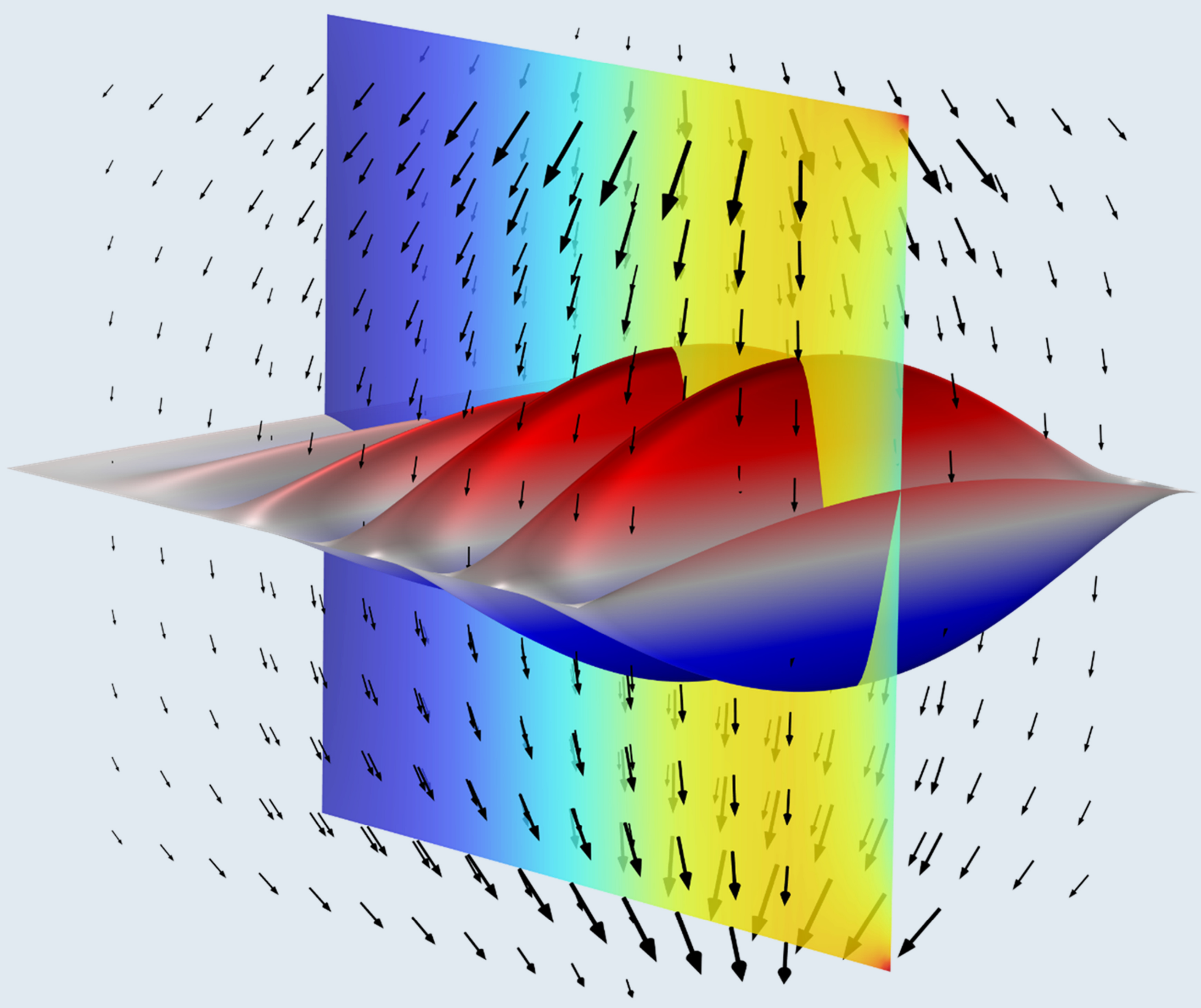

Quantum–Electromagnetic Coupling in Time Domain Simulations Using COMSOL Multiphysics®

This work analyzes the transport properties of nano-structures in the ballistic regime under the effect of electromagnetic fields.

G. M. Zampa, D. Mencarelli, L. Pierantoni
Information Engineering Department, Polytechnic University of Marche, Ancona, Italy

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® provides a useful platform for the solution of such a problem thanks to its high versatility and the potentiality to solve custom equation sets.

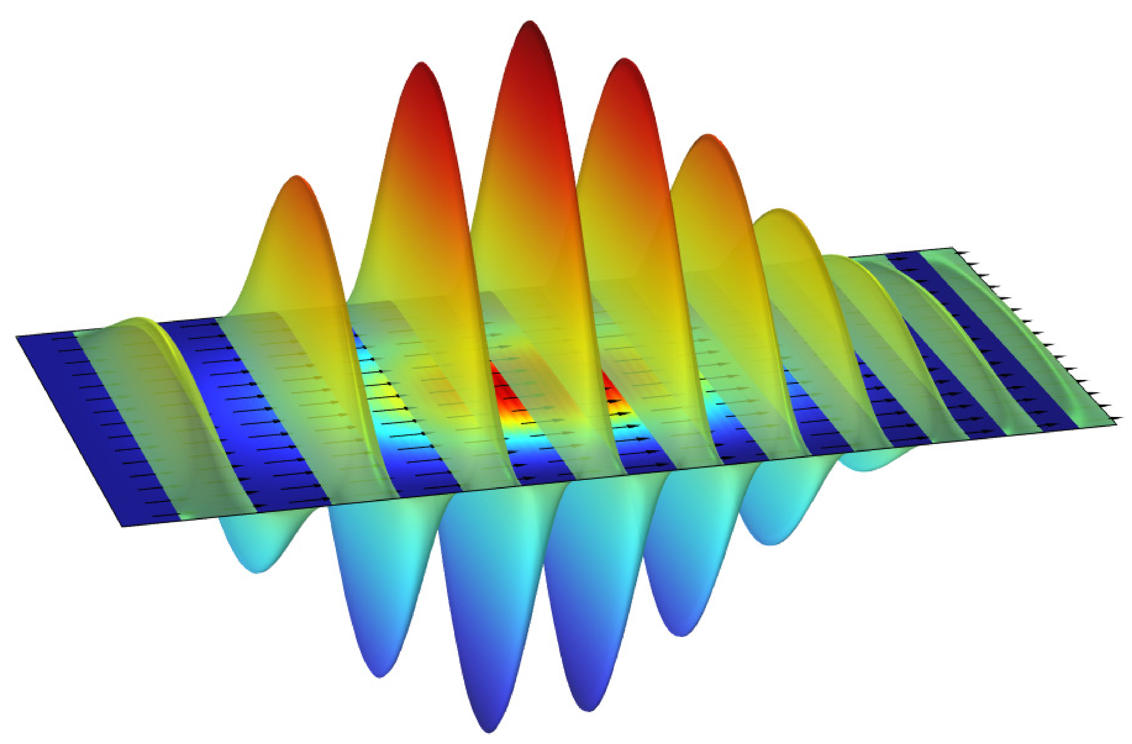

FIGURE 1: Self-generated electromagnetic field from a propagating gaussian quantum wave packet.

Theory

The Hamiltonian of a particle moving in an electromagnetic field is provided by:

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

where A is the vector potential, derived using the Coulomb Gauge. From the time-dependent Schrödinger equation it is possible to obtain the quantum current density (formula below) which is source for the EM radiation.

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

Implementation and Results

The coupling is realized in COMSOL Multiphysics® using the Coefficient Form PDE and the Electromagnetic Waves, Transient interfaces.

The behavior of a gaussian wave packet has been simulated without external electromagnetic field to estimate the self-generated field. 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 Figure (2).

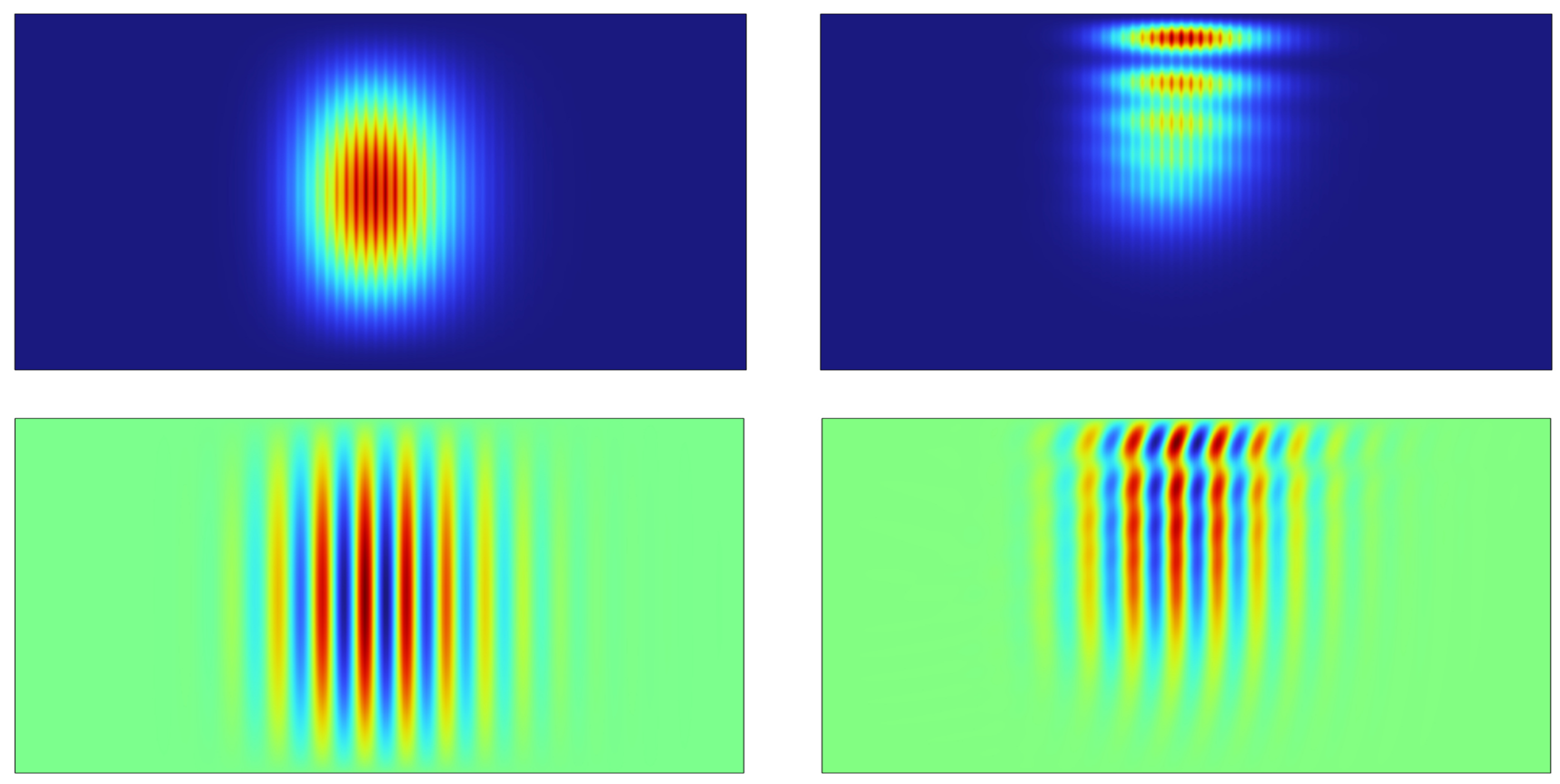

FIGURE 2: Quantum current density (top) and wave function (bottom) of a gaussian wave packet propagating with B_0 = 0 T (left) and B_0 = 0.5 T (right).

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.

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