# Real-time evolution of Maxwell systems in spinor representation

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## Motivation

The Yee algorithm [1] is a standard method to numerically solve for the classical electromagnetic field in arbitrary geometries and for external current and density sources. The algorithm is based on a finite-difference discretization on a real-space mesh for the electric field and a shifted mesh in space-time for the magnetic field. However, since the Maxwell equations have a symplectic structure and are first order in time, it is possible to transform them, by using the Riemann-Silberstein vector, into a matrix-spinor representation similar to the Dirac equation [2]. Such a spinor representation is advantageous for a coupled propagation of Maxwell's and Schrödinger's equations.

## Maxwell's equations in vacuum in Schrödinger form

The classical Maxwell's equations in vacuum are given by

$$\vec\nabla\cdot\vec E = 0\ , \quad (1) \qquad \vec\nabla\times\vec E = -\partial_t\vec B\ , \quad (3)$$

$$\vec\nabla\cdot\vec B = 0\ , \quad (2) \qquad \vec\nabla\times\vec B = \mu_0\epsilon_0\partial_t\vec E\ . \quad (4)$$

The equations (1) and (2) and equally (3) and (4) can be combined to one complex equation. With the definition of the complex Riemann-Silberstein vector for the electromagnetic field

$$\vec F^{(\mathrm{v})}(\vec r,t) = \sqrt{\epsilon_0/2}\ \vec E(\vec r,t) + i\sqrt{1/(2\mu_0)}\ \vec B(\vec r,t)\ , \tag{5}$$

the two Maxwell's equations (1) and (2) are equivalent to

$$\vec\nabla\cdot\vec F^{(\mathrm{v})} = 0\ . \tag{6}$$

The two remaining Maxwell's equations (3) and (4) can be formulated in terms of the Riemann-Silberstein vector in equation (5) in the form

$$i\partial_t\vec F^{(\mathrm{v})}(\vec r,t) = c_0\vec\nabla\times\vec F^{(\mathrm{v})}(\vec r,t)\ .$$

Using the identity of the cross product

$$\vec a\times\vec b = -i(\vec a\cdot\vec{\mathbf S})\vec b \qquad \text{with} \qquad \vec{\mathbf S} = \left(\mathbf S_\mathbf{x}\ ,\ \mathbf S_\mathbf{y}\ ,\ \mathbf S_\mathbf{z}\right)$$

$$\text{and}\quad \mathbf S_\mathbf{x} = \begin{bmatrix}0&0&0\\0&0&-i\\0&i&0\end{bmatrix}\ ,\quad \mathbf S_\mathbf{y} = \begin{bmatrix}0&0&i\\0&0&0\\-i&0&0\end{bmatrix}\ ,\quad \mathbf S_\mathbf{z} = \begin{bmatrix}0&-i&0\\-i&0&0\\0&0&0\end{bmatrix}\ ,$$

where $\mathbf S_\mathbf{x}$, $\mathbf S_\mathbf{y}$, and $\mathbf S_\mathbf{z}$ describe spin-1 matrices, we can express Maxwell's equations (3) and (4) in a form equivalent to the Schrödinger equation in quantum mechanics

$$i\hbar\partial_t\ \vec F^{(\mathrm{v})}(\vec r,t) = \hat{\mathcal H}^{(\mathrm{v})}\vec F^{(\mathrm{v})}(\vec r,t) \qquad \text{with} \qquad \hat{\mathcal H}^{(\mathrm{v})} = c_0\left(\vec{\mathbf S}\cdot\frac{\hbar}{\mathrm i}\vec\nabla\right)\ . \tag{7}$$

All important dynamical quantities of the electromagnetic field can be obtained in terms of bilinear expressions of the complex vector $\vec F$. By analogy with quantum mechanics, quantities like the total energy or the momentum of the electromagnetic field take a form that is reminiscent to quantum mechanical expectation values

$$E = \int d^3r\vec F^*(\vec r)\cdot\vec F(\vec r)\ , \qquad \vec P = \frac{1}{2ic_0}\int d^3r\vec F^*(\vec r)\times\vec F(\vec r)\ . \tag{8}$$

Hence, the formulation of Maxwell's equations given in equation (7) with the constraint of (6), has the advantage that standard quantum mechanical algorithms can be employed to solve Maxwell systems.

## References

[1] K. Yee, IEEE Transactions on Antennas and Propagation. **14** (1966), 302-307
[2] Bialynicki-Birula, Progress in Optics, Vol. XXXVI (1996), 245-294
[3] S. Ahmed Khan, Physica Scripta. **71** (2005), 440-442

## Maxwell's equations in a medium in Schrödinger form

In a similar way Maxwell's equations in a medium

$$\vec\nabla\cdot\vec D = 0\ , \quad (9) \qquad \vec\nabla\times\vec E = -\partial_t\vec B\ , \quad (11)$$

$$\vec\nabla\cdot\vec B = 0\ , \quad (10) \qquad \vec\nabla\times\vec H = \partial_t\vec D\ , \quad (12)$$

can also be written in a Schrödinger like form, where we use

$$\vec D(\vec r,t) = \epsilon(\vec r)\vec E(\vec r,t) \qquad \text{and} \qquad \vec H(\vec r,t) = \mu(\vec r)\vec B(\vec r,t)$$

for a linear isotropic medium, without free charge and current densities ($\rho = 0$ and $\vec j = 0$). The electric permittivity $\epsilon(\vec r)$ and magnetic permeability $\mu(\vec r)$ now depend on the position $\vec r$, but are still constant in time. Applying the same operations as in the vacuum considerations to combine equations (9) with (10) and (11) with (12), it is not possible to get a Schrödinger like form similar to equations (6) and (7) only with one Riemann-Silberstein vector $\vec F$. In this case, it is necessary to define two different Riemann-Silberstein vectors $\vec F_+$ and $\vec F_-$ to fulfill Maxwell's equations in a medium (9) - (12)

$$\vec F^{(\mathrm m)}_{\pm}(\vec r,t) = \sqrt{\epsilon(\vec r)/2}\ \vec E(\vec r,t) \pm i\sqrt{1/(2\mu(\vec r))}\ \vec B(\vec r,t)\ . \tag{13}$$

In contrast to the three dimensional Maxwell's equations in Schrödinger form in vacuum (6) and (7), the description of Maxwell's equations in Schrödinger representation in a medium is described by a six dimensional problem, since it includes both Riemann-Silberstein vectors (13). Therefore we define a six dimensional Spinor $\mathcal F^{(\mathrm m)}$ and the two auxiliary functions $c(\vec r)$ and $w(\vec r)$

$$\mathcal F^{(\mathrm m)}(\vec r,t) = \begin{pmatrix}\vec F^{(\mathrm m)}_+(\vec r,t)\\ \vec F^{(\mathrm m)}_-(\vec r,t)\end{pmatrix}\ , \qquad c(\vec r) = \sqrt{\frac{1}{\mu(\vec r)\epsilon(\vec r)}}\ , \qquad w(\vec r) = \sqrt{\frac{\mu(\vec r)}{\epsilon(\vec r)}}\ .$$

Finally, the operator $\mathcal H^{(\mathrm m)}$ for a position dependent medium is given by

$$\hat{\mathcal H}^{(m)} = \sqrt{c(\vec r)}\begin{bmatrix}1&0\\0&-1\end{bmatrix}\otimes\left(\vec{\mathbf S}\cdot\frac{\hbar}{i}\vec\nabla\right)\sqrt{c(\vec r)} + \frac{\hbar c(\vec r)}{2w(\vec r)}\begin{bmatrix}0&-i\\i&0\end{bmatrix}\otimes\left(\vec{\mathbf S}\cdot(\vec\nabla w(\vec r))\right)\ ,$$

and the electromagnetic fields $\vec E$ and $\vec B$ in a linear isotropic medium without free charge and current densities are described by the two equations

$$\vec\nabla\cdot\mathcal F^{(\mathrm m)}(\vec r,t) = 0\ , \tag{14}$$

$$i\hbar\partial_t\mathcal F^{(\mathrm m)}(\vec r,t) = \hat{\mathcal H}^{(m)}\cdot\mathcal F^{(\mathrm m)}(\vec r,t)\ . \tag{15}$$

Comparing this result with the Dirac equation for a relativistic electron theory, we obtain a similar structure for Maxwell's equations in a medium.

## Operator splitting for time evolution

Similar as in quantum mechanics, the time-evolution of the electromagnetic field can be expressed in terms of a time-evolution operator and takes the following form

$$\hat U(\Delta t) = e^{-\frac{i}{\hbar}\Delta t\hat{\mathcal H}^{(m)}} = e^{-\frac{i}{\hbar}\Delta t(\hat{\mathcal A}+\hat{\mathcal B})} \approx e^{-\frac{i}{\hbar}\Delta t\hat{\mathcal A}}e^{-\frac{i}{\hbar}\Delta t\hat{\mathcal B}}e^{\frac{1}{2\hbar^2}(\Delta t)^2[\hat{\mathcal A},\hat{\mathcal B}]}\ ,$$

where the operator $\mathcal H^{(\mathrm m)}$ can be separated into two operators $\mathcal A$, $\mathcal B$, and the exponential in $U(\Delta t)$ is approximated by the Baker-Campbell-Hausdorff formula

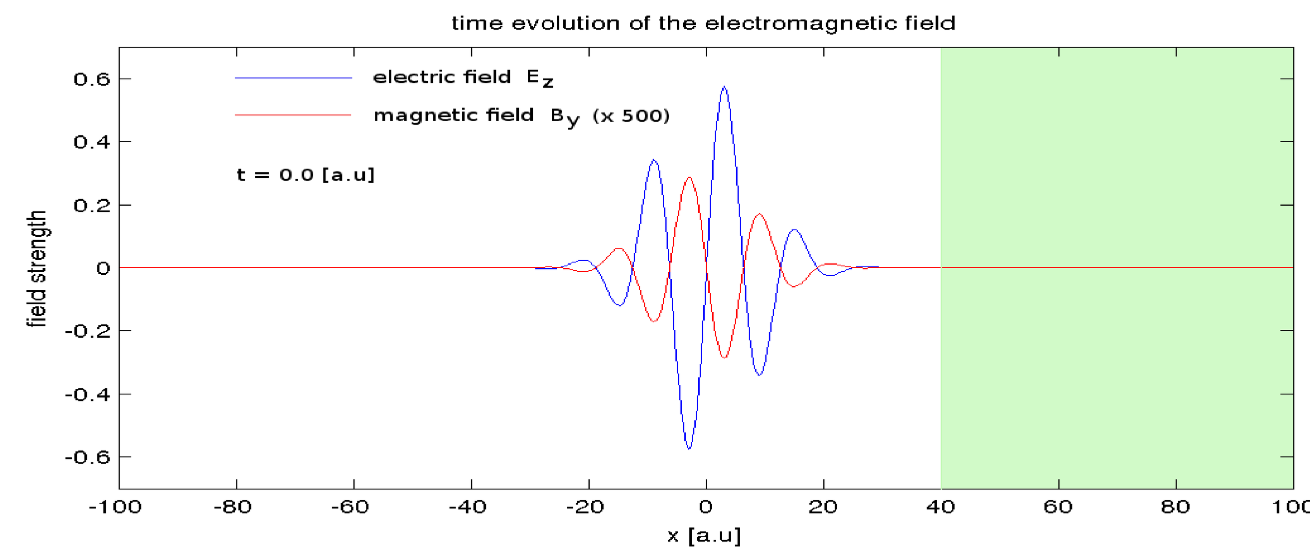
$$\hat{\mathcal A} = \begin{bmatrix}c\left(\vec{\mathbf S}\cdot\frac{\hbar}{i}\vec\nabla\right) & \mathbf 0\\ \mathbf 0 & -c\left(\vec{\mathbf S}\cdot\frac{\hbar}{i}\vec\nabla\right)\end{bmatrix}\ , \qquad \hat{\mathcal B} = \begin{bmatrix}\frac{\hbar}{2i}\vec{\mathbf S}\cdot(\vec\nabla c) & \frac{\hbar}{2i}\frac{c}{w}\vec{\mathbf S}\cdot(\vec\nabla w)\\ \frac{\hbar}{2i}\frac{c}{w}\vec{\mathbf S}\cdot(\vec\nabla w) & -\frac{\hbar}{2i}\vec{\mathbf S}\cdot(\vec\nabla c)\end{bmatrix}\ ,$$

$$[\hat{\mathcal A},\hat{\mathcal B}] = \begin{bmatrix}\frac{\hbar^2}{2}\vec{\mathbf S}\cdot\vec C & \mathbf 0\\ \mathbf 0 & \frac{\hbar^2}{2}\vec{\mathbf S}\cdot\vec C\end{bmatrix}\ , \qquad \vec C = (C_x, C_y, C_z)\ , \quad C_\zeta = (\partial_\zeta c)^2 - c\ \partial^2_\zeta c\ \ \text{with}\ \ \zeta\in\{\mathrm{x},\mathrm{y},\mathrm{z}\}\ .$$

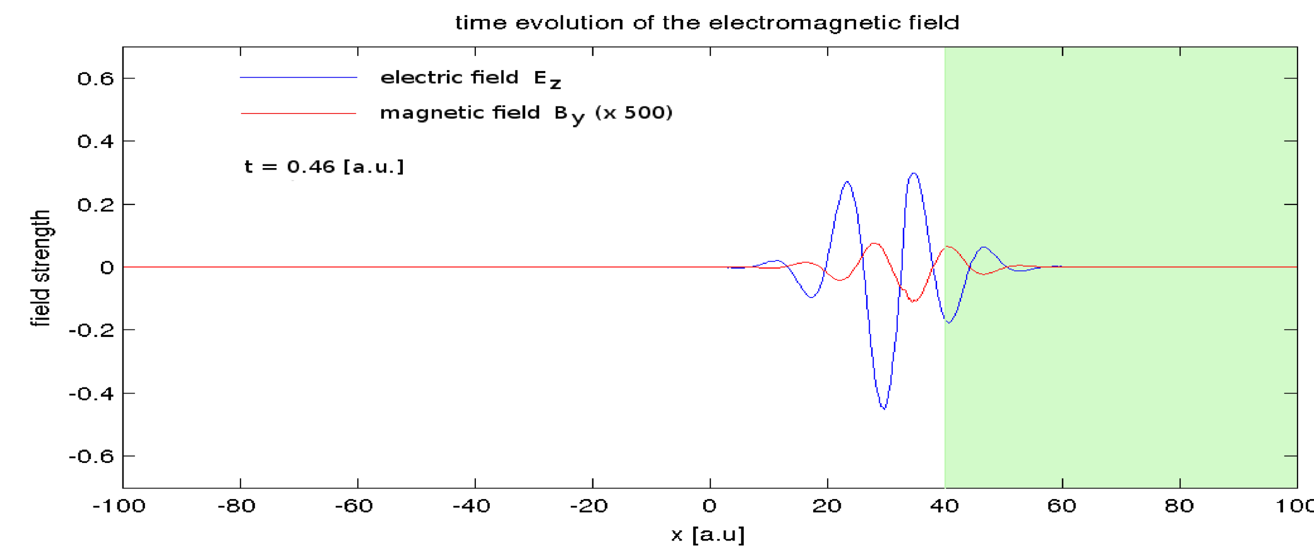
As before, the variables $c$ and $w$ depend on position $\vec r$, but they are constant in time.

## Numerical example

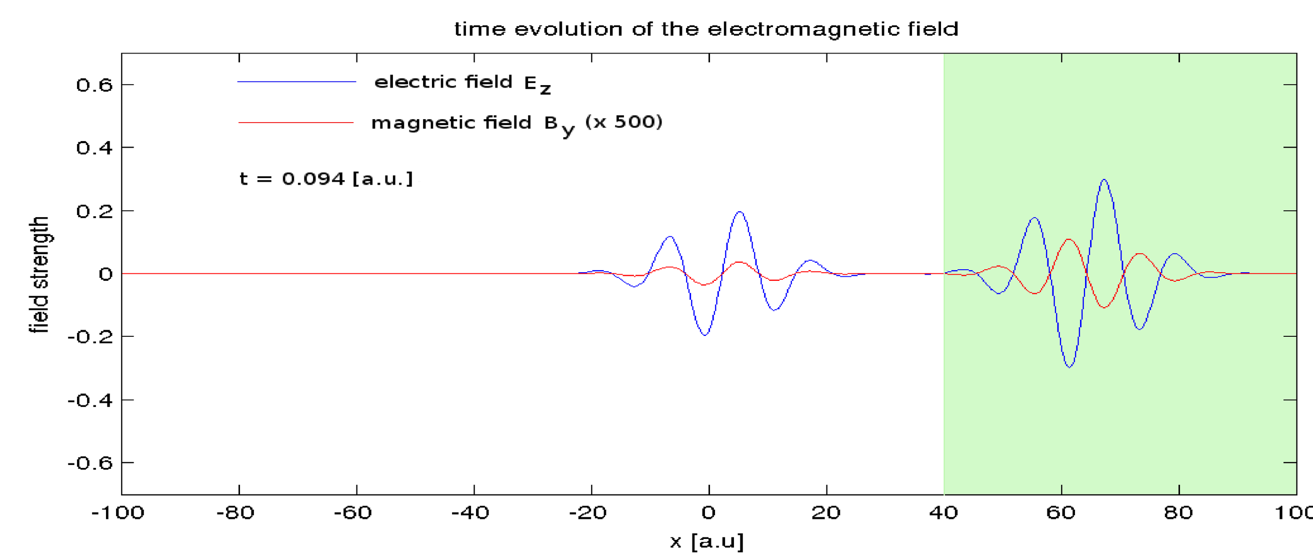
To illustrate the electromagnetic time evolution of equation (15) with the split operator method, we show the electric field propagation in x direction for a light pulse that hits a medium at $x \geq 40$.




The initial electromagnetic field in vacuum moves to the right with a speed of $c_0$.




When the wave reaches the medium one part passes the border of the medium and the intensity of the electric field and the propagation speed $c$ of the wave in the matter is reduced compared to the propagation in free space. Another part of the initial wave is reflected at the border of the medium, also with a lower intensity compared to the initial signal and travels with the vacuum speed $c_0$.




While the transmitted wave is in phase with the initial wave, the reflected wave shows a phase shift of $\pi$. This effect is well known from the electric field boundary conditions of classical electrodynamics. In contrast, there is no phase shift of the reflected magnetic wave. This is in accord with the magnetic field boundary conditions.

## Outlook

Maxwell's equations in a quantum-mechanical representation suggest to use the time evolution of the Riemann-Silberstein spinor in equation (15) with constraint (14) to consider coupled Maxwell-Schrödinger systems. An implementation of coupled Maxwell-Schrödinger systems in the real-time real-space code octopus is currently in preparation.