimensional nanoscale structures. J. Applied Physics 2005; 97: 104305. doi: 10.1063/1.1896437
13. Soriano A, Navarro EA, Porti JA, Such V. Analysis of the finite difference time domain technique to solve the Schrödinger equation for quantum devices. J. Applied Physics 2004; 95: 8011–8018. doi: 10.1063/1.1753661
14. Ren GB, Rorison JM. Eigenvalue problem of the Schroedinger equations via the finite-difference time-domain method. Phys. Rev. E (2004) 69, 036705. doi: 10.1103/PhysRevE.69.036705
15. Sullivan DM. Quantum Mechanics for Electrical Engineers. IEEE Press; 2012.
16. Kuzyk M, Watkins DS. The effects of geometry on the hyperpolarizability. J. Chem. Phys. 2006; 124: 244104. doi: 10.1063/1.2205859 PMID: 16821970
17. Zhou J, Kuzyk M, Watkins DS. Pushing the hyperpolarizability to the limit. Optics Letters 2006; 31: 2891. doi: 10.1364/OL.31.002891 PMID: 16969413
18. Zhou J, Szafrug UB, Watkins DS, Kuzyk MG. Optimizing potential energy functions for maximal intrinsic hyperpolarizability. Phys. Rev. A 2007; 76: 05381. doi: 10.1103/PhysRevA.76.05383
19. Burke CJ, Atherton TL, Lesnfsk J, Petschek RG. Optimizing the second hyperpolarizability with minimally parametrized potentials, J. Optical Society of America B 2013; 30: 1438–1445. doi: 10.1364/JOSAB.30.001438
20. Atherton TJ, Lesnfsky J, Wigger GA, Petschek RG. Maximizing the hyperpolarizability poorly determines the potential, J. Optical Society of America B 2012; 29: 513–520. doi: 10.1364/JOSAB.29.000513
21. Dai W, Li G, Nassar R, Su S. On the stability of the FDTD method for solving a time-dependent Schrödinger Equation. Numerical Methods for Partial Differential Equations 2006; 21: 1140–1154. doi: 10.1002/num.20082
22. Berenger JP. A perfectly matched layer for the absorption of electromagnetic waves. J. Comput. Phys. 1994; 114: 185–200. doi: 10.1006/jcph.1994.1159
23. Zheng C. A perfectly matched layer approach to the nonlinear Schrödinger wave equations. J. Compt. Phys. 2007; 227: 537–556. doi: 10.1016/j.jcp.2007.08.004
24. Sullivan DM, Wilson PM. Time-domain determination of transmission in quantum nanostructures. J. Applied Physics 2012; 112: 064325. doi:10.1063/1.4754812
25. Sullivan DM. Electromagnetic simulation using the FDTD method. 2nd Ed. IEEE Press; 2013.
26. Sullivan DM, Citrin DS. Time-domain simulation of two electrons in a quantum dot. J. Applied Physics 2001; 89: 3841–3846. doi:10.1063/1.1352559