

Discrete electrodynamics: potentials and quantum electronics

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Abstract

A general mathematical framework for the computational modelling of electromagnetic fields interacting with arbitrary quantum-electronic systems is described. The discretisation of space and time are taken as fundamental to the model, and the quantum-electronic systems with which the fields interact are taken to be discretised at each spatial mesh point. Maxwell equations are formulated on the discrete space using exact potentials and discrete forms of Stokes' Theorem. The discrete potentials interact with the quantum-electronic systems through the minimal coupling scheme (potential-momentum or $\mathbf{A} \cdot \mathbf{p}$ coupling). The entire scheme is essentially a finite-difference time-domain Maxwell-Bloch system (FDTD-MB) for potentials, with discrete exterior calculus (DEC) as the fundamental mathematical language.

1. Introduction

Maxwell-Bloch (MB) systems are generically composed of coupled systems of Maxwell equations and fundamental quantum-mechanical dynamical systems. They describe electromagnetic waves in general atomic media, including the effects of dispersion, dissipation, external pumping, active and passive nonlinearity and even resonance. While, in principle, the dynamical systems are infinite-dimensional, it is often a good approximation to retain only a few degrees of freedom in the dynamical systems that are closest to resonance with the electromagnetic wave. In this paper a general computational framework for multi-level Maxwell-Bloch systems will be described. The fundamental formulation is in terms of the vector potential coupling to the atomic dipoles, so-called minimal replacement coupling, rather than the conventional electric dipole coupling. It has already been noted elsewhere that the nonlinear optics of nonresonant finite-dimensional quantum systems may differ quantitatively depending on whether the vector potential or electric field defines the coupling [1].

The equations governing a spatially homogeneous ensemble of quantum systems (bound electrons in atoms) interacting with an electromagnetic wave consist of the Liouville equation for the dynamics of the quantum density matrix Γ

$$i\hbar\partial_t\Gamma = [H, \Gamma], \quad (1)$$

and Maxwell's equations for the electromagnetic potentials \mathbf{A} and Φ

$$\nabla^2\mathbf{A} - c^{-2}\partial_t^2\mathbf{A} = -\mu_0\partial_t\mathbf{P} \quad (2)$$

$$\nabla^2\Phi - c^{-2}\partial_t^2\Phi = \epsilon_0^{-1}\nabla\cdot\mathbf{P}, \quad (3)$$

where $\mathbf{A}(\mathbf{x}, t)$ is the vector potential, $\Phi(\mathbf{x}, t)$ is the scalar potential, $\mathbf{P}(\mathbf{x}, t)$ is the polarisation density induced in the atomic ensemble, and c is the velocity of light *in vacuo*. The gauge condition for the potentials is the Lorentz gauge

$$c^2\nabla\cdot\mathbf{A} + \partial_t\Phi = 0. \quad (4)$$

$\Gamma(\mathbf{x}, t)$ is the density matrix, and H is the Hamiltonian matrix given by

$$H = H_0 + \frac{e}{m}\mathbf{p} \cdot \mathbf{A} \quad (5)$$

where H_0 is the diagonal matrix of electron eigenenergies, $-e$ and m are the charge and mass of the electron, respectively, and \mathbf{p} is the momentum matrix. The polarisation density \mathbf{P} is given by

$$\mathbf{P} = -\frac{1}{2}Ne\text{Tr}\{\Gamma\mathbf{Q}\}, \quad (6)$$

where N is the number density of atoms, and \mathbf{Q} is the dipole displacement operator. The relation between the matrices \mathbf{p} and \mathbf{Q} is

$$\mathbf{p} = (i\hbar)^{-1}m[\mathbf{Q}, H_0]. \quad (7)$$

2. Discrete exterior calculus and FDTD

A well-established computational scheme for the study of Maxwell's equations is the finite-difference time-domain method (FDTD), in which the fields \mathbf{E} and \mathbf{H} are recursively updated in discrete time through Maxwell's field equations after approximating spatial derivatives by finite-difference formulae on a discrete spatial sampling grid. A FDTD scheme for Maxwell's field equations coupled to simple quantum dynamical systems similar to the above has been extensively studied in [2, 3]. The FDTD scheme can be adapted with very small modification to the recursive update of the potential system (2)-(3) with (1).

Further study of the FDTD approach suggests a more fundamental conclusion. If the potentials and fields are replaced entirely by discrete samples on a spatial mesh, and the finite-difference *approximations* to differential operators are replaced by *exact* discrete operators, then one has an exact analogy of continuum electrodynamics, but constrained to live in a purely discrete space. If, in addition, one requires the discrete fields and discrete operators to conform to the structure of *discrete exterior calculus* (DEC) [6, 7], then one has an exact correspondence between the electrodynamics in the discrete and continuous worlds.

The way in which this correspondence is established is to define the potentials Φ and \mathbf{A} to be a discrete 0-form and a discrete 1-form, respectively, and to define the discrete exterior operator \mathbf{d} that maps n -forms into $n + 1$ -forms by means of discrete versions of Stokes' Theorem. In this structure, 0-forms are imagined to live on the nodes of a regular spatial mesh, 1-forms live on the branches of the mesh, 2-forms live on the facets of the mesh cells, and 3-forms are densities located at the centres of mesh cells. It is convenient to define dual meshes, such that the mesh nodes of one mesh coincide with the cell centres of the other mesh. Each mesh has its own system of r -forms. In addition, the Hodge operator $*$ maps r -forms on one mesh to $3 - r$ -forms on the other. Thus, $\{\mathbf{d} : 0\text{-form} \rightarrow 1\text{-form}\}$ acts as a discrete analogue of the continuum operator of *gradient* (∇), $\{\mathbf{d} : 1\text{-form} \rightarrow 2\text{-form}\}$ acts as *curl* ($\nabla \times$), $\{\mathbf{d} : 2\text{-form} \rightarrow 3\text{-form}\}$ acts as *divergence* ($\nabla \cdot$). In addition, and very fundamentally, the \mathbf{d} -operator on forms satisfies $\mathbf{d}\mathbf{d} = 0$ at every grade. The action of the \mathbf{d} -operator is specified at each grade by a discrete form of Stokes' Theorem. Finally, the operator equivalent to the Laplacian ∇^2 is the discrete Laplacian $*\mathbf{d}*\mathbf{d}$. With these definitions for the potentials and operators, the potential wave equations have the discrete forms

$$(-*\mathbf{d}*\mathbf{d} + \mathbf{d}*\mathbf{d}*)\mathbf{A} - c^{-2}\partial_t^2\mathbf{A} = -\mu_0*\partial_t\mathbf{P} \quad (8)$$

$$*\mathbf{d}*\mathbf{d}\Phi - c^{-2}\partial_t^2\Phi = \epsilon_0^{-1}*\mathbf{d}\mathbf{P} \quad (9)$$

and the Lorentz gauge condition is

$$c^2\mathbf{d}*\mathbf{A} + \partial_t*\Phi = 0. \quad (10)$$

The polarisation \mathbf{P} in this formulation is a discrete 2-form on the dual mesh, so that $*\mathbf{P}$ is a discrete 1-form located on branches of the primary mesh (collocated with \mathbf{A}). The operators ∂_t are discretised by simple differencing at successive sampled times $t = m\Delta_t$, to complete the transission from a continuous space-time world to a totally discrete space-time world. With this entirely discrete structure, the geometrical embedding of the discrete mesh in the continuum can be abandoned, and the discrete system becomes an entity in its own right [8].

3. Lagrangian discrete electrodynamics

In what follows we adopt the following labelling system: mesh nodes will be labelled with an index L , and mesh branches with a label K . In a rectangular mesh the labels K separate into 3 sets according to whether the mesh branch is parallel to x , y or z of a reference cartesian frame. In a cartesian reference system $L = (l_1, l_2, l_3) : l_j \in \mathbf{Z}$. Since mesh branches join between nodes, then $K = (k_1, k_2, k_3) : k_j \in \mathbf{Z}$.

It can be demonstrated that the entire system is Lagrangian, which is to say that the electrodynamical equations are the Euler-Lagrange equations of a real Lagrangian variational functional S with respect to arbitrary variations in the discrete potentials Φ and \mathbf{A} . The action functional can be written in the form

$$S = \sum_{K', m'} S_{KK'}^m A_K^m A_{K'}^{m'} + \sum_{L', m'} R_{LL'}^m \Phi_L^m \Phi_{L'}^{m'} - \sum A_K^m J_K^m - \sum \Phi_L^m \rho_L^m \quad (11)$$

where K is a generalised index representing mesh branches, L is a generalised index representing mesh nodes, m represents discrete time, and the elements $S_{KK'}^m$ and $R_{LL'}^m$ represent a topology of mesh interactions.

The conventional FDTD time-updating scheme can then be recovered by the following algorithm for the trial functions of the action principle: assume the potentials are determined over the whole mesh at all times up to discrete time m , then take variations of the spatial distributions at time $m + 1$ to optimise the action functional S , thereby determining the potentials over the whole mesh at time $m + 1$, and repeat recursively. The Euler-Lagrange equations obtained from this variational procedure are

$$\sum_{K', m'} W_{KK'}^m A_{K'}^{m'} = -\mu_0 J_K^m \quad (12)$$

$$\sum_{L', m'} W_{LL'}^m \Phi_{L'}^{m'} = +\epsilon_0^{-1} \rho_L^m \quad (13)$$

where the discrete operator W is essentially the wave operator. The elements of $W_{KK'}^m$ are very sparse, with topological connections to determine the nonvanishing components. The operator elements are given by

$$W_{KK'}^m = h^{-2} F_{KK'} \delta^{mm'} - c^{-2} \Delta_t^{-2} D^{mm'} \delta_{KK'} \quad (14)$$

where F is the time-independent discrete Laplacian and D is the space-independent operator

$$F_{KK'} = \begin{cases} -6, & K' = K \\ 1, & K' \in \partial K \\ 0, & \text{otherwise} \end{cases}, \quad D^{mm'} = \begin{cases} -2, & m' = m \\ 1, & m' = m \pm 1 \\ 0, & \text{otherwise.} \end{cases} \quad (15)$$

The set ∂K represents those mesh branches that are parallel to mesh branch K and one mesh step away from K . In a practical updating scheme the scalar potential Φ is updated using the Lorentz condition (10); then Φ automatically satisfies the discrete wave equation (13) when \mathbf{A} is updated using (12).

There are significant discretisation issues associated with the description of the polarisation of the medium \mathbf{P} by means of model atomic dipoles located at the nodes of the primary mesh. Since dipoles are charges, they should appear at mesh nodes; however, the polarisation they produce is required to be specified at mesh branches, and the field (potential) driving them is similarly specified only at mesh branches, not at nodes. Also, a consistent embedding of the discrete sampling times in the continuum is required. For this reason, the differential Liouville equation is discretised in time by the implicit form

$$\Gamma^{m+1} - \Gamma^m = (i\hbar)^{-1} \Delta_t [H^m, \frac{1}{2}(\Gamma^{m+1} + \Gamma^m)] \quad (16)$$

where $H^m = (H_0 + (e/m)\mathbf{A}^m \cdot \mathbf{p})$, which embodies the idea that the potentials are sampled at the half-time points between the discrete times at which the density matrix Γ^m is sampled. Then $\mathbf{P}^m = -\frac{1}{2} Ne \text{Tr}\{\Gamma^m \mathbf{Q}\}$ locates the polarisations at half-time points between the potentials, which is consistent with their location from Maxwell's equations. This form has the advantage that the evolution of the discretised density matrix Γ^m is *unitary* ($\text{Tr}\{(\Gamma^m)^2\} = 1$ for all m), which contributes strongly to the stability of the time-stepping scheme. For the embedding of the spatial domain to the continuum, we adopt the device of spatially averaging the potential to obtain the driving potential for the atoms at mesh nodes, then averaging the resulting dipole polarisation to transfer it back to mesh branches, so that

$$\bar{A}_{xL}^m = \frac{1}{2} \sum_{K \in K_x(L)} A_K^m \quad (17)$$

$$\bar{P}_{K_x}^m = \frac{1}{2} \sum_{L \in L(K_x)} P_L^m \quad (18)$$

where x is a cartesian direction along mesh branches, K labels mesh branches, L labels mesh nodes, $K_x(L)$ is the set of two mesh branches located along x on either side of node L , and $L(K_x)$ is the set of two mesh nodes at either end of the mesh branch K_x along x .

4. Conclusions

A systematic computational scheme is developed for the description of electromagnetic waves interacting with materials described quantum mechanically. The scheme is essentially a finite-difference time-domain Maxwell-Bloch system. Features of the scheme are: potentials are taken to be the fundamental electrodynamical quantities rather than the electric and magnetic fields of conventional FDTD; space is discretised *a priori*, with conventional derivatives replaced by discrete exterior calculus operators and discrete Stokes' Theorems replacing conventional Maxwell equations; exact discrete Green's Theorems exist for domain truncation, domain decomposition and diakoptics [5]; idealised quantum electronic systems are located on spatial nodes to represent charge polarisations developed in the media.

While originally conceived as a purely numerical procedure for the modelling of nonlinear electrodynamics in polarisable media, the scheme is a complete electromagnetic theory in its own right, with discrete space-time substituting the conventional continuous space-time as the underlying configuration manifold, and discrete exterior calculus replacing the conventional calculus of continua. The isomorphism generated between operators of the discrete and continuous forms of this electrodynamics makes it possible to replicate all fundamental electrodynamical concepts in the discrete case, leading to many interesting questions about reproducing phenomena known from continuum electrodynamics in the purely discrete space-time world. These include the existence of discrete Green's theorems [5], and various theorems about conserved invariants of the discrete fields that mirror those in continuum electrodynamics, but which also play an important role in the stability of the discrete time evolution of the purely discrete systems.

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