

Qubit Lattice Algorithm Simulations of the Scattering of a Bounded Two Dimensional Electromagnetic Pulse from an Infinite Planar Dielectric Interface

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Abstract

Qubit lattice algorithm (QLA) simulations are performed for a two-dimensional (2D) spatially bounded pulse propagating onto a plane interface between two dielectric slabs. QLA is an initial value scheme that consists of a sequence of unitary collision and streaming operators, with appropriate potential operators, that recover Maxwell equations in inhomogeneous dielectric media to second order in the lattice discreteness. For the case of total internal reflection, there is transient energy transfer into the second medium due to the evanescent fields as the Poynting unit vector of the pulse is rotated from its incident to reflected direction. Because of the finite spatial extent of the pulse, a self-consistent Goos-Hanchen-type displacement along the interface is found without imposing any explicit interface boundary conditions on the fields. For normal incidence, the standard Fresnel coefficients are recovered for appropriately averaged QLA fields. Energy is conserved at all times to seven significant figures.

1 Introduction

Recently, we have been developing a qubit lattice algorithm (QLA) for the solution of Maxwell equations in dielectric media [1-6]. In principle, QLA is a quantum-inspired algorithm built from an interleaved sequence of unitary collision and streaming operators that act on a lattice representation of Maxwell equations, recovering the continuum dynamics to second order in the lattice spacing. QLA is not a direct finite difference representation of the field equations themselves. As a quantum algorithm, the QLA representation is ideal for direct encoding on a quantum computer [7-13]. Moreover, it exhibits ideal parallelization to all available cores on classical supercomputers. This efficiency arises because the collision operator acts purely locally at each lattice site, while the streaming operator simply shifts data to neighboring sites. When, spatial gradients in the dielectric medium are present such as interfaces or inhomogeneous regions, additional potential operators have

to be introduced into the collision-streaming sequence. These operators are typically non-unitary but sparse.

Previous QLA simulations [1-4] successfully considered the scattering of a 1D Gaussian pulse from localized dielectric structures. However, for non-local dielectrics the QLA studies were restricted to normal incidence because periodic boundary conditions are applied at the lattice boundaries. It is not straightforward to investigate oblique incidence using this 1D pulse scattering from infinite plasma slab interfaces. In addition, it was determined that for 1D QLA runs to rigorously conserve energy, an asymptotic scaling of the transition region between the two dielectrics is required. Thus, QLA simulations for initial 1D pulses did not permit us to study phenomena like total internal reflection and the Fresnel relations for reflected and transmitted fields. Nevertheless, the study of these incident 1D pulses interacting with small localized 2D and 3D dielectric objects yielded very interesting results [4] on the transient effects of reflections and transmissions from within the dielectric object itself while rigorously conserving the energy.

In the present paper, we consider a QLA for a 2D bounded pulse, where the non-zero domain of the pulse has finite measure in both spatial coordinates, Fig. 1. Specifically, we consider an incident bounded 2D electromagnetic TEM pulse onto a plane interface between two scalar dielectrics with refractive indexes n_1 and n_2 . The plane of incidence is defined by the standard Cartesian (x, y) coordinates with the two dielectric regions $0 \leq x < L, 0 \leq y < L/2$ and $0 \leq x < L, L/2 \leq y < L$. For p -polarization [8], the incident electric field, $\mathbf{E}$, is in the $x - y$ plane and the corresponding magnetic field, $\mathbf{H}$, is in the $-z$ -direction. For the initial 2D pulse we use its natural coordinate system - a rotated Cartesian system (ζ, χ) where the direction of incident propagation is $\hat{\zeta}$, the magnetic field is in the $-\hat{z}$ direction, and the electric field in the $\hat{\chi}$ direction. Thus the incident magnetic field amplitude is (Fig. 1)

$$H_z(\zeta, \chi) = -Exp \left[- \left(\frac{\zeta - \zeta_0}{\zeta_w} \right)^2 - \left(\frac{\chi - \chi_0}{\chi_w} \right)^2 \right] \cos(k\zeta). \quad (1)$$

Here ζ_w defines the extent of the packet in the ζ -direction, and similarly χ_w in the χ -direction. The two coordinate systems are related by the rotation matrix

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} \zeta \\ \chi \end{bmatrix} \quad (2)$$

where θ is the angle of incidence in the (x, y) -plane.

The electric field amplitude $E_\chi(\zeta, \chi)$ is related to the magnetic field amplitude H_z by the impedance of the medium, $Z = E_\chi/H_z$.

In Section 2, QLA simulations are presented which yield transient effects in total internal reflection of the pulse as well as the recovery of the spatial Goos-Hanchen [14] shift of the pulse along the interface. Details of the transient fields generated around the interface region are presented as the incident pulse is steered into the reflected pulse. The Fresnel conditions for normal incidence are considered in Section 3. In all these QLA simulations, total energy is conserved to at least 7 significant figures. For completeness we briefly summarize the QLA operators required to recover the Maxwell equations in the Appendix as well as some quantum information science ideas on how to deal with non-unitary operators for quantum computing.

2 Total Internal Reflection

Consider the electromagnetic propagation of this bounded pulse, Fig. 1, onto a slab dielectric interface at $y = L/2$. For $y < L/2$, the dielectric slab has refractive index $n_1 = 2$ while the

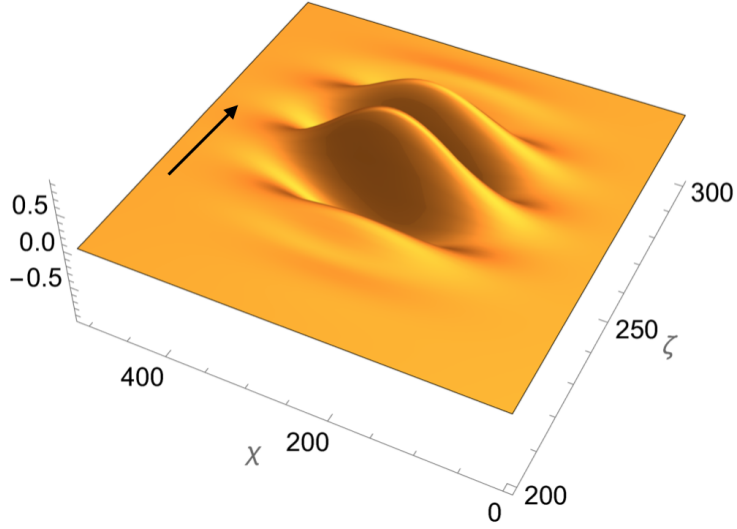


Figure 1: *Initial 2D magnetic field amplitude H_z that is bounded in both ζ and χ . The initial pulse propagates in the ζ -direction in dielectric n_1 , with dispersion relation $\omega/k = c/n_1$. The initial electric field amplitude $E_\chi = Z_1 H_z$. The square lattice has a spatial grid of side $L = 1024$.*

dielectric slab $y \geq L/2$ has refractive index $n_2 = 1$. The critical angle for total internal reflection is $\theta_c = 30^\circ$ [8]. For p-polarization, we first plot the time evolution of the transient energy in each dielectric slab when the angle of incidence $\theta = 25^\circ < \theta_c$ and when $\theta = 35^\circ > \theta_c$. The time-dependent electromagnetic energy in regions $y < L/2$ and $y \geq L/2$ is

$$\mathcal{E}_1(t) = \int_0^{L/2-1} dy \int_0^L dx [\epsilon_0 n_1^2 \mathbf{E}_1^2 + \mu_0 \mathbf{H}_1^2], \quad \mathcal{E}_2(t) = \int_{L/2}^L dy \int_0^L dx [\epsilon_0 n_2^2 \mathbf{E}_2^2 + \mu_0 \mathbf{H}_2^2]. \quad (3)$$

In *QLA*-units, the simulation time t is normalized by a factor $1/c$, where c is the speed of light in vacuum. From Fig. 2, the pulse for time $t < 18k$ remains within the dielectric n_1 , so that $\mathcal{E}_2(t) = 0$. It is important to note that since *QLA* is an initial value algorithm, no boundary or jump conditions are applied at $y = L/2$.

Case 1: $\theta = 25^\circ < \theta_c$

Because the pulse has a finite width, there is a finite interaction time with the dielectric interface during which there is a smooth temporal transition as it splits into transmitted and reflected components, as shown in the energy profiles, $\epsilon_2(25)$ and $\epsilon_1(25)$, of Fig. 2. For $t > 42K$ these pulses then propagate undistorted in their respective dielectric regions.

Case 2: $\theta = 35^\circ > \theta_c$

In our *QLA*-simulations for $\theta = 35^\circ > \theta_c$, we observe total internal reflection for $t > 60k$, with normalized energy $\epsilon_2(35) = 0$ and $\epsilon_1(35) = 1$, Fig. 2. During the intermediate interaction time-window $18k < t < 60K$, the finite pulse width leads to transient evanescent fields in the second dielectric n_2 associated with non-propagating energy transfer which nevertheless contributes to

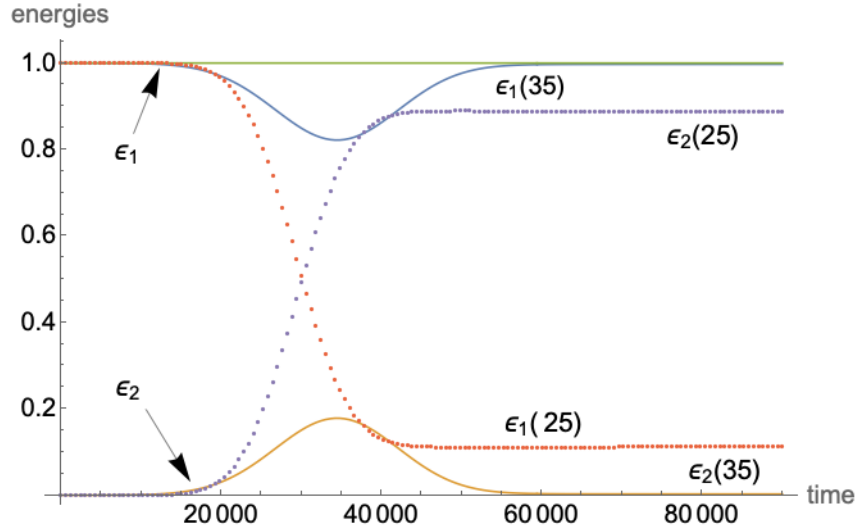


Figure 2: The time evolution of the normalized energy in dielectric n_1 , $\epsilon_1(t) = \mathcal{E}_1(t)/[\mathcal{E}_1(0) + \mathcal{E}_2(0)]$, and in dielectric n_2 , $\epsilon_2(t) = \mathcal{E}_2(t)/[\mathcal{E}_1(0) + \mathcal{E}_2(0)]$ for $\theta = 25^\circ < \theta_c$ - - - dashed curves, and for $\theta = 35^\circ > \theta_c$ - solid curves. At every time output, the total energy, $\mathcal{E}_1(t) + \mathcal{E}_2(t) = \text{const.}$ to the 7th significant figure. In these simulations $L = 1024$. Thus the $\epsilon_1(35)$ -plot is the time evolution of the normalized energy in the refractive index medium $n_1 = 2$ for angle of incidence $\theta = 35^\circ$.

the reflected pulse in the n_1 medium, along with a Goos-Hanchen [14]-like spatial shift along the interface. The time evolution of the $H_z > 0$ part of the profile is presented in Figs 3 and 4.

For $t \approx 30k$, Fig 3(e), there is a symmetry about the interface normal in the structure of the fields together with a peak in the transient total energy in the dielectric medium n_2 , all localized near the interface $y = L/2$, Fig. 2

We also see that there is a π -like phase change in the magnetic field H_z as the incident pulse in $n_1 = 2$ region is reflected from the beginning of the $n_2 = 1$ dielectric region. Figs 3 and 4 only plot the $H_z > 0$ surfaces, while Fig. 5 is a full 2D projection with green for that of the profile having $H_z < 0$ and red for $H_z > 0$. It can be seen that the leading edge of the incident pulse has $H_z < 0$ while the leading edge of the reflected pulse has $H_z > 0$.

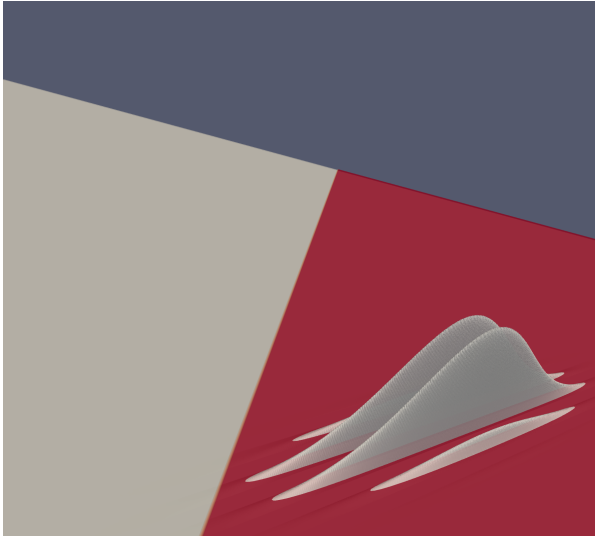
3 Fresnel Conditions for Normal Incidence

We now consider the normal incidence of our electromagnetic pulse from medium n_1 onto medium n_2 , with $n_1 < n_2$. In Fig 6 we plot the total energy reflected and transmitted from the $n_1 - n_2$ interface. For these runs, $n_1 = 1$. As $n_2 > n_1$ the transmitted energy decreases, while the reflected energy increases with the total energy remaining constant to 7 significant figures.

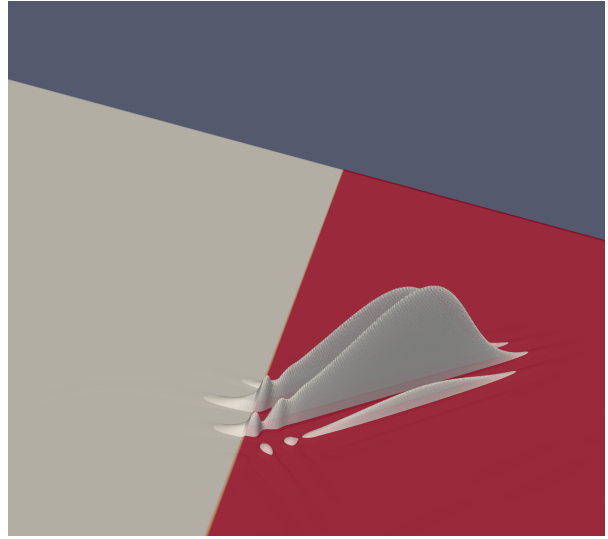
It can be readily shown that the Fresnel conditions for a simple plane wave incident, reflected and transmitted at a plane interface, for p-polarization, satisfy [15]

$$r_E \equiv \frac{E_r}{E_i} = \frac{n_2 - n_1}{n_1 + n_2} \quad , \quad t_E \equiv \frac{E_t}{E_i} = \frac{2n_1}{n_1 + n_2} \quad (4)$$

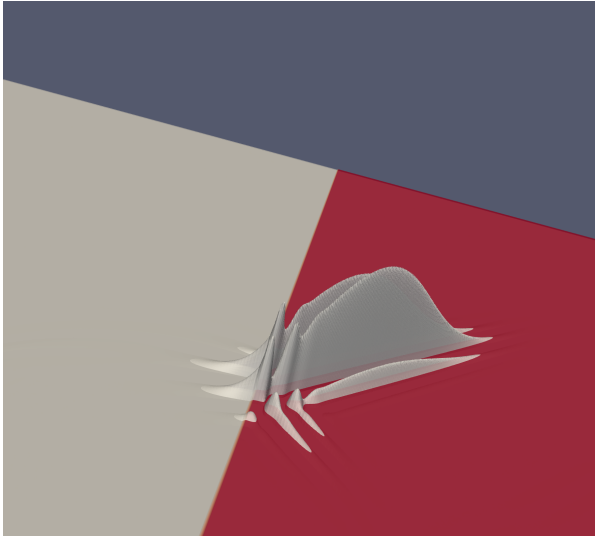
For normal incidence, the p-polarization and s-polarization are equivalent. Thus the reflected and incident electric fields are in opposite directions, so that $E_r/E_t < 0$. From Eq. (4), $(n_2 - n_1)/(n_1 +$



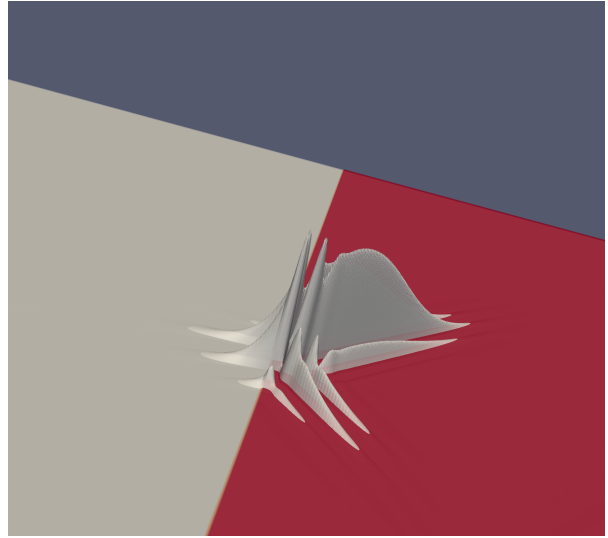
(a) $H_z > 0$ at $t = 0k$



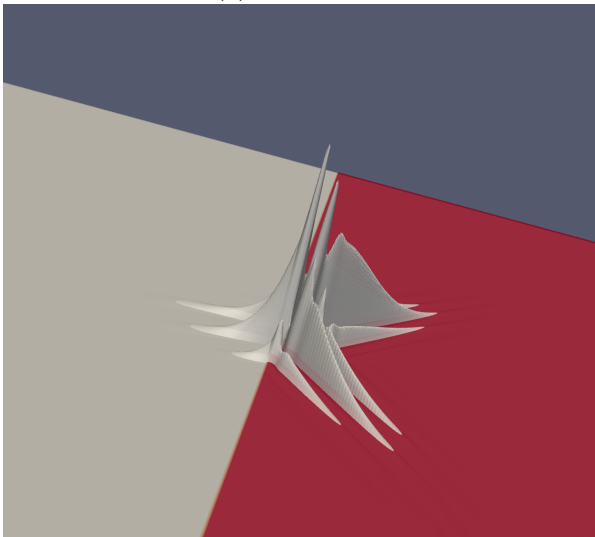
(b) $H_z > 0$ at $t = 12k$



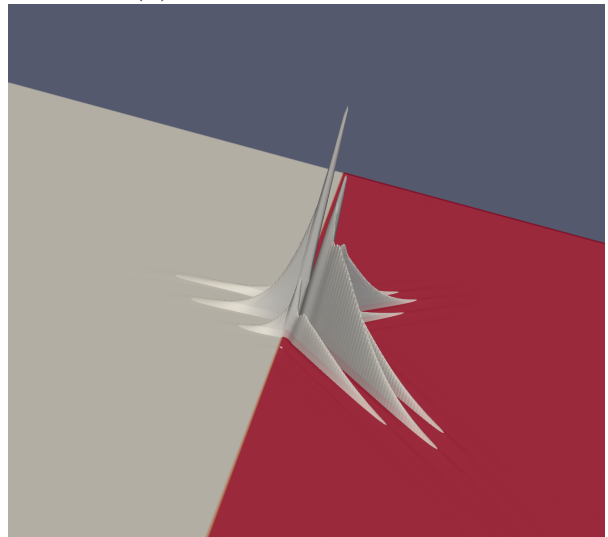
(c) $H_z > 0$ at $t = 18k$



(d) $H_z > 0$ at $t = 24k$



(e) $H_z > 0$ at $t = 30k$



(f) $H_z > 0$ at $t_2 = 36k$

Figure 3: Evolution of the magnetic field $H_z(x, \tilde{y}) > 0$ for $\theta = 35^\circ > \theta_c$. Red: region $n_1 = 2, y < L/2$. Grey: region $n_2 = 1, y \geq L/2$.

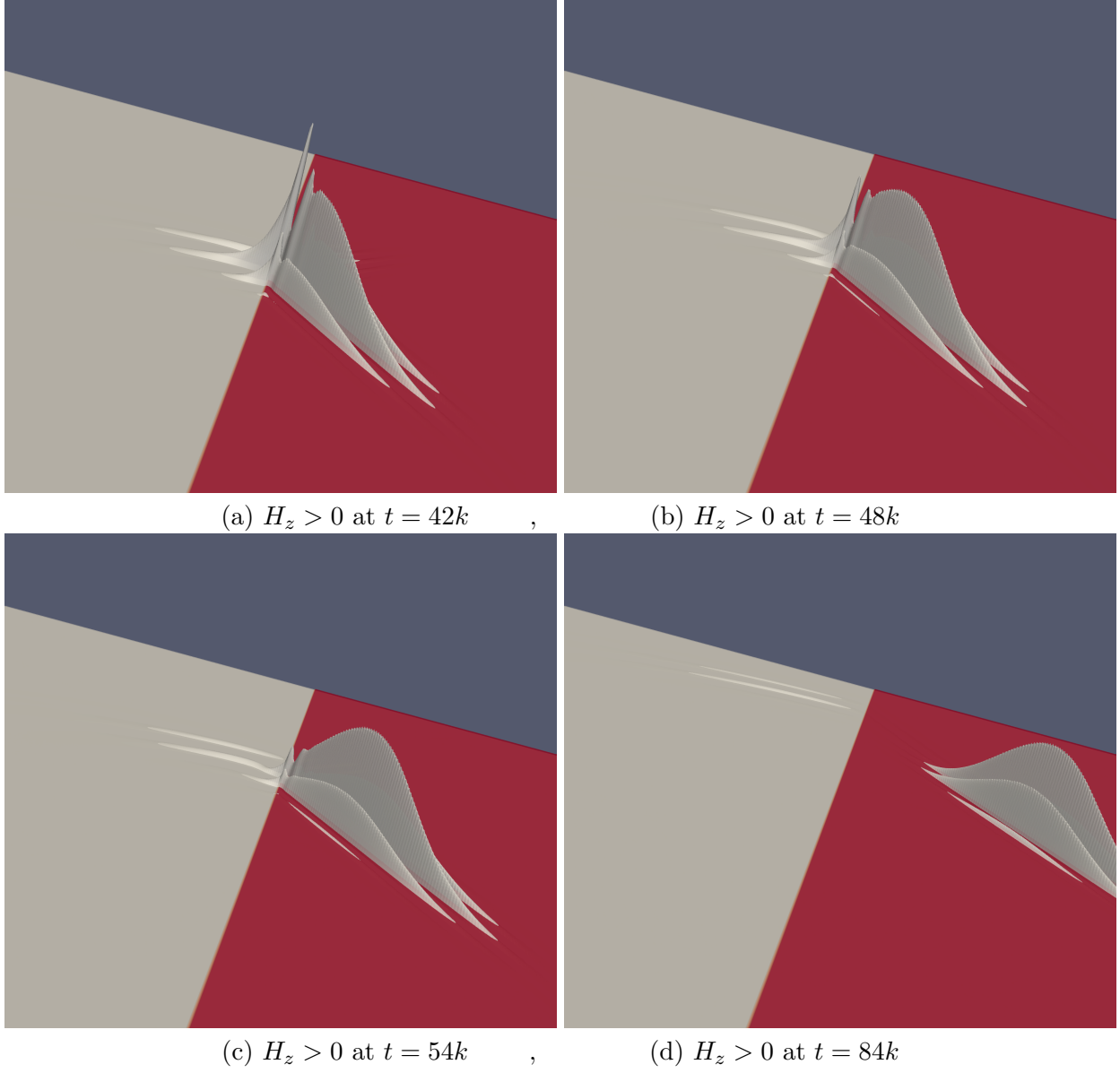
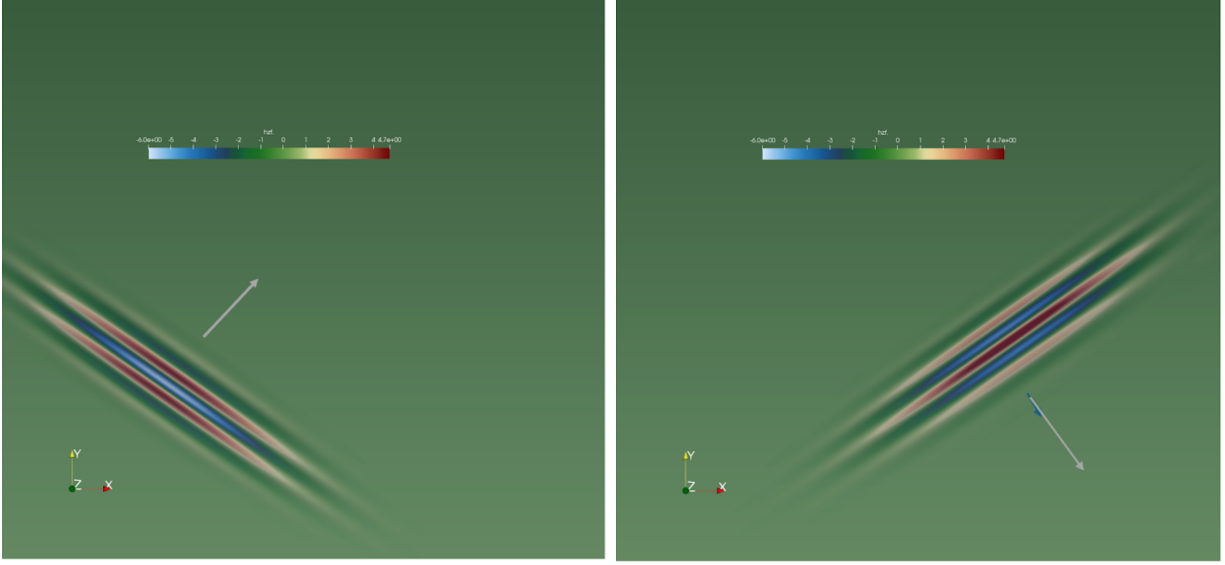


Figure 4: *Evolution of the magnetic field $H_z(x, y) > 0$ for $\theta = 35^\circ > \theta_c$ at later times. Red: region $n_1 = 2, y < L/2$. Grey: region $n_2 = 1, y \geq L/2$. The Goos-Hanchen [9] longitudinal boundary shift is clearly seen on comparing Fig 3b and 4c.*



(a) incident H_z at $t = 0$, (b) reflected H_z at $t = 72k$

Figure 5: (a) The initial magnetic field $H_z(x, y)$ at $t = 0$ as the pulse propagates to the plane dielectric boundary, and (b) the reflected $H_z(x, y)$ at $t = 72k$ as the pulse moves from the dielectric interface. The color coding for the H_z -profile is shown in the horizontal strip: blue-green for $H_z < 0$ and yellow-red for $H_z > 0$.

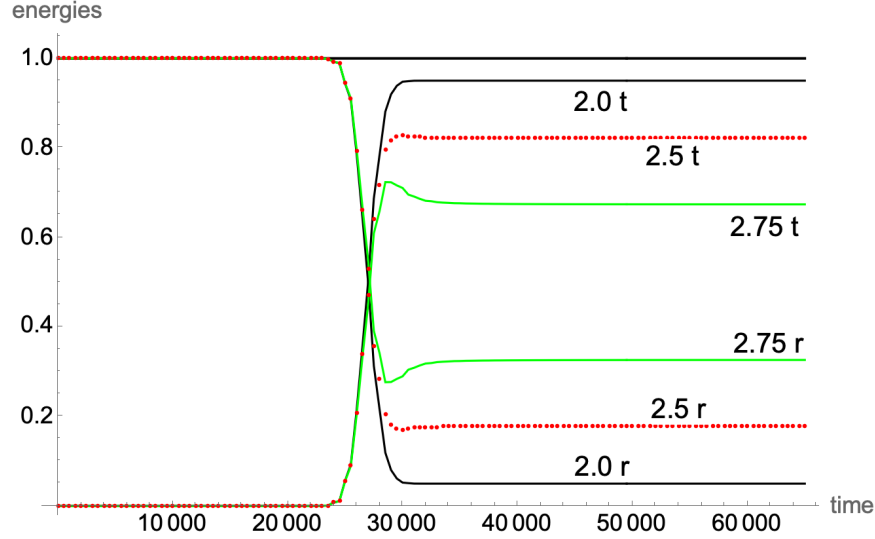


Figure 6: Normal incidence. The time evolution of the normalized reflected "r" and transmitted "t" energy from vacuum ($n_1 = 1$) into 3 different dielectrics $n_2 = 2.0, n_2 = 2.5, n_2 = 2.75$. (Nontrivial plots for time > 25000 when the pulse reaches the plane interface between the two dielectric slabs.) At every time output, the total energy $\mathcal{E}_1(t) + \mathcal{E}_2(t) = \text{const.}$ to the 7th significant figure. In these simulations $L = 1024$ and energies are normalized to the initial pulse total energy $\mathcal{E}_1(0) + \mathcal{E}_2(0) = \text{const.}$ Fig 2 and Fig 6 use different initial pulse locations since the pulse in Fig. 2 has half the speed of that in Fig. 6. The correlation of the time axes in these figures is not straightforward.

$n_2) > 0$ so that the ratio $E_r/E_i < 0$ stays negative. Alternatively, the reflected electric field undergoes a phase change of π when hitting an interface with $n_2 > n_1$.

For the magnetic field, in p-polarization, the incident, reflected, and transmitted fields are all in the same direction with the Fresnel ratio [15]

$$r_H \equiv \frac{H_r}{H_i} = \frac{n_2 - n_1}{n_1 + n_2} \quad , \quad t_H \equiv \frac{H_t}{H_i} = 1 + r_H \quad (5)$$

The QLA calculation of the Fresnel ratio is not straightforward for our initial bounded 2D electromagnetic pulse in its reflection and transmission. Since we are dealing with normal incidence all the propagation is quasi-1D : along the y -axis. We thus determine the position y_m where the corresponding electric and magnetic fields have their maxima and then average the fields over their finite extent in x : e.g, this average for the reflected fields is

$$\langle E_r \rangle = \int_0^L dx E_r(x, y_m) \quad \langle H_r \rangle = \int_0^L dx H_r(x, y_m). \quad (6)$$

Electric Field	r_E analytic	$\langle r_E \rangle_{QLA}$	t_E analytic	$\langle t_E \rangle_{QLA}$
$n_2 = 1.5$	0.2000	0.2119	0.8000	0.7881
$n_2 = 2.0$	0.3333	0.3507	0.6667	0.6493
$n_2 = 2.5$	0.4286	0.4280	0.5714	0.5720
$n_2 = 3.0$	0.5000	0.4916	0.5000	0.5084

Table 1: *The Fresnel coefficients, (4), for Normal Incidence from medium $n_1 = 1$ to various $n_2 > n_1$ dielectrics for the electric field. The QLA calculated Fresnel coefficients are derived using (6).*

Magnetic Field	r_H analytic	$\langle r_H \rangle_{QLA}$	t_H analytic	$\langle t_H \rangle_{QLA}$
$n_2 = 1.5$	0.2000	0.1815	1.200	1.1815
$n_2 = 2.0$	0.3333	0.2975	1.333	1.298
$n_2 = 2.5$	0.4286	0.4329	1.429	1.433
$n_2 = 3.0$	0.5000	0.5237	1.500	1.524

Table 2: *The Fresnel coefficients, (4), for Normal Incidence from medium $n_1 = 1$ to various $n_2 > n_1$ dielectrics for the magnetic field. The QLA calculated Fresnel coefficients are derived using (6).*

In Tables 1 and 2 we determine the Fresnel coefficients for normal incidence. For the incident theoretical plane wave, the Fresnel coefficients are immediately determined from the refractive indices, (4) and (5), with the reflection coefficients equal for the fields: $r_E = r_H$. For the QLA Fresnel coefficients, these are determined directly from the qubit amplitude solutions and then averaging the electric and magnetic field, without explicit references to the refractive indices themselves.

4 Summary and Conclusion

We have been somewhat in a quandary why QLA produces such excellent 2D and 3D scattering results for an incident 1D Gaussian pulse onto small dielectric objects but yet 1D-QLA could not handle the relatively simple textbook problem of 1D normal incidence of a wave packet onto a plane

dielectric slab interface. For this 1D problem, for energy conservation to hold, the 1D-QLA requires the scaling of the interface region to be such that the simulations now model a WKB-like scattering with very little electromagnetic reflection. Here we come to a possible resolution of this dilemma. Instead of restricting ourselves to only 1D, we have introduced a 2D Gaussian wave packet that cuts off in each of these two directions. Hence, even when restricting ourselves to 1D normal incidence, our incident pulse is 2D and thus making the QLA simulation 2D. We now find QLA can readily handle this 1D normal incidence problem and from it we recover the Fresnel conditions on reflection and transmission (and preserving energy conservation to the 7th significant figure).

In our full 2D QLA simulations we considered a p-polarized incident pulse with its $\mathbf{E}_i$ in the plane of incidence. For this polarization the magnetic field has only one component, perpendicular to the plane of incidence. Since QLA is an initial value code, we examined the transient rotation of the incident pulse propagation direction to that of the reflected pulse under total internal reflection. Not only are there transient and spatially concentrated energy spikes in the vicinity of the interface but there is a spatial shift in the pulse center as it hits the dielectric binterface and at which it reflects from the interface. This is clearly related to the Goos-Hanchen effect [15] which arises because of the finite-size of the pulse. In all the simulations reported here, a sharp boundary is assumed between the two dielectric (rather than our usual hyperbolic-tangent buffer region). Finally, we also find a π -like phase shift in the reflected magnetic field. It should be noted that in these simulations $\nabla \cdot \mathbf{H} = 0$ since $\mathbf{H} = H_z(x, y, t)\hat{z}$ while throughout the run $|\nabla \cdot \mathbf{D}|/D_{max} < O(10^{-19})$.

While theoretically one can determine a unitary QLA for the energy-conserving Maxwell equations through a Dyson map [5], it is non-trivial to explicitly determine the required unitary collision and potential operators. Thus for the QLA presented here to be encodable onto a quantum computer one must investigate unitary representations of potential operators like (15) in the Appendix.

Acknowledgments

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Appendix [6]

The time evolving subset of the Maxwell equations for non-magnetic inhomogeneous dielectric media is $\partial \mathbf{B} / \partial t = -\nabla \times \mathbf{E}$, and $\partial \mathbf{D} / \partial t = \nabla \times \mathbf{H}$, with $\mathbf{D} = \epsilon \cdot \mathbf{E}$ and $\mathbf{B} = \mu_0 \mathbf{H}$. The divergence subset

of Maxwell equations can be treated as initial conditions. If one works with the field $\mathbf{u} = (\mathbf{E}, \mathbf{H})^T$ then the matrix Maxwell equations representation

$$i \frac{\partial \mathbf{u}}{\partial t} = \mathbf{W}^{-1} \mathbf{M} \mathbf{u} \quad (7)$$

is non-unitary for inhomogeneous dielectric media since $\mathbf{W}^{-1}$ and $\mathbf{M}$ will no longer commute. Here $\mathbf{W}$ is a Hermitian 6×6 matrix for lossless media and $\mathbf{M}$ the Hermitian curl-matrix operator under standard boundary conditions:

$$\mathbf{W} = \begin{bmatrix} \epsilon_i \mathbf{I}_{3 \times 3} & 0_{3 \times 3} \\ 0_{3 \times 3} & \mu_0 \mathbf{I}_{3 \times 3} \end{bmatrix}, \quad \mathbf{M} = \begin{bmatrix} 0_{3 \times 3} & i \nabla \times \\ -i \nabla \times & 0_{3 \times 3} \end{bmatrix}. \quad (8)$$

where we work in a coordinate system where the Hermitian dielectric tensor is diagonal $\epsilon_i, i = x, y, z$.

There exists a Dyson map [5], [10]-[12]

$$\mathcal{U} = \mathbf{W}^{1/2} \mathbf{u} \quad (9)$$

that yields a unitary evolution for the $\mathcal{U}$ -field even for inhomogeneous dielectric media:

$$i \frac{\partial \mathcal{U}}{\partial t} = \mathbf{W}^{-1/2} \mathbf{M} \mathbf{W}^{-1/2} \mathcal{U} \quad (10)$$

since $\mathbf{W}^{-1/2} \mathbf{M} \mathbf{W}^{-1/2}$ is Hermitian. For non-magnetic materials, (9) is

$$\mathcal{U} = \left(\epsilon_0^{1/2} n_x E_x, \epsilon_0^{1/2} n_y E_y, \epsilon_0^{1/2} n_z E_z, \mu_0^{1/2} \mathbf{H} \right)^T. \quad (11)$$

where (n_x, n_y, n_z) is the vector (diagonal) refractive index, with $\epsilon_i = \epsilon_0 n_i^2, i = x, y, z$, and (10) for 2D $x - y$ spatially dependent fields is

$$\begin{aligned} \frac{\partial q_0}{\partial t} &= \frac{1}{n_x} \frac{\partial q_5}{\partial y}, & \frac{\partial q_1}{\partial t} &= -\frac{1}{n_y} \frac{\partial q_5}{\partial x}, & \frac{\partial q_2}{\partial t} &= \frac{1}{n_z} \left[\frac{\partial q_4}{\partial x} - \frac{\partial q_3}{\partial y} \right] \\ \frac{\partial q_3}{\partial t} &= -\frac{\partial(q_2/n_z)}{\partial y}, & \frac{\partial q_4}{\partial t} &= \frac{\partial(q_2/n_z)}{\partial x}, & \frac{\partial q_5}{\partial t} &= -\frac{\partial(q_1/n_y)}{\partial x} + \frac{\partial(q_0/n_x)}{\partial y}, \end{aligned} \quad (12)$$

with $\mathcal{U} \equiv (q_0, q_1, q_2, q_3, q_4, q_5)^T$.

Qubit Lattice Algorithm (QLA) for Eq. (12)

In moving to a qubit amplitude discrete representation, at this stage, one will need only 3 qubits per lattice site. For the 6 qubit amplitudes $(q_0, q_1, q_2, q_3, q_4, q_5)$. QLA consists of an appropriately chosen sequence of interleaved collision and streaming operators, where the collision operators act only locally at each lattice site while the streaming operators move these entangled amplitudes to neighboring lattice sites. QLA is modular in that each directional derivative can be handled independently. QLA is also perturbative with the lattice step size δ as perturbation parameter.

We now outline how to recover the $\partial/\partial x$ -derivatives in the amplitudes in (12). One sees coupling between the amplitudes $q_1 - q_5$ and between the amplitudes $q_2 - q_4$. We thus choose the unitary collision matrix $\hat{C}_X$ to have the form

$$C_X = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \cos \theta_1 & 0 & 0 & 0 & -\sin \theta_1 \\ 0 & 0 & \cos \theta_2 & 0 & -\sin \theta_2 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & \sin \theta_2 & 0 & \cos \theta_2 & 0 \\ 0 & \sin \theta_1 & 0 & 0 & 0 & \cos \theta_1 \end{bmatrix} \quad (13)$$

where the collision angles θ_1, θ_2 in these couplings are different for medium refractive indices $n_y \neq n_z$. We now stream 2 amplitudes along the x -axis, while keeping the other 4 amplitudes fixed. The appropriate streamed amplitudes are $q_1 - q_4$ and the other set $q_2 - q_5$ thus coupling the two post-collision pairs in $\hat{C}_X$. In particular, we define S_{14}^{x+} to stream the amplitudes q_1 and q_4 one lattice unit in the positive x -direction while keeping the remaining amplitudes q_0, q_2, q_3, q_5 unstreamed. Streaming is simply a shift operator and so is unitary. The final unitary collide-stream sequence for the x -direction is

$$\mathbf{U}_X = S_{25}^{x+} \cdot C_X^\dagger \cdot S_{25}^{x-} \cdot C_X \cdot S_{14}^{x-} \cdot C_X^\dagger \cdot S_{14}^{x+} \cdot C_X \cdot S_{25}^{x-} \cdot C_X \cdot S_{25}^{x+} \cdot C_X^\dagger \cdot S_{14}^{x+} \cdot C_X \cdot S_{14}^{x-} \cdot C_X^\dagger \quad (14)$$

. where $C_X^\dagger$ is the adjoint of C_X .

Similarly to recover the $\partial/\partial y$ derivatives on the amplitudes in (12). One sees that $q_0 - q_5$ are coupled, as are $q_2 - q_3$. The corresponding collision matrix C_Y will introduce a new collision angle θ_0 if dealing with a biaxial medium. The unitary streaming operator in the y -direction will stream the couplet $q_0 - q_3$ and the couplet $q_2 - q_5$ with the other qubits unstreamed.

However, we still need to recover terms that involve spatial derivatives on the refractive indices. In particular to recover the $\partial n_y/\partial x$ term we need to couple amplitudes $q_5 - q_1$, while to recover $\partial n_z/\partial x$ we couple $q_4 - q_2$. The resulting potential matrix is non-unitary with

$$V_X = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -\sin \beta_2 & 0 & \cos \beta_2 & 0 \\ 0 & \sin \beta_0 & 0 & 0 & 0 & \cos \beta_0 \end{bmatrix} \quad (15)$$

Similarly for the corresponding non-unitary V_Y for the recovery of $\partial n_x/\partial y$ and $\partial n_z/\partial y$. Thus the QLA time stepping initial value code evolves as

$$\mathcal{U}(t+1) = V_Y V_X \mathbf{U}_Y \mathbf{U}_X \mathcal{U}(t). \quad (16)$$

Note that one can readily find a weighted sum of unitary matrices to obtain V_X . First consider the simple unitary matrix from the structure of the matrix V_X :

$$U_{0X} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \cos[\beta_0] & 0 & 0 & 0 & -\sin[\beta_0] \\ 0 & 0 & \cos[\beta_2] & 0 & \sin[\beta_2] & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -\sin \beta_2 & 0 & \cos \beta_2 & 0 \\ 0 & \sin \beta_0 & 0 & 0 & 0 & \cos \beta_0 \end{bmatrix} \quad (17)$$

Another unitary matrix constructed from the structure of V_X , but which would eliminate the new off-diagonal elements in U_{0X} is U_{1X} :

$$U_{1X} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\cos[\beta_0] & 0 & 0 & 0 & \sin[\beta_0] \\ 0 & 0 & -\cos[\beta_2] & 0 & -\sin[\beta_2] & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -\sin \beta_2 & 0 & \cos \beta_2 & 0 \\ 0 & \sin \beta_0 & 0 & 0 & 0 & \cos \beta_0 \end{bmatrix} \quad (18)$$

so that the weighted sum of the unitary matrices $(U0_X + U1_X)/2$ yields

$$\frac{1}{2}(U0_X + U1_X) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -\sin \beta_2 & 0 & \cos \beta_2 & 0 \\ 0 & \sin \beta_0 & 0 & 0 & 0 & \cos \beta_0 \end{bmatrix}. \quad (19)$$

On comparing (19) with (15), one needs to find a weighted sum of unitary diagonal matrices to recover just the missing diagonal elements in (19). These two unitary diagonal matrices are simply the identity matrix $U2_X$ and $U3_X$:

$$U2_X = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad \text{and} \quad U3_X = \begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}. \quad (20)$$

Thus the LCU's to recover the potential operator V_X , (15), is

$$V_X = \frac{1}{2} [U0_X + U1_X + U2_X + U3_X]. \quad (21)$$

One finds a similar LCU decomposition of the external potential operator V_Y . Much work has been done in quantum computing in representing LCUs [16]-[19].

The LCU decomposition process is not unique. For example, one could analytically determine the Singular Value Decomposition of V_X into a product of 3 matrices, $V_X = UU.DD.VV$ where UU and VV are unitary and DD is non-unitary but diagonal. By renormalizing the DD -matrix by its maximal eigenvalue the resulting diagonal elements will have a maximal value of 1. This resulting matrix can be immediately split into the sum of 2 unitary operators.

The required 2D Maxwell equations (12) are recovered from our QLA sequence of operators provided the collision and external operator matrices are chosen:

$$\theta_0 = \frac{\delta}{4n_x}, \quad \theta_1 = \frac{\delta}{4n_y}, \quad \theta_2 = \frac{\delta}{4n_z}, \quad (22)$$

and

$$\beta_0 = \delta^2 \frac{\partial n_y / \partial x}{n_y^2}, \quad \beta_1 = \delta^2 \frac{\partial n_x / \partial y}{n_x^2}, \quad \beta_2 = \delta^2 \frac{\partial n_z / \partial x}{n_z^2}, \quad \beta_3 = \delta^2 \frac{\partial n_z / \partial y}{n_z^2} \quad (23)$$

on using symbolic manipulations. Note the ordering of these angles in the perturbation parameter

δ . Indeed, on passing to the continuum limit we recover the following equations

$$\begin{aligned}
\frac{\partial q_0}{\partial t} &= \frac{\delta^2}{\Delta t} \frac{1}{n_x} \frac{\partial q_5}{\partial y} + O\left(\frac{\delta^4}{\Delta t}\right) \\
\frac{\partial q_1}{\partial t} &= -\frac{\delta^2}{\Delta t} \frac{1}{n_y} \frac{\partial q_5}{\partial x} + O\left(\frac{\delta^4}{\Delta t}\right) \\
\frac{\partial q_2}{\partial t} &= \frac{\delta^2}{\Delta t} \frac{1}{n_z} \left[\frac{\partial q_4}{\partial x} - \frac{\partial q_3}{\partial y} \right] + O\left(\frac{\delta^4}{\Delta t}\right) \\
\frac{\partial q_3}{\partial t} &= -\frac{\delta^2}{\Delta t} \left[\frac{1}{n_z} \frac{\partial q_2}{\partial y} - \frac{\partial n_z / \partial y}{n_z^2} q_2 \right] + O\left(\frac{\delta^4}{\Delta t}\right) \\
\frac{\partial q_4}{\partial t} &= \frac{\delta^2}{\Delta t} \left[\frac{1}{n_z} \frac{\partial q_2}{\partial x} - \frac{\partial n_z / \partial x}{n_z^2} q_2 \right] + O\left(\frac{\delta^4}{\Delta t}\right) \\
\frac{\partial q_5}{\partial t} &= \frac{\delta^2}{\Delta t} \left[-\frac{1}{n_y} \frac{\partial q_1}{\partial x} + \frac{\partial n_y / \partial x}{n_y^2} q_1 + \frac{1}{n_x} \frac{\partial q_0}{\partial y} - \frac{\partial n_x / \partial y}{n_x^2} q_0 \right] + O\left(\frac{\delta^4}{\Delta t}\right)
\end{aligned} \tag{24}$$

which recover (12) under diffusion ordering ($\Delta t \approx \delta^2$) to second order in δ .

It is a nontrivial task to determine a QLA that is fully unitary. A non-unitary QLA creates no obstacle for its extreme parallelization on classical supercomputers.

Conservation of Instantaneous Total Electromagnetic Energy

The total electromagnetic energy $\mathcal{E}(t)$ for our Maxwell equations is a constant of the motion. In Dyson variables, $\mathcal{U}$, (11),

$$\mathcal{E}(t) = \int_0^L \int_0^L dx dy [\epsilon_0(n_x^2 E_x^2 + n_y^2 E_y^2 + n_z^2 E_z^2) + \mu_0 \mathbf{H}^2] = \|\mathcal{U}\|^2 = \text{const.} \tag{25}$$

where the total system is in a square box of length L . However, since our current QLA is not fully unitary, this energy must be monitored in our simulations $\mathcal{E}_{QLA}(t)$ since it is not a constant of the motion. We find in all the simulations reported in Sec. 2 and 3, the energy $\mathcal{E}_{QLA}(t)$ was indeed a constant.

Unitary representation of LCUs [20]

The state of a qubit is a linear combination of two orthogonal states $|0\rangle$ and $|1\rangle$. In matrix representation

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{26}$$

Here we shall discuss how to determine a unitary algorithm to determine the sum of qubit states $|q_0\rangle - a|q_1\rangle$. This can then be generalized to handle LCUs. Let unitary operators U and V be such that on the $|0\rangle$

$$U|0\rangle = |q_0\rangle, \quad V|0\rangle = |q_1\rangle. \tag{27}$$

Consider the initial state of the 2-qubit system to be $|00\rangle = |0\rangle \otimes |0\rangle$, where $\otimes$ is the tensor product. Now apply the rotation matrix $R(\phi)$ to the first qubit (reading from right to left of $|00\rangle$)

$$R(\phi)|0\rangle = \begin{bmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} \cos \phi \\ \sin \phi \end{bmatrix} = \cos \phi |0\rangle + \sin \phi |1\rangle \tag{28}$$

so that

$$R(\phi) |00\rangle = |0\rangle \otimes (\cos \phi |0\rangle + \sin \phi |1\rangle) \quad (29)$$

We now apply the U -matrix on the second qubit $|0\rangle$ provided the first qubit is $|0\rangle$, and V -matrix also on the second qubit $|0\rangle$ provided the first qubit is $|1\rangle$. Thus

$$U V R(\phi) |00\rangle = \cos \phi |q_0 0\rangle + \sin \phi |q_1 1\rangle. \quad (30)$$

Now apply the Hadamard gate, H , on the first qubit of (30), where

$$H |0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \quad , \quad H |1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) \quad (31)$$

so that with a little rearranging one obtains

$$H U V R(\phi) |00\rangle = \frac{\cos \phi |q_0\rangle + \sin \phi |q_1\rangle}{\sqrt{2}} \otimes |0\rangle + \cos \phi \frac{|q_0\rangle - \tan \phi |q_1\rangle}{\sqrt{2}} \otimes |1\rangle. \quad (32)$$

Thus, applying the 4 unitary operators on the $|00\rangle$ we obtain for the second qubit the desired state $|q_0\rangle - a |q_1\rangle$, provided the rotation angle ϕ is such that $\tan \phi = a$. We can uncouple this desired state from (32) by applying the non-unitary projection operator $P = |1\rangle \langle 1|$ on the first qubit of (32) since $\langle 1|0\rangle = 0$. Extending this to the linear combination of unitaries, we can determine a unitary set of operators which will, with some probability, recovery the desired LCU sum.