Unitary Quantum Lattice Simulations for Maxwell Equations in Vacuum and in Dielectric Media

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Utilizing the similarity between the spinor representation of the Dirac equation and the Maxwell equations that has been recognized since the early days of relativistic quantum mechanics, a quantum lattice (QLA) representation of unitary collision-stream operators of Maxwell’s equations is derived for both homogeneous and inhomogeneous media. A second order accurate 4-spinor scheme is developed and tested successfully for two dimensional (2D) propagation of a Gaussian pulse in a uniform medium while for normal (1D) incidence of an electromagnetic Gaussian wave packet onto a dielectric interface requires 8-component spinors. In particular, the well-known phase change, field amplitudes and profile widths are recovered by the QLA asymptotic profiles without the imposition of electromagnetic boundary conditions at the interface. The QLA simulations yield the time-dependent electromagnetic fields as the wave packet enters and straddles the dielectric boundary. QLA involves unitary interleaved non-commuting collision and streaming operators that can be coded onto a quantum computer – the non-commutation being the very reason why one perturbatively recovers the Maxwell equations.

1. Introduction

Dirac (1928) derived a relativistic covariant representation of the Schrödinger equation with positive definite probability density by, in essence, taking the square root of the Klein-Gordon wave equation. With the introduction of Dirac spinors, there were immediate attempts to connect Maxwell’s equations with the Dirac equation (Laporte & Uhlenbeck 1931, Oppenheimer 1931, Moses 1959), particularly with the introduction of the Riemann-Silberstein vector (Bialynicki-Birula 1996, Coffey 2008) for the electromagnetic field. More recent attempts have further coupled the Maxwell equations to various field theories (Yepez 2016, 2002, 2005; Kulyabov et. al. 2017, Jestadt et. al. 2018).

Here we will give an explicit unitary quantum lattice algorithm (QLA) for Maxwell equations in material media, building on our earlier QLA for solitons (L. Vahala et al. 2003, G. Vahala et al. 2003, 2004, 2005; Oganesov 2016a, 2016b, 2018) and Bose-Einstein condensates (Yepez et. al. 2009a, 2009b, G. Vahala et al. 2011, 2012a, 2012b, 2020; L. Vahala et. al. 2019a, 2019b). QLA are of much interest since its interleaved sequence of unitary collision and streaming operators can be immediately modeled by qubit gates. This permits immediate encoding onto a quantum computer. An interesting by-product of QLA is that these algorithms are also ideally parallelizable on classical supercomputers and typically lead to algorithms that can outperform standard classical algorithms in parallelization and numerical stability.

Consider Maxwell equations
where the external charge and current densities are $\rho$ and $J$. For linear isotropic material media, the electromagnetic fields obey the constitutive equations

$$
D(x,t) = \varepsilon(x,t) E(x,t) \quad , \quad B(x,t) = \mu(x,t) H(x,t)
$$

(2)

where the permittivity $\varepsilon(x,t) = \varepsilon_0 \varepsilon_r(x,t)$ and the permeability $\mu(x,t) = \mu_0 \mu_r(x,t)$. (The speed of light in a vacuum $c = (\mu_0 \varepsilon_0)^{-1/2}$). To rewrite the Maxwell equations into matrix form illustrative of the Dirac equation, it is convenient to introduce the two Riemann-Silberstein (RS) vectors (Bialynicki-Birula 1996, Jestadt et al. 2018, Khan 2005)

$$
F^t = \frac{1}{\sqrt{2}} \begin{bmatrix} \varepsilon E \pm i \frac{B}{\sqrt{\mu}} \end{bmatrix}
$$

(3)

for the two polarizations of the electromagnetic fields. In homogeneous media, there is no mixing of the polarizations, so the RS vectors remain uncoupled. In inhomogeneous media, there is coupling of the polarizations resulting in the need to use both RS vectors.

Following Khan (2002, 2005), we introduce

$$
\nu(x,t) = \frac{1}{\sqrt{\varepsilon \mu}}, \quad h(x,t) = \frac{\sqrt{\mu}}{\sqrt{\varepsilon}}
$$

(4)

so that the Maxwell equations are (Khan 2005)

$$
i \frac{\partial F^t}{\partial t} = \pm \nu \nabla \times F^t + \frac{1}{2} \nabla \nu \times F^t \pm \frac{\nu}{2h} \nabla h \times F^t + i \frac{\partial \ln \nu}{\partial t} F^t + \frac{\partial \ln h}{\partial t} F^t - i \sqrt{\frac{\nu h}{2}} J
$$

$$
\nabla \nabla F^t = \frac{1}{2\nu} \nabla \nabla F^t + \frac{1}{2h} \nabla h \nabla F^t + \sqrt{\frac{\nu h}{2}} \rho
$$

(5)

Polarization coupling occurs through either spatial or temporal time variations of $h(x,t)$. Eq. (4). In matrix form, Eq. (5) can be written as the time evolution of the 8-spinor components (Khan 2005)

$$
\frac{\partial}{\partial t} \begin{bmatrix} \Psi^- \\ \Psi^+ \end{bmatrix} = -\frac{1}{2} \frac{\partial \ln \nu}{\partial t} \begin{bmatrix} \Psi^- \\ \Psi^+ \end{bmatrix} + \frac{i}{2} \mathbf{M} \cdot \alpha + \frac{\partial \ln h}{\partial t} \begin{bmatrix} \Psi^- \\ \Psi^+ \end{bmatrix} + \begin{bmatrix} \mathbf{M} \cdot \nabla \pm \frac{\nabla \nu}{2\nu} \mathbf{\Sigma} \cdot \alpha \\ -i \frac{\mathbf{M} \cdot \nabla}{2h} \alpha \end{bmatrix} \begin{bmatrix} \Psi^- \\ \Psi^+ \end{bmatrix} - \begin{bmatrix} \Psi^- \\ \Psi^+ \end{bmatrix} + \begin{bmatrix} \Psi^- \\ \Psi^+ \end{bmatrix}
$$

(6)

with the Cartesian RS components and source matrices defined by
the 4x4 matrices $M$ in Eq. (6) are just the tensor product of the Pauli spin matrices with the 2x2 identity matrix $I_2$: $M = \tilde{\sigma} \otimes I_2$, with $M_z = \sigma_z \otimes I_2$. \( \tilde{\sigma} = (\sigma_x, \sigma_y, \sigma_z) \) and

\[
\begin{align*}
\sigma_x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, & \sigma_y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, & \sigma_z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\end{align*}
\]

Finally

\[
\begin{pmatrix} \bar{\sigma} \\ \bar{\sigma} \end{pmatrix} = \begin{pmatrix} 0 & \bar{\sigma} \\ \bar{\sigma} & 0 \end{pmatrix}
\]

and

\[
\begin{pmatrix} \bar{\sigma} \\ \bar{\sigma} \end{pmatrix} = \begin{pmatrix} \bar{\sigma} & 0 \\ 0 & \bar{\sigma} \end{pmatrix}.
\]

For homogeneous media,

\[
\nabla \psi = 0 = \nabla h = \frac{\partial \psi}{\partial t} = \frac{\partial h}{\partial t}
\]

so that Eq. (6) decouples to

\[
\frac{\partial \Psi^+}{\partial t} = -\nabla M \nabla \Psi^+ - W^+
\]

From Eq. (11) one can readily deduce Maxwell’s equations. Indeed, the sum of the 1st and 4th rows of Eq. (11) determines the time evolution of $F_y^+$, i.e., of the y-components of $E$ and $B$, while the difference of the 1st and 4th rows yields the time evolution of the x-component of $E$ and $B$. The sum of the 2nd and 3rd rows yields the time evolution of the z-component of $E$ and $B$. Finally, the divergence equations of the Maxwell equations come from the difference of the 2nd and 3rd rows.

2. Unitary Quantum Lattice Algorithm

2.1. Dirac Equation

What drew the attention of researchers from as early as 1931 was the similarity between the RS vector representation of Maxwell equations and the Dirac equation. One form of the Dirac equation for a free particle of mass $m$ is the 4-spinor evolution of $\psi$

\[
\frac{\partial \psi}{\partial t} - i \sum_{j=1}^{3} a_j \sigma_j \frac{\partial \psi}{\partial x_j} + i b \otimes I_2 m \psi
\]

where $a$ and $b$ are any Pauli spin matrices, with $a \neq b$. In particular (Yepez 2002, 2005, 2016) for the choice $a = \sigma_x$, $m = 0$, and suitable normalization, Eq. (12) for a massless particle reduces to

\[
\begin{pmatrix}
\psi_0 \\
\psi_1 \\
\psi_2 \\
\psi_3
\end{pmatrix}
= \begin{pmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}
\begin{pmatrix}
\psi_0 \\
\psi_1 \\
\psi_2 \\
\psi_3
\end{pmatrix}
+ i \begin{pmatrix}
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
-\psi_3 \\
\psi_2 \\
-\psi_1 \\
\psi_0
\end{pmatrix}
+ \begin{pmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
-\psi_3 \\
-\psi_2 \\
-\psi_1 \\
-\psi_0
\end{pmatrix}.
\]
2.2. Maxwell’s Equations for Propagation in 2D in Homogeneous Media

For homogeneous media, one needs only the 4-spinor components \(\{q_0, q_1, q_2, q_3\}\):

\[
\Psi^+ = \begin{pmatrix}
-F_x^+ + i F_y^+ \\
F_2^+ \\
F_2^+ \\
F_x^+ + i F_y^+
\end{pmatrix} = \begin{pmatrix}
q_0 \\
q_1 \\
q_2 \\
q_3
\end{pmatrix},
\]

Eq. (10) for homogeneous media (and with no external sources) reduces to (on setting \(c = 1\))

\[
\frac{\partial}{\partial t} \begin{pmatrix}
q_0 \\
q_1 \\
q_2 \\
q_3
\end{pmatrix} = -\frac{\partial}{\partial x} \begin{pmatrix}
q_2 \\
q_0 \\
q_3 \\
-q_1
\end{pmatrix} + i \frac{\partial}{\partial y} \begin{pmatrix}
q_2 \\
-q_0 \\
-q_3 \\
-q_1
\end{pmatrix} - \frac{\partial}{\partial z} \begin{pmatrix}
q_0 \\
q_1 \\
q_2 \\
-q_3
\end{pmatrix}
\]

Note the overall similarity with the Dirac equation for a massless particle, Eq. (13).

A QLA for the Maxwell equations, Eq. (15), can now be readily determined, building on the Dirac-QLA of Yepez (2002, 2005, 2016). Here we will concentrate on determining such an algorithm for 1D and 2D Maxwell equations. Consider the unitary collision operators

\[
C_x = \begin{pmatrix}
\cos \theta & 0 & \sin \theta & 0 \\
0 & \cos \theta & 0 & \sin \theta \\
-\sin \theta & 0 & \cos \theta & 0 \\
0 & -\sin \theta & 0 & \cos \theta
\end{pmatrix}, \quad C_y = \begin{pmatrix}
\cos \theta & 0 & i \sin \theta & 0 \\
0 & \cos \theta & 0 & i \sin \theta \\
i \sin \theta & 0 & \cos \theta & 0 \\
0 & i \sin \theta & 0 & \cos \theta
\end{pmatrix}
\]

and the unitary streaming operators \(S_{1,x}^{\text{eq}}, S_{1,x}^{\text{eq}}\) which shift the appropriate amplitudes \(\{q_j(x,y), j = 0, 3\}\) along the lattice in the x-direction by \(\pm 1\) lattice units:

\[
S_{1,x}^{\text{eq}} = \begin{pmatrix}
q_0(x,y,t) \\
q_1(x,y,t) \\
q_2(x,y,t) \\
q_3(x,y,t)
\end{pmatrix}, \quad S_{2,x}^{\text{eq}} = \begin{pmatrix}
q_0(x,y,t) \\
q_1(x,y,t) \\
q_2(x,y,t) \\
q_3(x,y,t)
\end{pmatrix}
\]

There are similar expressions for the unitary streaming operators in the y-direction: \(S_{1,y}^{\text{eq}}, S_{2,y}^{\text{eq}}\). For the x-direction, one now considers the following interleaved sequence of unitary operators:

\[
U_x = S_{1,x}^{\text{eq}} C_x S_{1,x}^{\text{eq}} C_x S_{2,x}^{\text{eq}} C_x S_{1,x}^{\text{eq}} C_x
\]

while for the y-direction we consider a slightly different sequence of interleaved operators

\[
U_y = S_{2,y}^{\text{eq}} C_y S_{2,y}^{\text{eq}} C_y S_{1,y}^{\text{eq}} C_y S_{2,y}^{\text{eq}} C_y
\]

The QLA time advancement of the 4-spinor components
yields the required evolution of the 4-spinor
\[
\begin{pmatrix}
q_0 \\
q_1 \\
q_2 \\
q_3
\end{pmatrix}_{t+\delta t} = U^\text{atk}_x U^\text{atk}_y U^\text{atk}_x U^\text{atk}_x
\begin{pmatrix}
q_0 \\
q_1 \\
q_2 \\
q_3
\end{pmatrix}_t
\]
\[\text{(20)}\]

provided we have diffusion scaling (time advancement $\delta t \ll \varepsilon^2$ with lattice spacing $\delta x = \delta y \ll \varepsilon$) and collision angle $\theta = \varepsilon / 4$. Equation (21) is just Maxwell equations for electromagnetic fields with 2D spatial dependence.

3. QLA Simulation of Propagation of Gaussian Wave Packet for the 2D Maxwell Equations in a Vacuum

First, we shall consider a Gaussian wave packet propagating in the $y$-direction with initial condition
\[
E_z(x, y, t=0) = E_0 \exp\left[-\frac{(y-y_0)^2}{\sigma^2}\right] \cos[k_y(y-y_0)]
\]
\[\text{(22)}\]

and the other field components zero: $E_x = 0 = E_y = B_y = B_z$. The QLA algorithm, Eq. (20), is solved on a 5000 x 5000 grid, with the small parameter $\varepsilon = 0.1$ and collision angle $\theta = \varepsilon / 4$. For parameters $E_0 = 0.01$, $\sigma^2 = 9000$, $k_y = 0.08$, the initial Gaussian wave packet for $E_z$ is
**FIGURE 1** The initial Gaussian wave packet for the electric field $E_z(t = 0)$, plotted at every tenth data point in the $x$- and $y$- directions. (i.e., the actual simulation grid is $500 < y' < 1500$, $0 < x' < 500$).

shown in Fig. 1, with $E_z(x, y, t) = \Re\left[q_1 + q_2\right]/2$. After 1000 time steps, the wave packet has propagated along the $y$-axis undistorted, Fig. 2:

**FIGURE 2** Gaussian wave packet $E_z$ at time $t = 1k$.

After $t = 30k$ time steps, under periodic boundary conditions, there is no discernable distortion in the wave packet, Fig. 3
Because the evolution equations for the spinor amplitudes $q_1$ and $q_2$ are different in Eq. (21), it is interesting to plot the difference $\Re\left[q_1 - q_2\right]$. This difference, as shown in Fig. 6, is negligible.

Finally we show the Gaussian wave packet after 130 k iterations. In Fig. 7 we plot the pulse itself.

FIGURE 3 Gaussian wave packet $F_z^-$ at $t = 30k$.

FIGURE 4 A plot of the difference in the spinor amplitudes $\Re[q_1 - q_2]$ at $t = 30k$.

FIGURE 5 The $F_z^-$-component of the Gaussian wave packet at $t = 130 K$. 
and see that the non-localization of the wave packet even after many periods is negligible: Fig. 6 for $0 < y < 320$, and Fig. 7 for $400 < y < 500$.

**FIGURE 6** A blow-up of the region $0 < y < 320$ of Fig. 5. The $E_z$-component here remains over 7 orders of magnitude below that of the Gaussian wave packet.

**FIGURE 7** A blow-up of the region $400 < y < 500$ of Fig. 5. The $E_z$-component here remains over 7 orders of magnitude below that of the Gaussian wave packet.

In our normalized units, $B_x = E_z$ and this is faithfully preserved in the QLA simulations.

4. QLA for 1D Maxwell equations in Inhomogenous Media
We now consider the case of normal incidence of an electromagnetic wave onto a dielectric boundary, permitting only a spatial dependence in \( y \). i.e., we consider an electromagnetic wave with non-zero components \( E_z, B_z \) propagating in a medium with refractive index \( n(y) \). Equations (6)-(8) reduce to the following 8-spinor representation which is conveniently written in the two polarization blocks of 4-spinor components:

\[
\begin{pmatrix}
    q_0 \\
    q_1 \\
    q_2 \\
    q_3 \\
    q_4 \\
    q_5 \\
    q_6 \\
    q_7
\end{pmatrix} = \frac{1}{n(y)} \begin{pmatrix}
    0 \\
    -i \frac{\partial}{\partial y} n'(y) \\
    -i \frac{\partial}{\partial y} n'(y) \\
    i \frac{\partial}{\partial y} n'(y) \\
    0 \\
    i \frac{\partial}{\partial y} n'(y) \\
    -i \frac{\partial}{\partial y} n'(y) \\
    0
\end{pmatrix} \begin{pmatrix}
    q_0 - q_6 \\
    q_1 \\
    q_2 - q_7 \\
    q_3 + q_4 \\
    q_4 - q_3 \\
    q_5 + q_6 \\
    q_6 + q_1 \\
    q_7 - q_2
\end{pmatrix}
\]

where \( n'(y) = \frac{dn}{dy} \), and

\[
\begin{pmatrix}
    q_0 \\
    q_1 \\
    q_2 \\
    q_3 \\
    q_4 \\
    q_5 \\
    q_6 \\
    q_7
\end{pmatrix} = \begin{pmatrix}
    -F_x^+ + i F_y^+ \\
    F_x^+ \\
    F_z^+ \\
    F_x^- + i F_y^- \\
    -F_x^- - i F_y^- \\
    F_z^- \\
    F_x^- \\
    F_z^- \\
\end{pmatrix}, \quad \text{with} \quad F^\pm = \frac{1}{\sqrt{2}} \left[ \sqrt{\varepsilon} \mathbf{E} \pm i \frac{\mathbf{B}}{\sqrt{\mu}} \right].
\]

The two RS vectors for the polarizations, \( F^+ \) and \( F^- \), are coupled by the spatial gradient in the refractive index \( n(y) = \sqrt{\mu_0 \varepsilon(y)} \). For simplicity, we shall consider normal wave incidence from a region of constant dielectric \( n_0 \) onto a region of constant dielectric \( n_1 \). These two dielectrics are connected by a thin boundary region [see Eq. (33) below for an explicit profile].

The QLA to reproduce the 1D Maxwell equations, Eq. (23), to second order accuracy has the following unitary collision operator,
which interleaved with the unitary streaming operator will recover the 1st term on the right-hand side of Eq. (23) provided

$$\theta = \frac{\varepsilon}{4n(y)}.$$  \hfill (26)

To recover the inhomogeneous dielectric factor $n'(y)$ in Eq. (23) we introduce the Hermitian operators

$$V_{11} = \begin{pmatrix}
\cos\alpha & \sin\alpha & 0 & 0 & 0 & 0 & 0 & 0 \\
-\sin\alpha & \cos\alpha & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \cos\alpha & \sin\alpha & 0 & 0 & 0 & 0 \\
0 & 0 & -\sin\alpha & \cos\alpha & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \cos\alpha & -\sin\alpha & 0 & 0 \\
0 & 0 & 0 & 0 & \sin\alpha & \cos\alpha & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \cos\alpha & -\sin\alpha \\
0 & 0 & 0 & 0 & 0 & 0 & \sin\alpha & \cos\alpha \\
\end{pmatrix}$$

$$V_{22} = \begin{pmatrix}
\cos\alpha & 0 & 0 & 0 & 0 & 0 & -\sin\alpha & 0 \\
0 & \cos\alpha & 0 & 0 & 0 & 0 & 0 & -\sin\alpha \\
0 & 0 & \cos\alpha & 0 & \sin\alpha & 0 & 0 & 0 \\
0 & 0 & 0 & \cos\alpha & 0 & \sin\alpha & 0 & 0 \\
0 & 0 & -\sin\alpha & 0 & \cos\alpha & 0 & 0 & 0 \\
\sin\alpha & 0 & 0 & 0 & 0 & 0 & \cos\alpha & 0 \\
0 & \sin\alpha & 0 & 0 & 0 & 0 & 0 & \cos\alpha \\
\end{pmatrix}$$ \hfill (27)

with the (complex) rotation angle

$$\alpha = -i e^2 \frac{n'(y)}{2n^2(y)}. \hfill (28)$$

Note that the operators $V_{11}$ and $V_{22}$ would be unitary if the rotation angle $\alpha$ was real. Now each of these Hermitian matrices can be decomposed into a sum of two unitary matrices: e.g., on normalizing $V_{11}$ so that $\|V_{11}\| \leq 1$ then one can rewrite
\[ V_{11} = \frac{1}{2} (U_{11}^{(1)} + U_{11}^{(2)}) \]

where \( U_{11}^{(1)} \) and \( U_{11}^{(2)} \) are now unitary

\[ U_{11}^{(1)} = V_{11} + i \sqrt{I - V_{11}^2}, \quad U_{11}^{(2)} = V_{11} - i \sqrt{I - V_{11}^2} \]

Childs & Wiebe (2012) have shown that one can encode linear combinations of unitary operators on quantum computers and that in some cases these algorithms will outperform the usual product of unitary operators algorithms.

The unitary interleaved sequence of collide-stream-potential operators

\[ U_{rr} = S^{23.67}_{\gamma} C_{\gamma} (\theta) S^{23.67}_{\gamma} C_{\gamma}^{\dagger} (\theta) S_{\gamma}^{01.45} C_{\gamma} (\theta) S_{\gamma}^{01.45} C_{\gamma}^{\dagger} (\theta) \]

\[ U_{rr}^{\alpha} = S^{23.67}_{\gamma} C_{\gamma} (\theta) S_{\gamma}^{23.67} C_{\gamma} (\theta) S_{\gamma}^{01.45} C_{\gamma} (\theta) S_{\gamma}^{01.45} C_{\gamma} (\theta) \]

are thus augmented with the Hermitian operators that can be decomposed into a sum of two unitary matrices which can still be encoded onto a quantum computer

\[ \tilde{q}(t + i) = V_{21} V_{11}^{\dagger} U_{11} \tilde{q}(t) \]

where \( \tilde{q} \) is the 8-spinor, Eq. (24).

5. QLA Simulations for 1D Inhomogeneous Dielectric Media

We now discuss some 1D QLA simulations of electromagnetic wave propagation from a region of refractive index \( n_0 \) into a region with refractive index \( n_i \). The refractive index profile is modeled by the hyperbolic tangent - function

\[ n(y) = \frac{n_0 + n_i}{2} - \frac{n_0 - n_i}{2} \tanh \left( \beta \left( y - L \right) \right) \]

where \( \beta \) controls the thickness of the boundary region between the two media. Some care needs to be taken with the perturbation parameter \( \varepsilon \), as the collide-stream unitary operators have \( \theta = O(\epsilon) \) while the operators controlling the media refractive interface have \( \alpha = O(\epsilon^2) \); one order of \( \epsilon \) will come implicitly from the scaling of \( n'(y) \). For the simulations reported here, the boundary region between the two media is centered at \( L_m = 16000 \) (lattice units) with the end of the grid at \( L_{end} = 2L_m \). Periodic boundary conditions are enforced by adding a small buffer region after \( L_{end} \) so that the refractive index is periodic as shown in Fig. 8(a)
5.1. Electromagnetic Pulse Propagation for \( n_0 < n_1 \)

First, consider a simple non-oscillatory pulse propagating from the region of refractive index
\( n_0 = 1 \) towards the region with \( n_1 = 3 \), with \( \varepsilon = 0.3 \). The initial electric and magnetic field profiles are chosen to be solutions of the Maxwell equations with \( B_y(y,0) = n(y)E_z(y,0) \). Hence, when propagating in the vacuum region the \( E_z \) and \( B_x \) profiles overlap, Fig. 9(a) and (b), where \( t = 20,000 \) time iteration:

\[
\begin{align*}
(a) \quad t &= 0 \\
(b) \quad t &= 20k
\end{align*}
\]

FIGURE 9 The propagation of an electromagnetic pulse from vacuum into a dielectric region with \( n_1 = 3 \). Interface at \( y = 16000 \). Initially the field components overlap: \( E_z(\text{blue}), B_x(\text{red}) \). The unitary QLA reproduces the Maxwell equations as the profiles propagate undistorted in the vacuum, as seen after 20,000 time iterations (\( t = 20k \), (b).

In Fig. 10 (\( t = 28k \)) the pulse has penetrated the interface (\( y = 16000 \)) resulting in the non-overlap of the electromagnetic \( E_z(\text{blue}), B_x(\text{red}) \) fields. Moreover, at \( t = 32k \), we notice that the \( E_z(\text{blue}) \) field undergoes a \( \pi \)-phase change for \( y < 16000 \). This is in accordance with standard electromagnetic boundary layer theory for a plane wave incident on a dielectric discontinuity: the ratio of the reflected to incident electric field \( \frac{E_{\text{refl}}}{E_{\text{inc}}} = \left( \frac{n_0 - n_1}{n_0 + n_1} \right) \) with \( n_0 = 1, n_1 = 3 \) (Jackson 1998)

\[
\begin{align*}
(a) \quad t &= 28K \\
(b) \quad t &= 32K
\end{align*}
\]

FIGURE 10 The effect of the boundary region on the pulse as it is straddles the two media. (a) \( t = 28k \) : a separation starts to occur between the \( E_z(\text{blue}), B_x(\text{red}) \) fields, with (b) showing an inversion in the \( E_z(\text{blue}) \) at \( t = 32k \).
FIGURE 11 The reflected and transmitted fields. The reflected fields suffer a π-phase change since \( n_0 < n_i \). Interface centered at \( y = 16000 \). The transmitted fields are in phase but with amplitudes in the ratio of \( n_i / n_0 = 3 \), and with pulse width reduced by \( n_i / n_0 \) since the speed of the transmitted pulse is reduced by this factor. This is readily seen on comparing (a) \( t = 40k \), and (b) \( t = 60k \). Note the ratio of the fields \( |B_x / E_z| = n \), where \( n \) is the refractive index of that medium.

5.2. Electromagnetic Pulse Propagation for \( n_0 > n_i \)

It is instructive to also consider the effect of this pulse propagating from high to low refractive index. Since the pulse speed in \( n_0 = 3 \) is a factor of 3 slower when compared with the speed in the low refractive index medium, the corresponding time outputs are a factor of 3 greater within medium \( n_o \):

FIGURE 12 The propagation of a pulse from \( n_0 = 3 \) towards \( n_i = 1 \). Note that \( B_x / E_z = n_0 = 3 \) for \( y < 16000 \).

At the dielectric interface, it is now the magnetic field components \( B_x \) that undergoes a π-phase change while the electric field component \( E_z \) does not (Fig. 13):
FIGURE 13  The reflected and transmitted pulse for propagation from large to smaller refractive index.

(a)  $t = 84k$: here the pulse is straddling the interface between the two dielectric media. Note that for $y > 16000$ the $E_z$ (blue), $B_x$ (red) profiles overlay each other;

(b)  $t = 96k$: for $y < 16000$ there is a $\pi$-phase change in the reflected magnetic component $B_x$ (red). The axes had to be shifted because of the larger width of the transmitted pulse.

At $t = 120$ K, Fig. 14 shows that the transmitted pulse has its width and speed of propagation increased by $n_i/n_0$.

FIGURE 14  The reflected and transmitted pulse for propagation from $n_0 \rightarrow n_i$ with $n_i/n_0 = 3$ at $t = 120k$. For the reflected pulse, there is no phase change in $E_z$ (blue) but a $\pi$-phase change in $B_x$ (red). The speed of the transmitted pulse is a factor of $n_i/n_0$ greater than the incident (or reflected) pulse. The boundary between the media is at $y = 16000$. For the transmitted pulse, the $E_z$ (blue), $B_x$ (red) fields are equal and so overlay each other.

5.3. Propagation of a Gaussian Wave Packet for $n_o < n_i$

Finally we show the reflection/transmission of a Gaussian wave packet as it propagates from a low-to-high refractive medium: $n_0 = 1$ to $n_i = 3$. In the vacuum region, $n_0 = 1$, $B_x = E_z$ so that these fields again overlay each other, Fig. 15. This overlay continues throughout the Gaussian packet’s evolution through the vacuum region $y < 16000$ as can be seen in Fig. 15(b).
FIGURE 15  (a) The initial Gaussian wave packet as it propagates from a vacuum $n_0 = 1$ to a higher refractive region for $y > 16000$ with refractive index $n_1 = 3$. Initially $E_z = B_x$ so the profiles overlay each other: $E_z \text{ (blue)}, B_x \text{ (red)}$. (b) The Gaussian wave packet at $t = 20K$ as it approaches the boundary for the higher refractive index medium.

In Fig. 16 the Gaussian packet, at $t = 28K$, is straddling the two dielectric media (interface at $y = 16000$). The $E_z \text{ (blue)}, B_x \text{ (red)}$ profiles no longer overlay near the interface and the wavelength of the packet oscillations in the denser medium are decreased over the vacuum wavelength.

FIGURE 16 The Gaussian wave packet at $t = 28K$ as it straddles the boundary between the two dielectrics: $n_0 = 1$ for $y < 16000$ and $n_1 = 3$ for $y > 16000$. 
The transient reflected and transmitted Gaussian wave packets are seen in Fig. 17, at $t = 32K$. Many features of the asymptotic profiles are becoming evident at this early stage: for the transmitted packet, the $E_z^{(\text{blue})}, B_y^{(\text{red})}$ profiles are in phase with $B_y = n_1 E_z$ and the wavelength of the transmitted packet is reduced by the factor $n_1 / n_0 = 3$. For the reflected packet one is clearly in a transient stage close to the interface but a phase difference of $\pi$ is evident for $y < 15000$. An asymptotic snapshot of the reflected and transmitted packets is seen in Fig. 18 at $t = 40K$.

![Figure 17](image17.png)

![Figure 18](image18.png)

6. Summary and Conclusions

Utilizing the similarity of the spinor representation of the Dirac equation to the Maxwell equations, we have extended our studies in unitary QLA [8-23]. In particular, using the Pauli spin $\frac{1}{2}$-matrices, we have expressed Khan’s Riemann-Silberstein representation of the Maxwell equations in a unitary spinor lattice representation. The QLA is readily determined for the 1D and 2D spatial dependence of the electromagnetic fields. For homogeneous media, the QLA requires only 4 spinor components per spatial lattice node, while for inhomogeneous media the two polarizations of the electromagnetic fields are coupled requiring the use of the two Riemann-Silberstein vectors and an 8-spinor representation. The QLA can be shown to be 2nd order accurate under diffusion ordering.
To attain this ordering we must introduce a small parameter \( \varepsilon \) into the unitary collision operators. In our earlier works of QLA for the Nonlinear Schrödinger equation and Bose-Einstein condensation for spinor fields, the introduction of the required small parameter can be accomplished by an appropriate scaling of the spinor order parameter wave functions that appear in the nonlinear Bose-Bose interaction potential (Vahala et. al. 2003, 2005, 2022, 2012, 2019a, 2020). For the Maxwell representation, this is not possible. By appropriately scaling the fields relative to the lattice spatial unit the QLA will still hold for sufficiently small \( \varepsilon \).

To benchmark the QLA we have considered two problems: (1) electromagnetic propagation in a 2D homogeneous medium, and (2) electromagnetic propagation in 1D inhomogeneous media. In 2D homogeneous medium, we have tested propagation in the x-direction and y-direction separately. This was done since the Pauli spin \( \frac{1}{2} \) matrices \( \sigma_x \) are real while \( \sigma_y \) are purely imaginary, resulting in a different collide-stream interleaved sequence in these directions to recover the 2D QLA Maxwell equations. Since the results were essentially the same, we have only presented the results for y-propagation. In 1D inhomogeneous media, we have studied the problem of a 1D normally incident electromagnetic wave onto a sharp (but continuous) transition region between two different dielectric media. For a Gaussian pulse this problem would be very difficult to solve analytically. Of course, if the dielectric boundary region became a strict discontinuity, the standard electromagnetic texts solve this boundary value problem for a plane wave, yielding the appropriate phase shifts in the reflected wave and the corresponding amplitude ratios. Provided the boundary layer is sufficiently thin, the QLA simulations agree with the analytic results for an incident plane wave onto a dielectric discontinuity.

It is interesting to compare our 1D QLA, which utilizes simple unitary collision and streaming operators based on the Pauli spin \( \frac{1}{2} \) matrices, with the Jestadt et. al. algorithm [2014, 2018] based on the bosonic spin-1 matrices. Consequently they only consider the 3-spinor components

\[
\Phi^t = \begin{pmatrix}
-F_x^t + i F_y^t \\
F_y^t \\
-F_x^t + i F_y^t
\end{pmatrix}.
\]

This representation recovers the time-dependent parts of Maxwell’s equations, but not the divergence equations \( \nabla \cdot \mathbf{D} = \rho \) , \( \nabla \cdot \mathbf{B} = 0 \). These two equations will have to be imposed as constraints. For 1D propagation these constraints are easily satisfied, but their representation in 3D is nontrivial. For closure, Jestadt [2014] invoke the Baker-Campbell-Hausdorff expansion to approximate the exponential operator in the commutator of their kinetic-potential operators and their inhomogeneous medium operator. This commutator depends on the second derivative on the refractive index \( n''(y) \) with respect to \( y \). In our QLA, it is the interleaving of the non-commuting unitary collide-stream operators that yields the Maxwell equations - if we had ignored the non-commutative property of the collision and streaming operators then our sequence would have resulted in the identity operator itself. Extension of QLA for Maxwell equations to 3D is expected to follow the standard procedures we have utilized in earlier QLA for 1D and 3D simulations of the Nonlinear Schrodinger equation [Vahala et. al. 2003, 2011, 2012, 2019a, 2019b, 2020, 2020]. Other spinor representations of Maxwell equations were also attempted by Moses (1959), Coffey (2008) and Kulyabov et al. (2017).

The vista for further applications is boundless as the field of electromagnetic wave propagation in different dielectric media, like a 3D magnetized plasma lies before us.
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