Quantum–Electromagnetic coupling in time domain simulations using COMSOL Multiphysics®

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Abstract
This work analyzes the transport properties of nanostructures in the ballistic regime under the effect of electromagnetic fields using a coupled Quantum-Electromagnetic solver implemented completely in the COMSOL Multiphysics® environment.

Keywords: Multiphysics simulation, Quantum, EM fields.

Introduction

The coupling of the Schrödinger and Maxwell equations allows to predict the self-generated electromagnetic (EM) field for a quantum charged particle moving in a domain.
Such problem is really challenging, and it must be investigated to simulate the behavior of a particle in an EM field. COMSOL Multiphysics® provide a useful platform for the solution of such a problem thanks to its high versatility and the potentiality to solve custom equation sets.

Theory

The Hamiltonian of a particle moving in an electromagnetic field is provided by eq. (1)

$$H = \frac{(\boldsymbol{p} - q\boldsymbol{A})^2}{2m} + q\phi \tag{1}$$

where $\boldsymbol{A}$ and ϕ are the vector and scalar potentials respectively, derived using the Lorentz Gauge as in eq. (2).

$$\begin{cases} \nabla^2 \boldsymbol{A} - \frac{1}{c^2}\partial_t^2 \boldsymbol{A} = -\mu \boldsymbol{J} \\ \nabla^2 \phi - \frac{1}{c^2}\partial_t^2 \phi = -\frac{\rho}{\varepsilon} \end{cases} \tag{2}$$

From the time-dependent Schrödinger equation it is possible to calculate the quantum charge distribution (ρ) and current density ($\boldsymbol{J}$) defined as follows in eq. (3) and eq. (4).

$$\boldsymbol{J} = q\left[\frac{\hbar}{2im}(\psi^*\nabla\psi - \psi\nabla\psi^*) - \frac{q}{m}|\psi|^2\boldsymbol{A}\right] \tag{3}$$

$$\rho = q|\psi|^2 \tag{4}$$

Methods

The coupling is realized in COMSOL Multiphysics® 6.1 using both the Coefficient Form PDE and the Electromagnetic Waves, Transient interfaces.
The Schrödinger equation has been solved in a 2D domain representing the nanomaterial device (e.g., graphene) while the Electromagnetic field has been solved in a 3D domain including the 2D layer.
The coupling has been achieved by means of a general extrusion mapping of the quantum current calculated from eq. (3) to a surface current density in the Electromagnetic Waves, Transient interface.
To solve the Schrödinger equation without an extremely large domain to prevent boundary reflections, an absorbing region with low reflections is necessary. That condition has been implemented using an imaginary potential defined by eq. (5) as in [1].

$$V = iA\left(\cosh\frac{x}{x_0}\right)^{-2} \tag{5}$$

Simulation Results

The behavior of a gaussian wave packet has been simulated without external electromagnetic field to estimate the self-generated field as shown in Fig. (1).

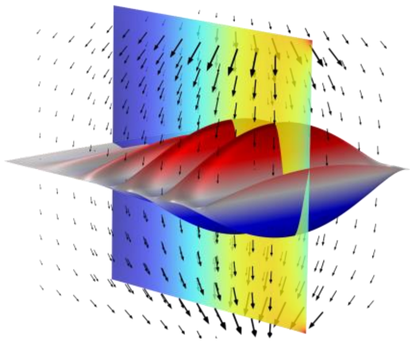

Figure 1. Propagating quantum gaussian wave-packet with self-generated electromagnetic field (black arrows).

Subsequently it has been considered an external constant magnetic field of B_0 = 0.5 T along the y-axis. Such field rotate the direction of the wave packet as expected from classical electrodynamics of a charged particle due to the Lorentz force as shown in Fig. (2).

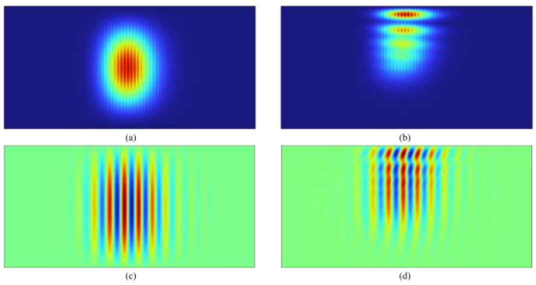

Figure 2. Quantum current density (a) and wave function (c) of a gaussian wave packet propagating with B_0 = 0 T and (b), (d) with B_0 = 0.5 T.

Conclusions

This work presented a quantum–electromagnetic coupling in time domain simulations. This coupling could be of great interest in the simulation of the coherent quantum electric transport especially for ballistic device design and optimization.

In future work this model will be employed in the optimization of device geometry considering coherent quantum transport properties.

References

[1] Zampa, G. M., Mencarelli, D., Pierantoni, L. (2023). A full-wave time-dependent Schrödinger equation approach for the modeling of asymmetric transport in geometric diodes. Physica B: Condensed Matter, 661, 414917.