Including Quantum Effects in Electromagnetic System--An FDTD Solution to Maxwell-Schrödinger Equations

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Abstract — **In this paper a novel approach to include quantum effects, described by Schrödinger equation in tempo and spatial domains, into electromagnetic system analysis, which uses an extended finite-difference time-domain (FDTD) technique to solve the Maxwell's equations. An iterative numerical scheme that marches in time provides a complete solution that describes the interactions between electromagnetic field and electron movement under quantum effects. An example is given to include electron tunneling current through a potential barrier and the good agreement between the extended FDTD method and the analytical solution proves its accuracy. This technique is expected to become an important tool analyzing nano-scale circuit.**

Index Terms — **Maxwell's equations, Schrödinger's equation, FDTD solution, nano circuit, quantum effects, tunneling current.**

I. Introduction

Rapid technology development in material, semiconductor and electronic industry has prompted demand for new analysis technique for electrical circuitry in nano-scale where quantum effects have to be considered. As the device dimension shrinks further down to nanometer sized structure, the quantum effects should be included into system analysis. In certain cases, like in a quantum-dot (QD) configuration, the quantum effects are dominant [1] and this requires new mathematical approach to analyze such devices. Transistors in the size of tens of nanometer (FinFET) and other single-electron transistor (SET) devices have been reported and studied, mostly by experimental measurement [2,3]. The stipulation for a complete theoretical analysis and corresponding numerical scheme that can include all physical interactions is forthcoming and would be playing an important role in future nano-scale circuit design and analysis.

Maxwell's equations are the fundamental governing principles for electromagnetic interaction and they are valid in both macro- and microscopic scale [4]. There are many techniques for solving the equations, both in frequency and time domain, recently many work are reported using FDTD method [5]. Electronic devices perform their designed functions by various ways of charged carrier movement and those charged particles become "quantum" when the physical sizes are reduced to nano-scale, leading to the need of Schrödinger equation, the governing equation for quantum mechanics. To provide a complete description of an electromagnetic system that includes quantum effects and interactions between the charged particles and the electromagnetic fields, one has to combine both sets of equations and solve them simultaneously.

Mathematically, Maxwell's equations and Schrödinger's equation are time- and spatial-domain differential equations and they can be solved numerically using different kinds of numerical schemes, yet a consistent numerical method that can combine the two sets of equations for nano-scale analysis has not been reported. Poisson-Schrödinger problem has been reported to discuss a static solution that includes quantum effects inside an electric system [6,7]. Such approaches are not adequate for dynamic system, especially when considering a complete system that could include other circuit elements.

In this paper, Maxwell's equations are solved with extension to include additional current [8,9], and Schrödinger equation is solved by a similar finite-difference scheme. Both equation sets are coupled by the current that is generated by the carrier movement and it is related to the electromagnetic field and wave function corresponding to the carriers.

II. Combining Maxwell's Equations for Electromagnetic System and Quantum Effects Described by Schrödinger Equation

The well-known Maxwell equations, listed below, describe the behaviors of electromagnetic system or circuit in time and spatial domains:

$$\nabla \times \vec{E} = -\mu \frac{\partial \vec{H}}{\partial t} \tag{1.a}$$

$$\nabla \times \vec{H} = \varepsilon \frac{\partial \vec{E}}{\partial t} + \sigma \vec{E} + \vec{J}_s \tag{1.b}$$

The extra current term, $\vec{J}_s$, in (1.b) could be from other current-contributing elements and its inclusion provides flexibility to many FDTD analyses of hybrid system as discussed in details in [10].

Schrödinger equation, which is in both time and spatial domains as well, is the governing equation for system's quantum effects,

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(\vec{r},t)}{\partial^2 \vec{r}} + U(\vec{r},t)\Psi(\vec{r},t) = i\hbar \frac{\partial \Psi(\vec{r},t)}{\partial t} \tag{2}$$

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Introducing filed vector potential $\mathbf{A}$, which relates to electrical and magnetic fields equations $\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} - \nabla \cdot \Phi$ and $\vec{H} = \nabla \times \vec{A} / \mu_0$, Schrödinger equation can be expressed as

$$i\hbar \frac{\partial \Psi}{\partial t} = [-\frac{\hbar^2}{2m}\Delta + \frac{i\hbar q}{mc}\nabla \cdot \vec{A} + \frac{q^2}{2mc^2}\vec{A}^2 + q\Phi]\Psi \quad (3)$$

Since the probability of finding an electron at location $\vec{r}$ is proportional to $|\Psi(\vec{r})|^2$, we could use $e|\Psi(\vec{r})|^2$ and $\vec{j}|\Psi(\vec{r})|^2$ to represent the charge density and current density, respectively.

Current $\vec{J}_s$ is due to the current density of electron movement and by definition it can be expressed as:

$$\vec{J}_S = e\vec{j} = e\hat{v}|\Psi|^2 = \frac{e|\Psi|^2}{m}(-i\hbar\nabla - \frac{e}{c}\vec{A}) \quad (4)$$

where e is the electron charge, Φ is the electrical potential, $\vec{j}$ is electron probability density and Ψ is the wave function solved from (3).

Once the wave-function is solved from (3), and both $\mathbf{A}$ and Φ are calculated (see equations below), current density $\vec{J}_s$ can then be calculated from (4), thus realizing the coupling between electromagnetic field in (1) and the quantum effects in (3). Based on the interactions of these physical quantities: *E, H, J_s, A, Φ, Ψ*, we can solve them alternately in the time domain on a special grid, therefore providing a complete time-domain solution to the electromagnetic fields and associated current. In this paper, second-order finite differential method is utilized to solve the Maxwell-Schrödinger equations and their numerical solutions provide a complete analysis of the electromagnetic system that includes quantum effects.

III. FDTD NUMERICAL SCHEME

To obtain FDTD formulae for Maxwell and Schrödinger equations, all the equations, (1) and (3), are discretized in both time and space. As commonly used in FDTD solution to Maxwell equations, Yee cell is employed to describe the physical quantities of each node and all the involved variables are shown in the Figure 1.

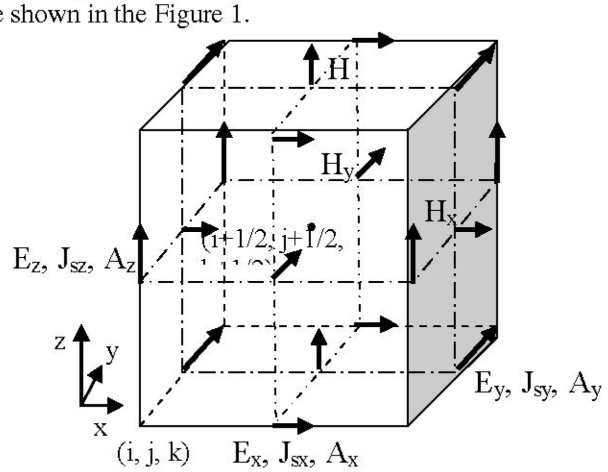

Figure 1. A Yee cell with all the variable locations.

When $m=(i,j+ ½,k+ ½)$, $(i+ ½,j,k+ ½)$, $(i+ ½,j+ ½,k)$, respectively, and $CQ(m) = \frac{\Delta t}{\mu(m)}$, the FDTD discretization of magnetic field components are:

$$H_x^{n+\frac{1}{2}}(m) = H_x^{n-\frac{1}{2}}(m) - CQ(m)\cdot[\frac{E_z^n(i,j+1,k+\frac{1}{2}) - E_z^n(i,j,k+\frac{1}{2})}{\Delta y} - \frac{E_y^n(i,j+\frac{1}{2},k+1) - E_y^n(i,j+\frac{1}{2},k)}{\Delta z}] \quad (5.a)$$

$$H_y^{n+\frac{1}{2}}(m) = H_y^{n-\frac{1}{2}}(m) - CQ(m)\cdot[\frac{E_x^n(i+\frac{1}{2},j,k+1) - E_x^n(i+\frac{1}{2},j,k)}{\Delta z} - \frac{E_z^n(i+1,j,k+\frac{1}{2}) - E_z^n(i,j,k+\frac{1}{2})}{\Delta x}] \quad (5.b)$$

$$H_z^{n+\frac{1}{2}}(m) = H_z^{n-\frac{1}{2}}(m) - CQ(m)\cdot[\frac{E_y^n(i+1,j+\frac{1}{2},k) - E_y^n(i,j+\frac{1}{2},k)}{\Delta x} - \frac{E_x^n(i+\frac{1}{2},j+1,k) - E_x^n(i+\frac{1}{2},j,k)}{\Delta y}] \quad (5.c)$$

When $m=(i+½,j,k)$, $(i,j+½,k)$, $(i,j,k+½)$, respectively, and

$$CA(m) = \frac{1 - \frac{\sigma(m)\Delta t}{2\varepsilon(m)}}{1 + \frac{\sigma(m)\Delta t}{2\varepsilon(m)}} \quad CB(m) = \frac{\frac{\Delta t}{\varepsilon(m)}}{1 + \frac{\sigma(m)\Delta t}{2\varepsilon(m)}}$$

$$E_x^{n+1}(m) = CA(m)E_x^n(m) - CB(m)\cdot[\frac{H_z^{n+\frac{1}{2}}(i+\frac{1}{2},j+\frac{1}{2},k) - H_z^{n+\frac{1}{2}}(i+\frac{1}{2},j-\frac{1}{2},k)}{\Delta y} - \frac{H_y^{n+\frac{1}{2}}(i+\frac{1}{2},j,k+\frac{1}{2}) - H_y^{n+\frac{1}{2}}(i+\frac{1}{2},j,k-\frac{1}{2})}{\Delta z} - J_{sx}^{n+\frac{1}{2}}(m)] \quad (6.a)$$

$$E_y^{n+1}(m) = CA(m)E_y^n(m) - CB(m)\cdot[\frac{H_x^{n+\frac{1}{2}}(i,j+\frac{1}{2},k+\frac{1}{2}) - H_x^{n+\frac{1}{2}}(i,j+\frac{1}{2},k-\frac{1}{2})}{\Delta z} - \frac{H_z^{n+\frac{1}{2}}(i+\frac{1}{2},j+\frac{1}{2},k) - H_z^{n+\frac{1}{2}}(i-\frac{1}{2},j+\frac{1}{2},k)}{\Delta x} - J_{sy}^{n+\frac{1}{2}}(m)] \quad (6.b)$$

$$E_z^{n+1}(m) = CA(m)E_z^n(m) - CB(m)\cdot[\frac{H_y^{n+\frac{1}{2}}(i+\frac{1}{2},j,k+\frac{1}{2}) - H_y^{n+\frac{1}{2}}(i-\frac{1}{2},j,k+\frac{1}{2})}{\Delta x} - \frac{H_x^{n+\frac{1}{2}}(i,j+\frac{1}{2},k+\frac{1}{2}) - H_x^{n+\frac{1}{2}}(i,j-\frac{1}{2},k+\frac{1}{2})}{\Delta y} - J_{sz}^{n+\frac{1}{2}}(m)] \quad (6.c)$$

For arbitrary (i,j,k), and if $\alpha = \frac{i\hbar\Delta t}{2m}$, $\beta = \frac{2e\Delta t}{mc}$, $\gamma = \frac{2\alpha}{\Delta x^2} + \frac{2\alpha}{\Delta y^2} + \frac{2\alpha}{\Delta z^2}$, $\lambda = \frac{e^2\Delta t}{im\hbar c^2}$, and c is the speed of light, (3) can be discretized as:

$$\Psi^{n+1}(i,j,k)=\alpha[\frac{\Psi^{n}(i+1,j,k)+\Psi^{n}(i-1,j,k)}{\Delta x^{2}}+$$
$$\frac{\Psi^{n}(i,j+1,k)+\Psi^{n}(i,j-1,k)}{\Delta y^{2}}+\frac{\Psi^{n}(i,j,k+1)+\Psi^{n}(i,j,k-1)}{\Delta z^{2}}]-\gamma\Psi^{n}(i,j,k)$$
$$+\{\beta[\frac{A_{x}^{n}(i+\frac{1}{2},j,k)-A_{x}^{n}(i-\frac{1}{2},j,k)}{\Delta x}+\frac{A_{y}^{n}(i,j+\frac{1}{2},k)-A_{y}^{n}(i,j-\frac{1}{2},k)}{\Delta y}+$$
$$\frac{A_{z}^{n}(i,j,k+\frac{1}{2})-A_{z}^{n}(i,j,k-\frac{1}{2})}{\Delta z}]+$$
$$\lambda[(\frac{A_{x}^{n}(i+\frac{1}{2},j,k)+A_{x}^{n}(i-\frac{1}{2},j,k)}{2})^{2}+(\frac{A_{y}^{n}(i,j+\frac{1}{2},k)+A_{y}^{n}(i,j-\frac{1}{2},k)}{2})^{2}$$
$$+(\frac{A_{z}^{n}(i,j,k+\frac{1}{2})+A_{z}^{n}(i,j,k-\frac{1}{2})}{2})^{2}+e\Phi^{n}(\mathrm{i,j,k})]\}\Psi^{n}(i,j,k)+\Psi^{n-1}(i,j,k) \tag{7}$$

For current relation in (4), once the latest electromagnetic field, vector potential and electrical potential and wave function are known, it can be calculated by

$$J_{x}^{n+\frac{1}{2}}(i+\frac{1}{2},j,k)=-\frac{e}{m}\mathrm{Re}[(\frac{\Psi^{n+\frac{1}{2}}(i+1,j,k)+\Psi^{n+\frac{1}{2}}(i,j,k)}{2})^{*}\cdot$$
$$(i\hbar\frac{\Psi^{n+\frac{1}{2}}(i+1,j,k)-\Psi^{n+\frac{1}{2}}(i,j,k)}{\Delta x}+$$
$$\frac{e}{c}A_{x}^{n+\frac{1}{2}}(i+\frac{1}{2},j,k)(\frac{\Psi^{n+\frac{1}{2}}(i+1,j,k)+\Psi^{n+\frac{1}{2}}(i,j,k)}{2}))] \tag{8a}$$

$$J_{y}^{n+\frac{1}{2}}(i,j+\frac{1}{2},k)=-\frac{e}{m}\mathrm{Re}[(\frac{\Psi^{n+\frac{1}{2}}(i,j+1,k)+\Psi^{n+\frac{1}{2}}(i,j,k)}{2})^{*}\cdot$$
$$(i\hbar\frac{\Psi^{n+\frac{1}{2}}(i,j+1,k)-\Psi^{n+\frac{1}{2}}(i,j,k)}{\Delta y}+$$
$$\frac{e}{c}A_{y}^{n+\frac{1}{2}}(i,j+\frac{1}{2},k)(\frac{\Psi^{n+\frac{1}{2}}(i,j+1,k)+\Psi^{n+\frac{1}{2}}(i,j,k)}{2}))] \tag{8b}$$

$$J_{z}^{n+\frac{1}{2}}(i,j,k+\frac{1}{2})=-\frac{e}{m}\mathrm{Re}[(\frac{\Psi^{n+\frac{1}{2}}(i,j,k+1)+\Psi^{n+\frac{1}{2}}(i,j,k)}{2})^{*}\cdot$$
$$(i\hbar\frac{\Psi^{n+\frac{1}{2}}(i,j,k+1)-\Psi^{n+\frac{1}{2}}(i,j,k)}{\Delta z}+$$
$$\frac{e}{c}A_{z}^{n+\frac{1}{2}}(i,j,k+\frac{1}{2})(\frac{\Psi^{n+\frac{1}{2}}(i,j,k+1)+\Psi^{n+\frac{1}{2}}(i,j,k)}{2}))] \tag{8c}$$

where $\Psi^{n+\frac{1}{2}}(i,j,k)=\dfrac{\Psi^{n+1}(i,j,k)+\Psi^{n}(i,j,k)}{2}$.

To ensure stability for FDTD solution of Maxwell's and Schrödinger equations, a time step must satisfy the following requirement

$$\Delta t \le \min(\frac{\delta}{\sqrt{3}c},k\delta^{2}) \tag{9}$$

where c is the speed of light and k is an arbitrary constant. It can be proved that when (9) is satisfied, both Maxwell's and Schrödinger FDTD equations are stable and convergent.

After the above derivation, the new FDTD algorithm to combine numerical solution of Maxwell's and Schrödinger equations into a combined description can be written in the following pseudo coding format:

Start: for $\forall t \in (-\infty,0]$, $\vec{E}=0$, $\vec{H}=0$, $|\Psi|^{2}=1$.

Procedure:

1) assuming $\vec{E}_{ijk}^{n}$, $\vec{H}_{ijk}^{n-1/2}$, Ψ_{ijk}^{n}, Ψ_{ijk}^{n-1} are known from previous steps;

2) updating $\vec{H}_{ijk}^{n+\frac{1}{2}}=F(\vec{E}_{ijk}^{n},\vec{H}_{ijk}^{n-\frac{1}{2}})$ using (5);

3) vector potential $A_{ijk}^{n+1/2}$ can be calculated from the latest $H_{ijk}^{n+1/2}$ from $\vec{H}=\nabla\times\vec{A}/\mu_{0}$;

4) electrical potential $\Phi_{ijk}^{n+1/2}$ is calculated from E_{ijk}^{n}, $A_{ijk}^{n+1/2}$, and $A_{ijk}^{n-1/2}$ from $\vec{E}=-\frac{1}{c}\frac{\partial\vec{A}}{\partial t}-\nabla\cdot\Phi$;

5) updating $\Psi_{ijk}^{n+1}=F(A_{ijk}^{n},\Phi_{ijk}^{n},\Psi_{ijk}^{n},\Psi_{ijk}^{n-1})$ using (7);

6) updating current J_{s} using (8);

7) updating $\vec{E}_{ijk}^{n+1}=F(\vec{E}_{ijk}^{n},\vec{H}_{ijk}^{n+\frac{1}{2}},\vec{J}_{ijk}^{n+\frac{1}{2}})$ using (6);

8) $n=n+1$, go back to Step 1) until finish time.

IV. RESULTS AND DISCUSSIONS

A three-dimensional test case that includes a section of insulator material, in the dimension of 5nmx5nmx1nm in near $0K$ temperature, connected to an external voltage source is computed using the numerical scheme described in this paper. The voltage source is modeled with the equivalent lumped circuit model in [9] and the potential barrier inside the nano-scale material is approximated as a square potential barrier. There are electron stores on both sides of the material, with different Fermi levels, and the tunneling current through the barrier can be calculated by analytical method, as derived in [11]. An exponential ramping voltage is applied to the material and the calculated current is shown in Figure 2.

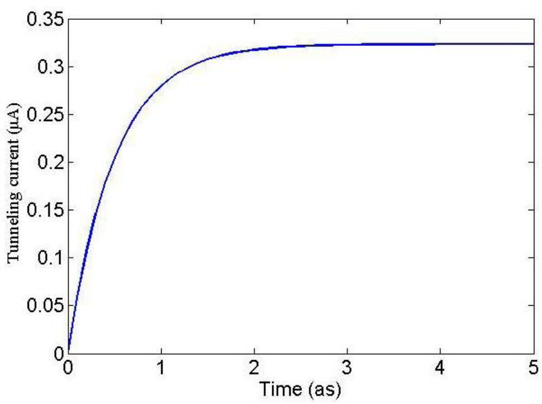

Figure 2. Tunneling current through the potential barrier.

Both analytical and numerical tunneling currents have been calculated, and they agree to each very well. The excellent agreement is a good indicator that the algorithm described in this paper has good numerical accuracy and stability. The stability of the algorithm is guaranteed by the selection of time step Δt in (11) and more detailed discussions on the numerical scheme will be given in future correspondences.

When the potential barrier height between the two electron stores is varied between $3.1eV$ and $4eV$, and the electron energy is $3eV$, the tunneling current is plotted against the variation, as shown in Figure 3.

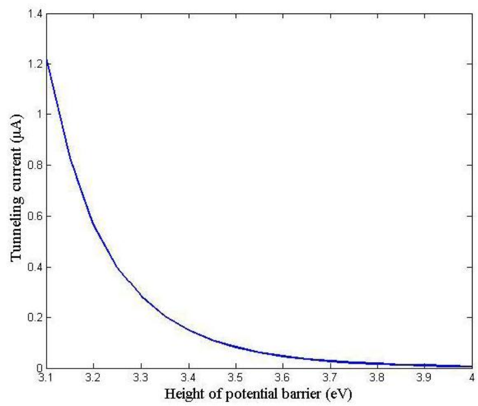

Figure 3. Tunneling current variation with the height of potential barrier.

The iterative FDTD solution to Maxwell and Schrödinger equations can be used to analyze electrodynamic system or circuit that includes quantum effects. Such circuit example could be a GaAs SET that includes a QD and a numerical scheme proposed in this paper would definitely be required when the device circuit model parameters are to be extracted for the purpose of circuit simulation.

The test case used in this paper is relatively simple, but it does show some versatile features of the newly developed numerical approach. The square potential barrier model is a simple approximation to the actual physical state, in order to get an analytical tunneling current solution, and there are other approximations that do not assume the square form [12]. When the configuration of the structure becomes more complicated, it is not possible to get any analytical comparison, in such cases, experimental measurement data have to be obtained.

V. Conclusion

In this paper a novel approach is proposed to include quantum effects in electromagnetic system numerical analysis. The combination of FDTD solutions to Maxwell's and Schrödinger equations in both time and spatial domains leads to the potential for future complete analysis of nano-scale structures and devices where quantum effects can not be ignored. More detailed study of the numerical technique, from mathematical point of view and from practical application side, are expected to perfect this novel approach. Future research work will concentrate on the expansion of the technique to practical nanometer scale circuit analysis.

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