Quantum simulation of dissipation for Maxwell equations in dispersive media

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Abstract

The dissipative character of an electromagnetic medium breaks the unitary evolution structure that is present in lossless, dispersive optical media. In dispersive media, dissipation appears in the Schrödinger representation of Maxwell equations as a sparse diagonal operator occupying an r-dimensional subspace. A first order Suzuki-Trotter approximation for the evolution operator enables us to isolate the non-unitary operators (associated with dissipation) from the unitary operators (associated with lossless media). The unitary operators can be implemented through qubit lattice algorithm (QLA) on n qubits, based on the discretization and the dimensionality of the pertinent fields. However, the non-unitary-dissipative part poses a challenge both physically and computationally on how it should be implemented on a quantum computer. In this paper, two dilation algorithms are considered for handling the dissipative operators. The first algorithm is based on treating the classical dissipation as a linear amplitude damping-type completely positive trace preserving (CPTP) quantum channel where an unspecified environment interacts with the system of interest and produces the non-unitary evolution. Therefore, the combined system-environment is now closed, and must undergo unitary evolution in the dilated space. The unspecified environment can be modeled by just one ancillary qubit, resulting in an implementation scaling of $O(2^{n-1}n^2)$ elementary gates for the total system-environment unitary evolution operator. The second algorithm approximates the non-unitary operators by the Linear Combination of Unitaries (LCU). On exploiting the diagonal structure of the dissipation, we obtain an optimized representation of the non-unitary part, which requires $O(2^n)$ elementary gates. A connection of our results with the non-linear-in-normalization-only (NINO) quantum channels is also presented.

Keywords: Maxwell equations, Dissipation, Non-unitary dynamics, Quantum channels, Unitary dilation method, Quantum simulation.

1. Introduction

Electromagnetic waves are ubiquitous in natural and artificial environments and play a useful role in a variety of applications ranging from communications to heating of thermonuclear fusion plasma. The propagation of waves through different dielectric and magnetic media is usually studied using computational models, the implementation of which on classical computers is not cost effective either in terms of available resources or in computational run time. However, the possibility that quantum computers could overcome the limitations of classical computing [1, 2] has been the motivation behind research on the application of quantum information science (QIS) to traditionally classical fields. In this direction, Maxwell equations, which mediate the physics of propagation and scattering of electromagnetic waves in complex media, are appropriate for quantum implementation due to their linear nature and that can be recast into a form that is similar to the Dirac or Schrödinger equations of quantum mechanics [3–6]. Recent studies on a fully unitary representation of Maxwell equations in a simple dielectric have been the basis of qubit lattice algorithms (QLA) suitable for implementing on quantum computers [6–9].

Current quantum computers are optimized to unitary operations. Such operators naturally occur for closed quantum systems obeying the Schrödinger equation

$$i\frac{\partial |\psi\rangle}{\partial t} = \hat{H}(\boldsymbol{r})\,|\psi\rangle \quad \text{with} \quad \hat{H} = \hat{H}^{\dagger}. \tag{1}$$

where $|\psi\rangle$ is the wave function and $\hat{H}$ is the Hermitian generator of dynamics. Time evolution of $|\psi\rangle$ is,

$$|\psi(t)\rangle = \hat{\mathcal{U}}\,|\psi(0)\rangle\,, \tag{2}$$

where $\hat{\mathcal{U}} = \exp\{-it\hat{H}\}$ is the unitary evolution operator. For simplicity we assume $\hat{H}$ to be time-independent.

Classical, linear and energy conserving systems admit a Schrödinger representation analogous to Eq.(1), where unitary evolution corresponds to energy conservation. Then, it is possible to simulate the classical unitary dynamics through a series of unitary quantum gates in pursuit of higher computational efficiency compared to classical algorithms.

However, realistic systems exhibit dissipation (energy loss), prohibiting a straightforward application to quantum computers. For these classical systems the Schrödinger-like evolution equation is still valid but the generator of the dynamics is now non-Hermitian, $\hat{H} \neq \hat{H}^{\dagger}$, and possibly time-dependent, breaking the unitary evolution.

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Quantum systems which include dissipation and decoherence due to interactions with an environment are classified as open systems. In QIS, open systems can be studied using Kraus representation for the evolution of the open system density matrix ρ_S [10],

$$\rho_S(t) = \sum_\mu \hat{K}_\mu \rho_S(0) \hat{K}_\mu^\dagger, \quad \sum_\mu \hat{K}_\mu^\dagger \hat{K}_\mu = I, \tag{3}$$

For an open system interacting with a stationary environment density matrix $\rho_E = |e_0\rangle\langle e_0|$, the Kraus operators can be defined as,

$$\hat{K}_\mu = \langle \mu | \hat{\mathcal{U}}_{S+E} | e_0 \rangle, \tag{4}$$

where $\hat{\mathcal{U}}_{S+E}$ in Eq.(4) is the unitary evolution operator for the closed, composite system-environment $\rho_S \otimes \rho_E$. The representation in Eq.(3) is completely positive (CP), trace preserving (TP), and can always describe the time-dependent density matrix of an open system ρ_S [11].

In recent years, the concept of dilation theory of operators has been used to embed the non-unitary evolution of open quantum systems into the unitary framework appropriate for quantum computers [12–14]. In these studies, a non-unitary operator is considered as a projection of a unitary operator in an extended Hilbert space [15]. This extension of the Hilbert space requires introducing ancillary qubits in order to appropriately represent the extended closed system. Following this line of thought, the authors in Refs.[16–18] have proven that Maxwell equations in a passive, dissipative and dispersive medium have a Hermitian Schrödinger structure, as in Eq.(1), by extending the Hilbert space of the primary electromagnetic fields $\boldsymbol{E}, \boldsymbol{H}$ with appropriate set of auxiliary fields that are derived using functional analysis techniques. However, the resulting Hermitian Hamiltonian operator $\hat{H}$ has a complex structure that is not suitable for implementing on a quantum computer. Therefore, for a quantum implementation of Maxwell equations in lossy and dispersive media a quantum representation that is compatible with the principles of QIS is required.

In this paper, we develop probabilistic dilation algorithms for simulating electromagnetic wave propagation in dissipative and dispersive electromagnetic media by expressing the non-unitary Suzuki-Trotter evolution of Maxwell equations within the framework of quantum channels.

In Sec. 2.1, we formulate a quantum Schrödinger equation representation of Maxwell equations in dispersive media by introducing auxiliary electromagnetic fields which are related to the wave polarization and to the polarization density current. In Sec. 2.2, we examine the appearance of dissipation in the Maxwell-Schrödinger equation which leads to an anti-Hermitian component within the Hamiltonian, generating non-unitary Suzuki-Trotter evolution dynamics.

In Sec. 3 we formulate the classical electromagnetic dissipation as a post-selective augmented quantum amplitude damping-type channel [13]. The respective set of Kraus operators form the basis of the dilation model with one ancillary qubit as the environmental state. In Secs. 3.1 and 3.2, a quantum circuit for the probabilistic simulation of dissipative dynamics is presented along with the implementation scaling for the system-environment unitary operator into elementary quantum gates. Considerations about the simulation error ε of the total evolution and the connection with the optimal time step and success probability are discussed. Section 3.3 provides insights on an alternative deterministic, evaluation of the non-unitary dynamics based on the positive only non-linear quantum channels. We consider some expected outcomes from this approach.. Finally, in Sec. 4, we show the means to reduce the implementation cost of the dilated unitary evolution of dissipative systems using the LCU method.

2. Quantum representation of Maxwell equations in dispersive media

We consider a six-vector formulation of the electromagnetic fields $\boldsymbol{u} = (\boldsymbol{E}, \boldsymbol{H})^T$ and their respective intensities $\boldsymbol{d} = (\boldsymbol{D}, \boldsymbol{B})^T$ given by constitutive equations for a general dispersive medium [6],

$$\boldsymbol{d}(\boldsymbol{r}, t) = \hat{W}(\boldsymbol{r})\boldsymbol{u}(\boldsymbol{r}, t) + \int_0^t \hat{G}(\boldsymbol{r}, t-\tau)\boldsymbol{u}(\boldsymbol{r}, \tau). \tag{5}$$

The instantaneous optical response of the medium is given by the 6×6 matrix $\hat{W} = diag(\epsilon(\boldsymbol{r}), \mu(\boldsymbol{r}))$. The susceptibility kernel $\hat{G}$ yields the linear dispersive response of the medium, accounting for both dissipation and memory effects.

The corresponding source-free Maxwell equations are,

$$\boldsymbol{\nabla} \cdot \boldsymbol{d}(\boldsymbol{r}, t) = 0, \quad i\frac{\partial \boldsymbol{d}(\boldsymbol{r}, t)}{\partial t} = \hat{M}\boldsymbol{u}(\boldsymbol{r}, t), \tag{6}$$

where the Maxwell operator $\hat{M}$,

$$\hat{M} = i\begin{bmatrix} 0 & \boldsymbol{\nabla}\times \\ -\boldsymbol{\nabla}\times & 0 \end{bmatrix} \tag{7}$$

is Hermitian in $L^2(\mathcal{V} \subseteq \mathbb{R}^3, \mathbb{C})$ under the imposed Dirichlet boundary condition,

$$\boldsymbol{n}(\boldsymbol{r}) \times \boldsymbol{u}_1 = 0 \text{ on the boundary } \partial\mathcal{V}, \tag{8}$$

where $\boldsymbol{n}$ is the outward pointing normal at the boundary. The form of the constitutive relation (5) satisfies five physical postulates [19]: determinism, linearity, causality, locality in space, and invariance under time translations. In an inhomogeneous and dispersion-less medium, the unitary form of Maxwell equations has been obtained in [6].

For a medium that is dispersive and dissipative and is described by a scalar permittivity and permeability, the general constitutive relations in the frequency domain are [18],

$$\epsilon(\boldsymbol{r}, \omega) = \epsilon_0\Big(1 + \sum_{l=1}^{N_e} \frac{\Omega_{e,l}^2(\boldsymbol{r})}{\omega_{e,l}^2(\boldsymbol{r}) - i\gamma_{e,l}(\boldsymbol{r})\omega - \omega^2}\Big), \tag{9}$$

$$\mu(\boldsymbol{r}, \omega) = \mu_0\Big(1 + \sum_{l=1}^{N_m} \frac{\Omega_{m,l}^2(\boldsymbol{r})}{\omega_{m,l}^2(\boldsymbol{r}) - i\gamma_{m,l}(\boldsymbol{r})\omega - \omega^2}\Big). \tag{10}$$

Equations (9) and (10) describe the phenomenological Lorentz oscillator response model of bound charges in materials. Ω_e

and Ω_m are the characteristic frequencies of the oscillator, whereas ω_e, ω_m are the resonant frequencies. Finally, the $\gamma_{e,l}(\boldsymbol{r})$, $\gamma_{m,l}(\boldsymbol{r}) \geq 0$ are the relaxation-dissipation rates. If $\gamma_e = 0$ and $\gamma_m = 0$, the medium is dispersive but lossless and for $\omega_e = 0$ and $\omega_m = 0$, we retrieve the Drude model for a simple metal. The connection between the susceptibility kernel $\hat{G}$ in Eq.(5) and the constitutive relations (9),(10) in the frequency domain is,

$$\hat{G}(\boldsymbol{r},t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\begin{bmatrix}\epsilon(\boldsymbol{r},\omega)-\epsilon_0 & 0\\ 0 & \mu(\boldsymbol{r},\omega)-\mu_0\end{bmatrix}e^{-i\omega t}\,d\omega \quad (11)$$

Below, in Sec. 2.1, we re-express the time dependent Maxwell equations (6) for a Lorentz medium as a Schrödinger equation with Hermitian structure. When the medium is lossless, the unitary evolution, as expected, represents the conservation of the electromagnetic energy. The effect of dissipation is considered in Sec. 2.2.

2.1. *Schrödinger representation of Maxwell equations in a lossless Lorentz medium*

We define the following auxiliary fields [18],

$$\mathbb{P}_l(\boldsymbol{r},t) = \frac{1}{2\pi}\int_0^t\int_{-\infty}^{\infty}\frac{e^{-i\omega(t-\tau)}}{\omega_{e,l}^2-\omega^2}\boldsymbol{E}(\boldsymbol{r},\tau)d\,\omega d\,\tau, \quad (12)$$

and,

$$\mathbb{M}_l(\boldsymbol{r},t) = \frac{1}{2\pi}\int_0^t\int_{-\infty}^{\infty}\frac{e^{-i\omega(t-\tau)}}{\omega_{m,l}^2-\omega^2}\boldsymbol{H}(\boldsymbol{r},\tau)d\,\omega d\,\tau \quad (13)$$

which are related to the electric $\boldsymbol{P}$ and magnetic $\boldsymbol{M}$ polarizability of the medium,

$$\boldsymbol{P}(\boldsymbol{r},t) = \epsilon_0\sum_{l=1}^{N_e}\Omega_{e,l}^2\mathbb{P}_l, \quad \boldsymbol{M}(\boldsymbol{r},t) = \mu_0\sum_{l=1}^{N_m}\Omega_{m,l}^2\mathbb{M}_l. \quad (14)$$

Maxwell equations (6), together with the evolution equations for the auxiliary fields (12),(13) yield the following closed system of partial differential equations,

$$\begin{aligned} i\frac{\partial\boldsymbol{u}}{\partial t} &= \hat{W}_0^{-1}\hat{M}\boldsymbol{u} - i\sum_{l=1}^{N}\hat{\Omega}_l^2\boldsymbol{\mathcal{P}}_{l,t},\\ i\frac{\partial\boldsymbol{\mathcal{P}}_l}{\partial t} &= i\boldsymbol{\mathcal{P}}_{l,t}, \qquad l=1,2...N,\\ i\frac{\partial\boldsymbol{\mathcal{P}}_{l,t}}{\partial t} &= i\boldsymbol{u} - i\hat{\omega}_l^2\boldsymbol{\mathcal{P}}_l, \qquad l=1,2...N, \end{aligned} \quad (15)$$

where $\boldsymbol{u} = (\boldsymbol{E},\boldsymbol{H})^T$, $\boldsymbol{\mathcal{P}}_l = (\mathbb{P}_l,\mathbb{M}_l)^T$, $N = max\{N_e,N_m\}$, and the diagonal matrices $\hat{\Omega}_l^2$ and $\hat{\omega}_l^2$ are,

$$\hat{\Omega}_l^2 = \begin{bmatrix}\Omega_{e,l}^2 & 0\\ 0 & \Omega_{m,l}^2\end{bmatrix}, \quad \hat{\omega}_l^2 = \begin{bmatrix}\omega_{e,l}^2 & 0\\ 0 & \omega_{m,l}^2\end{bmatrix}. \quad (16)$$

Upon applying the Dyson transform [6],

$$\hat{\rho} = diag(\hat{W}_0^{1/2}, \hat{W}_0^{1/2}\hat{\Omega}_l\hat{\omega}_l, W_0^{1/2}\hat{\Omega}_l), \quad (17)$$

to Eq.(15), we obtain a Hermitian Maxwell-Schrödinger representation,

$$i\frac{\partial}{\partial t}\begin{bmatrix}\hat{W}_0^{1/2}\boldsymbol{u}\\ \hat{W}_0^{1/2}\hat{\Omega}_l\hat{\omega}_l\boldsymbol{\mathcal{P}}_l\\ W_0^{1/2}\hat{\Omega}_l\boldsymbol{\mathcal{P}}_{l,t}\end{bmatrix} = \begin{bmatrix}c\hat{M} & 0 & -i\hat{\Omega}_l\\ 0 & 0 & i\hat{\omega}_l\\ i\hat{\Omega}_l & -i\hat{\omega}_l & 0\end{bmatrix}\begin{bmatrix}W_0^{1/2}\boldsymbol{u}\\ \hat{W}_0^{1/2}\hat{\Omega}_l\hat{\omega}_l\boldsymbol{\mathcal{P}}_l\\ W_0^{1/2}\hat{\Omega}_l\boldsymbol{\mathcal{P}}_{l,t}\end{bmatrix}, \quad (18)$$
$l = 1,2,...,N.$

This evolution equation can be compactly written as,

$$i\frac{\partial\boldsymbol{\psi}}{\partial t} = \hat{D}_0\boldsymbol{\psi}, \quad \hat{D}_0 = \hat{D}_0^{\dagger}, \quad (19)$$

with the initial condition $\boldsymbol{\psi}_0 = (\hat{W}_0^{1/2}\boldsymbol{u}_0, 0, 0)^T$. The state vector $\boldsymbol{\psi}$ includes all the physically relevant electromagnetic fields that are necessary to understand propagation and scattering of waves in a lossless Lorentz medium. A generalization of Eq.(18) to a tensorial Lorentz medium can be found in [20].

A quantum implementation of unitary evolution operator $\exp\{-it\hat{D}_0\}$ that results from Eq.(19), has been delineated in [21] for the special case of magnetized plasma based on a qubit lattice algorithm (QLA). A QLA consists of an interleaved sequence of non-commuting collision $\hat{C}$ and streaming $\hat{S}$ operators that recover the Maxwell-Schrödinger equation (18) to second order diffusion scheme $\delta t \sim \delta^2$, $\delta\boldsymbol{r} = (\delta x, \delta y, \delta z) \sim \delta$. We define δ to be the Cartesian grid spacing between the (N_x, N_y, N_z) number of grid points along the principal axes that cover the entire domain Ω.

We express the state vector $\boldsymbol{\psi}$, as a n-qubit superposition state, where $n = \log_2 d$ and $d = (6+12N)N_xN_yN_z$ is the dimensionality of the state after discretization. The total number of qubits n can be divided into two registers of $n_q = \log_2(6+12N)$ and $n_p = \log_2(N_xN_yN_z)$ qubits, representing the amplitude and spatial gridding, respectively. The advantage of QLA implementation is that the collision operators $\hat{C}$, for the homogeneous case, act only locally as controlled rotations on the amplitude n_p register; hence their implementation cost is $O(n_q^2) = constant$, whereas the streaming $\hat{S}$ operators can be considered as a quantum walk in the n_p register that can be implemented in $O(n_p^2)$ single qubit and contolled-NOT (CNOT) operations [6, 22].

The unitary evolution of Eq.(19) leads to the conservation of the extended electromagnetic energy E_{total} which is the norm of the state vector $\|\boldsymbol{\psi}\|^2$,

$$\begin{aligned} E_{total}(t) &= \frac{1}{2}\|\boldsymbol{\psi}\|^2 = \frac{1}{2}\hat{W}_0\int_{\Omega}\|\boldsymbol{u}\|^2 d\,\boldsymbol{r}\\ &+ \frac{1}{2}\hat{W}_0\sum_{l=1}^{N}\int_{\Omega}\hat{\Omega}_l^2\left(\hat{\omega}_l^2\|\boldsymbol{\mathcal{P}}_l\|^2 + \left\|\boldsymbol{\mathcal{P}}_{l,t}\right\|^2\right)d\,\boldsymbol{r}. \end{aligned} \quad (20)$$

The first term on the right hand side of (20) is the vacuum electromagnetic energy,

$$E_{el}(t) = \frac{1}{2}\int_{\Omega}\epsilon_0\left(\|\boldsymbol{E}\|^2 + \mu_0\|\boldsymbol{H}\|^2\right)d\,\boldsymbol{r} \leq E_{total}(0) = E_{el}(0). \quad (21)$$

Energy expression (20) is valid beyond the plane-wave, harmonic and semi-harmonic approximations for the fields as imposed by Landau and Brillouin [23].

2.2. Dissipative Medium

For a dissipative medium, in Eqs.(9) and (10) $\gamma_{e,l} \geq 0$ and $\gamma_{m,l} \geq 0$. Consequently, the denominators in Eqs.(12) and (13) include the appropriate factors of $-i\gamma_{e,l}$ and $-i\gamma_{m,l}$, respectively. As a result, the Hermitian structure of the Schrödinger evolution equation (19) is lost. While the first two Maxwell equations in (15) are not affected by dissipation, the third equation reads,

$$i\frac{\partial \boldsymbol{\mathcal{P}}_{l,t}}{\partial t} = i\boldsymbol{u} - i\hat{\omega}_l^2\boldsymbol{\mathcal{P}}_l - i\hat{\gamma}_l\boldsymbol{\mathcal{P}}_{l,t}, \qquad l = 1, 2...N, \tag{22}$$

where,

$$\hat{\gamma}_l = \begin{bmatrix} \gamma_{e,l} & 0 \\ 0 & \gamma_{m,l} \end{bmatrix}. \tag{23}$$

The dissipative counterpart to Eq.(19) has the form,

$$i\frac{\partial \boldsymbol{\psi}}{\partial t} = [\hat{D}_0 - i\hat{D}_{diss}]\boldsymbol{\psi}. \tag{24}$$

The diagonal matrix $\hat{D}_{diss} = diag(0, 0, \hat{\gamma}_l)$ is Hermitian and positive definite ($\gamma_{e,l} \geq 0$ and $\gamma_{m,l} \geq 0$) so the anti-Hermitian term $-i\hat{D}_{diss}$ is purely dissipative. As a consequence, the generator of the dynamics in Eq.(24) is non-Hermitian so that the evolution operator $\hat{\mathcal{U}}(t) = \exp\{-it[\hat{D}_0 - i\hat{D}_{diss}]\}$ is non-unitary. On the face of it, this non-unitarity poses a challenge for implementation on a quantum computer.

For an infinitesimal time step δt, starting at $t = 0$, a first order Suzuki-Trotter approximation of the non-unitary operator $\hat{\mathcal{U}}(t)$ yields,

$$\exp\{-i\delta t[\hat{D}_0 - i\hat{D}_{diss}]\} = e^{-i\delta t\hat{D}_0}e^{-\delta t\hat{D}_{diss}} + O(\delta t^2). \tag{25}$$

This allows us to separate out the non-unitary term $\exp\{-\delta t\hat{D}_{diss}\}$.

The diagonal dissipative operator $\hat{D}_{diss}$ contains at most $6N$ positive elements $(\gamma_{e,l}, \gamma_{m,l})$, $l = 1, \ldots N$. Then,

$$\exp\{-\delta t\hat{D}_{diss}\} = \hat{K}_0 = diag(I_{6\times 6}, I_{6N\times 6N}, \hat{\Gamma}), \tag{26}$$

where,

$$\hat{\Gamma} = \begin{bmatrix} e^{-\delta t\gamma_{e,l}}I_{3\times 3} & 0 \\ 0 & e^{-\delta t\gamma_{m,l}}I_{3\times 3} \end{bmatrix}. \tag{27}$$

The dimensions of the diagonal sub-matrix $\hat{\Gamma}$ are $6N \times 6N$. The non-unitary operator $\exp\{-\delta t\hat{D}_{diss}\}$ has been denoted as K_0 because it will represent the first Kraus operator in the quantum channel description Eq.(3) of classical dissipation that follows in the next section.

3. Dissipation in the context of quantum channels

In the density matrix framework, the Suzuki-Trotter evolution (25) is,

$$\bar{\rho}(\delta t) = e^{-i\delta t\hat{D}_0}\hat{K}_0\rho(0)\hat{K}_0^\dagger e^{i\delta t\hat{D}_0}, \tag{28}$$

where the initial density matrix $\rho(0)$ is,

$$\rho(0) = |\psi_0\rangle\langle\psi_0|, \quad |\psi_0\rangle = \frac{1}{\sqrt{E_0}}\sum_{j=0}^{d-1}\psi_{0j}|j\rangle. \tag{29}$$

From Eq.(21), the initial energy is $E_0 = \langle\psi_0|\psi_0\rangle = \frac{1}{2}\sum_j \epsilon_0 E_j^2 + \mu_0 H_j^2$. By construction, the initial state $|\psi_0\rangle$ is a pure state. It should be noted that $\bar{\rho}(\delta t)$ is not a proper quantum mechanical density matrix, as the operation $\hat{K}_0\rho(0)\hat{K}_0^\dagger$ is not trace preserving (TP). Non-TP quantum channels emerge when a measurement is performed in the environment and selecting over a specific outcome [10]. Consequently, we can think of classical dissipation as a post-selective outcome from the interaction between a quantum represented lossless system and an unspecified environment. Accordingly, to retrieve the TP property we augment Eq.(28) with the term,

$$\hat{K}_1\rho(0)\hat{K}_1, \tag{30}$$

where the second Kraus operator $\hat{K}_1$ satisfies $\hat{K}_1^\dagger\hat{K}_1 = I_{d\times d} - \hat{K}_0^\dagger\hat{K}_0$, and has an upper-triangular form,

$$\hat{K}_1 = \begin{bmatrix} 0 & \sqrt{I_{r\times r} - \hat{\Gamma}^2} \\ 0 & 0 \end{bmatrix}, \tag{31}$$

with $r = 6NN_xN_yN_z$ being the dimension of the dynamic space occupied by dissipation. The operator $\hat{K}_1$ corresponds to a transition – a quantum jump from the dissipative state of interest to a different state. The operators $\hat{K}_0$ and $\hat{K}_1$ are the multi-dimensional analogs of the amplitude damping channel operators [10]. The augmented quantum dissipative evolution for the open quantum system is,

$$\rho_{aug}(\delta t) = e^{-i\delta t\hat{D}_0}\rho_{diss}(\delta t)e^{i\delta t\hat{D}_0}, \tag{32}$$

where,

$$\rho_{diss}(\delta t) = \hat{K}_0\rho(0)\hat{K}_0^\dagger + \hat{K}_1\rho(0)\hat{K}_1^\dagger. \tag{33}$$

The operator $e^{-i\delta t\hat{D}_0}$ has been defined in Eq.(18).

The constructed linear CPTP quantum channel in Eqs.(32),(33) that supports dissipation describes the evolution of the linear dynamics of an open quantum system, generated by the effective Hamiltonian $\hat{H}_{eff}$,

$$\hat{H}_{eff} = \hat{D}_0 - i\hat{L}^\dagger\hat{L}, \quad \hat{L} = \begin{bmatrix} 0 & \sqrt{\hat{\gamma}_r} \\ 0 & 0 \end{bmatrix}. \tag{34}$$

The diagonal matrix $\hat{\gamma}_r$, defined in (23), represents dissipation in the r-dimensional subspace. The operator $\hat{L}$ is called the Lindblad jump operator [24]. The generated Gorini–Kossakowski–Sudarshan–Lindblad (GKSL) master equation [24, 25] is then,

$$\frac{\partial\rho}{\partial t} = -i\hat{H}_{eff}\rho + i\rho\hat{H}_{eff}^\dagger + 2\hat{L}\rho\hat{L}^\dagger. \tag{35}$$

For an infinitesimal time evolution $0 \to \delta t$, the density matrix evolution, to first order in δt, can be generated through the master equation (35) for the classical, non-Hermitian operator,

$$\rho(\delta t) = \hat{E}_0\rho(0)\hat{E}_0^\dagger + \hat{E}_1\rho(0)\hat{E}_1^\dagger, \tag{36}$$

with

$$\hat{E}_0 = I_{d\times d} - i\delta t\hat{D}_0 - \delta t\hat{D}_{diss}, \quad \hat{E}_1 = \sqrt{2\delta t}\hat{L}. \tag{37}$$

By expanding in a Taylor series the Kraus operators in the augmented evolution Eq.(32) we obtain,

$$\rho_{aug}(\delta t) = \rho(\delta t) + O(\delta t^2). \tag{38}$$

Equation (38) confirms that treating the classical non-Hermitian operator $\hat{D}_0 - i\hat{D}_{diss}$ as a quantum effective Hamiltonian generates, to first order, the same dynamics with the quantum channel of Eqs.(32),(33). In the following section, we establish that this minimal augmented form is sufficient to capture the classical dissipative dynamics.

3.1. The algorithm

Since the set of Kraus operators $\hat{K}_0$ and $\hat{K}_1$ in Eq.(33) define a linear CPTP quantum channel, they are contractions [12]. Thus, a guaranteed minimal unitary dilation $\hat{\mathcal{U}}_{diss}$ can be formulated for the Suzuki-Trotter evolution (25) of the open quantum system,

$$\hat{\mathcal{U}}_{diss} = \begin{bmatrix} \hat{K}_0 & -\hat{K}_1^\dagger \\ \hat{K}_1 & \hat{\mathcal{X}}\hat{K}_0\hat{\mathcal{X}} \end{bmatrix}, \tag{39}$$

without resorting to block-encoding techniques that introduce a failure error. The operator $\hat{\mathcal{X}}$ is an appropriate extension of the Pauli $\hat{X}$ operator to d-dimensions. The unitary $\hat{\mathcal{U}}_{diss}$ is a $2d \times 2d$ matrix operator acting on $n+1$ qubits. The ancillary qubit represents the environment; the lossless system together with the environment form a closed conservative system that evolves under the unitary operator $\hat{\mathcal{U}}_{diss}$. This minimal dilation is related to the Sz. Nagy dilation [15] of $\hat{K}_0$ by a rotational transformation.

We consider the qubit environment to be stationary with density matrix $\rho_E = |0\rangle\langle 0|$, and the initial state in the dilated space $|\Psi_0\rangle$ to be separable,

$$|\Psi_0\rangle = |0\rangle |\psi_0\rangle . \tag{40}$$

The action of $\hat{\mathcal{U}}_{diss}$ on the composite initial state (40) yields,

$$|0\rangle \hat{K}_0 |\psi_0\rangle + |1\rangle \hat{K}_1 |\psi_0\rangle . \tag{41}$$

Next, we apply a controlled $e^{-i\delta t\hat{D}_0}$ operation to (41) with respect to the 0-bit environment qubit, leading to the composite state,

$$|0\rangle e^{-i\delta t\hat{D}_0} \hat{K}_0 |\psi_0\rangle + |1\rangle \hat{K}_1 |\psi_0\rangle . \tag{42}$$

Subsequently, a projective measurement of the first qubit with operator $P_0 = |0\rangle\langle 0| \otimes I_{d\times d}$ followed by tracing out the environment, leads to the non-unitary Suzuki-Trotter evolution equation (25) for the lossy, dispersive medium. The steps in Eqs.(40)-(42) along with the post selection of the output state are illustrated in the quantum circuit in Fig. 1.

To first order in δt, the probability $p_0(\delta t) = \langle\psi_0|\hat{K}_0^2|\psi_0\rangle$ for a successful post-selection is,

$$p_0(\delta t) = 1 - 2\delta t \sum_{q=d-r}^{d-1} \gamma_q \frac{|\psi_{0q}|^2}{E_0}. \tag{43}$$

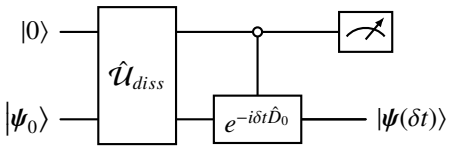

Figure 1: Quantum circuit for simulation of the non-unitary classical evolution (25) in a dissipative and dispersive electromagnetic medium.

where $p_0(\delta t)$ is bounded $p_{0min}(\delta t) \le p_0(\delta t) \le p_{0max}(\delta t)$,

$$p_{0min}(\delta t) = 1 - 2\gamma_{max}\delta t \sum_{q=d-r}^{d-1} \frac{|\psi_{0q}|^2}{E_0}, \tag{44}$$

$$p_{0max}(\delta t) = 1 - 2\gamma_{min}\delta t \sum_{q=d-r}^{d-1} \frac{|\psi_{0q}|^2}{E_0}, \tag{45}$$

with $r = 6NN_xN_yN_z$, $\gamma_{max} = \max\{\gamma_{e,l}, \gamma_{m,l}\}$, and $\gamma_{min} = \min\{\gamma_{e,l}, \gamma_{m,l}\}$, $l = 1, \ldots, r$. From (43), the optimal time-step δt for a high success post-selection out of the output state (42) requires,

$$\delta t << \frac{1}{2\sum_{q=d-r}^{d-1} \gamma_q \frac{|\psi_{0q}|^2}{E_0}}. \tag{46}$$

Based on (44), the upper bound on δt is,

$$\delta t_{phys} = \frac{1}{2\gamma_{max}\sum_{q=d-r}^{d-1} \frac{|\psi_{0q}|^2}{E_0}}, \tag{47}$$

with $\delta t << \delta t_{phys}$, where the time step δt_{phys} corresponds to the fast time scale $1/\gamma_{max}$ associated with dissipation – since $\sum_{q=d-r}^{d-1} \frac{|\psi_{0q}|^2}{E_0} \sim r/d \sim 1/2$, $\delta t_{phys} \sim 1/\gamma_{max}$. Thus, for an accurate modeling of dissipation we have to select a simulation time step that is smaller that the fastest time scale. We have realized this physical conclusion solely from the quantum operational requirement of a highly successive post-selection process. However, a fine-meshing in the temporal domain directly affects the number of Trotter steps N_t required for a complete simulation time $t_{total} = N_t\delta t$ within an error ε,

$$\varepsilon = \left\| \hat{\mathcal{U}} - (e^{-i\delta t\hat{D}_0}\hat{K}_0)^{N_t} \right\| = O\Big(\frac{2^n\gamma_{max}t_{total}^2}{N_t}\Big), \tag{48}$$

which reflects the trade-off between the smallness of the time step δt and the number of repetitions N_t for the desired error scaling. For example, for constant error scaling $\varepsilon = O(1)$, the number of Trotter steps scale as $N_t \sim 2^n$, resulting in an exponentially large number of repetitions of the quantum circuit. This, in turn, implies that we need an exponentially large number of post-selections, $1/p_0^{N_t}$ for simulating the dissipative dynamics to within a desired error.

Considering a more sophisticated Trotter error scaling [26] can lead to an optimized selection between the quantities $\varepsilon, N_t, \delta t$ and $p_0(\delta t)$.

3.2. Implementation of the $\hat{\mathcal{U}}_{diss}$ operator

The explicit form of $\hat{\mathcal{U}}_{diss}$ in Eq.(39) is,

$$\hat{\mathcal{U}}_{diss} = \begin{bmatrix} I_{(d-r)\times(d-r)} & 0 & 0 & 0 \\ 0 & \hat{\Gamma} & -\sqrt{I_{r\times r} - \hat{\Gamma}^2} & 0 \\ 0 & \sqrt{I_{r\times r} - \hat{\Gamma}^2} & \hat{\Gamma} & 0 \\ 0 & 0 & 0 & I_{(d-r)\times(d-r)} \end{bmatrix}, \tag{49}$$

where the diagonal operator $\hat{\Gamma}$ is given in Eq.(27). Setting $\cos\theta_l/2 = \hat{\Gamma}_{ll}$, we can decompose $\hat{\mathcal{U}}_{diss}$ into r two-level unitary y-rotations, $\hat{\mathcal{R}}_y(\theta_l)$, acting on $n+1$ qubits,

$$\hat{\mathcal{U}}_{diss} = \prod_{l=1}^{r} \hat{\mathcal{R}}_y(\theta_l). \tag{50}$$

Hence, to leading order, we can implement $\hat{\mathcal{U}}_{diss}$ in $O(rn^2)$ CNOTs and a single qubit rotations $\hat{R}_y(\theta_l)$. Since $d = (6 + 12N)N_xN_yN_z = 6N_xN_yN_z + 2r = 2^n$ then $r = 2^{n-1}(1 - \frac{1}{1+2N})$, and the implementation of $\hat{\mathcal{U}}_{diss}$ is achieved using $O(2^{n-1}n^2)$ simple gates.

The decomposition of $\hat{\mathcal{U}}_{diss}$ into a product of two-level rotations Eq.(50) acting on $n+1$ qubits is related to multiplex rotations. Following [27], a multiplex rotation acting on $n+1$ qubits can be implemented in $O(4^{n+1})$ CNOTs and single qubit $\hat{R}_y$ rotations. The two crucial aspects that enable us to implement the product structure Eq.(50) in an exponentially better way are, firstly that the dissipation subspace $\mathcal{H}_r$ has a smaller dimension $r < d$ compared to the overall system, and secondly the Hilbert space $\mathcal{H}_r$ structure of the classical system enables decomposition into separate spaces through a direct sum, $\mathcal{H}_r = \bigoplus_{l=1}^{r} \mathcal{H}_l$. The latter is not always possible in quantum systems and is the cause of the Strinespring scaling [28] in the amplitude damping dilation of [13] compared to our one-qubit amplitude damping dilation.

3.3. Connection with non-linear quantum channels

The quantum circuit of Fig. 1 produces the normalized classical evolved density matrix,

$$\rho(\delta t) = \frac{e^{-i\delta t\hat{D}_0}\hat{K}_0\rho(0)\hat{K}_0^\dagger e^{i\delta t\hat{D}_0}}{\langle\psi_0|\hat{K}_0^2|\psi_0\rangle}, \tag{51}$$

after a deterministic evolution followed by a successful post-selective projective measurement that introduces a probabilistic aspect to our algorithm along with the pertinent errors (see the discussion at the end of Sec.3.2).

It is possible to obtain the desired result of Eq.(51) purely deterministically by employing a non-linear in normalization only (NINO) evolution quantum channel[29–32],

$$\rho_0 \to \rho(\delta t) = \frac{\Phi(\rho_0)}{Tr[\Phi(\rho_0)]}, \tag{52}$$

where the linear map Φ in Eq.(52) is,

$$\Phi(\rho_0) = e^{-i\delta t\hat{D}_0}\hat{K}_0\rho(0)\hat{K}_0^\dagger e^{i\delta t\hat{D}_0}. \tag{53}$$

NINO channels are weakly non-linear quantum channels that have found applications in quantum information processes such as fast quantum purification [29], amplification [32], mixed state evolution in Parity-Time ($\mathcal{PT}$) symmetric systems [33] and state discrimination [31] as well as implicit application in the theory of classical dynamical systems [34].

The generated non-linear extension of GKSL equation for the dynamics of the open quantum system is,

$$\frac{\partial\rho}{\partial t} = -i\hat{H}_{eff}\rho = i\rho\hat{H}_{eff} - \rho\hat{D}_{diss} + 2R\rho, \tag{54}$$

with

$$R = Tr(\hat{D}_{diss}\rho). \tag{55}$$

From classical perspective, the quantity R is the instantaneous Laypunov exponent [34] that translates into relaxation exponent in our case due to the existence of dissipation.

Comparing the master equation Eq.(35) and its non-linear counterpart Eq.(55) we deduce two important differences: (1) Equation (55) conserves the trace non-linearly without any jump operators, in contrast with Eq.(33) where the jump operator $\hat{L}$ has been introduced in Eq.(34). Thus, Eq.(51) is derived deterministically without the post-selection error overhead. (2) The linear CPTP channel preserves the trace though the condition $\hat{D}_{diss} = \hat{L}^\dagger\hat{L}$ which implies that the non-Hermitian operator $-i\hat{D}_{diss}$ has to describe only dissipative processes (all eigenvalues of $\hat{D}_{diss}$ are positive). NINO channels support both dissipation and amplification, by relaxing the (CP) condition to simple positivity (P) [31]. Hence, it may be possible to simulate active electromagnetic media and meta-materials with combined gain and loss exploiting the PTP NINO channels.

4. An optimized approach

In the previous section, we succeeded in showing the pathway to convert the non-unitary, diagonal, dissipative Kraus operator $\hat{K}_0 = \exp\{-\delta t\hat{D}_{diss}\}$ into $O(2^{n-1}n^2)$ elementary unitary gates, based on the constructed interconnection between dissipative and post-selective open quantum systems and classical dissipation. A different approach is to refrain from associating classical dissipation with a quantum process but treat $\hat{K}_0$ with the Linear Combination of Unitary (LCU) method [35]. Specifically, $\hat{K}_0$ can be written as a sum of two unitary matrices,

$$\hat{K}_0 = \frac{1}{2}(\hat{K}_{0z} + \hat{K}_{0z}^\dagger), \tag{56}$$

where,

$$\hat{K}_{0z} = \begin{bmatrix} I_{(d-r)\times(d-r)} & 0 \\ 0 & e^{-i\theta_l/2} \end{bmatrix}, \quad l = 1, 2, ..., r. \tag{57}$$

As in Sec. 3.2, we have set $\cos\theta_l/2 = \hat{\Gamma}_{ll}$. It is important to realize that the unitary components in Eq.(56) remain diagonal. In order to apply the LCU method (Lemma 6 in [35]), we need one auxiliary qubit as in the dilation process of Sec. 3. We

introduce the unitary operators,

$$\hat{U}_{prep} : |0\rangle \rightarrow \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \tag{58}$$

$$\hat{U}_{select} = |0\rangle\langle 0| \otimes \hat{K}_{0z} + |1\rangle\langle 1| \otimes \hat{K}_{0z}^{\dagger}, \tag{59}$$

where $\hat{U}_{prep} = \hat{H}$ is the Hadamard gate. We can probabilistically implement $\hat{K}_0$ using the unitary dilated operator,

$$\hat{\mathcal{U}}_{diss} = (\hat{H} \otimes I_{d\times d})\hat{U}_{select}(\hat{H} \otimes I_{d\times d}). \tag{60}$$

The action of $\hat{\mathcal{U}}_{diss}$ on the initial state $|0\rangle|\psi_0\rangle$ is,

$$\hat{\mathcal{U}}_{diss}|0\rangle|\psi_0\rangle = |0\rangle\hat{K}_0|\psi_0\rangle + \frac{1}{2}|1\rangle(\hat{K}_{0z} - \hat{K}_{0z}^{\dagger})|\psi_0\rangle. \tag{61}$$

Again, a measurement on the first qubit provides the desired result. The quantum circuit representation for simulation of the Suzuki-Trotter dynamics (25), taking into consideration Eqs.(60) and (61), is depicted in Fig.2. The probability of

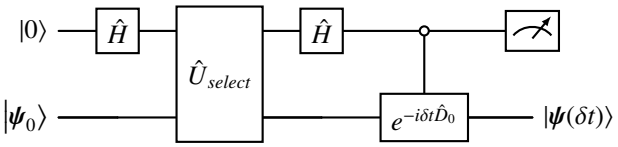

Figure 2: Quantum circuit for simulation of the non-unitary classical evolution (25) in a dissipative and dispersive medium using the LCU method.

measuring the 0-bit value qubit in the output state (61) is $p_0 = \langle\psi_0|\hat{K}_0^2|\psi_0\rangle$. This obeys the same bounds ((44), (45)) as in Sec. 3.1.

The remaining question is whether the implementation cost of $\hat{U}_{select}$ scales favorably compared to that of $\hat{\mathcal{U}}_{diss}$ from the previous section. Given the definition in (59), $\hat{U}_{select}$ is a $2d\times 2d$ diagonal operator,

$$\hat{U}_{select} = \begin{bmatrix} \hat{K}_{0z} & 0 \\ 0 & \hat{K}_{0z}^{\dagger} \end{bmatrix}, \tag{62}$$

which contains r two-level z-rotations $\hat{\mathcal{R}}_z(\theta_l)$ compared to the r two-level y-rotations $\hat{\mathcal{R}}_y(\theta_l)$ of Eq.(49). As a result, the diagonal nature of $\hat{U}_{select}$ allows for an implementation in $2^n(1-\frac{1}{1+2N})-3$ alternating CNOTs and single-qubit $\hat{R}_z(\theta_l)$ rotations [36]. Thus, to leading order, a quadratic improvement is achieved as compared to the scaling of the physical dilation in (50). The LCU method produces the same dilation method, specialized for diagonal operators, as in [14].

When $\{\gamma_{e,l},\ \gamma_{m,l}\}$ are homogeneous and few in numbers, their values appear repetitively in the diagonal matrix $\hat{U}_{select}$ following discretization. It is then possible to further reduce the implementation cost of $\hat{U}_{select}$ to polynomial scaling $O[p(n)]$, [37].

5. Conclusions

An effective simulation of dynamics in dissipative classical systems is inherently challenging for quantum computers due to the loss of unitary evolution. In this paper, we have focused on dissipative and dispersive electromagnetic media in which energy loss appears as an anti-Hermitian, diagonal part in the Schrödinger representation of Maxwell equations. Using the Suzuki-Trotter approximation, we untangle the unitary evolution from the non-unitary, enabling us to concentrate exclusively on the non-unitary evolution.

The interconnection between the dissipation in dispersive electromagnetic media and the dissipation in open quantum systems serves as a first step in a dilation process which relies on an augmented Kraus representation (32) and the direct sum structure of the dissipative r-dimensional subspace. In this way, we only need one ancillary qubit to model the environment, in contrast to the respective formulation of non-unitary quantum evolution through quantum channels [13]. This physical dilation requires $O(2^{n-1}n^2)$ CNOTs and one qubit y-rotations. The second algorithm does not use the physical connection between classical and quantum processes but implements the non-unitary evolution through the LCU Lemma in $O(2^n)$ CNOTs and one qubit z-rotations. However, while the second method is quadratically better, it lacks the physical interpretation which is essential when the anti-Hermitian part in the Hamiltonian does not correspond to pure dissipation but also accommodates amplification (gain) effects. In such cases, a physical dilation based on the construction of the proper quantum channel for the classical dynamics may be advantageous in terms of physical information that can be extracted from the quantum implementation, compared to the LCU dilation. This is evident in Sec.3.3 where the PTP NINO quantum operations are considered.

Combining the results from Secs. 3, 4 and those in reference [6] in conjunction with a quantum simulation implementation of Maxwell equations for the lossless case, (possibly with QLA) we can realize a full wave simulation of electromagnetic wave propagation and scattering in complex media, such as magnetized plasmas and meta-materials, in a quantum computer. In this way, we are enabling quantum computing to make an impact in the field of computational electromagnetism for applications. Our set up, Eqs.(5) and (6), considers minimal assumptions while respecting Kramer-Kroning causality relations [23] in the whole frequency spectrum and extending beyond $\mathcal{PT}$-symmetric models [38].

Finally, it is important to note that, when computationally feasible, both methods can be applied to other classical dissipative systems by diagonalizing the Hermitian dissipative operator $\hat{D}_{diss}$ in the respective Schrödinger equation (24) as $\hat{D}_{diss} = \hat{V}\hat{\Delta}\hat{V}^{\dagger}$. Then the diagonal operator $\hat{\Delta}$ leads to a diagonal non-unitary part as in Eq.(25), which can be implemented using the techniques described in this paper and in Ref.[14]. The implementation cost of unitary operators $\hat{V}, \hat{V}^{\dagger}$ is directly related to the dimension of the dissipative subspace.

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