Efficient Modelling of Quantum Nanostructures

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***Abstract*- Calculation of the higher order modes for the Time Dependent Schrödinger's equation (TDSE). The Imaginary Time Propagation (ITP) method is used to solve the TDSE where this reduces the computational effort required to solve the TDSE. Also using the adjoint variable method the energy level sensitivity for higher order modes has been calculated for the same simulation.**

I. Introduction

The description of the dynamics for the non-relativistic quantum system is done using the Schrödinger's equation where one needs to solve a differential equation specifying the boundary conditions and calculating the energy levels and the wave functions of the system.

Imaginary Time Propagation Method (ITP) [1] is used to solve the time dependent Schrodinger equation (TDSE). This approach is mainly useful to solve the quantum structure with 3D Hamiltonian which may require beyond the available computational sources. The ITP method is shown to be a good candidate for this type of problem as it is a fast method to obtain the wave function and the energy levels.

The ITP method is only utilized in extracting the fundamental model for the TDSE. We propose a novel approach where we succeeded to calculate both the wave functions and the energy levels of the higher order modes.

Accurate modeling of the quantum structures is of great importance. In addition, sensitivity analysis has an important role, especially in tolerance and yield analyses. Sensitivity analysis of the wavefunctions and energy level with respect to all the design parameters is important in analyzing any optical quantum structure. This sensitivity is essential to calculate the sensitivity of many essential parameters such as the gain in quantum lasers, and the absorption in quantum photodetectors. One of the direct known methods in calculating this sensitivity is based on using the perturbation approach using central finite difference method (CFD). This technique is an accurate approach but requires high computational effort as it solves the eigen value problem 2N times where N is the number of the tested design parameters. The Adjoint Variable Method (AVM) can be applied on these types of problems to reduce the computational cost [2], [3].

In this work, we propose an efficient approach to estimate the wavefunctions and energy levels for all the states in quantum structures using the ITP method propose the methodology. In addition, we also present an efficient technique to obtain the sensitivity of the wavefunctions and energy levels based on the AVM.

II. Theoretical Analysis and Methodology

The general form of the TDSE can be written as shown below

$$\boldsymbol{H}\left|\psi(\mathrm{t})\right\rangle = j\hbar\frac{d}{dt}\left|\psi(\mathrm{t})\right\rangle \tag{1}$$

where ψ is the wave function. $\boldsymbol{H}$ is the Hamiltonian matrix and $\hbar$ is plank's constant. This equation can be solved numerically using various approach. Caley's approximation is considered as one of the most suitable approaches due to its second order accuracy and its unconditional stability. Using this approach (1) can be written as

$$\left|\psi(\mathrm{t}+\Delta\mathrm{t})\right\rangle = \left(\frac{1-\frac{j\boldsymbol{H}}{\hbar}\Delta t}{1+\frac{j\boldsymbol{H}}{\hbar}\Delta t}\right)\left|\psi(\mathrm{t})\right\rangle \tag{2}$$

where Δt is the time step. The system of equations in (2) can be solved in the form of system equation written as

$$\boldsymbol{A}_n\psi_{n+1} = \boldsymbol{B}_n\psi_n \tag{3}$$

where n is the order of time step. This system of equations can be solved iteratively at each time step. In the ITP method, the transformation of $-jt = \tau$ is utilized for the time steps. Finite difference discretization is utilized for the system in (3). The time evolution of the wave using this approach can be described as

$$\psi(x,y,\tau) = \Sigma g_i e^{\frac{-\tau E_i}{\hbar}}\varphi_i \tag{4}$$

where φ_i is the wave function of *i th* eigen function and E_i is the energy level associated with this eigenfunctiion. ψ is the total wavefunction at any time instant. The coefficient of the eigenfunction is given by

$$g_i = \frac{\iint_{x,y}\varphi_i(x,y)\psi_{ex}(x,y)\,\mathrm{dxdy}}{\iint_{x,y}\varphi_i^T(x,y)\varphi_i(x,y)\,\mathrm{dxdy}} \tag{5}$$

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where ψ_{ex} is initial excitation of the ITP and $\psi_{ex} = \psi(x, y, \tau)$ .Therefore after propagation with time, the wavefunction which has the smallest energy level will dominate. Initially, the state that will be dominating is the ground state function. Extracting higher order modes can be done by subtracting the fundamental mode previously calculated from the initial excitation and then repeating the simulation with excitation excluding the fundamental mode.

$$\psi_{i+1} = \psi_{ex} - \sum_i g_i \varphi_i \tag{6}$$

To calculate the energy levels, (4) can be utilized to obtain the following expression

$$\ln\left|\phi_{n+1}(x,y)\right\rangle = -\frac{\tau E_i}{\hbar} \ln\left|\phi_n(x,y)\right\rangle \tag{7}$$

By integration, we get

$$E = -\frac{\hbar}{\tau} \frac{\ln\left\langle\phi_{n+1}(x,y)\middle|\phi_{n+1}(x,y)\right\rangle}{\ln\left\langle\phi_{n+1}(x,y)\middle|\psi(x,y)\right\rangle} \tag{8}$$

Sensitivity of the energy levels with respect to the *s*th design parameters can be obtained as [3].

$$\left\langle \frac{\partial E_i}{\partial p_s} \right\rangle = \frac{\left\langle \varphi_i \middle| \frac{\partial \boldsymbol{H}}{\partial p_j} \middle| \varphi_i \right\rangle}{\left\langle \varphi_i \middle| \varphi_i \right\rangle} \times \frac{4\,jm}{\hbar \Delta t} \tag{9}$$

III. NUMERICAL EXAMPLES

The quantum wire in this example is a rectangle shape as shown in Fig.1 where the domain dimensions are X and Y and the dimensions of the rectangle shape is l and w. The energy level of the wire is noted as E in eV. The quantum wire in this example is a rectangular with dimensions l × w = 3×6 nm with a height of E= 0.2 eV. The simulation parameters in this case has a spatial step size of Δx = Δy =0.1 nm and $\Delta t = 20\times10^{-18}$ s and 8000 iterations were done to extract the fundamental mode and 4000 iterations were done to extract the 1st order mode. The excitation in this case is done with also done using a summation of a symmetric and anti-symmetric Gaussian pulse. The Fundamental mode is shown in Fig.2 and the 1st order mode is shown in Fig.3. To get the third order mode the excitation is a gaussian wavelet with 8000 iteration for the fundamental mode and 2200 iteration for the 2nd order mode with dt= $\Delta t = 8\times10^{-18}$ s. E_0=0.03267 eV, E_1=0.05625 eV and E_2=0.09492 eV which agree with the values calculated from the Time Independent Schrödinger's Equation (TISE). Another example of a square wire is also abanlayzed with same accuracy in getting the wavefunctions and energy level. In this example, the energy level (eigen value) sensitivity with respect to the voltage barrier height for a square wire is calculated for both the fundamental mode and 1st order mode are shown in Figures 3 and 4 respectively. The wire's dimensions is 3×3 nm. A sweep on the energy barrier is done from 0.2 eV to 0.7 eV. The AVM results shown are compared to the CFD results and the results calculated from TISE and show identical values.

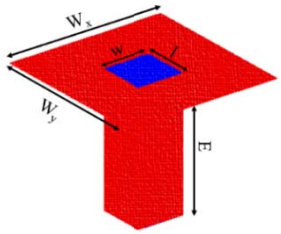

Fig.1. 2D Finite Quantum Wire

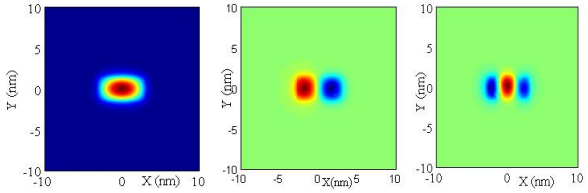

Fig.2.Wave Functions from TDSE using ITP

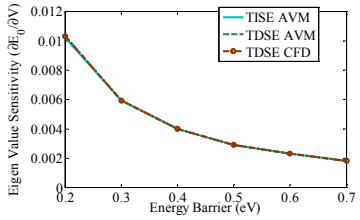

Fig.3. Energy level sensitivity $\partial E_0/\partial V$

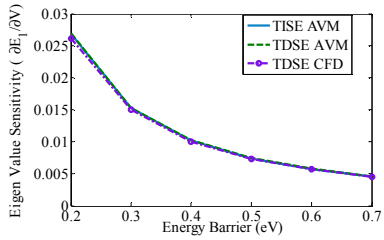

Fig.4. Energy level sensitivity $\partial E_1/\partial V$

IV. CONCLUSION

Higher order modes were calculated using a novel approach for the ITP method. The energy level sensitivity of the fundamental and higher order modes are presented as an example to our approach. Similarly the wave function (eigen vector) sensitivity can be calculated.

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