Matrix Representations of Discrete Differential Operators and Operations in Electromagnetism

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Abstract

Metamaterials with periodic structures are building blocks of various photonic and electronic materials. Numerical simulations, which based on the solutions of the three dimensional Maxwell's equations, play an important role to explore and design these novel artificial materials. To solve the governing equations, Yee's finite difference scheme has been widely used to discretize the Maxwell equations. However, studies of Yee's scheme from the viewpoints of matrix computation remain sparse. To fill the gap, we derive the explicit matrix representations of the differential operators $\nabla\times$, ∇^2, $\nabla(\nabla\cdot)$, and some of the resulting differential equations. These matrix representations inspire us to develop efficient eigenvalue solvers to the Maxwell equations and assist us to assert why the divergence free conditions hold in Yee's scheme.

Keywords: Maxwell's equations, Yee's discretization scheme, matrix representation, curl, divergence, gradient, periodic structures, simple cubic lattice, face centered cubic lattice.

1. Introduction

Properties of electromagnetic waves can be modeled by the three dimensional (3D) Maxwell equations

⟨eq:2nd_Maxwell_eq⟩

$$\nabla \times E = \mathrm{i}\omega B, \tag{1a}$$ eq:curl_E_B

$$\nabla \times H = -\mathrm{i}\omega D, \tag{1b}$$ eq:curl_E_H

$$\nabla \cdot B = 0, \tag{1c}$$?eq:divergent_free_B?

$$\nabla \cdot D = 0. \tag{1d}$$?eq:divergent_free_D?

Here, E is the electric field, H is the magnetic field, and ω is the frequency of time. Furthermore, the magnetic flux density B and the electric flux density D

satisfy the constitutive relations

$$B = \mu H + \zeta E \quad \text{and} \quad D = \varepsilon E + \xi H, \tag{2}$$ eq:couple_relation

where μ is the magnetic permeability, ε is the electric permittivity, and ζ and ξ are magnetoelectric parameters. Materials modelled by Eq. (1) can be characterized by μ and ε as follows [13].

- $\mu > 0$, $\varepsilon > 0$, and $\zeta = \xi = 0$. Most dielectric materials belong to this category. The governing equations in (1) can be reformulated as

  $$\nabla \times \mu^{-1} \nabla \times E = \omega^2 \varepsilon E, \quad \nabla \cdot (\varepsilon E) = 0,$$

  where ε is the material dependent piecewise constant.

- $\mu > 0$ and $\varepsilon < 0$. This category includes dispersive metallic materials, ferroelectric materials, and doped semiconductors. In dispersive metallic materials [2, 3, 4, 14, 15, 20], ε is not a piecewise constant but dependents on the frequency ω. That is, $\varepsilon(\mathbf{x}, \omega)$. Such materials can exhibit negative permittivity at certain frequencies, such as below the plasma frequency.

- $\mu < 0$ and $\varepsilon < 0$. This category represents the left-handed material or negative-index materials. It is worth mentioning that there is no such material in nature. To expand the material properties including the negative refractive index, artificial metamaterials which made of periodic structures has been proposed [16, 17] firstly. Such metamaterials open up a completely new research area. For example, bi-isotropic and bianisotropic media are two important classes of metamaterials [21]. The associated B and D satisfy the magnetoelectric coupling in (2) [18, p. 26], [21, p. 44].

- $\mu < 0$ and $\varepsilon > 0$. This category consist of some ferrite materials with negative permeability. However, the deduced the magnetic responses, fade away above microwave frequencies quickly.

Furthermore, for periodic structures, the Bloch Theorem [12] suggests that the electric and magnetic fields E and H satisfy the quasi-periodic conditions

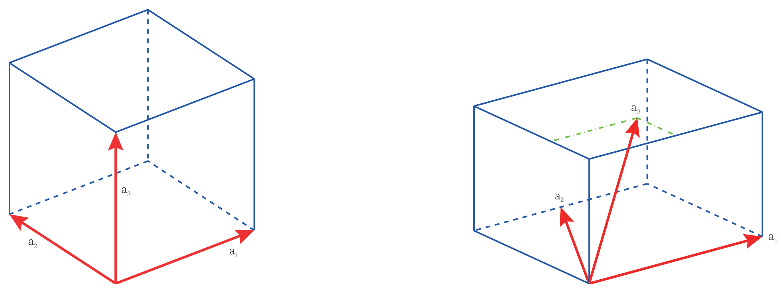
$$E(\mathbf{x} + \mathbf{a}_\ell) = e^{\mathrm{i}2\pi \mathbf{k}\cdot \mathbf{a}_\ell} E(\mathbf{x}), \; H(\mathbf{x} + \mathbf{a}_\ell) = e^{\mathrm{i}2\pi \mathbf{k}\cdot \mathbf{a}_\ell} H(\mathbf{x}), \; \ell = 1, 2, 3. \tag{3}$$ pbc

Here, $2\pi\mathbf{k}$ is the Bloch wave vector in the first Brillouin zone and $\mathbf{a}_\ell$'s are the lattice translation vectors that span the primitive cell which extends periodically to form the magnetoelectric materials. Figure 1 shows two types of lattice translation vectors that are of particular interests. The first type is the simple cubic (SC) lattice, whose lattice translation vectors are

$$\mathbf{a}_1 = a[1, 0, 0]^\top, \; \mathbf{a}_2 = a\,[0, 1, 0]^\top, \; \mathbf{a}_3 = a\,[0, 0, 1]^\top, \tag{4}$$ eq:lattice_vector_sc

where a is the lattice constant. The second type is the face centered cubic (FCC) lattice, whose lattice translation vectors are

$$\mathbf{a}_1 = \frac{a}{\sqrt{2}}[1, 0, 0]^\top, \; \mathbf{a}_2 = \frac{a}{\sqrt{2}}[\frac{1}{2}, \frac{\sqrt{3}}{2}, 0]^\top, \; \mathbf{a}_3 = \frac{a}{\sqrt{2}}[\frac{1}{2}, \frac{1}{2\sqrt{3}}, \sqrt{\frac{2}{3}}]^\top. \tag{5}$$?eq:lattice_vector_fcc?



(a) (b)

Figure 1: The translation vectors of (a) simple cubic and (b) face centered cubic lattice.

⟨fig:lattice⟩

Physics breakthroughs and engineering innovations of magnetoelectric metamaterials heavily rely on the numerical solutions of the Maxwell equations [5, 10, 11, 19]. Yee's discretization scheme [22] is one key tool among various numerical methods. Despite of the wide use of Yee's scheme, the discrete counterparts of the continuous differential operators and the related properties have not documented systematically to the best of our knowledge. This article fills the gap by deriving the discrete differential operators in Maxwell's equation and asserting several differential equations from the viewpoints of matrix representations. We also demonstrate how these matrix representations inspire the development of numerical schemes to the simulations of the magnetoelectric materials.

Throughout this paper, we denote the transpose and the conjugate transpose of a matrix by the superscript $\top$ and $*$, respectively. For the matrix operations, we denote $\otimes$ the Kronecker product of two matrices. We denote the imaginary number $\sqrt{-1}$ by i and the identity matrix of order n by I_n. The $\mathrm{vec}(\cdot)$ is the operator that vectorizes a matrix by stacking the columns of the matrix.

This paper is outlined as follow. We first derive the explicit matrix representations of the single curl operator in Section 3. Second, based on the matrix representations derived in Section 3, we give the eigenvalue problem in different material settings. Third, we assert the divergence free conditions hold in Section 5. Discretizations and a property of some second order operators are derived and verified in Section 6. Finally, we conclude this paper in Section 7.

2. Yee's Discretization Scheme

?⟨sec:yee⟩?

We outline how Yee's discretization scheme [22] is applied to solve the Maxwell equations (1). In this article, we focus on the SC lattice. However, similar derivations can be applied to the FCC lattice. The grid points are located on the edges and faces of primitive cell as shown in Figure 2. In our

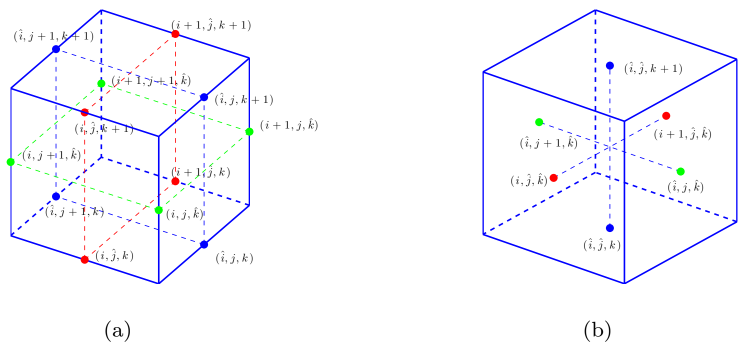


Figure 2: The grid points are located on the (a) edges and (b) faces of primitive cell in Yee's scheme. The figure also shows the corresponding indices.
⟨fig:grids⟩

derivation, we let $E = [E_1, E_2, E_3]^\top$, $H = [H_1, H_2, H_3]^\top$, $B = [B_1, B_2, B_3]^\top$, and $D = [D_1, D_2, D_3]^\top$ and then rewrite Eqs. (1a) and (1b) as

$$\begin{cases} \partial_y E_3 - \partial_z E_2 = \mathrm{i}\omega B_1, \\ \partial_z E_1 - \partial_x E_3 = \mathrm{i}\omega B_2, \\ \partial_x E_2 - \partial_y E_1 = \mathrm{i}\omega B_3, \end{cases} \tag{6}$$ eq:double_curl_E_1

and

$$\begin{cases} \partial_y H_3 - \partial_z H_2 = -\mathrm{i}\omega D_1, \\ \partial_z H_1 - \partial_x H_3 = -\mathrm{i}\omega D_2, \\ \partial_x H_2 - \partial_y H_1 = -\mathrm{i}\omega D_3. \end{cases} \tag{7}$$ eq:double_curl_E_2

In Yee's scheme, Eqs. (6) and (7) are discretized at the centers of cell faces and edges, respectively, by using the following notations.

Let δ_x, δ_y, and δ_z denote the grid length along the x, y, and z axial directions, respectively. Let n_1, n_2, and n_3 be the numbers of grid points in x, y, and z directions, respectively, and we define $n = n_1 n_2 n_3$. The approximate function values due to the first order central finite differences are represented by the grid points indexed by i, j, and k and the "half grid points" indexed by $\hat{i} = i + \frac{1}{2}$, $\hat{j} = j + \frac{1}{2}$, and $\hat{k} = k + \frac{1}{2}$. For simplicity, we represent an arbitrary point $(r\delta_x, s\delta_y, t\delta_z)$ in the computational domain by $\mathbf{x}(r, s, t)$, where $r, s, t \in \mathbb{R}$. That is,

$$\mathbf{x}(r, s, t) = (r\delta_x, s\delta_y, t\delta_z). \tag{8}$$?eq:notation_x?

For $i = 0, \ldots, n_1 - 1$, $j = 0, \ldots, n_2 - 1$, and $k = 0, \ldots, n_3 - 1$, we further define $F(r, s, t)$ to denote approximate value of function F at the point $\mathbf{x}(r, s, t)$. Next, by using the vectorization function of a matrix $F_\ell \in \mathbb{C}^{m_1 \times m_2 \times m_3}$, for $\ell = 1, 2, 3$

that

$$\operatorname{vec}(F_\ell) = \begin{bmatrix} \operatorname{vec}(F_\ell(1:m_1, 1:m_2, 1)) \\ \operatorname{vec}(F_\ell(1:m_1, 1:m_2, 2)) \\ \vdots \\ \operatorname{vec}(F_\ell(1:m_1, 1:m_2, m_3)) \end{bmatrix},$$

we define

$$\mathbf{f} = \begin{bmatrix} \mathbf{f}_1^\top & \mathbf{f}_2^\top & \mathbf{f}_3^\top \end{bmatrix}^\top \in \mathbb{C}^{3m_1m_2m_3}$$

with $\mathbf{f}_\ell = \operatorname{vec}(F_\ell)$, for $\ell = 1, 2, 3$.

3. Explicit Matrix Representation of the Curl Operator

⟨sec:discrete_double_curl⟩ We derive the explicit matrix representation form of the single curl operator $\nabla\times$ discretized by Yee's scheme [22]. In particular, (i) the matrix form of $\nabla \times E = \mathrm{i}\omega B$ in (1a) is derived in Section 3.1 and (ii) the matrix form of $\nabla \times H = -\mathrm{i}\omega D$ in (1b) is derived in Section 3.2.

3.1. Matrix representation of $\nabla \times E$

⟨sec:curl_E⟩ In this subsection, we derive the matrix representation of Yee's discretization for (6) by taking central finite differences at the central face points $\mathbf{x}(i, \hat{j}, \hat{k})$, $\mathbf{x}(\hat{i}, j, \hat{k})$, and $\mathbf{x}(\hat{i}, \hat{j}, k)$, respectively. The finite differences leads to the results:

⟨eq:disc_curl_H⟩

$$\mathrm{i}\omega B_1(i, \hat{j}, \hat{k}) = \frac{E_3(i, j+1, \hat{k}) - E_3(i, j, \hat{k})}{\delta_y} - \frac{E_2(i, \hat{j}, k+1) - E_2(i, \hat{j}, k)}{\delta_z}, \quad \text{(9a)}$$ eq:Dsface1

$$\mathrm{i}\omega B_2(\hat{i}, j, \hat{k}) = \frac{E_1(\hat{i}, j, k+1) - E_1(\hat{i}, j, k)}{\delta_z} - \frac{E_3(i+1, j, \hat{k}) - E_3(i, j, \hat{k})}{\delta_x}, \quad \text{(9b)}$$ eq:Dsface2

$$\mathrm{i}\omega B_3(\hat{i}, \hat{j}, k) = \frac{E_2(i+1, \hat{j}, k) - E_2(i, \hat{j}, k)}{\delta_x} - \frac{E_1(\hat{i}, j+1, k) - E_1(\hat{i}, j, k)}{\delta_y}, \quad \text{(9c)}$$ eq:Dsface3

for $i = 0, 1, \ldots, n_1 - 1$, $j = 0, 1, \ldots, n_2 - 1$, and $k = 0, 1, \ldots, n_3 - 1$. Since the matrix representation derivation of the single curl $\nabla \times (\cdot)$ involves the partial derivatives, we separate the discretization of the partial derivatives with respect to x, y, and z in the following three parts. Note that the key point to form the corresponding matrix is to explore the periodic properties associated with the lattice translation vectors that define the structure of the target material.

Part 3.1.1. Partial derivative with respect to x for E. Consider the finite difference

$$\frac{E_2(i+1, \hat{j}, k) - E_2(i, \hat{j}, k)}{\delta_x} \quad \text{and} \quad \frac{E_3(i+1, j, \hat{k}) - E_3(i, j, \hat{k})}{\delta_x} \qquad (10)$$ eq:disc_pxE2_pxE3

in (9c) and (9b), respectively. By applying the periodic condition (3) along the lattice translation vector $\mathbf{a}_1$ defined in (4), we have

$$E_2(n_1, \hat{j}, k) = e^{\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_1} E_2(0, \hat{j}, k) \text{ and } E_3(n_1, j, \hat{k}) = e^{\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_1} E_3(0, j, \hat{k}),$$

which implies that the discretizations in (10) can be represented as

$$\delta_x^{-1} K_{\mathbf{a}_1,n_1} E_2(0 : n_1 - 1, \hat{j}, k), \quad \text{and} \quad \delta_x^{-1} K_{\mathbf{a}_1,n_1} E_3(0 : n_1 - 1, j, \hat{k})$$

for $j = 0, 1, \ldots, n_2 - 1$ and $k = 0, 1, \ldots, n_3 - 1$, where

$$K_{\mathbf{a},m} = \begin{bmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \\ e^{\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}} & & & -1 \end{bmatrix} \in \mathbb{C}^{m\times m}. \tag{11}$$ eq:mtx_K_m

This means that the matrix representations of the discretizations for $\partial_x E_2$ and $\partial_x E_3$ in (10) are $C_1\mathbf{e}_2$ and $C_1\mathbf{e}_3$, respectively. Here,

$$C_1 = \delta_x^{-1} \left(I_{n_3} \otimes I_{n_2} \otimes K_{\mathbf{a}_1,n_1} \right) \in \mathbb{C}^{n\times n}.$$

Part 3.1.2. Partial derivative with respect to y for E. Consider the finite difference

$$\frac{E_1(\hat{i}, j+1, k) - E_1(\hat{i}, j, k)}{\delta_y} \quad \text{and} \quad \frac{E_3(i, j+1, \hat{k}) - E_3(i, j, \hat{k})}{\delta_y} \tag{12}$$ eq:disc_pyE1_pyE3_face

in (9c) and (9a), respectively. By applying the quasi-periodic condition (3) along the lattice translation vector $\mathbf{a}_2$ defined in (4), we have

$$E_1(\hat{i}, n_2, k) = e^{\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_2} E_1(\hat{i}, 0, k) \quad \text{and} \quad E_3(i, n_2, \hat{k}) = e^{\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_2} E_3(i, 0, \hat{k}),$$

which implies that the discretizations in (12) can be represented as

$$K_2 \mathrm{vec}(E_1(\hat{0} : \hat{n}_1 - 1, 0 : n_2 - 1, k)) \text{ and } K_2 \mathrm{vec}(E_3(0 : n_1 - 1, 0 : n_2 - 1, \hat{k})),$$

respectively, for $k = 0, 1, \ldots, n_3 - 1$ and

$$K_2 = \frac{1}{\delta_y} \begin{bmatrix} -I_{n_1} & I_{n_1} & & \\ & \ddots & \ddots & \\ & & -I_{n_1} & I_{n_1} \\ e^{\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_2} I_{n_1} & & & -I_{n_1} \end{bmatrix} = \delta_y^{-1} \left(K_{\mathbf{a}_2,n_2} \otimes I_{n_1} \right).$$

Or equivalently, the matrix representations of the discretizations in (12) are $C_2\mathbf{e}_1$ and $C_2\mathbf{e}_3$, respectively. Here,

$$C_2 = \delta_y^{-1} \left(I_{n_3} \otimes K_{\mathbf{a}_2,n_2} \otimes I_{n_1} \right).$$

Part 3.1.3. Partial derivative with respect to z for E. Consider the finite difference

$$\frac{E_1(\hat{\imath},j,k+1)-E_1(\hat{\imath},j,k)}{\delta_z} \quad \text{and} \quad \frac{E_2(i,\hat{\jmath},k+1)-E_2(i,\hat{\jmath},k)}{\delta_z} \tag{13}$$ eq:disc_pzE1_pzE2_face

in (9b) and (9a), respectively. By applying the quasi-periodic condition (3) along the lattice translation vector $\mathbf{a}_3$ defined in (4), we have

$$E_1(\hat{\imath},j,n_3)=e^{\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_3}E_1(\hat{\imath},j,0) \quad \text{and} \quad E_2(i,\hat{\jmath},n_3)=e^{\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_3}E_2(i,\hat{\jmath},0),$$

which implies that the discretizations in (13) can be represented as $C_3\mathbf{e}_1$ and $C_3\mathbf{e}_2$, respectively. Here,

$$\begin{aligned} C_3 &= \frac{1}{\delta_z}\begin{bmatrix} -I_{n_1\times n_2} & I_{n_1\times n_2} & & \\ & \ddots & \ddots & \\ & & -I_{n_1\times n_2} & I_{n_1\times n_2} \\ e^{\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_3}I_{n_1\times n_2} & & & -I_{n_1\times n_2}\end{bmatrix} \\ &= \delta_z^{-1}\left(K_{\mathbf{a}_3,n_3}\otimes I_{n_2}\otimes I_{n_1}\right). \end{aligned}$$

Part 3.1.4. A short summary. We have shown that the discretization of $\nabla\times E=\mathrm{i}\omega B$ at central face points can be represented by the following matrix representation

$$C\mathbf{e}=\mathrm{i}\omega\mathbf{b}, \tag{14}$$ eq:mtx_form_curl_E

where

$$C=\begin{bmatrix} 0 & -C_3 & C_2 \\ C_3 & 0 & -C_1 \\ -C_2 & C_1 & 0\end{bmatrix}. \tag{15}$$ eq:mtx_D_C

Part 3.1.5. A property of C_1, C_2 and C_3. The following theorem asserts that C_1, C_2 and C_3 are normal and commute with each other. See appendix for the proof of the theorem.

⟨thm:commute_prop⟩ **Theorem 1.** *For C_1, C_2 and C_3 defined in Subsection 3.1, it holds that*

$$C_i^*C_j=C_jC_i^* \quad \text{and} \quad C_iC_j=C_jC_i, \quad \text{for } i,j=1,2,3. \tag{16}$$?eq:commute?

3.2. Matrix representation of $\nabla\times H=-\mathrm{i}\omega D$

⟨sec:curl_H⟩ We derive the matrix representations of the three equations in (7) by the central finite differences at the central edge points $\mathbf{x}(\hat{\imath},j,k)$, $\mathbf{x}(i,\hat{\jmath},k)$, and $\mathbf{x}(i,j,\hat{k})$, respectively. These finite differences are given below.

?⟨eq:disc_curl_E⟩?

$$-\mathrm{i}\omega D_1(\hat{\imath},j,k) = \frac{H_3(\hat{\imath},\hat{\jmath},k)-H_3(\hat{\imath},\hat{\jmath}-1,k)}{\delta_y} - \frac{H_2(\hat{\imath},j,\hat{k})-H_2(\hat{\imath},j,\hat{k}-1)}{\delta_z}, \tag{17a}$$ eq:Dsedge1

$$-\mathrm{i}\omega D_2(i,\hat{\jmath},k) = \frac{H_1(i,\hat{\jmath},\hat{k})-H_1(i,\hat{\jmath},\hat{k}-1)}{\delta_z} - \frac{H_3(\hat{\imath},\hat{\jmath},k)-H_3(\hat{\imath}-1,\hat{\jmath},k)}{\delta_x}, \tag{17b}$$ eq:Dsedge2

$$-\mathrm{i}\omega D_3(i,j,\hat{k}) = \frac{H_2(\hat{\imath},j,\hat{k})-H_2(\hat{\imath}-1,j,\hat{k})}{\delta_x} - \frac{H_1(i,\hat{\jmath},\hat{k})-H_1(i,\hat{\jmath}-1,\hat{k})}{\delta_y}, \tag{17c}$$ eq:Dsedge3

for $i=0,1,\ldots,n_1-1$, $j=0,1,\ldots,n_2-1$, and $k=0,1,\ldots,n_3-1$. The matrix representation of $\nabla\times H$ are then derived in the following three parts, with a short summery showing the matrix representation of $\nabla\times H=-\mathrm{i}\omega D$.

The derivation in this subsection is based on the following three lemmas, whose proofs are given in the appendix.

⟨lem:pero_H23_x⟩ **Lemma 2** (Periodicity of $H_2(\hat{\imath},j,\hat{k})$ and $H_3(\hat{\imath},\hat{\jmath},k)$)**.** *By* (9b), (9c), *and the periodicity of E_ℓ, for $\ell=1,2,3$, we have*

$$H_2(\widehat{-1},j,\hat{k}) = e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_1}H_2(\hat{n}_1,j,\hat{k}),\quad H_3(\widehat{-1},\hat{\jmath},k) = e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_1}H_3(\hat{n}_1,\hat{\jmath},k),$$

for $j=0,1,\ldots,n_2-1$ and $k=0,1,\ldots,n_3-1$.

⟨lem:pero_H1H3_y⟩ **Lemma 3** (Periodicity of $H_1(i,\hat{\jmath},\hat{k})$ and $H_3(\hat{\imath},\hat{\jmath},k)$)**.** *By* (9a), (9c), *and the periodicity of E_ℓ, for $\ell=1,2,3$, we have*

$$H_1(0:n_1-1,\widehat{-1},\hat{k}) = e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_2}H_1(0:n_1-1,\hat{n}_2-1,\hat{k}) \text{ and}$$
$$H_3(\hat{0}:\hat{n}_1-1,\widehat{-1},k) = e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_2}H_3(\hat{0}:\hat{n}_1-1,\hat{n}_2-1,k),$$

for $k=0,1,\ldots,n_3-1$.

⟨lem:pero_H12_z⟩ **Lemma 4** (Periodicity of $H_1(i,\hat{\jmath},\hat{k})$ and $H_2(\hat{\imath},j,\hat{k})$)**.** *By* (9a), (9b), *and the periodicity of E_ℓ, for $\ell=1,2,3$, we have*

$$\begin{aligned}&H_1(0:n_1-1,\hat{0}:\hat{n}_2-1,\widehat{-1})\\ &= e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_3}H_1(0:n_1-1,\hat{0}:\hat{n}_2-1,\hat{n}_3-1) \text{ and}\end{aligned} \tag{18}$$?eq:pero_H1_z?

$$\begin{aligned}&H_2(\hat{0}:\hat{n}_1-1,0:n_2-1,\widehat{-1})\\ &= e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_3}H_2(\hat{0}:\hat{n}_1-1,0:n_2-1,\hat{n}_3-1).\end{aligned} \tag{19}$$ eq:pero_H2_z

Now, we show the details of the derivation in the following three parts.

Part 3.2.1. Partial derivative with respect to x for H. Consider the finite difference

$$\frac{H_2(\hat{\imath},j,\hat{k})-H_2(\hat{\imath}-1,j,\hat{k})}{\delta_x} \quad\text{and}\quad \frac{H_3(\hat{\imath},\hat{\jmath},k)-H_3(\hat{\imath}-1,\hat{\jmath},k)}{\delta_x} \tag{20}$$ eq:disc_pxH2_pxH3

in (17c) and (17b), respectively. Lemma 2 suggests that the matrix representations of the discretizations in (20) are

$$-\delta_x^{-1} K^*_{\mathbf{a}_1,n_1} H_2(\hat{0} : \hat{n}_1 - 1, j, \hat{k}) \quad \text{and} \quad -\delta_x^{-1} K^*_{\mathbf{a}_1,n_1} H_3(\hat{0} : \hat{n}_1 - 1, \hat{j}, k).$$

In other words, the matrix representations of the discretizations for $\partial_x H_2$ at $\mathbf{x}(i, j, \hat{k})$ and $\partial_x H_3$ at $\mathbf{x}(i, \hat{j}, k)$ are $-C_1^* \mathbf{h}_2$ and $-C_1^* \mathbf{h}_3$, respectively.

Part 3.2.2. Partial derivative with respect to y for H. Consider the finite difference

$$\frac{H_1(i, \hat{j}, \hat{k}) - H_1(i, \hat{j} - 1, \hat{k})}{\delta_y} \quad \text{and} \quad \frac{H_3(\hat{i}, \hat{j}, k) - H_3(\hat{i}, \hat{j} - 1, k)}{\delta_y} \tag{21}$$ eq:disc_pyH1_pyH3

in (17c) and (17a), respectively. Lemma 3 suggests that the matrix representations of the discretizations in (21) are

$$\begin{aligned} &- K_2^* \text{vec}\left(H_1(0 : n_1 - 1, \hat{0} : \hat{n}_2 - 1, \hat{k})\right), \\ &- K_2^* \text{vec}\left(H_3(\hat{0} : \hat{n}_1 - 1, \hat{0} : \hat{n}_2 - 1, k)\right), \end{aligned}$$

for $k = 0, 1, \ldots, n_3 - 1$. In other words, the matrix representation of the discretizations for $\partial_y H_1$ and $\partial_y H_3$ are $-C_2^* \mathbf{h}_1$ and $-C_2^* \mathbf{h}_3$, respectively.

Part 3.2.3. Partial derivative with respect to z for H. Consider the finite difference

$$\frac{H_1(i, \hat{j}, \hat{k}) - H_1(i, \hat{j}, \hat{k} - 1)}{\delta_z} \quad \text{and} \quad \frac{H_2(\hat{i}, j, \hat{k}) - H_2(\hat{i}, j, \hat{k} - 1)}{\delta_z} \tag{22}$$ eq:disc_pzH1_pzH2

in (17b) and (17a), respectively. Lemma 4 suggests that the matrix representations of the discretizations in (22) are $-C_3^* \mathbf{h}_1$ and $-C_3^* \mathbf{h}_2$.

Part 3.2.4. A short summary. Combining the aforementioned results, the discretization of $\nabla \times H = -\mathrm{i}\omega D$ can be represented by the following matrix representation

$$C^* \mathbf{h} = -\mathrm{i}\omega \mathbf{d}. \tag{23}$$ eq:mtx_form_curl_H

4. Resulting Eigenvalue Problems

?⟨sec:eigvalue_prob⟩? Based on the explicit matrix representations derived in Section 3, we can write down the eigenvalue problem corresponding to different material settings.

4.1. Photonic Crystal

For the photonic crystals with $\mu = 1$, we have $\zeta = \xi = 0$. That is,

$$\mathbf{b} = \mathbf{h}, \quad \mathbf{d} = B_\varepsilon \mathbf{e}, \tag{24}$$ eq:bd_PC

where B_ε is the discrete counterpart of ε. By substituting (14) with using (24) into (23), the discretizations of (1a) and (1b) form the following general eigenvalue problem (GEP)

$$A\mathbf{e} = \lambda B_\varepsilon \mathbf{e}, \quad \lambda = \omega^2, \tag{25}$$ eq:generalize_eigprob

where

$$A = C^* C. \tag{26}$$?eq:mtx_A?

4.2. Complex Media

For the complex media, from (2), the vector $[\mathbf{b}^\top, \mathbf{d}^\top]^\top$ can be rewritten as

$$\begin{bmatrix} \mathbf{b} \\ \mathbf{d} \end{bmatrix} = \begin{bmatrix} D_\zeta & B_\mu \\ -B_\varepsilon & -D_\xi \end{bmatrix} \begin{bmatrix} \mathbf{e} \\ \mathbf{h} \end{bmatrix} \equiv C_{\varepsilon,\mu,\xi,\zeta} \begin{bmatrix} \mathbf{e} \\ \mathbf{h} \end{bmatrix}, \tag{27}$$ eq:relation_bd_eh

where B_μ, D_ζ and D_ξ are the discrete counterparts of μ, ζ and ξ, respectively. Combining the results in (14), (23) and (27), the discretizations of (1a) and (1b) form the following general eigenvalue problem

$$\begin{bmatrix} C & 0 \\ 0 & C^* \end{bmatrix} \begin{bmatrix} \mathbf{e} \\ \mathbf{h} \end{bmatrix} = \mathrm{i}\omega C_{\varepsilon,\mu,\xi,\zeta} \begin{bmatrix} \mathbf{e} \\ \mathbf{h} \end{bmatrix}. \tag{28}$$ eq:GEP_complex_media

5. Divergence free condition

⟨sec:div_free⟩ This sections shows that, under a certain assumptions, the divergence free conditions corresponding to the photonic crystals and complex media are automatically satisfied in Yee's scheme.

5.1. $\nabla \cdot (\varepsilon E) = 0$ in photonic crystal

⟨sec:div_free_PC⟩ We consider the photonic crystal GEP (25) in terms of the electric field E in this section. In this case, there is only one divergence free condition $\nabla \cdot (\varepsilon E) = 0$. Let the discrete operator $\nabla_h \times^*$ denote the discretization of $\nabla \times H$ at the centers of cell edges and $\nabla_{h,\mathbf{e}} \cdot$ denote the discretization of divergence operator $\nabla \cdot E$ at the vertices due to Yee's scheme. That is,

$$\begin{aligned} (\nabla_{h,\mathbf{e}} \cdot E)(i,j,k) =& \frac{E_1(\hat{i},j,k) - E_1(\hat{i}-1,j,k)}{\delta_x} + \frac{E_2(i,\hat{j},k) - E_2(i,\hat{j}-1,k)}{\delta_y} \\ &+ \frac{E_3(i,j,\hat{k}) - E_3(i,j,\hat{k}-1)}{\delta_z} \end{aligned} \tag{29}$$ eq:discrete_div

for $i = 0, 1, \ldots, n_1 - 1$, $j = 0, 1, \ldots, n_2 - 1$ and $k = 0, 1, \ldots, n_3 - 1$. Similar to the derivations of the matrix representation for $\nabla \times H = -\mathrm{i}\omega D$ in Section 3.2, the discretization of $\nabla \cdot E$ in (29) can be represented by the matrix representation

$$-N_c^* \mathbf{e},$$

where $N_c = \begin{bmatrix} C_1^\top & C_2^\top & C_3^\top \end{bmatrix}^\top$. This representation suggests that the discrete version of the divergence free constrain $\nabla \cdot (\varepsilon E) = 0$ can be written as

$$N_c^* \left(B_\varepsilon \mathbf{e} \right) = 0. \tag{30}$$ eq:discrete_divergence_free

On the other hand, we have (i) the identity

$$\nabla_{h,\mathbf{e}} \cdot (\nabla_h \times^*) = 0 \tag{31}$$ eq:div_curl

from a straightforward calculation and (ii) $C^* \mathbf{h}$ as the matrix representation of $\nabla_h \times^*$ on the centers of cell edges from Section 3.2. Based on these two facts, Eq. (31) further suggests that

$$N_c^* C^* = 0. \tag{32}$$ eq:GHCHeq0

Now, multiplying (25) by N_c^* and using (32), we can see that

$$\lambda \left(N_c^* B_\varepsilon \mathbf{e} \right) = 0.$$

This observation implies that the divergence free constrain (30) holds provided the corresponding eigenvalue $\lambda \neq 0$.

5.2. $\nabla \cdot B = 0$ and $\nabla \cdot D = 0$ in complex media

⟨sec:div_free_cm⟩ We consider the case of complex media in this section. From (9), the discrete values of B_ℓ, $\ell = 1, 2, 3$, are defined at the central face points. In order to match these discrete values of B_ℓ in the discretization of $\nabla \cdot B$, we discretize $\nabla \cdot B$, denoted by $\nabla_{h,\mathbf{b}} \cdot$, at the cubic central points $\mathbf{x}(\hat{\imath}, \hat{\jmath}, \hat{k})$. Note that this is different from the discretization of $\nabla \cdot E$ that is performed at the vertices in (29). By doing so, we can see that the discrete counterpart of the operator $\nabla \cdot B$ can be written as

$$\begin{aligned} (\nabla_{h,\mathbf{b}} \cdot B)(\hat{\imath}, \hat{\jmath}, \hat{k}) = & \frac{B_1(i+1, \hat{\jmath}, \hat{k}) - B_1(i, \hat{\jmath}, \hat{k})}{\delta_x} + \frac{B_2(\hat{\imath}, j+1, \hat{k}) - B_2(\hat{\imath}, j, \hat{k})}{\delta_y} \\ & + \frac{B_3(\hat{\imath}, \hat{\jmath}, k+1) - B_3(\hat{\imath}, \hat{\jmath}, k)}{\delta_z}, \end{aligned} \tag{33}$$?eq:discrete_div_H?

for $i = 0, 1, \ldots, n_1 - 1$, $j = 0, 1, \ldots, n_2 - 1$ and $k = 0, 1, \ldots, n_3 - 1$. Or, in the matrix form $C_1 \mathbf{b}_1 + C_2 \mathbf{b}_2 + C_3 \mathbf{b}_3$. In other words, the discrete version of the divergence free constraint $\nabla \cdot B = 0$ is

$$C_1 \mathbf{b}_1 + C_2 \mathbf{b}_2 + C_3 \mathbf{b}_3 = 0. \tag{34}$$ eq:div_free_B

Similarly, the discretization of $\nabla \cdot D$ at the vertices suggests that the discrete version of the divergence free constrain $\nabla \cdot D = 0$ is

$$C_1^* \mathbf{d}_1 + C_2^* \mathbf{d}_2 + C_3^* \mathbf{d}_3 = 0. \tag{35}$$ eq:div_free_D

Now, we show that the discrete divergence free constrains (34) and (35) due to Yee's scheme hold under a mild assumption. The proof is given by using the following notation: $N_l^* = \begin{bmatrix} C_1 & C_2 & C_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & C_1^* & C_2^* & C_3^* \end{bmatrix}$. By the definition of C in (15) and Theorem 1, it holds that

$$N_l^* \begin{bmatrix} C & 0 \\ 0 & C^* \end{bmatrix} = 0.$$

That is, $\text{span}\{N_l\}$ is a left null space of $\text{diag}(C, C^*)$. Consequently, if $[\mathbf{b}^\top, \mathbf{d}^\top]^\top$ belongs to a subspace $\mathcal{S}_l$ generated by the left singular vectors corresponding to all positive singular values of $\text{diag}(C, C^*)$, we have

$$N_l^* \begin{bmatrix} \mathbf{b} \\ \mathbf{d} \end{bmatrix} = 0. \tag{36}$$ eq:discrete_div_free_BD

In other words, Eq. (36) suggests that the discrete divergence free constrains (34) and (35) hold under the assumption of $[\mathbf{b}^\top, \mathbf{d}^\top]^\top \in \mathcal{S}_l$.

5.3. Eigensolvers with incorporated divergence free conditions

⟨sec:div_free_cond_and_es⟩ The derivations in Sections 5.1 and 5.2 also inspire us to develop eigenvalue solvers that the divergence free conditions are incorporated. Such eigenvalue solvers are based on the eigendecomposition of A in the simulations of photonic crystal and singular value decomposition of C in the simulations complex media. Details are given below.

Eigensolver for photonic crystal. If we set $\tilde{\mathbf{e}} = B_\varepsilon \mathbf{e}$, then Eq. (30) implies that

$$N_c^* \tilde{e} = 0.$$

That is, $\tilde{\mathbf{e}}$ is orthogonal to the subspace $\mathcal{N}_c$ spanned by N_c. From Theorem 1, $\mathcal{N}_c$ is a null space of $A = C^*C$. Since A is Hermitian positive semidefinite, the invariant subspace $\mathcal{R}_A$ of A corresponding to all positive eigenvalues is orthogonal to $\mathcal{N}_c$. This tells us that if we take $\tilde{\mathbf{e}} \in \mathcal{R}_A$, then the divergence free constrain in (30) is automatically satisfied. In [8], the eigendecomposition of A is derived as

$$A = Q \text{diag}\left(0, \Lambda\right) Q^* = Q_r \Lambda Q_r^*.$$

Then, the invariant subspace $\text{span}\{B_\varepsilon^{-1} Q_r\}$, which is equivalent to $B_\varepsilon^{-1} \mathcal{R}_A$, is used to reduce the GEP (25) into a null space free eigenvalue problem (NSFEP-PC). Therefore, any eigenvector $\mathbf{e}$ computed by solving the NFSEP-PC automatically satisfies the divergence free constrain (30).

Eigensolver for complex media. It has been shown that the singular value decomposition (SVD) of C is

$$C = P \text{diag}(\Sigma_r, 0) Q^* = P_r \Sigma_r Q_r^*, \tag{37}$$ eq:svd_C

where P, Q are unitary and Σ_r is a diagonal matrix with positive diagonal entries [1]. Using the SVD of C defined in (37), we can see that that the subspace $\mathcal{S}_l$ defined in Subsection 5.2 is equal to

$$\mathcal{S}_l = \text{span}\left\{\text{diag}\left(P_r, Q_r\right)\right\}. \tag{38}$$?eq:nonzero_svd_space?

Combing the results in (27) and assuming $C_{\varepsilon,\mu,\xi,\zeta}$ is nonsingular, we see that, if

$$\begin{bmatrix}\mathbf{e}\\ \mathbf{h}\end{bmatrix} \in \text{span}\left\{C^{-1}_{\varepsilon,\mu,\xi,\zeta}\text{diag}\left(P_r, Q_r\right)\right\}, \tag{39}$$ eq:div_free_subsp

the divergence free constrains (36) are automatically satisfied. Based on the subspace defined in (39), a null space free method is developed to reduce the GEP (28) into a null space free eigenvalue problem (NFSEP-CM) [1]. So that the eigenvector $[\mathbf{e}^\top, \mathbf{h}^\top]^\top$ computed by solving the NFSEP-CM is automatically satisfies the divergence free constrains (36).

6. Discretizations of $\nabla(\nabla\cdot)$ and ∇^2 and their applications

⟨sec:second_order⟩ We derive the matrix representations of the second order differential operators $\nabla(\nabla\cdot)$ and ∇^2 due to Yee's scheme in Sections 6.1 and 6.2. These matrix representations have two applications. First, as shown in Sections 6.3, the matrix representations immediately that the discrete counterpart of the well-known curl of the curl indentity. Second, as shown in 6.5, these matrix representations further inspire us to develop efficient methods to solve the linear systems embedded in the shift-and-invert type eigenvalue solvers for various photonic crystal simulators. In the derivations, we let $\nabla_h\left(\nabla_{h,\mathbf{e}}\cdot E\right)$ and $\nabla_h^2 E$ denote the discrete $\nabla\left(\nabla\cdot E\right)$ and $\nabla^2 E$ due to Yee's scheme, respectively.

6.1. Discretization of $\nabla(\nabla\cdot E)$

⟨sec:mtx_nabla⟩ From Section 5.1, the discretization of $F = \nabla\cdot E$ at the vertices in (29) leads to

$$\mathbf{f} = -N_c^*\mathbf{e}. \tag{40}$$ eq:mtx_form_div

Denoting $G = \nabla(\nabla\cdot E) = \nabla F$, we discretize $\partial_x F$, $\partial_y F$ and $\partial_z F$ at $\mathbf{x}(\hat{i},j,k)$, $\mathbf{x}(i,\hat{j},k)$ and $\mathbf{x}(i,j,\hat{k})$, respectively, to obtain the following finite differences.

⟨eq:discrete_grad⟩

$$G_1(\hat{i},j,k) = \frac{F(i+1,j,k) - F(i,j,k)}{\delta_x}, \tag{41a}$$ {?}

$$G_2(i,\hat{j},k) = \frac{F(i,j+1,k) - F(i,j,k)}{\delta_y}, \tag{41b}$$ {?}

$$G_3(i,j,\hat{k}) = \frac{F(i,j,k+1) - F(i,j,k)}{\delta_z}, \tag{41c}$$ {?}

for $i = 0, 1, \ldots, n_1 - 1$, $j = 0, 1, \ldots, n_2 - 1$ and $k = 0, 1, \ldots, n_3 - 1$. From (29), we can see that F has the following quasi-periodic properties

$$
\begin{aligned}
F(n_1, j, k) &= e^{\mathrm{i}2\pi \mathbf{k}\cdot\mathbf{a}_1} F(0, j, k),\\
F(i, n_2, k) &= e^{\mathrm{i}2\pi \mathbf{k}\cdot\mathbf{a}_2} F(i, 0, k),\\
F(i, j, n_3) &= e^{\mathrm{i}2\pi \mathbf{k}\cdot\mathbf{a}_3} F(i, j, 0).
\end{aligned}
$$

Applying these quasi-periodic properties, the discretization of $G = \nabla F$ in (41) leads to the matrix form

$$\mathbf{g} = N_c \mathbf{f}. \tag{42}$$
eq:mtx_form_grad

Finally, substituting (40) into (42), we get the matrix representation of the discretization for $G = \nabla(\nabla \cdot E)$ that

$$\mathbf{g} = -N_c N_c^* \mathbf{e}.$$

6.2. Discretization of ∇^2

⟨sec:mtx_nabla_sqr⟩ First, we rewrite $\nabla^2 E_1$ as $\nabla \cdot (\nabla E_1)$ and set $F = \nabla E_1$. For the discretized $F_1 = \partial_x E_1$, $F_2 = \partial_y E_1$ and $F_3 = \partial_z E_1$ at $\mathbf{x}(i, j, k)$, $\mathbf{x}(\hat{i}, \hat{j}, k)$ and $\mathbf{x}(\hat{i}, j, \hat{k})$, respectively, we have

$$F_1(i, j, k) = \frac{E_1(\hat{i}, j, k) - E_1(\hat{i} - 1, j, k)}{\delta_x}, \tag{43a}$$
eq:grad_1

$$F_2(\hat{i}, \hat{j}, k) = \frac{E_1(\hat{i}, j + 1, k) - E_1(\hat{i}, j, k)}{\delta_y}, \tag{43b}$$
eq:grad_2

$$F_3(\hat{i}, j, \hat{k}) = \frac{E_1(\hat{i}, j, k + 1) - E_1(\hat{i}, j, k)}{\delta_z}, \tag{43c}$$
eq:grad_3

for $i = 0, 1, \ldots, n_1 - 1$, $j = 0, 1, \ldots, n_2 - 1$ and $k = 0, 1, \ldots, n_3 - 1$. By the quasi-periodic condition (3), the discretizations in (43a), (43b) and (43c) can be represented as the matrix forms

$$\mathbf{f}_1 = -C_1^* \mathbf{e}_1,\ \mathbf{f}_2 = C_2 \mathbf{e}_1,\ \mathbf{f}_3 = C_3 \mathbf{e}_1, \tag{44}$$
eq:mtx_form_grad_2

respectively. Similar to (29), we discrete $\nabla \cdot F$ at the central edge points $\mathbf{x}(\hat{i}, j, k)$ to obtain

$$
\begin{aligned}
(\nabla_h \cdot F)(\hat{i}, j, k) = & \frac{F_1(i + 1, j, k) - F_1(i, j, k)}{\delta_x} + \frac{F_2(\hat{i}, \hat{j}, k) - F_2(\hat{i}, \hat{j} - 1, k)}{\delta_y}\\
& + \frac{F_3(\hat{i}, j, \hat{k}) - F_3(\hat{i}, j, \hat{k} - 1)}{\delta_z},
\end{aligned} \tag{45}
$$
eq:discrete_div_2

for $i = 0, 1, \ldots, n_1 - 1$, $j = 0, 1, \ldots, n_2 - 1$ and $k = 0, 1, \ldots, n_3 - 1$. By the quasi-periodic properties, the discretization in (45) results in the matrix representation

$$C_1 \mathbf{f}_1 - C_2^* \mathbf{f}_2 - C_3^* \mathbf{f}_3. \tag{46}$$
eq:mtx_form_div_3

Now, substituting (44) into (46), we obtain the matrix form of the discretization for $\nabla^2 E_1$ as

$$-\left(C_1 C_1^* + C_2^* C_2 + C_3^* C_3\right)\mathbf{e}_1 = -N_c^* N_c \mathbf{e}_1. \tag{47}$$
eq:Lap_e1

A similar derivation can show that the matrix representations of discretized $\nabla^2 E_2$ and $\nabla^2 E_3$ are

$$-N_c^* N_c \mathbf{e}_2 \quad \text{and} \quad -N_c^* N_c \mathbf{e}_3, \tag{48}$$
eq:Lap_e23

respectively. Finally, by combining (47) and (48), we can see that the matrix form of the discrete $\nabla^2 E$ is

$$-\left(I_3 \otimes N_c^* N_c\right)\mathbf{e}.$$

6.3. Discrete curl of curl identify

⟨sec:curl_curl⟩ We assert the discrete counterpart of the curl of curl identify

$$\nabla \times \nabla \times E = \nabla\left(\nabla \cdot E\right) - \nabla^2 E. \tag{49}$$
?eq:transform?

We have shown that C^*C, $-N_c N_c^*$ and $-I_3 \otimes (N_c^* N_c)$ are the matrix representations of discrete operations $\nabla_h \times^* \nabla_h \times$, $\nabla_h\left(\nabla_{h,\mathbf{e}} \cdot\right)$ and ∇_h^2 in Yee's scheme, respectively. On the other hand, Theorem 1 implies that

$$C^*C = I_3 \otimes (N_c^* N_c) - N_c N_c^*. \tag{50}$$
eq:mtx_double_curl

It is thus clear that Eq. (50) is the explicit matrix representation of the discretization

$$\nabla_h \times^* \nabla_h \times E = \nabla_h\left(\nabla_{h,\mathbf{e}} \cdot E\right) - \nabla_h^2 E. \tag{51}$$
?eq:diff_double_curl?

6.4. Application to the kernel of the single curl

⟨sec:huge_kernel⟩ It is worth mentioning that, by taking conjugate transpose of (32), we have

$$C N_c = 0. \tag{52}$$
eq:null_space_A

Since C and N_c are the matrix representations of the discretizations of single curl operator $\nabla\times$ in Section 3.1 and the gradient operator ∇ in (42), respectively, it is clear that Eq. (52) is the explicit matrix representation of the discretization

$$\nabla_h \times \nabla_h \equiv 0, \tag{53}$$
eq:disc_curl_grad

where $\nabla_h\times$ denotes the discretization of $\nabla\times$ in Section 3.1. In other words, for any vector $\mathbf{f}$, (53) suggests that $\nabla_h \mathbf{f}$ is a null vector of $\nabla_h\times$. Or equivalently, Eq. (53) implies that the kernel of the discrete single curl with the quasi-periodicity constrain is huge.

6.5. Applications to the eigensolvers

⟨sec:app_to_prec_sys⟩ To solve the GEP (25) by the shift-and-invert Lanczos method, we need to solve the linear system

$$(C^*C - D)\mathbf{x} = \mathbf{b} \tag{54}$$ eq:LinearSystem

in each iteration for a certain diagonal matrix D. As suggested in [6, 9], $M = C^*C - \sigma I$, where σ is a constant, is an efficient preconditioner. The matrix equation (50) actually suggests an efficient way to solve the preconditioned linear system

$$(C^*C - \sigma I)\mathbf{y} = \mathbf{d}.$$

Furthermore, for the dispersive metallic photonic crystals [2, 3, 4, 14, 15, 20], the Yee's discretization results a rational eigenvalue problem

$$C^*C\mathbf{e} = \lambda^2 B_\varepsilon(\lambda)\mathbf{e}, \tag{55}$$ eq:rational_eigprob

where $B_\varepsilon(\lambda)$ is diagonal. The diagonal entries of $B_\varepsilon(\lambda)$ are rational functions with variable λ. The most expensive computational task in solving (55) is a series of linear systems in the form of (54). Again, such linear systems can be efficiently solved by the iterative method with preconditioner $M = C^*C - \sigma I$ [7] by applying equation (50).

7. Conclusion

⟨sec:conclusion⟩ Solving the Maxwell equations by Yee's scheme is one essential tool for studying electromagnetism. Our goal is to deepen the understanding of such scheme from the viewpoint of matrix computation. This article is summarized in Tables 1 to 3. Table 1 summarizes the explicit matrix representations of the differential operators and operations that are related to the Maxwell equations modeling the metamaterials. As summarized in Table 2, we have asserted three second-order discrete operators due to Yee's scheme and discussed their roles in solving the Maxwell equations. First, in Section 5.1, we have asserted the discrete counterpart of the continuous divergence of curl $\nabla\cdot\nabla\times = 0$ in Eq. (31). The fact also implies that the divergence free constrain (30) holds for the nonzero eigenvalues that are of interest. Second, in Section 6.4, we have asserted the discrete counterpart of the continuous curl of gradient identify $\nabla \times \nabla\phi = 0$ in Eq. (53). The result suggests that there is large kernel of the discrete curl operator $\nabla_h\times$. For the eignevalue problem (28) formed by the curl operator, such large kernel can downgrade the convergence of the eigenvalue solvers. Fortunately, as discussed in Section 5.3, a null space free eigenvalue problem developed in [1] overcomes this issue by deflating the null space. Third, in Section 6.3, we have asserted the discrete counterpart of the continuous curl of curl identify $\nabla\times\nabla\times E = \nabla(\nabla\cdot E) - \nabla^2 E$ in Eq. (50). Then, in Section 6.5, we have shown how the results can be applied to develop efficient methods for the linear systems embedded in the eigenvalue solvers. For photonic crystal and complex media,

Cont. operator	$\nabla \times H$	$\nabla \times E$	$\nabla \cdot E$	$\nabla \cdot B$	$\nabla \cdot D$
Disc. operator	$\nabla_h \times^*$	$\nabla_h \times$	$\nabla_{h,\mathbf{e}} \cdot$		
Matrix form	$C^*\mathbf{h}$	$C\mathbf{e}$	$-N_c^*\mathbf{e}$	$[C_1, C_2, C_3]\mathbf{b}$	$-N_c^*\mathbf{d}$
Discretized pts	$\mathbf{x}(\hat{i}, j, k)$	$\mathbf{x}(i, \hat{j}, \hat{k})$	$\mathbf{x}(i, j, k)$	$\mathbf{x}(\hat{i}, \hat{j}, \hat{k})$	$\mathbf{x}(i, j, k)$
	$\mathbf{x}(i, \hat{j}, k)$	$\mathbf{x}(\hat{i}, j, \hat{k})$			
	$\mathbf{x}(i, j, \hat{k})$	$\mathbf{x}(\hat{i}, \hat{j}, k)$			
Reference	Sec. 3.2	Sec. 3.1	Sec. 5.1	Sec. 5.2	Sec. 5.2
Cont. operator	$\nabla \times \nabla \times E$				
Matrix form	$C^*C\mathbf{e}$				

Cont. operator	$\nabla \cdot E$	∇F	∇E_1	$\nabla \cdot F$
Disc. operator	$\nabla_{h,\mathbf{e}} \cdot$	∇_h		
Matrix form	$-N_c^*\mathbf{e}$	$N_c\mathbf{f}$	$[-C_1 \;\; C_2^* \;\; C_3^*]^* \, \mathbf{e}_1$	$C_1\mathbf{f}_1 - C_2^*\mathbf{f}_2 - C_3^*\mathbf{f}_3$
Discretized pts	$\mathbf{x}(i, j, k)$	$\mathbf{x}(\hat{i}, j, k)$	$\mathbf{x}(i, j, k)$	$\mathbf{x}(\hat{i}, j, k)$
		$\mathbf{x}(i, \hat{j}, k)$	$\mathbf{x}(\hat{i}, \hat{j}, k)$	
		$\mathbf{x}(i, j, \hat{k})$	$\mathbf{x}(\hat{i}, \hat{j}, k)$	
Reference	Sec. 6.1	Sec. 6.1	Sec. 6.2	Sec. 6.2
Cont. operator	$\nabla(\nabla \cdot E)$		$\nabla^2 E$	
Matrix form	$-N_c N_c^* \mathbf{e}$		$-[I_3 \otimes (N_c^* N_c)]\mathbf{e}$	

Table 1: Explicit matrix representations and discretization points of the differential operators and operations within the Maxwell equations.

⟨tab:mtx_rep_summary⟩

Continuous operator	$\nabla \cdot (\nabla \times E) = 0$	$\nabla \times \nabla F = 0$
Discrete operator	$\nabla_{h,\mathbf{e}} \cdot (\nabla_h \times^* E) = 0$	$\nabla_h \times (\nabla_h \mathbf{f}) = 0$
Matrix form	(32)	(52)
Indication	Div. free constraint (30) holds in Yee's scheme	$\nabla_h \times$ has large kernel
Reference	Section 5.1	Sections 6.4, 5.3, [1]

Continuous operator	$\nabla \times \nabla \times E = \nabla (\nabla \cdot E) - \nabla^2 E$
Discrete operator	$\nabla_h \times^* \nabla_h \times E = \nabla_h (\nabla_{h,\mathbf{e}} \cdot E) - \nabla_h^2 E$
Matrix form	$C^* C = I_3 \otimes (N_c^* N_c) - N_c N_c^*$ in (50)
Application	Efficient linear solvers within eigensolvers
Reference	Sections 6.3 and 6.5

Table 2: Second order operators and their indications or application.

⟨tab:ContDiscEqs_summary⟩

	Photonic crystal	Complex media
Eigenvalue prob.	(25)	(28)
Constraint	$\nabla \cdot (\varepsilon E) = 0$	$\nabla \cdot B = 0, \ \ \nabla \cdot D = 0$
Matrix form	$N_c^*(B_\varepsilon \mathbf{e}) = 0$	$N_l^* \left[\mathbf{b}^* \ \ \mathbf{d}^*\right]^* = 0$
Condition	$\mathbf{e} \in \mathrm{span}\left\{B_\varepsilon^{-1} Q_r\right\}$	$[\mathbf{e}^* \ \ \mathbf{h}^*]^* \in \mathrm{span}\{C_{\varepsilon,\mu,\xi,\zeta}^{-1}\mathrm{diag}\,(P_r, Q_r)\}$
Reference	Section 5.3 and [8]	Section 5.3 and [1].

Table 3: Subjects in the derivations regarding why the divergence free constraints are automatically satisfied in the eigenvalue solvers due to Yee's scheme.

⟨tab:DivFree_summary⟩

Table 3 shows the eigenvalue problems, the corresponding divergence free constrains and their explicit matrix representations. As discussed in Section 5.3, the eigensolver developed in [8] and [1] can lead to the eigenvectors satisfying the conditions shown in the table and thus the divergence free conditions are satisfied.

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Appendix

Proof of Theorem 1 .
By the definition of $K_{\mathbf{a},m}$ in (11), it is easily verified that

$$K_{\mathbf{a},m}^* K_{\mathbf{a},m} = K_{\mathbf{a},m} K_{\mathbf{a},m}^*$$

which implies that

$$C_i^* C_i = C_i C_i^* \quad \text{for } i = 1, 2, 3. \tag{56}$$?eq:normal?

On the other hand, using the property

$$(A_1 \otimes A_2 \otimes A_3)(B_1 \otimes B_2 \otimes B_3) = (A_1 B_1) \otimes (A_2 B_2) \otimes (A_3 B_3),$$

and the definitions of C_ℓ, $\ell = 1, 2, 3$, we have $C_i^* C_j = C_j C_i^*$ and $C_i C_j = C_j C_i$ for $i \neq j$. $\square$

Proof of Lemma 2.
By the periodic condition (3), we have

$$\begin{aligned} E_1(\widehat{-1}, j, k) &= e^{-\mathrm{i}2\pi \mathbf{k}\cdot\mathbf{a}_1} E_1(\hat{n}_1 - 1, j, k), \\ E_3(0, j, \hat{k}) &= e^{-\mathrm{i}2\pi \mathbf{k}\cdot\mathbf{a}_1} E_3(n_1, j, \hat{k}), \\ E_3(-1, j, \hat{k}) &= e^{-\mathrm{i}2\pi \mathbf{k}\cdot\mathbf{a}_1} E_3(n_1 - 1, j, \hat{k}). \end{aligned}$$

From (9b), we have

$$
\begin{aligned}
&H_2(\widehat{-1}, j, \hat{k}) \\
=&e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_1}\left(\frac{E_1(\hat{n}_1-1,j,k+1)-E_1(\hat{n}_1-1,j,k)}{\delta_z}-\frac{E_3(n_1,j,\hat{k})-E_3(n_1-1,j,\hat{k})}{\delta_x}\right) \\
=&e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_1}H_2(\hat{n}_1-1,j,\hat{k}).
\end{aligned}
$$

Similarly, it holds that $H_3(\widehat{-1},\hat{j},k)=e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_1}H_3(\hat{n}_1,\hat{j},k)$. □

Proof of Lemma 3.
By the periodic condition (3), we have

$$
\begin{aligned}
E_2(i,\widehat{-1},k) &= e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_2}E_2(i,\hat{n}_2-1,k), \\
E_3(i,0,\hat{k}) &= e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_2}E_3(i,n_2,\hat{k}), \\
E_3(i,-1,\hat{k}) &= e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_2}E_3(i,n_2-1,\hat{k}).
\end{aligned}
$$

From (9a), we have

$$
\begin{aligned}
&H_1(i,\widehat{-1},\hat{k}) \\
&= \frac{E_3(i,0,\hat{k})-E_3(i,-1,\hat{k})}{\delta_y}-\frac{E_2(i,\widehat{-1},k+1)-E_2(i,\widehat{-1},k)}{\delta_z} \\
&= e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_2}\left(\frac{E_3(i,n_2,\hat{k})-E_3(i,n_2-1,\hat{k})}{\delta_y}\right. \\
&\quad\left.-\frac{E_2(i,\hat{n}_2-1,k+1)-E_2(i,\hat{n}_2-1,k)}{\delta_z}\right) \\
&= e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_2}H_1(i,\hat{n}_2-1,\hat{k}),
\end{aligned}
$$

which implies that

$$
H_1(0:n_1-1,\widehat{-1},\hat{k}) = e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_2}H_1(0:n_1-1,\hat{n}_2-1,\hat{k}).
$$

Finally, by using the same technique, we can show that

$$
H_3(\hat{0}:\hat{n}_1-1,\widehat{-1},k) = e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_2}H_3(\hat{0}:\hat{n}_1-1,\hat{n}_2-1,k),
$$

which complete the proof. □

Proof of Lemma 4.
By the periodic condition (3), we have

$$
\begin{aligned}
E_2(i,\hat{j},0) &= e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_3}E_2(i,\hat{j},n_3), \\
E_2(i,\hat{j},-1) &= e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_3}E_2(i,\hat{j},n_3-1), \\
E_3(i,j,\widehat{-1}) &= e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_3}E_3(i,j,\hat{n}_3-1).
\end{aligned}
$$

From (9a), we have

$$
\begin{aligned}
&H_1(i,\hat{j},\widehat{-1}) \\
&= \frac{E_3(i,j+1,\widehat{-1}) - E_3(i,j,\widehat{-1})}{\delta_y} - \frac{E_2(i,\hat{j},0) - E_2(i,\hat{j},-1)}{\delta_z} \\
&= e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_3}\left(\frac{E_3(i,j+1,\hat{n}_3-1) - E_3(i,j,\hat{n}_3-1)}{\delta_y}\right. \\
&\quad \left. - \frac{E_2(i,\hat{j},n_3) - E_2(i,\hat{j},n_3-1)}{\delta_z}\right) \\
&= e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_3} H_1(i,\hat{j},\hat{n}_3-1).
\end{aligned}
$$

That is

$$
H_1(0:n_1-1,\hat{0}:\hat{n}_2-1,\widehat{-1}) = e^{-\mathrm{i}2\pi\mathbf{k}\cdot\mathbf{a}_3} H_1(0:n_1-1,\hat{0}:\hat{n}_2-1,\hat{n}_3-1).
$$

The periodicity shown in (19) can be proved similarly. □

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