Multiscale and Multiphysics Modeling Techniques for Nanoelectronic Devices

Project hybrid QM/EM modeling: length vs. velocity gauge

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1 Introduction

In this project, you will implement a finite-difference time-domain (FDTD) scheme capable of simulating a system in which both electromagnetic (EM) and quantum mechanical (QM) phenomena occur. To keep the problem tractable, the situation considered here will be one-dimensional (1-D) both electromagnetically and quantum mechanically. Along the way, you are encouraged to get in a scientific state of mind and thoroughly investigate interesting physical situations with different numerical schemes all having their pros and cons.

2 Problem description

A linearly polarized plane wave traveling along the x-axis is incident on two thin sheets parallel to the yz-plane and of infinite extent in the yz-plane. The electric field is directed along the y-axis. Both sheets have a thickness L_x and actually consist of quantum dots located in a uniform, rectangular grid in the y- and z-directions with pitch L_y and L_z respectively. The edges of the sheets, which are parallel to the yz-plane, are modeled as infinite potential barriers. In the y- and z- direction the quantum dots are modeled as 2-D harmonic oscillators and the electrons inside the quantum dot have an effective mass m^* and charge q. A unit cell of the problem setting (for which $|y| \leq L_y/2$) is depicted in Fig. 1. In Appendix A, you can find some suggested starting values for the several parameters encountered in this project.

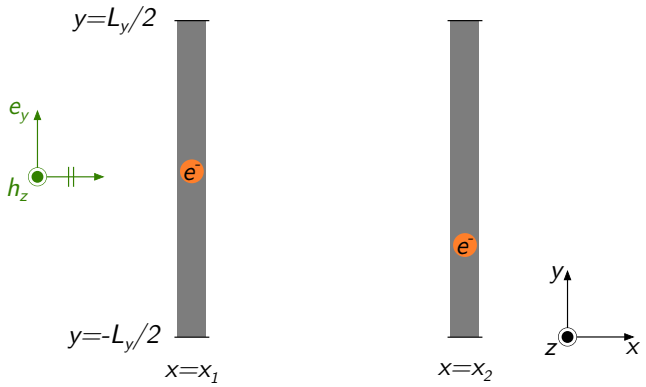

Figure 1: A y-polarized electromagnetic plane wave is incident on two infinite thin sheets made of quantum dots (only one unit cell for which $|y| \leq L_y/2$ is shown).

The problem is now adapted so that both the QM system and the EM system can be treated as 1-D. First, assume that the quantum dots do not interact with each other. The 3-D wave function for one such quantum dot is given by:

$$\psi(x, y, z, t) = \xi(x)\phi(y, t)\chi(z), \tag{1}$$

where it was taken into account that no excitation happens in the x- or z- directions. Hence, $\xi(x)$ and $\chi(z)$ are simply eigenfunctions of a particle-in-a-box and a harmonic oscillator, respectively. The wave function ψ is normalized to contain n non-interacting electrons per quantum dot, i.e.,

$$n = \int_{-L_z/2}^{L_z/2} \int_{-L_y/2}^{L_y/2} \int_{-L_x/2}^{L_x/2} |\xi(x)|^2 |\phi(y, t)|^2 |\chi(z)|^2 \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z \,, \tag{2}$$

and $\phi(y, t)$ is normalized to one. Consequently, $\phi(y, t)$ is modeled as:

$$\jmath\hbar \frac{\partial \phi(y, t)}{\partial t} = (H_0 + H_{\text{int}})\phi(y, t), \tag{3}$$

where

$$H_0 = -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial y^2} + V, \tag{4}$$

$$H_{\text{int}} = \frac{\jmath\hbar q}{2m^*} \left(\boldsymbol{a} \cdot \frac{\partial}{\partial y} \boldsymbol{u}_y + \frac{\partial \boldsymbol{u}_y \cdot \boldsymbol{a}}{\partial y} \right) + \frac{q^2}{2m^*} \boldsymbol{a}^2 + q\varphi, \tag{5}$$

where V represents the harmonic oscillator potential along y and where $\boldsymbol{a}$ and φ are the well-known electromagnetic vector and scalar potential, respectively.

The quantum current density in the nanosheets is given by

$$\boldsymbol{j}_q = \frac{q\hbar}{m^*} \operatorname{Im}\{\psi^* \boldsymbol{\nabla} \psi\} - \frac{q^2}{m} \boldsymbol{a} |\psi|^2 \tag{6}$$

$$= \frac{q\hbar}{m^*} |\xi(x)|^2 |\chi(z)|^2 \operatorname{Im}\left\{ \phi^*(y, t) \frac{\partial \phi(y, t)}{\partial y} \right\} \boldsymbol{u}_y - \frac{q^2}{m^*} |\xi(x)|^2 |\phi(y, t)|^2 |\chi(z)|^2 \boldsymbol{a} \quad [\mathrm{A\,m^{-2}}] \tag{7}$$

and is a source for electromagnetic fields. As the quantum dots are repeated in the y- and z-directions and no current can flow in the x-direction, we average the influence of the quantum current over one quantum dot and assume this is the current density everywhere in the sheet. It is also assumed that the vector potential $\boldsymbol{a}$ is uniform across the nanosheet. This yields:

$$\boldsymbol{j}_q^{1-\mathrm{D}} = \frac{q\hbar N}{m} \int_{-L_y/2}^{L_y/2} \operatorname{Im}\left\{ \phi^* \frac{\partial \phi}{\partial y} \right\} \mathrm{d}y \, \boldsymbol{u}_y - \frac{q^2}{m} N \boldsymbol{a}, \tag{8}$$

where the bulk particle density in the sheet is defined as:

$$N = \frac{n}{L_x L_y L_z} \quad [\text{particles}/\mathrm{m}^3]. \tag{9}$$

As the 1-D quantum current density is uniform in a sheet of infinite extent, the electromagnetic fields generated by it will be plane waves, which are linearly polarized along the y-direction. This justifies, a posteriori, the 1-D interaction Hamiltonian H_{int} of (5).

3 Discretization of the equations

In this section, we derive the necessary FDTD update equations to perform a hybrid QM/EM simulation for the situation described in Section 2 but only for a scalar EM potential.

3.1 1-D Schrödinger equation

The 1-D Schrödinger equation with only a scalar potential is given by:

$$\jmath\hbar\frac{\partial\phi}{\partial t} = -\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial y^2}\phi + V\phi + q\varphi\phi, \tag{10}$$

where we have omitted the explicit dependence on y and t. The resulting FDTD scheme is easily obtained by splitting the equation in its real and imaginary parts, staggering these parts in time and applying second-order accurate central differences to the time derivative and fourth-order accurate central differences to the spatial derivative. This results in:

$$\phi_{\mathrm{Re}}|_j^{n+\frac{1}{2}} = \phi_{\mathrm{Re}}|_j^{n-\frac{1}{2}} - \frac{\hbar\Delta t}{2m^*}\frac{-\phi_{\mathrm{Im}}|_{j-2}^n + 16\phi_{\mathrm{Im}}|_{j-1}^n - 30\phi_{\mathrm{Im}}|_j^n + 16\phi_{\mathrm{Im}}|_{j+1}^n - \phi_{\mathrm{Im}}|_{j+2}^n}{12\Delta y^2} + \frac{\Delta t}{\hbar}\Big(q\varphi|_j^n + V|_j\Big)\phi_{\mathrm{Im}}|_j^n, \tag{11}$$

$$\phi_{\mathrm{Im}}|_j^{n+1} = \phi_{\mathrm{Im}}|_j^n + \frac{\hbar\Delta t}{2m^*}\frac{-\phi_{\mathrm{Re}}|_{j-2}^{n+\frac{1}{2}} + 16\phi_{\mathrm{Re}}|_{j-1}^{n+\frac{1}{2}} - 30\phi_{\mathrm{Re}}|_j^{n+\frac{1}{2}} + 16\phi_{\mathrm{Re}}|_{j+1}^{n+\frac{1}{2}} - \phi_{\mathrm{Re}}|_{j+2}^{n+\frac{1}{2}}}{12\Delta y^2} - \frac{\Delta t}{\hbar}\left(q\varphi|_j^{n+\frac{1}{2}} + V|_j\right)\phi_{\mathrm{Re}}|_j^{n+\frac{1}{2}}. \tag{12}$$

Note that φ is needed at different time-steps for updating ϕ_{Re} and ϕ_{Im}. If the wave function stays sufficiently far away from the boundary of the computational domain, we can use Dirichlet boundary conditions, i.e., $\phi(-L_y/2) = \phi(L_y/2) = 0$.

3.2 1-D electromagnetic fields

Maxwell's curl equations for a plane wave traveling in the x-direction with linear polarization along the y-axis are given by:

$$\epsilon\frac{\partial e_y}{\partial t} = -\frac{\partial h_z}{\partial x} - j_y, \tag{13}$$

$$\mu\frac{\partial h_z}{\partial t} = -\frac{\partial e_y}{\partial x}. \tag{14}$$

Staggering h_z and e_y along the time- and x-axes, and using second-order finite differences for the derivatives, yields:

$$h_z|_{i+\frac{1}{2}}^{n+\frac{1}{2}} = h_z|_{i+\frac{1}{2}}^{n-\frac{1}{2}} - \frac{\Delta t}{\mu\Delta x}\left(e_y|_{i+1}^n - e_y|_i^n\right), \tag{15}$$

$$e_y|_i^{n+1} = e_y|_i^n - \frac{\Delta t}{\epsilon\Delta x}\left(h_z|_{i+\frac{1}{2}}^{n+\frac{1}{2}} - h_z|_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right) - \frac{\Delta t}{\epsilon}j_y|_i^{n+\frac{1}{2}}. \tag{16}$$

To terminate the computational domain, one can use a first-order Sommerfeld Absorbing Boundary Condition (ABC):

$$e_y|_0^{n+1} = e_y|_1^n + \frac{1-S}{1+S}\left(e_y|_0^n - e_y|_1^{n+1}\right), \tag{17}$$

$$e_y|_{n_x}^{n+1} = e_y|_{n_x-1}^n + \frac{1-S}{1+S}\left(e_y|_{n_x}^n - e_y|_{n_x-1}^{n+1}\right), \tag{18}$$

where n_x is the number of cells in the x-direction and $S = c\Delta t/\Delta x$.

3.3 Feedback with quantum current density

Assume a nanoplate is placed at the center $x = i\Delta_x$ of a grid cell of width Δx along the x-axis (with plate thickness $L_x < \Delta x$). To correctly add the 1-D quantum current density defined in Section 2 to Maxwell's equations, we start from Ampère's law in integral representation:

$$\oint_C \boldsymbol{h}\cdot\mathrm{d}\boldsymbol{l} = \epsilon\iint_{\mathcal{S}}\frac{\partial\boldsymbol{e}}{\partial t}\cdot\boldsymbol{u}_n\,\mathrm{d}\mathcal{S} + \iint_{\mathcal{S}}\boldsymbol{j}_q^{1-\mathrm{D}}\cdot\boldsymbol{u}_n\,\mathrm{d}\mathcal{S}, \tag{19}$$

where we integrated over a rectangle $\mathcal{S}$ (with boundary $C = \partial\mathcal{S}$) in the xz-plane centered at $(x, z) = (i\Delta x, 0)$ and with side lengths Δx and L_z. Assuming a linearly polarized plane wave of which the e_y-component does not exhibit spatial variation in $\mathcal{S}$, reduces Ampère's law to:

$$\int_{-L_z/2}^{L_z/2} h_z|_{i-\frac{1}{2}}^{n+\frac{1}{2}}\,\mathrm{d}z + \int_{L_z/2}^{-L_z/2} h_z|_{i+\frac{1}{2}}^{n+\frac{1}{2}}\,\mathrm{d}z = \epsilon L_z \Delta x \frac{e_y|_i^{n+1} - e_y|_i^n}{\Delta t} + L_z \int_{-Lx/2}^{L_x/2} \boldsymbol{j}_q^{1-\mathrm{D}} \cdot \boldsymbol{u}_y\,\mathrm{d}x\,. \tag{20}$$

As the h_z-component does not exhibit z-dependence and the current density is uniform in the nanoplate, this further reduces to:

$$e_y|_i^{n+1} = e_y|_i^n - \frac{\Delta t}{\epsilon \Delta x}\left(h_z|_{i+\frac{1}{2}}^{n+\frac{1}{2}} - h_z|_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right) - \frac{\Delta t L_x}{\epsilon \Delta x}\boldsymbol{j}_q^{1-\mathrm{D}}|_i^{n+\frac{1}{2}} \cdot \boldsymbol{u}_y. \tag{21}$$

Using the midpoint rule (aka rectangle method) for the integration, the quantum current density (8) – without vector potential – is discretized [1] as follows:

$$\boldsymbol{j}_q^{1-\mathrm{D}}|_i^{n+\frac{1}{2}} = \frac{q\hbar N}{2m}\sum_{j=0}^{n_y}\left(\phi_{\mathrm{Re}}|_j^{n+\frac{1}{2}}\left(\phi_{\mathrm{Im}}|_{j+1}^{n+1} + \phi_{\mathrm{Im}}|_{j+1}^{n}\right) - \phi_{\mathrm{Re}}|_{j+1}^{n+\frac{1}{2}}\left(\phi_{\mathrm{Im}}|_j^{n+1} + \phi_{\mathrm{Im}}|_j^{n}\right)\right)\boldsymbol{u}_y. \tag{22}$$

4 Assignment and deadline

1. Perform the following tasks by writing a Python3 program that can execute the required computations:

   (a) Consider a single quantum dot with a harmonic oscillator (HO) potential $V(y) = m^*{\omega_{\mathrm{HO}}}^2 y^2/2$, initialize the electron in a coherent state centered at $y = 0$ (i.e., its ground state) and implement the 4-th order accurate FDTD scheme presented in Section 3.5.2 for the Schrödinger equation in the length (l) gauge (long wavelength approximation). For now, there is no coupling from QM to EM.

   (b) Excite the QM wave function by an electromagnetic plane wave with a temporal profile of a:

   - Gaussian pulse: $e_y = E_0^{(g)} \exp\left((t - t_0)^2/\left(2{\sigma_t}^2\right)\right)$,
   - monochromatic sine wave: $e_y = E_0^{(s)} \sin(\omega_{\mathrm{EM}} t) f(t)$ where $f(t)$ is a ramping function that ensures that the source is turned on smoothly.

   As there is no coupling from QM to EM yet, there is no need to calculate the EM fields induced by the quantum current.

   (c) Compute the expectation value of the position, kinetic momentum and kinetic energy as a function of time. Also check that the wave function satisfies the continuity equation.

   (d) Convert (3) to the velocity (vel) gauge (long wavelength approximation). Construct and implement an FDTD scheme that is still 4th-order accurate in space and with a real and imaginary part of the wave function that are still staggered in time. The new scheme will be implicit, necessitating the inversion of a pentadiagonal matrix in each time step. To do this efficiently, utilise the sparse linear algebra package of scipy: `https://docs.scipy.org/doc/scipy/reference/sparse.linalg.html`. You are free to use a direct solver or an iterative one.

   (e) Repeat steps (b)–(c) for the velocity gauge.

   (f) Consider now a single sheet of quantum dots as described in Section 2. In this case, the QM part of the system couples back to the EM part. Implement the FDTD scheme for the hybrid QM/EM system (with full coupling between EM and QM) as explained in Section 3.5.2 of the syllabus and in Section 3 of this document, but only for a single sheet for now. You can choose to use either the length gauge or the velocity gauge scheme (or both).

   (g) Add the second layer of quantum dots some distance away from the first one.

[1] Make this derivation yourself, as you will need it to check the continuity equation

2. Make sure that the program is easy to use, as it will be tested by us. You can submit multiple python files for the different kinds of simulations or you can write a single program that can perform all of the tasks described above. Please do not waste precious time on making a GUI, instead focus your (coding) efforts on making the program efficient and easy to read.

3. Perform simulations for a single quantum dot (with only forward coupling from EM to QM), a single sheet of quantum dots (with full forward-backward coupling between QM and EM) and two sheets of quantum dots (with full forward-backward coupling between QM and EM). Investigate the behavior of the wave function *and* the EM fields for different parameters (think about interesting simulation set-ups) with an emphasis on the difference between the length and velocity gauges, the difference between coupling and no coupling from QM to EM and the difference between a single sheet and two sheets.

4. Write a (short) report that contains (at least):

   - A derivation of the update scheme in the velocity gauge.
   - A description of how to use your program.
   - A thorough analysis and discussion of the obtained results. Show figures only of your most interesting results and give clear descriptions of the simulation set-up. The results should be easily reproducible by us. Make sure that each graph/figure conveys valuable information. Be creative in how you present your data.

5. Upload your written report (PDF-file) + the Python code(s) via "Ufora-tools: Assignments" before **Wednesday, May 31, 2023 at 11.59pm**.

6. Note that — as always — self-efficacy and engineering spirit are encouraged, with extra marks for creative ideas that focus on the QM/EM modeling aspects of the problem.

Appendix A: Suggested values

parameter	value
L_x	$0.5\,\mathrm{nm}$
L_y	$100\,\mathrm{nm}$
N	$9.0\,\mathrm{nm}^{-3}$
m^*	$0.15\,m_\mathrm{e} = 1.366\,407 \times 10^{-31}\,\mathrm{kg}$
q	$-1.602\,177 \times 10^{-19}\,\mathrm{C}$
ω_HO	$10 \times 10^{12}\,\mathrm{rad\,s^{-1}}$
$E_0^{(g)}$	$5.0 \times 10^{6}\,\mathrm{V\,m^{-1}}$
$E_0^{(s)}$	$1.0 \times 10^{5}\,\mathrm{V\,m^{-1}}$
σ_t	$10.0\,\mathrm{fs}$
t_0	$20.0\,\mathrm{fs}$
ω_EM	$\alpha\omega_\mathrm{HO}$, with $0.9 < \alpha < 1.1$
Δx	$1.0\,\mu\mathrm{m}$
sheet separation	$47.0\,\mu\mathrm{m}$
Δy	$0.5\,\mathrm{nm}$
simulation time	$5\,\mathrm{ps}$

Table 1: Some possible values for several of the parameters.