EIGENDECOMPOSITION OF THE DISCRETE DOUBLE-CURL OPERATOR WITH APPLICATION TO FAST EIGENSOLVER FOR THREE DIMENSIONAL PHOTONIC CRYSTALS *

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Abstract. This article focuses on the discrete double-curl operator arising in the Maxwell equation that models three dimensional photonic crystals with face centered cubic lattice. The discrete double-curl operator is the degenerate coefficient matrix of the generalized eigenvalue problems (GEVP) due to the Maxwell equation. We derive an eigendecomposition of the degenerate coefficient matrix and explore an explicit form of orthogonal basis for the range and null spaces of this matrix. To solve the GEVP, we apply these theoretical results to project the GEVP to a standard eigenvalue problem (SEVP), which involves only the eigenspace associated with the nonzero eigenvalues of the GEVP and therefore the zero eigenvalues are excluded and will not degrade the computational efficiency. This projected SEVP can be solved efficiently by the inverse Lanczos method. The linear systems within the inverse Lanczos method are well-conditioned and can be solved efficiently by the conjugate gradient method without using a preconditioner. We also demonstrate how two forms of matrix-vector multiplications, which are the most costly part of the inverse Lanczos method, can be computed by fast Fourier transformation due to the eigendecomposition to significantly reduce the computation cost. Integrating all of these findings and techniques, we obtain a fast eigenvalue solver. The solver has been implemented by MATLAB and successfully solves each of a set of 5.184 million dimension eigenvalue problems within 50 to 104 minutes on a workstation with two Intel Quad-Core Xeon X5687 3.6 GHz CPUs.

Key words. The Maxwell equation, discrete double-curl operator, eigendecomposition, fast Fourier transform, photonic crystals, face centered cubic lattice.

AMS subject classifications. 65F15, 65T50, 15A18, 15A23.

1. Introduction.

We study the band structures of three-dimensional (3D) photonic crystals in the full space by considering the Maxwell equations

$$\begin{cases} \nabla \times H = \varepsilon \partial_t E, \\ \nabla \times E = -\mu_0 \partial_t H, \\ \nabla \cdot (\varepsilon E) = 0, \\ \nabla \cdot H = 0. \end{cases} \tag{1.1}$$

Here, H, E, μ_0, and ε represent the time-harmonic magnetic field, the time-harmonic electric field, the magnetic constant, and the material dependent piecewise constant permittivity, respectively. By separating the time and space variables and eliminating the magnetic field H, Eqs. (1.1) become the differential eigenvalue problem

$$\begin{cases} \nabla \times \nabla \times E = \lambda \varepsilon E, \\ \nabla \cdot (\varepsilon E) = 0, \end{cases} \tag{1.2}$$

where $\lambda = \mu_0 \omega^2$ is the unknown eigenvalue and ω stands for the frequency of time [22, Chap. 2].

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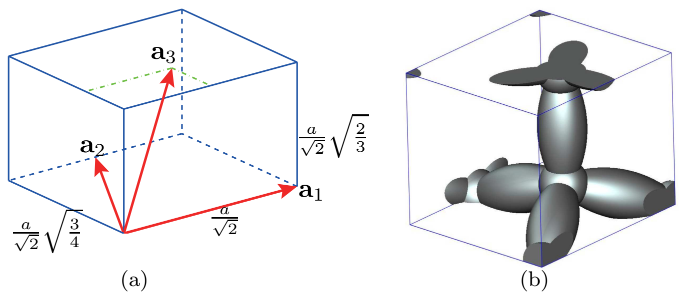


FIG. 1.1. *(a) The primitive cell and lattice translation vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$. Any pair of the vectors make an angle of $\frac{\pi}{3}$. The length, width and height of the primitive cell are $\frac{a}{\sqrt{2}}$, $\frac{a}{\sqrt{2}}\sqrt{\frac{3}{4}}$, and $\frac{a}{\sqrt{2}}\sqrt{\frac{2}{3}}$, respectively. (b) A schema of diamond structure with sp^3-like configuration within a single primitive cell.*

Supported by the Bloch theorem [23], the spectrum of the periodic setting in the full space is the union of all spectra of quasi-periodic problems in one primitive cell. Therefore, we consider a primitive cell as the computational domain of Eq. (1.2). Note that such primitive cell is spanned by the lattice translation vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ and we assume the primitive cell extends the target 3D periodic structure. In particular, for a Bloch wave vector $2\pi\mathbf{k}$ in the first Brillouin zone [22], we are interested in finding Bloch eigenfunctions E for Eq. (1.2) that satisfies the quasi-periodic condition [33]

$$E(\mathbf{x} + \mathbf{a}_\ell) = e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_\ell} E(\mathbf{x}), \tag{1.3}$$

for $\ell = 1, 2, 3$. Two examples of lattice translation vectors are (i) the simple cubic (SC) lattice vectors with $\mathbf{a}_\ell$ being the ℓ-th unit vectors in $\mathbb{R}^3$, $\ell = 1, 2, 3$; and (ii), as shown in Figure 1.1, the face-centered cubic (FCC) lattice vectors with

$$\mathbf{a}_1 = \frac{a}{\sqrt{2}}[1,0,0]^\top,\ \mathbf{a}_2 = \frac{a}{\sqrt{2}}\left[\frac{1}{2}, \frac{\sqrt{3}}{2}, 0\right]^\top,\ \text{and } \mathbf{a}_3 = \frac{a}{\sqrt{2}}\left[\frac{1}{2}, \frac{1}{2\sqrt{3}}, \sqrt{\frac{2}{3}}\right]^\top, \tag{1.4}$$

in which a is a lattice constant. Note that pairwise angles formed by $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ are $\frac{\pi}{2}$ and $\frac{\pi}{3}$ in SC and FCC lattices, respectively.

It has been shown that the photonic crystals with FCC lattice have a larger photonic band gap, compared with SC lattice [8], and larger band gaps are favored in many innovative practical applications [3, 13, 25, 31]. Therefore, in this paper, we focus on 3D photonic crystals with FCC lattice. Despite their broad applications, numerical simulations based on the numerical solutions to Eq. (1.2) with FCC lattice in 3D remain a challenge. To predict the shape of photonic crystals achieving maximal band gap, one needs to solve a sequence of eigenvalue problems associated with different geometric shape parameters and Bloch wave vectors. This is a very time consuming process as many large-scale eigenvalue problems need to be solved. It is thus of great interest to develop a fast eigensolver for the target eigenvalue problems, so that we can significantly shorten the computational time and thereby make the already widely used numerical simulations an even powerful tool.

Many numerical methods have been proposed to discretize the Maxwell equations. Examples include finite difference methods [7, 8, 26, 36], finite volume methods [9, 10, 24], finite element methods [2, 5, 6, 15, 21, 27], the Whitney form [1, 35], the co-volume discretization [30], the mimetic discretization [20], and edge element methods [12, 28, 29, 32]. In this paper, we use Yee's finite difference scheme [36] to discrete the Maxwell equations.

Discretizing Eq. (1.2) on a primitive cell with FCC lattice vectors (1.4) by Yee's scheme leads to a generalized eigenvalue problem (GEVP)

$$A\mathbf{x} = \lambda B\mathbf{x}, \tag{1.5}$$

where $A \in \mathbb{C}^{3n\times 3n}$ is Hermitian positive semi-definite and B is positive and diagonal. The matrix A is the discrete double-curl operator of $\nabla\times\nabla\times$ and the diagonal elements in B are the material dependent dielectric constants. To solve the GEVP (1.5), however, is not an easy task due to the following numerical challenges. First, the multiplicity of the zero eigenvalue of (1.5) is one third of the dimension of A [4, 8, 19]. As we are interested in finding a few of the smallest positive eigenvalues, the large dimension of the null space leads to several numerical difficulties [8, 16]. Second, the eigenvectors of A associated with the SC lattice are mutually *independent* to the 3D grid point indices i, j, and k. Consequently, the standard FFT can be applied to compute the associated photonic band gap in the SC lattice [11, 17]. However, the FCC case has no such luxury. Due to the skew lattice vectors (1.4), the eigenvectors of A associated with the FCC lattice are mutually *dependent* to the the indices i, j, and k. The standard FFT technique thus becomes infeasible for these periodic coupling eigenvectors as the periodic properties of the FCC lattice is much more complicated than that of SC lattice.

To tackle these challenging problems, we make the following contributions to derive an eigendecomposition of A and then to develop a fast eigensolver for the GEVP.

- We derive the eigendecompositions of discretization matrices of the partial derivative and double-curl operators explicitly. Then we assert that an orthogonal basis Q_r spans the range of A and $B^{-1}Q_r\Lambda_r^{1/2}$ spans the invariant subspace corresponding to all nonzero eigenvalues of (1.5) with a positive diagonal Λ_r.
- By applying the basis $B^{-1}Q_r\Lambda_r^{1/2}$, the GEVP can be reduced to a standard eigenvalue problem (SEVP) $A_r\mathbf{y} = \lambda\mathbf{y}$ and the GEVP and SEVP have the same positive eigenvalues. As $A_r = \Lambda_r^{1/2}Q_r^*B^{-1}Q_r\Lambda_r^{1/2}$ is an $2n\times 2n$ Hermitian and positive definite matrix, the SEVP can be solved by the inverse Lanczos method *without* being affected by zero eigenvalues. Moreover, the coefficient matrix A_r is well-conditioned. In each Lanczos step, the conjugate gradient method can be used to solve the associated linear system efficiently without any preconditioner.
- To solve the linear system in the inverse Lanczos method, two types of matrix-vector multiplications $Q_r^*\mathbf{p}$ and $Q_r\mathbf{q}$ are the most costly part of the computation. We successfully derive a variant FFT for the computations of $Q_r^*\mathbf{p}$ and $Q_r\mathbf{q}$, which significantly reduce the computational cost.
- As the null space of (1.5) can be deflated by the intrinsic mathematical properties of A and the computational bottleneck can be accelerated by FFT, we study the efficiency of the proposed inverse Lanczos method. This new method can be realized by MATLAB easily and the numerical results show several promising timing results. For example, our MATLAB implementation

can find the target positive eigenvalues of a sequence of 5.184 million dimension GEVP in the form of (1.5) within 50 to 104 minutes.

This paper is outlined as follows. In Section 2, we illustrate the degenerate coefficient matrix A corresponding to the discrete double-curl operator with FCC lattices. In Section 3, we find an eigendecomposition of A and give explicit representations of orthogonal basis for range and null spaces of A. We develop the inverse projective Lanczos method and an efficient way to compute the associated matrix-vector multiplications in Sections 4 and 5, respectively. Numerical experiments to validate and measure the timing performance of the proposed schemes are demonstrated in Section 6. Finally, we conclude the paper in Section 7.

Throughout this paper, we let $\top$ and $*$ denote the transpose and the conjugate transpose of a matrix by the superscript, respectively. For the matrix operations, we let $\otimes$ and $\oplus$ denote the Kronecker product and direct sum of two matrices, respectively. The imaginary number $\sqrt{-1}$ is written as $\imath$ and the identity matrix of order n is written as I_n. The conjugate of a complex scalar $z \in \mathbb{C}$ and a complex vector $\mathbf{z} \in \mathbb{C}^n$ are represented by $\bar{z}$ and $\bar{\mathbf{z}}$, respectively. The $\mathrm{vec}(\cdot)$ is the operator that vectorizes a matrix by stacking the columns of the matrix.

2. Discrete Double-Curl Operator with FCC Lattice. We use Yee's scheme [36] to discretize Eq. (1.2) in the primitive cell that is illustrated in Figure 1.1. As the details of discretization are complicated, we refer readers to [18] that describes the whole discretization process in details. Let n_1, n_2 and n_3 be the multiples of 6 and denote numbers of grid points in x-, y- and z-axis, respectively, and $n = n_1 n_2 n_3$. The mesh size in three axes are chosen by

$$\delta_x = \frac{a}{\sqrt{2}} \frac{1}{n_1}, \quad \delta_y = \frac{a}{\sqrt{2}} \sqrt{\frac{3}{4}} \frac{1}{n_2}, \quad \delta_z = \frac{a}{\sqrt{2}} \sqrt{\frac{2}{3}} \frac{1}{n_3}. \tag{2.1}$$

The resulting large-scale $3n \times 3n$ Hermitian and degenerate matrix associated with the double-curl operator $\nabla \times \nabla \times$ is of the form

$$A = C^* C \in \mathbb{C}^{3n \times 3n}, \tag{2.2}$$

where

$$C = \begin{bmatrix} 0 & -C_3 & C_2 \\ C_3 & 0 & -C_1 \\ -C_2 & C_1 & 0 \end{bmatrix} \in \mathbb{C}^{3n \times 3n}, \tag{2.3a}$$

$$C_1 = I_{n_2 n_3} \otimes K_1 \in \mathbb{C}^{n \times n}, \; C_2 = I_{n_3} \otimes K_2 \in \mathbb{C}^{n \times n}, \; C_3 = K_3 \in \mathbb{C}^{n \times n}, \tag{2.3b}$$

$$K_1 = \frac{1}{\delta_x} \begin{bmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \\ e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_1} & & & -1 \end{bmatrix} \in \mathbb{C}^{n_1 \times n_1}, \tag{2.4a}$$

$$K_2 = \frac{1}{\delta_y} \begin{bmatrix} -I_{n_1} & I_{n_1} & & \\ & \ddots & \ddots & \\ & & -I_{n_1} & I_{n_1} \\ e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_2} J_2 & & & -I_{n_1} \end{bmatrix} \in \mathbb{C}^{(n_1 n_2)\times(n_1 n_2)}, \tag{2.4b}$$

$$K_3 = \frac{1}{\delta_z} \begin{bmatrix} -I_{n_1 n_2} & I_{n_1 n_2} & & \\ & \ddots & \ddots & \\ & & -I_{n_1 n_2} & I_{n_1 n_2} \\ e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_3} J_3 & & & -I_{n_1 n_2} \end{bmatrix} \in \mathbb{C}^{n\times n}, \tag{2.4c}$$

$$J_2 = \begin{bmatrix} 0 & e^{-\imath 2\pi \mathbf{k}\cdot\mathbf{a}_1} I_{n_1/2} \\ I_{n_1/2} & 0 \end{bmatrix} \in \mathbb{C}^{n_1\times n_1}, \text{ and} \tag{2.5a}$$

$$J_3 = \begin{bmatrix} 0 & e^{-\imath 2\pi \mathbf{k}\cdot\mathbf{a}_2} I_{\frac{1}{3}n_2} \otimes I_{n_1} \\ I_{\frac{2}{3}n_2} \otimes J_2 & 0 \end{bmatrix} \in \mathbb{C}^{(n_1 n_2)\times(n_1 n_2)}. \tag{2.5b}$$

Note that these matrices are associated with particular operators as shown below.

(i) The block cyclic matrices K_1, K_2, and K_3 are the finite difference discretizations associated with quasi-periodic conditions. The entries $-I$ and I in the same row of K_ℓ, $\ell = 1, 2, 3$, correspond to the regular finite differences. The entries $e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_1}$ and -1 in the last row of K_1 are associated with the quasi-periodic condition along $\mathbf{a}_1$. Similarly, $e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_2} J_2$ and $-I_{n_1}$ in K_2 are associated with the quasi-periodic condition along $\mathbf{a}_1$ and $\mathbf{a}_2$. The matrices $e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_3} J_3$ and $-I_{n_1 n_2}$ in K_3 are associated with the quasi-periodic condition along $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$.

(ii) The matrices C_1, C_2, and C_3 are the discretizations of the operators ∂_x, ∂_y and ∂_z, respectively, at the central face points $((i+\frac{1}{2})\delta_x, (j+\frac{1}{2})\delta_y, k\delta_z)$, $(i\delta_x, (j+\frac{1}{2})\delta_y, (k+\frac{1}{2})\delta_z)$, and $((i+\frac{1}{2})\delta_x, j\delta_y, (k+\frac{1}{2})\delta_z)$.

(iii) The matrices C_1^*, C_2^* and C_3^* are the discretizations of the operators $-\partial_x$, $-\partial_y$ and $-\partial_z$, respectively, at the central edge points $((i+\frac{1}{2})\delta_x, j\delta_y, k\delta_z)$, $(i\delta_x, (j+\frac{1}{2})\delta_y, k\delta_z)$, and $(i\delta_x, j\delta_y, (k+\frac{1}{2})\delta_z)$.

(iv) The matrices C^*C, $I_3 \otimes (G^*G)$, and GG^* are the discretizations of the operators $\nabla\times\nabla\times$, $-\nabla^2$, and $-\nabla(\nabla\cdot)$ at the central edge points, respectively. Here,

$$G = [C_1^\top, C_2^\top, C_3^\top]^\top. \tag{2.6}$$

3. Eigendecomposition of the Discrete Operators. In the following two sub-sections, we derive eigendecompositions of the discrete partial derivative operators C_ℓ's and then the discrete double-curl operator $A = C^*C$ in *explicit* forms.

3.1. Eigendecomposition of the partial derivative operators. To find an eigendecomposition of C_ℓ defined in (2.3a), our approach is divided into the following steps. First, we find the eigenpairs of K_1, K_2, and K_3 defined in (2.4). By using these eigenpairs, we show that the matrices C_1, C_2, and C_3 can be diagonalized by a common unitary matrix. Combining these results, we obtain the eigendecompositions of C_ℓ.

THEOREM 3.1 (Eigenpairs of K_1). *The eigenpairs of K_1 in (2.4a) are $\left(\delta_x^{-1}(e^{\theta_i}-1),\ \mathbf{x}_i\right)$, where*

$$\theta_i = \frac{\imath 2\pi(i+\mathbf{k}\cdot\mathbf{a}_1)}{n_1}, \tag{3.1}$$

$$\mathbf{x}_i = \begin{bmatrix} 1 & e^{\theta_i} & e^{2\theta_i} & \cdots & e^{(n_1-1)\theta_i} \end{bmatrix}^\top, \tag{3.2}$$

for $i = 1,\dots,n_1$.

Proof. Verify $\delta_x K_1 \mathbf{x}_i = \left(e^{\theta_i}-1\right)\mathbf{x}_i$ directly, for $i=1,\dots,n_1$. □

THEOREM 3.2 (Eigenpairs of K_2). *The eigenpairs of K_2 in (2.4b) are*

$$\left(\delta_y^{-1}(e^{\theta_{i,j}}-1),\ \mathbf{y}_{i,j}\otimes\mathbf{x}_i\right),$$

where $\mathbf{x}_i$ is given in (3.2) and

$$\theta_{i,j} = \frac{\imath 2\pi(j-\frac{i}{2}+\mathbf{k}\cdot\hat{\mathbf{a}}_2)}{n_2} \quad \textit{with} \quad \hat{\mathbf{a}}_2 = \mathbf{a}_2 - \frac{1}{2}\mathbf{a}_1, \tag{3.3}$$

$$\mathbf{y}_{i,j} = \begin{bmatrix} 1 & e^{\theta_{i,j}} & e^{2\theta_{i,j}} & \cdots & e^{(n_2-1)\theta_{i,j}} \end{bmatrix}^\top, \tag{3.4}$$

for $i=1,\dots,n_1$, and $j=1,\dots,n_2$.

Proof. Suppose $(\lambda, [y_1,\cdots,y_{n_2}]^\top\otimes\mathbf{x}_i)$ is an eigenpair of K_2. From (2.4b) it satisfies that

$$y_2 - y_1 = \lambda\delta_y y_1, \tag{3.5a}$$

$$\vdots$$

$$y_{n_2} - y_{n_2-1} = \lambda\delta_y y_{n_2-1}, \tag{3.5b}$$

$$y_1 e^{\imath 2\pi\mathbf{k}\cdot\mathbf{a}_2} J_2\mathbf{x}_i - y_{n_2}\mathbf{x}_i = \lambda\delta_y y_{n_2}\mathbf{x}_i. \tag{3.5c}$$

By the definition of J_2 in (2.5a), Eq. (3.5c) implies that

$$y_1 e^{\imath 2\pi\mathbf{k}\cdot\mathbf{a}_2} e^{-\imath 2\pi\mathbf{k}\cdot\mathbf{a}_1} e^{\frac{n_1}{2}\theta_i} - y_{n_2} = \lambda\delta_y y_{n_2}, \tag{3.6a}$$

$$y_1 e^{\imath 2\pi\mathbf{k}\cdot\mathbf{a}_2} e^{-\frac{n_1}{2}\theta_i} - y_{n_2} = \lambda\delta_y y_{n_2}. \tag{3.6b}$$

Plugging θ_i in (3.1) into (3.6), we show that two equations of (3.6) are equivalent to

$$y_1 e^{\imath 2\pi(\mathbf{k}\cdot\hat{\mathbf{a}}_2 - \frac{i}{2})} - y_{n_2} = \lambda\delta_y y_{n_2}. \tag{3.7}$$

Combining the results in (3.5a), (3.5b), (3.7), and using Theorem 3.1, we get $\lambda = \delta_y^{-1}(e^{\theta_{i,j}}-1)$ and $y_{s+1} = e^{s\theta_{i,j}}$, for $s=0,\dots,n_2-1$, which completes the proof. □

THEOREM 3.3 (Eigenpairs of K_3). *The eigenpairs of K_3 in (2.4c) are*

$$(\delta_z^{-1}(e^{\theta_{i,j,k}}-1),\ \mathbf{z}_{i,j,k}\otimes\mathbf{y}_{i,j}\otimes\mathbf{x}_i),$$

where $\mathbf{x}_i$ and $\mathbf{y}_{i,j}$ are given in (3.2) and (3.4), respectively, and

$$\theta_{i,j,k} = \frac{\imath 2\pi(k-\frac{1}{3}(i+j)+\mathbf{k}\cdot\hat{\mathbf{a}}_3)}{n_3} \quad \textit{with} \quad \hat{\mathbf{a}}_3 = \mathbf{a}_3 - \frac{1}{3}\left(\mathbf{a}_1+\mathbf{a}_2\right), \tag{3.8}$$

$$\mathbf{z}_{i,j,k} = \begin{bmatrix} 1 & e^{\theta_{i,j,k}} & e^{2\theta_{i,j,k}} & \cdots & e^{(n_3-1)\theta_{i,j,k}} \end{bmatrix}^\top, \tag{3.9}$$

for $i=1,\dots,n_1$, $j=1,\dots,n_2$ and $k=1,\dots,n_3$.

Proof. Assume that $(\lambda, [z_1, \cdots, z_{n_3}]^\top \otimes \mathbf{y}_{i,j} \otimes \mathbf{x}_i)$ is an eigenpair of K_3. By the definition of K_3 in (2.4c), it satisfies that

$$z_2 - z_1 = \lambda \delta_z z_1, \tag{3.10a}$$
$$\vdots$$
$$z_{n_3} - z_{n_3-1} = \lambda \delta_z z_{n_3-1}, \tag{3.10b}$$
$$z_1 e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_3} J_3(\mathbf{y}_{i,j} \otimes \mathbf{x}_i) - z_{n_3}(\mathbf{y}_{i,j} \otimes \mathbf{x}_i) = \lambda \delta_z z_{n_3}(\mathbf{y}_{i,j} \otimes \mathbf{x}_i). \tag{3.10c}$$

By the definitions of J_3 in (2.5b) and $\mathbf{y}_{i,j}$ in (3.4), Eq. (3.10c) implies that

$$z_1 e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_3} e^{-\imath 2\pi \mathbf{k}\cdot\mathbf{a}_2} e^{\frac{2}{3} n_2 \theta_{i,j}} - z_{n_3} = \lambda \delta_z z_{n_3}, \tag{3.11a}$$
$$z_1 e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_3} e^{-\frac{n_2}{3}\theta_{i,j}} J_2 \mathbf{x}_i - z_{n_3}\mathbf{x}_i = \lambda \delta_z z_{n_3}\mathbf{x}_i. \tag{3.11b}$$

By the definitions of J_2 in (2.5a) and $\mathbf{x}_i$ in (3.2), Eq. (3.11b) implies that

$$z_1 e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_3} e^{-\frac{n_2}{3}\theta_{i,j}} e^{-\frac{n_1}{2}\theta_i} - z_{n_3} = \lambda \delta_z z_{n_3}, \tag{3.12a}$$
$$z_1 e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_3} e^{-\frac{n_2}{3}\theta_{i,j}} e^{-\imath 2\pi \mathbf{k}\cdot\mathbf{a}_1} e^{\frac{n_1}{2}\theta_i} - z_{n_3} = \lambda \delta_z z_{n_3}. \tag{3.12b}$$

From the definitions of θ_i and $\theta_{i,j}$ in (3.1) and (3.3), respectively, the exponents in (3.11a), (3.12a), and (3.12b) satisfy

$$\imath 2\pi \mathbf{k}\cdot\mathbf{a}_3 - \imath 2\pi \mathbf{k}\cdot\mathbf{a}_2 + \frac{2}{3} n_2 \theta_{i,j} = \imath 2\pi \mathbf{k}\cdot\hat{\mathbf{a}}_3 - \imath 2\pi \frac{(i+j)}{3} + \imath 2\pi j, \tag{3.13a}$$
$$\imath 2\pi \mathbf{k}\cdot\mathbf{a}_3 - \frac{1}{3} n_2 \theta_{i,j} - \frac{n_1}{2}\theta_i = \imath 2\pi \mathbf{k}\cdot\hat{\mathbf{a}}_3 - \imath 2\pi \frac{(i+j)}{3}, \text{ and} \tag{3.13b}$$
$$\imath 2\pi \mathbf{k}\cdot\mathbf{a}_3 - \frac{1}{3} n_2 \theta_{i,j} - \imath 2\pi \mathbf{k}\cdot\mathbf{a}_1 + \frac{n_1}{2}\theta_i = \imath 2\pi \mathbf{k}\cdot\hat{\mathbf{a}}_3 - \imath 2\pi \frac{(i+j)}{3} + \imath 2\pi i. \tag{3.13c}$$

Plugging (3.13a), (3.13b), and (3.13c) into (3.11a), (3.12a), and (3.12b), respectively, we see that Eq. (3.10c) can be reduced to

$$z_1 e^{\imath 2\pi (\mathbf{k}\cdot\hat{\mathbf{a}}_3 - \frac{(i+j)}{3})} - z_{n_3} = \lambda \delta_z z_{n_3}. \tag{3.14}$$

Combining the results in (3.10a), (3.10b) with (3.14), and using Theorem 3.1, we get $\lambda = \delta_z^{-1}(e^{\theta_{i,j,k}} - 1)$, and $z_{s+1} = e^{s\theta_{i,j,k}}$, for $s = 0, \ldots, n_3 - 1$. $\square$

It is worth noting that the sub-vectors $\mathbf{y}_{i,j}$ and $\mathbf{z}_{i,j,k}$ in the eigenvectors of K_2 and K_3 in Theorems 3.2 and 3.3 depend on the indices (i, j) and (i, j, k), respectively. Such coupling relations are due to the periodic structure over the skew lattice translation vectors in (1.4). These coupling relations complicates the derivation of the eigendecomposition. However, as C_ℓ's consists of K_ℓ's, we can suitably use the eigenvectors of K_ℓ's to form the eigenvectors of C_ℓ's. This idea is developed as follows.

Now, we proceed to show that C_1, C_2, and C_3 in (2.3a) can be diagonalized by the following unitary matrix

$$T = \frac{1}{\sqrt{n_1 n_2 n_3}} \begin{bmatrix} T_1 & T_2 & \cdots & T_{n_1} \end{bmatrix} \in \mathbb{C}^{n \times n}. \tag{3.15}$$

Here $T_i = \begin{bmatrix} T_{i,1} & T_{i,2} & \cdots & T_{i,n_2} \end{bmatrix} \in \mathbb{C}^{n \times (n_2 n_3)}$ and

$$T_{i,j} = \begin{bmatrix} \mathbf{z}_{i,j,1} \otimes \mathbf{y}_{i,j} \otimes \mathbf{x}_i & \mathbf{z}_{i,j,2} \otimes \mathbf{y}_{i,j} \otimes \mathbf{x}_i & \cdots & \mathbf{z}_{i,j,n_3} \otimes \mathbf{y}_{i,j} \otimes \mathbf{x}_i \end{bmatrix} \in \mathbb{C}^{n \times n_3}$$

for $i = 1, \ldots, n_1$, $j = 1, \ldots, n_2$, and $k = 1, \ldots, n_3$.

THEOREM 3.4. *The matrix T defined in* (3.15) *is unitary.*

Proof. Let $\varphi_s = \frac{\imath 2\pi s}{m}$ for $s = 1, \ldots, m$. By a simple calculation, we have

$$1 + e^{(\varphi_{s_2}-\varphi_{s_1})} + e^{2(\varphi_{s_2}-\varphi_{s_1})} + \cdots + e^{(m-1)(\varphi_{s_2}-\varphi_{s_1})} = m\delta_{s_1,s_2}, \tag{3.16}$$

where δ_{s_1,s_2} denotes the Kronecker delta. From the definitions of θ_i, $\theta_{i,j}$, and $\theta_{i,j,k}$ in (3.1), (3.3), and (3.8), respectively, it follows that

$$\theta_{i_2} - \theta_{i_1} = \frac{\imath 2\pi(i_2 + \mathbf{k}\cdot\mathbf{a}_1)}{n_1} - \frac{\imath 2\pi(i_1 + \mathbf{k}\cdot\mathbf{a}_1)}{n_1} = \frac{\imath 2\pi(i_2 - i_1)}{n_1}, \tag{3.17a}$$

$$\theta_{i_1,j_2} - \theta_{i_1,j_1} = \frac{\imath 2\pi(j_2 - \frac{i_1}{2} + \mathbf{k}\cdot\hat{\mathbf{a}}_2)}{n_2} - \frac{\imath 2\pi(j_1 - \frac{i_1}{2} + \mathbf{k}\cdot\hat{\mathbf{a}}_2)}{n_2} = \frac{\imath 2\pi(j_2 - j_1)}{n_2}, \tag{3.17b}$$

$$\begin{aligned}\theta_{i_1,j_1,k_2} - \theta_{i_1,j_1,k_1} &= \frac{\imath 2\pi(k_2 - \frac{i_1+j_1}{3} + \mathbf{k}\cdot\hat{\mathbf{a}}_3)}{n_3} - \frac{\imath 2\pi(k_1 - \frac{i_1+j_1}{3} + \mathbf{k}\cdot\hat{\mathbf{a}}_3)}{n_3} \\ &= \frac{\imath 2\pi(k_2 - k_1)}{n_3}.\end{aligned} \tag{3.17c}$$

By the definitions of $\mathbf{x}_i$, $\mathbf{y}_{i,j}$ and $\mathbf{z}_{i,j,k}$ in (3.2), (3.4), and (3.9), respectively, and using (3.16) and (3.17), we have $\mathbf{x}_{i_1}^*\mathbf{x}_{i_2} = n_1\delta_{i_1,i_2}$, $\mathbf{y}_{i_1,j_1}^*\mathbf{y}_{i_1,j_2} = n_2\delta_{j_1,j_2}$, $\mathbf{z}_{i_1,j_1,k_1}^*\mathbf{z}_{i_1,j_1,k_2} = n_3\delta_{k_1,k_2}$. This implies that if $(i_1, j_1, k_1) \neq (i_2, j_2, k_2)$, then

$$\begin{aligned}&\left(\mathbf{z}_{i_1,j_1,k_1} \otimes \mathbf{y}_{i_1,j_1} \otimes \mathbf{x}_{i_1}\right)^* \left(\mathbf{z}_{i_2,j_2,k_2} \otimes \mathbf{y}_{i_2,j_2} \otimes \mathbf{x}_{i_2}\right) \\ &= \left(\mathbf{z}_{i_1,j_1,k_1}^*\mathbf{z}_{i_2,j_2,k_2}\right)\left(\mathbf{y}_{i_1,j_1}^*\mathbf{y}_{i_2,j_2}\right)\left(\mathbf{x}_{i_1}^*\mathbf{x}_{i_2}\right) = 0\end{aligned}$$

and $\left(\mathbf{z}_{i,j,k} \otimes \mathbf{y}_{i,j} \otimes \mathbf{x}_i\right)^* \left(\mathbf{z}_{i,j,k} \otimes \mathbf{y}_{i,j} \otimes \mathbf{x}_i\right) = n_1 n_2 n_3$. Therefore, T is unitary. ∎

Define

$$\Lambda_{n_1} = \delta_x^{-1}\mathrm{diag}\left(e^{\theta_1} - 1, e^{\theta_2} - 1, \cdots, e^{\theta_{n_1}} - 1\right), \tag{3.18}$$

$$\Lambda_{i,n_2} = \delta_y^{-1}\mathrm{diag}\left(e^{\theta_{i,1}} - 1, e^{\theta_{i,2}} - 1, \cdots, e^{\theta_{i,n_2}} - 1\right), \tag{3.19}$$

$$\Lambda_{i,j,n_3} = \delta_z^{-1}\mathrm{diag}\left(e^{\theta_{i,j,1}} - 1, e^{\theta_{i,j,2}} - 1, \cdots, e^{\theta_{i,j,n_3}} - 1\right). \tag{3.20}$$

By the results of Theorems 3.1 to 3.4, we have

$$\begin{aligned}C_1 T_{i,j} &= (I_{n_2 n_3} \otimes K_1)\, T_{i,j} = \frac{e^{\theta_i} - 1}{\delta_x} T_{i,j}, \\ C_2 T_i &= (I_{n_3} \otimes K_2)\, T_i = T_i\left(\Lambda_{i,n_2} \otimes I_{n_3}\right), \\ C_3 T_{i,j} &= K_3 T_{i,j} = T_{i,j}\Lambda_{i,j,n_3},\end{aligned}$$

and therefore the following theorem holds.

THEOREM 3.5 (Eigendecompositions of C_i's). *The unitary matrix T defined in* (3.15) *leads to the eigendecompositions of C_1, C_2, and C_3 in the forms*

$$C_1 T = T\Lambda_{\mathbf{x}},\ C_2 T = T\Lambda_{\mathbf{y}},\ \textit{and}\ C_3 T = T\Lambda_{\mathbf{z}}, \tag{3.21}$$

where $\Lambda_{\mathbf{x}} = \Lambda_{n_1} \otimes I_{n_2 n_3}$, $\Lambda_{\mathbf{y}} = (\oplus_{i=1}^{n_1}\Lambda_{i,n_2}) \otimes I_{n_3}$, *and* $\Lambda_{\mathbf{z}} = \oplus_{i=1}^{n_1} \oplus_{j=1}^{n_2} \Lambda_{i,j,n_3}$.

3.2. Eigendecomposition of the double-curl operator. Now, we proceed to find the eigendecomposition of the discrete double-curl operator $A = C^*C$ defined in (2.2). We first define several intermediate diagonal matrices and show that these matrices are positive definite and invertible in a particular space in Lemma 3.6. These matrices will be used later to describe the eigendecomposition of A. Then we demonstrate an explicit representation of the corresponding range and null spaces of A. The eigendecomposition of A is finally presented in Theorem 3.7 by applying Lemma 3.6 and the representation of the range and null spaces.

Based on the diagonal matrices $\Lambda_{\mathbf{x}}$, $\Lambda_{\mathbf{y}}$, and $\Lambda_{\mathbf{z}}$ defined in (3.21), we define

$$\Lambda_q = \Lambda_{\mathbf{x}}^*\Lambda_{\mathbf{x}} + \Lambda_{\mathbf{y}}^*\Lambda_{\mathbf{y}} + \Lambda_{\mathbf{z}}^*\Lambda_{\mathbf{z}} \text{ and} \tag{3.22a}$$

$$\Lambda_p = \Lambda_s\Lambda_s^* = (\Lambda_{\mathbf{x}} + \Lambda_{\mathbf{y}} + \Lambda_{\mathbf{z}})(\Lambda_{\mathbf{x}} + \Lambda_{\mathbf{y}} + \Lambda_{\mathbf{z}})^*. \tag{3.22b}$$

As shown in Section 3.1, these diagonal matrices actually depend on the Bloch wave vector $2\pi\mathbf{k}$. To determine the band gap of a photonic crystals with FCC lattice, we need to solve a sequence of eigenvalue problems. These eigenvalue problems are associated with the Bloch wave vectors $2\pi\mathbf{k}$ which trace the perimeter of the irreducible Brillouin zone formed by the corners $X = \frac{2\pi}{a}\Omega[0,1,0]^\top$, $U = \frac{2\pi}{a}\Omega\left[\frac{1}{4},1,\frac{1}{4}\right]^\top$, $L = \frac{2\pi}{a}\Omega\left[\frac{1}{2},\frac{1}{2},\frac{1}{2}\right]^\top$, $G = [0,0,0]^\top$, $W = \frac{2\pi}{a}\Omega\left[\frac{1}{2},1,0\right]^\top$, and $K = \frac{2\pi}{a}\Omega\left[\frac{3}{4},\frac{3}{4},0\right]^\top$, where

$$\Omega = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 & 0 \\ -\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{3}} \\ \frac{2}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & \frac{2}{\sqrt{6}} \end{bmatrix}.$$

To conduct the mathematical analysis in Lemma 3.6 and Theorem 3.7, we consider the wave vectors $2\pi\mathbf{k}$ with $\mathbf{k} \in \mathcal{B}$, where

$$\mathcal{B} = \left\{ \mathbf{k} = (\mathrm{k}_1,\mathrm{k}_2,\mathrm{k}_3)^\top \neq \mathbf{0} \;\middle|\; 0 \le \mathrm{k}_1 \le \frac{\sqrt{2}}{a}, 0 \le \mathrm{k}_2 < \frac{2\sqrt{2}}{\sqrt{3}a}, 0 \le \mathrm{k}_3 < \frac{\sqrt{3}}{a}, \text{ and } \mathbf{k} \neq \frac{\sqrt{2}}{a}\left[1, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{6}}\right]^\top \right\}.$$

Furthermore, in Lemma 3.8 and Theorem 3.9, we prove the results that are similar to Lemma 3.6 and Theorem 3.7 for the case $\mathbf{k} = \mathbf{0}$. Note that $\mathcal{B}$ contains the Brillouin zone and it easy to verify that $(2\pi)^{-1}X$, $(2\pi)^{-1}U$, $(2\pi)^{-1}L$, G, $(2\pi)^{-1}W$, and $(2\pi)^{-1}K \in \mathcal{B}$.

Lemma 3.6. *For each $\mathbf{k} \in \mathcal{B}$, Λ_q and $3\Lambda_q - \Lambda_p$ are positive definite.*

Proof. The $((i-1)n_2n_3 + (j-1)n_3 + k)$-th diagonal element $\mu_{i,j,k}$ of Λ_q is equal to

$$\mu_{i,j,k} = \left|\frac{e^{\imath\theta_i} - 1}{\delta_x}\right|^2 + \left|\frac{e^{\imath\theta_{i,j}} - 1}{\delta_y}\right|^2 + \left|\frac{e^{\imath\theta_{i,j,k}} - 1}{\delta_z}\right|^2$$

for $i = 1,\ldots,n_1$, $j = 1,\ldots,n_2$ and $k = 1,\ldots,n_3$. This implies that $\mu_{i,j,k} = 0$ if and only if $\theta_i/(\imath 2\pi)$, $\theta_{i,j}/(\imath 2\pi)$, and $\theta_{i,j,k}/(\imath 2\pi)$ are integers. By a tedious calculation (see Theorem A.1 in the appendix), one can show that these conditions hold only if $\mathbf{k} = \sqrt{2}/a[1, 1/\sqrt{3}, 1/\sqrt{6}]^\top$. Therefore, Λ_q is nonsingular for $\mathbf{k} \in \mathcal{B}$.

From (2.3a) and (2.6), it holds that

$$C^*C = I_3 \otimes (G^*G) - GG^*. \tag{3.23}$$

Let $T_1 = [T^\top \ \ T^\top \ \ T^\top]^\top$. From (3.23) and the results of Theorem 3.5, we have

$$\begin{aligned} T_1^* C C^* T_1 &= 3T^* \left(C_1 C_1^* + C_2 C_2^* + C_3 C_3^*\right) T \\ &\quad - T^* \left(C_1 + C_2 + C_3\right) \left(C_1 + C_2 + C_3\right)^* T = 3\Lambda_q - \Lambda_p. \end{aligned}$$

Now, we show that $C^* T_1$ is of full column rank. Suppose that $C^* T_1 \mathbf{v} = 0$, that is, $(C_3^* - C_2^*) T\mathbf{v} = (C_1^* - C_3^*) T\mathbf{v} = (C_2^* - C_1^*) T\mathbf{v} = 0$. From Theorem 3.5, it follows that $\left(\Lambda_{\mathbf{z}}^* - \Lambda_{\mathbf{y}}^*\right) \mathbf{v} = \left(\Lambda_{\mathbf{x}}^* - \Lambda_{\mathbf{z}}^*\right) \mathbf{v} = \left(\Lambda_{\mathbf{y}}^* - \Lambda_{\mathbf{x}}^*\right) \mathbf{v} = 0$. Suppose that the $((i-1)n_2 n_3 + (j-1)n_3 + k)$-th element of $\mathbf{v}$ is nonzero. Then we have

$$\frac{\sin\theta_i}{\delta_x} = \frac{\sin\theta_{i,j}}{\delta_y} = \frac{\sin\theta_{i,j,k}}{\delta_z}$$

and

$$\frac{\cos\theta_i - 1}{\delta_x} = \frac{\cos\theta_{i,j} - 1}{\delta_y} = \frac{\cos\theta_{i,j,k} - 1}{\delta_z}, \tag{3.24}$$

which imply that

$$\begin{aligned} \left(\frac{\sin\theta_i}{\delta_x}\right)^2 + \left(\frac{\cos\theta_i - 1}{\delta_x}\right)^2 &= \left(\frac{\sin\theta_{i,j}}{\delta_y}\right)^2 + \left(\frac{\cos\theta_{i,j} - 1}{\delta_y}\right)^2 \\ &= \left(\frac{\sin\theta_{i,j,k}}{\delta_z}\right)^2 + \left(\frac{\cos\theta_{i,j,k} - 1}{\delta_z}\right)^2 \end{aligned}$$

and then

$$\frac{\cos\theta_i - 1}{\delta_x} = \frac{\delta_x}{\delta_y}\frac{\cos\theta_{i,j} - 1}{\delta_y} = \frac{\delta_x}{\delta_z}\frac{\cos\theta_{i,j,k} - 1}{\delta_z}. \tag{3.25}$$

From (2.1), it is easily seen that $\delta_x \neq \delta_y$ or $\delta_x \neq \delta_z$. Therefore, it holds from (3.24) and (3.25) that $\cos\theta_j = \cos\theta_{i,j} = \cos\theta_{i,j,k} = 1$. That is, $\theta_i/(\imath 2\pi)$, $\theta_{i,j}/(\imath 2\pi)$ and $\theta_{i,j,k}/(\imath 2\pi)$ must be integers. This contradicts that $\mathbf{k} \in \mathcal{B}$. Thus, $C^* T_1$ is of full column rank which implies that $3\Lambda_q - \Lambda_p$ is positive definite. $\square$

The range and null spaces of A are derived as follows. First, we assert that Q_0 forms an orthogonal basis for the null space of A, where

$$Q_0 = \begin{bmatrix} T\Lambda_{\mathbf{x}} \\ T\Lambda_{\mathbf{y}} \\ T\Lambda_{\mathbf{z}} \end{bmatrix} \in \mathbb{C}^{3n\times n}. \tag{3.26}$$

The orthogonality of Q_0 holds as Lemma 3.6 suggests that $Q_0^* Q_0 = \Lambda_q > 0$. Using the definition of A in (2.2), the eigendecompositions of C_ℓ in Theorem 3.5, and the fact that C_ℓ are normal and commute with each other (see Theorem A.2 in appendix), we can show that Q_0 spans the null space of A as

$$AQ_0 = A\begin{bmatrix} T\Lambda_{\mathbf{x}} \\ T\Lambda_{\mathbf{y}} \\ T\Lambda_{\mathbf{z}} \end{bmatrix} = A\begin{bmatrix} C_1 T \\ C_2 T \\ C_3 T \end{bmatrix} = 0. \tag{3.27}$$

Next, we form the orthogonal basis for the range space of A. Considering the full column rank matrix T_1 and taking the orthogonal projection of T_1 with respect to Q_0, we have

$$\left(I - Q_0 \Lambda_q^{-1} Q_0^*\right) T_1 = \begin{bmatrix} T\left(\Lambda_q - \Lambda_{\mathbf{x}}\Lambda_s^*\right) \\ T\left(\Lambda_q - \Lambda_{\mathbf{y}}\Lambda_s^*\right) \\ T\left(\Lambda_q - \Lambda_{\mathbf{z}}\Lambda_s^*\right) \end{bmatrix} \Lambda_q^{-1},$$

where Λ_s is defined in (3.22b). That is, Q_1 belongs to the range space of A, where

$$Q_1 = \left(I - Q_0\Lambda_q^{-1}Q_0^*\right) T_1\Lambda_q = \begin{bmatrix} T\left(\Lambda_q - \Lambda_{\mathbf{x}}\Lambda_s^*\right) \\ T\left(\Lambda_q - \Lambda_{\mathbf{y}}\Lambda_s^*\right) \\ T\left(\Lambda_q - \Lambda_{\mathbf{z}}\Lambda_s^*\right) \end{bmatrix}. \tag{3.28}$$

It is then natural to form the rest part of the orthogonal basis for the range space of A as the curl of T_1 by defining

$$Q_2 = C^*T_1 = \begin{bmatrix} T\left(\Lambda_{\mathbf{z}}^* - \Lambda_{\mathbf{y}}^*\right) \\ T\left(\Lambda_{\mathbf{x}}^* - \Lambda_{\mathbf{z}}^*\right) \\ T\left(\Lambda_{\mathbf{y}}^* - \Lambda_{\mathbf{x}}^*\right) \end{bmatrix}. \tag{3.29}$$

In short, we have shown that Q_0 and $[Q_1\ Q_2]$ are orthogonal bases for the null and range space of A, respectively.

In the next theorem, we derive the eigendecompositions of A and GG^*. Note that A and G are defined in (2.2) and (2.6), respectively.

Theorem 3.7. *Define*

$$Q = \begin{bmatrix} Q_0 & Q_1 & Q_2 \end{bmatrix} \mathit{diag}\left(\Lambda_q^{-\frac{1}{2}}, \left(3\Lambda_q^2 - \Lambda_q\Lambda_p\right)^{-\frac{1}{2}}, \left(3\Lambda_q - \Lambda_p\right)^{-\frac{1}{2}}\right). \tag{3.30}$$

Then Q is unitary. Furthermore,

$$Q^*AQ = \mathit{diag}\left(0, \Lambda_q, \Lambda_q\right) \ \ \mathit{and} \ \ Q^*GG^*Q = \mathit{diag}\left(\Lambda_q, 0, 0\right). \tag{3.31}$$

Proof. Since

$$\Lambda_{\mathbf{x}}^*\left(\Lambda_{\mathbf{z}}^* - \Lambda_{\mathbf{y}}^*\right) + \Lambda_{\mathbf{y}}^*\left(\Lambda_{\mathbf{x}}^* - \Lambda_{\mathbf{z}}^*\right) + \Lambda_{\mathbf{z}}^*\left(\Lambda_{\mathbf{y}}^* - \Lambda_{\mathbf{x}}^*\right) = 0, \tag{3.32a}$$

$$\Lambda_{\mathbf{x}}^*\left(\Lambda_q - \Lambda_{\mathbf{x}}\Lambda_s^*\right) + \Lambda_{\mathbf{y}}^*\left(\Lambda_q - \Lambda_{\mathbf{y}}\Lambda_s^*\right) + \Lambda_{\mathbf{z}}^*\left(\Lambda_q - \Lambda_{\mathbf{z}}\Lambda_s^*\right) = \Lambda_s^*\Lambda_q - \Lambda_q\Lambda_s^* = 0, \tag{3.32b}$$

$$\left(\Lambda_{\mathbf{z}} - \Lambda_{\mathbf{y}}\right)\left(\Lambda_q - \Lambda_{\mathbf{x}}\Lambda_s^*\right) + \left(\Lambda_{\mathbf{x}} - \Lambda_{\mathbf{z}}\right)\left(\Lambda_q - \Lambda_{\mathbf{y}}\Lambda_s^*\right) + \left(\Lambda_{\mathbf{y}} - \Lambda_{\mathbf{x}}\right)\left(\Lambda_q - \Lambda_{\mathbf{z}}\Lambda_s^*\right) = 0, \tag{3.32c}$$

and $T^*T = I_n$, it follows that the matrices Q_0, Q_1, and Q_2 in (3.30) are mutually orthogonal. Furthermore, we can directly verify that

$$Q_0^*Q_0 = \Lambda_q, \quad Q_1^*Q_1 = 3\Lambda_q^2 - \Lambda_q\Lambda_p, \quad Q_2^*Q_2 = 3\Lambda_q - \Lambda_p. \tag{3.33}$$

By Lemma 3.6, it follows that Q_0, Q_1, and Q_2 are of full column rank. Therefore, by (3.32), Q in (3.30) is unitary.

Eq. (3.27) shows that Q_0 forms an orthogonal basis for the null space of A. Eqs. (3.32a) and (3.32b) lead to

$$G^*Q_1 = 0 \ \text{ and } \ G^*Q_2 = 0. \tag{3.34}$$

From Theorem 3.5, (3.34), and the fact $\sum_{\ell=1}^{3} C_\ell^* C_\ell T = T\Lambda_q$, it follows that

$$AQ_1 = \left(I_3 \otimes (G^*G) - GG^*\right)Q = \left(I_3 \otimes G^*G\right)Q_1 = \left[I_3 \otimes \left(\sum_{\ell=1}^{3} C_\ell^* C_\ell\right)\right] Q_1 = Q_1\Lambda_q.$$

Similarly,

$$AQ_2 = (I_3 \otimes (G^*G) - GG^*)\, Q_2 = (I_3 \otimes (G^*G))\, Q_2 = Q_2\Lambda_q.$$

Consequently, we have proved that $Q^*AQ = \mathrm{diag}\,(0, \Lambda_q, \Lambda_q)$.

Finally, from (3.22) and Theorem 3.5, we have

$$GG^*Q_0 = \begin{bmatrix} C_1 \\ C_2 \\ C_3 \end{bmatrix} \begin{bmatrix} C_1^* & C_2^* & C_3^* \end{bmatrix} \begin{bmatrix} T\Lambda_{\mathbf{x}} \\ T\Lambda_{\mathbf{y}} \\ T\Lambda_{\mathbf{z}} \end{bmatrix} = \begin{bmatrix} C_1T \\ C_2T \\ C_3T \end{bmatrix} \Lambda_q = Q_0\Lambda_q. \tag{3.35}$$

Combining (3.35) with (3.34), we show that $Q^*GG^*Q = \mathrm{diag}\,(\Lambda_q, 0, 0)$. □

Now, we consider the case that $\mathbf{k} = \mathbf{0}$.

LEMMA 3.8. *If $\mathbf{k} = \mathbf{0}$, then Λ_q and $3\Lambda_q - \Lambda_p$ have rank $n-1$. Furthermore, $\Lambda_q(j,j) = 0$ and $\Lambda_p(j,j) = 0$ for $j = (n_1-1)n_2n_3 + (3n_3+1)\frac{n_1}{2} - (n_1+1)n_3$.*

Proof. From (3.1), (3.18), and the definition of $\Lambda_{\mathbf{x}}$ in Theorem 3.5, it holds that $\Lambda_{\mathbf{x}}(i,i) = 0$, for $i = (n_1-1)n_2n_3+1, \ldots, n$; otherwise, they are nonzero. That is, $\Lambda_q(i,i) > 0$ for $i = 1, \ldots, (n_1-1)n_2n_3$. From (3.3), (3.19), and the definition of $\Lambda_{\mathbf{y}}$ in Theorem 3.5, it holds that, for $(n_1-1)n_2n_3 + 1 \le i \le n$, $\Lambda_{\mathbf{y}}(i,i) = 0$ only when $i = (n_1-1)n_2n_3+n_3(\frac{n_1}{2}-1)+1, \ldots, (n_1-1)n_2n_3+n_3\frac{n_1}{2}$. Otherwise, they are nonzero, which means the associated $\Lambda_q(i,i) > 0$. Furthermore, from (3.8), (3.20), and the definition of $\Lambda_{\mathbf{z}}$ in Theorem 3.5, it holds that, for $(n_1-1)n_2n_3 + n_3(\frac{n_1}{2}-1)+1 \le i \le (n_1-1)n_2n_3 + n_3\frac{n_1}{2}$, $\Lambda_z(j,j) = 0$ with $j = (n_1-1)n_2n_3 + (3n_3+1)\frac{n_1}{2} - (n_1+1)n_3$. It implies that Λ_q has rank $n-1$ and $\Lambda_q(j,j) = 0$. Similar to the proof of Lemma 3.6, we have $3\Lambda_q - \Lambda_p$ being of rank $n-1$ and $\Lambda_p(j,j) = 0$. □

We define two notations that are used in the following theorem. For a given a matrix $F \in \mathbb{C}^{n\times n}$, let $F_c \in \mathbb{C}^{n\times(n-1)}$ (or $F_{rc} \in \mathbb{C}^{(n-1)\times(n-1)}$) be the submatrices of F that the the jth column is deleted (or both the jth column and the jth row are deleted). Here, j is defined in Lemma 3.8.

THEOREM 3.9. *Let $\mathbf{k} = \mathbf{0}$ and define*

$$\widehat{Q}_0 = \left[\begin{bmatrix} T\Lambda_{\mathbf{x},c} \\ T\Lambda_{\mathbf{y},c} \\ T\Lambda_{\mathbf{z},c} \end{bmatrix}, \frac{1}{\sqrt{n}} I_3 \otimes \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}\right], \widehat{Q}_1 = \begin{bmatrix} T\left(\Lambda_q - \Lambda_{\mathbf{x}}\Lambda_s^*\right)_c \\ T\left(\Lambda_q - \Lambda_{\mathbf{y}}\Lambda_s^*\right)_c \\ T\left(\Lambda_q - \Lambda_{\mathbf{z}}\Lambda_s^*\right)_c \end{bmatrix}, \widehat{Q}_2 = \begin{bmatrix} T\left(\Lambda_{\mathbf{z}}^* - \Lambda_{\mathbf{y}}^*\right)_c \\ T\left(\Lambda_{\mathbf{x}}^* - \Lambda_{\mathbf{z}}^*\right)_c \\ T\left(\Lambda_{\mathbf{y}}^* - \Lambda_{\mathbf{x}}^*\right)_c \end{bmatrix}.$$

Let

$$\widehat{Q} = \begin{bmatrix} \widehat{Q}_0 & \widehat{Q}_1 & \widehat{Q}_2 \end{bmatrix} \mathit{diag}\left((\Lambda_q)_{rc}^{-\frac{1}{2}} \oplus I_3, \left(3\Lambda_q^2 - \Lambda_q\Lambda_p\right)_{rc}^{-\frac{1}{2}}, (3\Lambda_q - \Lambda_p)_{rc}^{-\frac{1}{2}}\right).$$

Then $\widehat{Q}$ is unitary. Furthermore,

$$\widehat{Q}^* A \widehat{Q} = \mathit{diag}\,(0, (\Lambda_q)_{rc}, (\Lambda_q)_{rc}).$$

4. Inverse Projective Lanczos Method. The eigendecomposition of the discrete double-curl operator derived in Theorem 3.7 is actually a powerful tool to solve the GEVP (1.5). Via this eigendecomposition, we can form the eigendecomposition of A in terms of its range space. This particular decomposition allows us to project GEVP into a standard eigenvalue problem (SEVP) that is equipped with several attractive computational properties as shown below.

The eigendecomposition (3.31) suggests that Q_r forms an orthogonal basis for the range space of A, where

$$Q_r = \left[Q_1 \left(3\Lambda_q^2 - \Lambda_q\Lambda_p\right)^{-\frac{1}{2}} \quad Q_2 \left(3\Lambda_q - \Lambda_p\right)^{-\frac{1}{2}} \right] \equiv \left(I_3 \otimes T\right) \Lambda \tag{4.1}$$

and

$$\Lambda = \begin{bmatrix} \left(\Lambda_q - \Lambda_{\mathbf{x}}\Lambda_s^*\right)\left(3\Lambda_q^2 - \Lambda_q\Lambda_p\right)^{-\frac{1}{2}} & \left(\Lambda_{\mathbf{z}}^* - \Lambda_{\mathbf{y}}^*\right)\left(3\Lambda_q - \Lambda_p\right)^{-\frac{1}{2}} \\ \left(\Lambda_q - \Lambda_{\mathbf{y}}\Lambda_s^*\right)\left(3\Lambda_q^2 - \Lambda_q\Lambda_p\right)^{-\frac{1}{2}} & \left(\Lambda_{\mathbf{x}}^* - \Lambda_{\mathbf{z}}^*\right)\left(3\Lambda_q - \Lambda_p\right)^{-\frac{1}{2}} \\ \left(\Lambda_q - \Lambda_{\mathbf{z}}\Lambda_s^*\right)\left(3\Lambda_q^2 - \Lambda_q\Lambda_p\right)^{-\frac{1}{2}} & \left(\Lambda_{\mathbf{y}}^* - \Lambda_{\mathbf{x}}^*\right)\left(3\Lambda_q - \Lambda_p\right)^{-\frac{1}{2}} \\ & \end{bmatrix}.$$

This basis, together with the fact $\Lambda_r = \operatorname{diag}(\Lambda_q, \Lambda_q) > 0$, leads to the fact that $A = Q_r\Lambda_r Q_r^*$. In addition, $B^{-1/2}Q_r\Lambda_r^{\frac{1}{2}}$ forms a basis for the invariant subspace of $B^{-1/2}AB^{-1/2}$ corresponding to the *nonzero* eigenvalues of the GEVP (1.5). Letting

$$\mathbf{x} = B^{-1}Q_r\Lambda_r^{\frac{1}{2}}\mathbf{y} \tag{4.2}$$

and substituting $\mathbf{x}$ into (1.5), we have

$$A\left(B^{-1}Q_r\Lambda_r^{\frac{1}{2}}\mathbf{y}\right) = \lambda\left(Q_r\Lambda_r^{\frac{1}{2}}\mathbf{y}\right). \tag{4.3}$$

Pre-multiplying (4.3) by $\Lambda_r^{-\frac{1}{2}}Q_r^*$ and using the facts that $A = Q_r\Lambda_r Q_r^*$ and $Q_r^*Q_r = I_{2n}$, we can form the SEVP

$$A_r\mathbf{y} = \lambda\mathbf{y}, \tag{4.4}$$

where $A_r = \Lambda_r^{\frac{1}{2}}Q_r^*B^{-1}Q_r\Lambda_r^{\frac{1}{2}}$.

This SEVP has the following computational advantages. First, while both of the GEVP and SEVP have the same $2n$ positive eigenvalues, the dimension of the GEVP and SEVP are $3n \times 3n$ and $2n \times 2n$, respectively. The SEVP is a smaller eigenvalue problem. More importantly, as we are interested in several of the smallest positive eigenvalues among all of the $2n$ positive eigenvalues in SEVP, we can find these desired eigenvalues efficiently by the standard inverse Lanczos method [14]. In contrast, the GEVP contains n zero eigenvalues and $2n$ positive eigenvalues. This large null space usually causes numerical inefficiency [17].

Second, to solve the SEVP by the inverse Lanczos method, we need to solve the linear system

$$Q_r^*B^{-1}Q_r\mathbf{u} = \mathbf{c} \tag{4.5}$$

at each Lanczos step for a certain $\mathbf{u}$ and $\mathbf{c}$. The conjugate gradient (CG) method [14] fits this Hermitian positive definite system nicely. In addition, as shown in Theorem 4.1, we can bound the condition number $\kappa(Q_r^*B^{-1}Q_r)$ associated with (4.5) and then estimate the convergence performance of the CG method. In practice, the condition number is small as demonstrated in Section 6 and there is therefore no need to find a preconditioner for (4.5).

Third, to solve (4.5) by the CG method, the most costly computation is the matrix-vector multiplication in terms of the coefficient matrix $Q_r^*B^{-1}Q_r$ or particularly the matrix-vector multiplications $T^*\mathbf{p}$ and $T\mathbf{q}$ for certain vectors $\mathbf{p}$ and $\mathbf{q}$ due to the definition of Q_r in (4.1). At the first glance, the components in the three coordinates are coupled together in the matrix T. Consequently, these matrix-vector multiplications are general dense operations with cost $\mathcal{O}(n^2)$. However, as discussed in Section 5, these matrix-vector multiplications can be performed by a sequence of diagonal matrix-vector multiplications and one-dimensional FFT with cost $\mathcal{O}(k)$ and $\mathcal{O}(k\log(k))$, respectively, for $k = n_1, n_2$, or n_3.

Now, we assert an upper bound of $\kappa(Q_r^* B^{-1} Q_r)$ in Theorem 4.1 and summarize the aforementioned ideas by proposing the inverse projective Lanczos method (IPL) to solve the GEVP (1.5) in Algorithm 1.

THEOREM 4.1. *Let Q_r be defined in* (4.1). *Then*

$$\kappa\left(Q_r^* B^{-1} Q_r\right) \le \kappa(B^{-1}). \tag{4.6}$$

Proof. Since $Q_r^* Q_r = I_{2n}$, it implies that

$$\lambda_{\max}\left(Q_r^* B^{-1} Q_r\right) = \max_{\|\mathbf{z}\|_2=1} \mathbf{z}^* Q_r^* B^{-1} Q_r \mathbf{z} \le \max_{\|\tilde{\mathbf{z}}\|_2=1} \tilde{\mathbf{z}}^* B^{-1} \tilde{\mathbf{z}} = \lambda_{\max}(B^{-1}), \tag{4.7}$$

and

$$\lambda_{\min}\left(Q_r^* B^{-1} Q_r\right) = \min_{\|\mathbf{z}\|_2=1} \mathbf{z}^* Q_r^* B^{-1} Q_r \mathbf{z} \ge \min_{\|\tilde{\mathbf{z}}\|_2=1} \tilde{\mathbf{z}}^* B^{-1} \tilde{\mathbf{z}} = \lambda_{\min}(B^{-1}). \tag{4.8}$$

From (4.7) and (4.8), the result of (4.6) is proved. □

Algorithm 1 inverse projective Lanczos method for solving (1.5)

1: Compute $\Lambda_{\mathbf{x}}$, $\Lambda_{\mathbf{y}}$ and $\Lambda_{\mathbf{z}}$ in Theorem 3.5;
2: Compute Λ_q, Λ_p and Λ_s in (3.22);
3: Compute Λ in (4.1);
4: Apply the inverse Lanczos method to solve the following SEVP

$$\operatorname{diag}\left(\Lambda_q^{\frac{1}{2}}, \Lambda_q^{\frac{1}{2}}\right) \Lambda^* \left(I_3 \otimes T^*\right) B^{-1} \left(I_3 \otimes T\right) \Lambda \operatorname{diag}\left(\Lambda_q^{\frac{1}{2}}, \Lambda_q^{\frac{1}{2}}\right) \mathbf{y} = \lambda \mathbf{y};$$

5: Compute $\mathbf{x} = B^{-1}\left(I_3 \otimes T\right) \Lambda \operatorname{diag}\left(\Lambda_q^{\frac{1}{2}}, \Lambda_q^{\frac{1}{2}}\right) \mathbf{y}$.

5. Fast Matrix-Vector Multiplication for $T^*\mathbf{p}$ and $T\mathbf{q}$.

The most expensive computational cost for solving (4.5) by CG method has been pinned down to the matrix-vector multiplications $T^*\mathbf{p}$ and $T\mathbf{q}$. To derive fast algorithms to compute these multiplications, our strategy is to rewrite each of the eigenvector entries in K_ℓ's as a multiplication of diagonal matrix and a periodical matrix. Then we carefully explore the recursive and periodical matrix representations, so that we can rewrite the multiplication of $T^*\mathbf{p}$ and $T\mathbf{q}$ as a sequence of operations involving diagonal and FFT matrices, which can significantly reduce the computational cost.

First, we rewrite θ_i, $\theta_{i,j}$, $\theta_{i,j,k}$ and $\mathbf{x}_i$, $\mathbf{y}_{i,j}$, and $\mathbf{z}_{i,j,k}$ in Theorems 3.1 to 3.3 as follows.

$$\theta_i = \frac{\imath 2\pi i}{n_1} + \frac{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_1}{n_1} \equiv \theta_{\mathbf{x},i} + \varepsilon_{\mathbf{x}},$$
$$\theta_{i,j} = \frac{\imath 2\pi j}{n_2} + \frac{\imath 2\pi}{n_2}\left\{\mathbf{k}\cdot\hat{\mathbf{a}}_2 - \frac{i}{2}\right\} \equiv \theta_{\mathbf{y},j} + \varepsilon_{\mathbf{y},i},$$
$$\theta_{i,j,k} = \frac{\imath 2\pi k}{n_3} + \frac{\imath 2\pi}{n_3}\left\{\mathbf{k}\cdot\hat{\mathbf{a}}_3 - \frac{1}{3}(i+j)\right\} \equiv \theta_{\mathbf{z},k} + \varepsilon_{\mathbf{z},i+j}.$$

and

$$\mathbf{x}_i = E_{\mathbf{x}}\begin{bmatrix}1 & e^{\theta_{\mathbf{x},i}} & \cdots & e^{(n_1-1)\theta_{\mathbf{x},i}}\end{bmatrix}^\top \equiv E_{\mathbf{x}}\mathbf{u}_{\mathbf{x},i}, \tag{5.1a}$$
$$\mathbf{y}_{i,j} = E_{\mathbf{y},i}\begin{bmatrix}1 & e^{\theta_{\mathbf{y},j}} & \cdots & e^{(n_2-1)\theta_{\mathbf{y},j}}\end{bmatrix}^\top \equiv E_{\mathbf{y},i}\mathbf{u}_{\mathbf{y},j}, \tag{5.1b}$$
$$\mathbf{z}_{i,j,k} = E_{\mathbf{z},i+j}\begin{bmatrix}1 & e^{\theta_{\mathbf{z},k}} & \cdots & e^{(n_3-1)\theta_{\mathbf{z},k}}\end{bmatrix}^\top \equiv E_{\mathbf{z},i+j}\mathbf{u}_{\mathbf{z},k}, \tag{5.1c}$$

where $E_{\mathbf{x}} = \operatorname{diag}\left(1, e^{\varepsilon_{\mathbf{x}}}, \cdots, e^{(n_1-1)\varepsilon_{\mathbf{x}}}\right)$, $E_{\mathbf{y},i} = \operatorname{diag}\left(1, e^{\varepsilon_{\mathbf{y},i}}, \cdots, e^{(n_2-1)\varepsilon_{\mathbf{y},i}}\right)$ and $E_{\mathbf{z},i+j} = \operatorname{diag}\left(1, e^{\varepsilon_{\mathbf{z},i+j}}, \cdots, e^{(n_3-1)\varepsilon_{\mathbf{z},i+j}}\right)$. From (5.1) we denote

$$U_{\mathbf{x}} = \begin{bmatrix}\mathbf{u}_{\mathbf{x},1} & \mathbf{u}_{\mathbf{x},2} & \cdots & \mathbf{u}_{\mathbf{x},n_1}\end{bmatrix}, \tag{5.2a}$$
$$U_{\mathbf{y}} = \begin{bmatrix}\mathbf{u}_{\mathbf{y},1} & \mathbf{u}_{\mathbf{y},2} & \cdots & \mathbf{u}_{\mathbf{y},n_2}\end{bmatrix}, \tag{5.2b}$$
$$U_{\mathbf{z}} = \begin{bmatrix}\mathbf{u}_{\mathbf{z},1} & \mathbf{u}_{\mathbf{z},2} & \cdots & \mathbf{u}_{\mathbf{z},n_3}\end{bmatrix}. \tag{5.2c}$$

5.1. Matrix-vector multiplication for $T^*\mathbf{p}$. For a given vector $\mathbf{p} \in \mathbb{C}^{n_1 n_2 n_3}$, we denote $\mathbf{p}$ recursively by letting $\mathbf{p} = \begin{bmatrix}\mathbf{p}_1^\top & \cdots & \mathbf{p}_{n_3}^\top\end{bmatrix}^\top$, $\mathbf{p}_k = \begin{bmatrix}\mathbf{p}_{1,k}^\top & \cdots & \mathbf{p}_{n_2,k}^\top\end{bmatrix}^\top \in \mathbb{C}^{n_1 n_2}$, and $\mathbf{p}_{j,k} = \begin{bmatrix}p_{1,j,k} & \cdots & p_{n_1,j,k}\end{bmatrix}^\top \in \mathbb{C}^{n_1}$ for $j = 1, \ldots, n_2$ and $k = 1, \ldots, n_3$. Let $P = \begin{bmatrix}\mathbf{p}_1 & \mathbf{p}_2 & \cdots & \mathbf{p}_{n_3}\end{bmatrix}$ and $P_k = \begin{bmatrix}\mathbf{p}_{1,k} & \cdots & \mathbf{p}_{n_2,k}\end{bmatrix}$.

By the properties of tensor products, we have

$$\begin{aligned}(\mathbf{z}_{i,j,k}\otimes\mathbf{y}_{i,j}\otimes\mathbf{x}_i)^*\mathbf{p} &= (\mathbf{y}_{i,j}\otimes\mathbf{x}_i)^*\begin{bmatrix}\mathbf{p}_1 & \mathbf{p}_2 & \cdots & \mathbf{p}_{n_3}\end{bmatrix}\bar{\mathbf{z}}_{i,j,k} \\ &= (\mathbf{y}_{i,j}\otimes\mathbf{x}_i)^* P\bar{\mathbf{z}}_{i,j,k}\end{aligned} \tag{5.3}$$

and

$$(\mathbf{y}_{i,j}\otimes\mathbf{x}_i)^*\mathbf{p}_k = \mathbf{x}_i^*\begin{bmatrix}\mathbf{p}_{1,k} & \cdots & \mathbf{p}_{n_2,k}\end{bmatrix}\bar{\mathbf{y}}_{i,j} = \mathbf{x}_i^* P_k\bar{\mathbf{y}}_{i,j}, \tag{5.4}$$

for $k = 1, \ldots, n_3$. From (5.3), (5.1c), and (5.2c), it follows that

$$\begin{aligned}T_{i,j}^*\mathbf{p} &\equiv \begin{bmatrix}\mathbf{z}_{i,j,1}\otimes\mathbf{y}_{i,j}\otimes\mathbf{x}_i & \mathbf{z}_{i,j,2}\otimes\mathbf{y}_{i,j}\otimes\mathbf{x}_i & \cdots & \mathbf{z}_{i,j,n_3}\otimes\mathbf{y}_{i,j}\otimes\mathbf{x}_i\end{bmatrix}^*\mathbf{p} \\ &= \begin{bmatrix}(\mathbf{y}_{i,j}\otimes\mathbf{x}_i)^* P\,\overline{\mathbf{z}_{i,j,1}} \\ (\mathbf{y}_{i,j}\otimes\mathbf{x}_i)^* P\,\overline{\mathbf{z}_{i,j,2}} \\ \vdots \\ (\mathbf{y}_{i,j}\otimes\mathbf{x}_i)^* P\,\overline{\mathbf{z}_{i,j,n_3}}\end{bmatrix} = \begin{bmatrix}\mathbf{z}_{i,j,1}^* P^\top\left(\overline{\mathbf{y}_{i,j}\otimes\mathbf{x}_i}\right) \\ \mathbf{z}_{i,j,2}^* P^\top\left(\overline{\mathbf{y}_{i,j}\otimes\mathbf{x}_i}\right) \\ \vdots \\ \mathbf{z}_{i,j,n_3}^* P^\top\left(\overline{\mathbf{y}_{i,j}\otimes\mathbf{x}_i}\right)\end{bmatrix} \\ &= \begin{bmatrix}\mathbf{z}_{i,j,1} & \mathbf{z}_{i,j,2} & \cdots & \mathbf{z}_{i,j,n_3}\end{bmatrix}^* P^\top\left(\overline{\mathbf{y}_{i,j}\otimes\mathbf{x}_i}\right) \\ &= U_{\mathbf{z}}^* E_{\mathbf{z},i+j}^* P^\top\left(\overline{\mathbf{y}_{i,j}\otimes\mathbf{x}_i}\right),\end{aligned}$$

which implies that

$$T_i^*\mathbf{p} = \begin{bmatrix}T_{i,1}^*\mathbf{p} \\ T_{i,2}^*\mathbf{p} \\ \vdots \\ T_{i,n_2}^*\mathbf{p}\end{bmatrix} = \begin{bmatrix}U_{\mathbf{z}}^* E_{\mathbf{z},i+1}^* P^\top\left(\overline{\mathbf{y}_{i,1}\otimes\mathbf{x}_i}\right) \\ U_{\mathbf{z}}^* E_{\mathbf{z},i+2}^* P^\top\left(\overline{\mathbf{y}_{i,2}\otimes\mathbf{x}_i}\right) \\ \vdots \\ U_{\mathbf{z}}^* E_{\mathbf{z},i+n_2}^* P^\top\left(\overline{\mathbf{y}_{i,n_2}\otimes\mathbf{x}_i}\right)\end{bmatrix}. \tag{5.5}$$

From the definition of P and the result in (5.4), the vectors $P^\top\left(\overline{\mathbf{y}_{i,j}\otimes\mathbf{x}_i}\right)$ for $j = 1,\ldots,n_2$ in (5.5) can be calculated by

$$\begin{aligned}
&\left(\mathbf{p}_k^\top\left[\begin{array}{cccc}\overline{\mathbf{y}_{i,1}\otimes\mathbf{x}_i} & \overline{\mathbf{y}_{i,2}\otimes\mathbf{x}_i} & \cdots & \overline{\mathbf{y}_{i,n_2}\otimes\mathbf{x}_i}\end{array}\right]\right)^\top \\
&= \begin{bmatrix}\mathbf{y}_{i,1}\otimes\mathbf{x}_i & \mathbf{y}_{i,2}\otimes\mathbf{x}_i & \cdots & \mathbf{y}_{i,n_2}\otimes\mathbf{x}_i\end{bmatrix}^*\mathbf{p}_k = \begin{bmatrix}\mathbf{x}_i^*P_k\bar{\mathbf{y}}_{i,1}\\ \vdots \\ \mathbf{x}_i^*P_k\bar{\mathbf{y}}_{i,n_2}\end{bmatrix} = \begin{bmatrix}\mathbf{y}_{i,1}^*P_k^\top\bar{\mathbf{x}}_i\\ \vdots \\ \mathbf{y}_{i,n_2}^*P_k^\top\bar{\mathbf{x}}_i\end{bmatrix}\\
&= \begin{bmatrix}\mathbf{y}_{i,1} & \cdots & \mathbf{y}_{i,n_2}\end{bmatrix}^* P_k^\top\bar{\mathbf{x}}_i
\end{aligned} \tag{5.6}$$

for $k = 1,\ldots,n_3$. Let

$$\begin{bmatrix}\xi_{1,k} & \xi_{2,k} & \cdots & \xi_{n_1,k}\end{bmatrix} = P_k^*\begin{bmatrix}\mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_{n_1}\end{bmatrix} = \left(P_k^*E_{\mathbf{x}}\right)U_{\mathbf{x}} \tag{5.7}$$

for $k = 1,\ldots,n_3$ and

$$\begin{aligned}
\begin{bmatrix}\eta_{i,1} & \eta_{i,2} & \cdots & \eta_{i,n_2}\end{bmatrix} &= \left(\begin{bmatrix}\mathbf{y}_{i,1} & \cdots & \mathbf{y}_{i,n_2}\end{bmatrix}^*\begin{bmatrix}P_1^\top\bar{\mathbf{x}}_i & P_2^\top\bar{\mathbf{x}}_i & \cdots & P_{n_3}^\top\bar{\mathbf{x}}_i\end{bmatrix}\right)^*\\
&= \left(\begin{bmatrix}\xi_{i,1} & \xi_{i,2} & \cdots & \xi_{i,n_3}\end{bmatrix}^\top E_{\mathbf{y},i}\right)U_{\mathbf{y}}
\end{aligned} \tag{5.8}$$

for $i = 1,\ldots,n_1$. Then, by (5.6),

$$\mathbf{p}_k^\top\left[\begin{array}{cccc}\overline{\mathbf{y}_{i,1}\otimes\mathbf{x}_i} & \overline{\mathbf{y}_{i,2}\otimes\mathbf{x}_i} & \cdots & \overline{\mathbf{y}_{i,n_2}\otimes\mathbf{x}_i}\end{array}\right] = \left[\begin{array}{cccc}\overline{\eta_{i,1,k}} & \overline{\eta_{i,2,k}} & \cdots & \overline{\eta_{i,n_2,k}}\end{array}\right]$$

for $k = 1,\ldots,n_3$, where $\eta_{i,j,k}$ is the kth component of $\eta_{i,j}$. This implies that

$$P^\top\left(\overline{\mathbf{y}_{i,j}\otimes\mathbf{x}_i}\right) = \begin{bmatrix}\mathbf{p}_1^\top\left(\overline{\mathbf{y}_{i,j}\otimes\mathbf{x}_i}\right)\\ \mathbf{p}_2^\top\left(\overline{\mathbf{y}_{i,j}\otimes\mathbf{x}_i}\right)\\ \vdots\\ \mathbf{p}_{n_3}^\top\left(\overline{\mathbf{y}_{i,j}\otimes\mathbf{x}_i}\right)\end{bmatrix} = \begin{bmatrix}\overline{\eta_{i,j,1}}\\ \overline{\eta_{i,j,2}}\\ \vdots\\ \overline{\eta_{i,j,n_3}}\end{bmatrix} = \overline{\eta_{i,j}}. \tag{5.9}$$

Substituting (5.9) into (5.5), we have

$$T_i^*\mathbf{p} = \begin{bmatrix}U_{\mathbf{z}}^*E_{\mathbf{z},i+1}^*\overline{\eta_{i,1}}\\ U_{\mathbf{z}}^*E_{\mathbf{z},i+2}^*\overline{\eta_{i,2}}\\ \vdots\\ U_{\mathbf{z}}^*E_{\mathbf{z},i+n_2}^*\overline{\eta_{i,n_2}}\end{bmatrix} = \operatorname{vec}\left(U_{\mathbf{z}}^*\left[\begin{array}{ccc}E_{\mathbf{z},i+1}^*\overline{\eta_{i,1}} & \cdots & E_{\mathbf{z},i+n_2}^*\overline{\eta_{i,n_2}}\end{array}\right]\right) \equiv \operatorname{vec}\left(Z_i\right). \tag{5.10}$$

By the definition of T in (3.15) and the result in (5.10), we obtain

$$T^*\mathbf{p} = \frac{1}{\sqrt{n_1n_2n_3}}\operatorname{vec}\left(\begin{array}{ccc}Z_1 & \cdots & Z_{n_1}\end{array}\right). \tag{5.11}$$

We summarize this new way to compute $T^*\mathbf{p}$ in Algorithm 2.

5.2. Matrix-vector multiplication for $T\mathbf{q}$. For a given vector $\mathbf{q}\in\mathbb{C}^n$, we denote $\mathbf{q}$ recursively by letting $\mathbf{q} = \begin{bmatrix}\mathbf{q}_1^\top & \cdots & \mathbf{q}_{n_1}^\top\end{bmatrix}^\top$ with $\mathbf{q}_i = \begin{bmatrix}\mathbf{q}_{i,1}^\top & \cdots & \mathbf{q}_{i,n_2}^\top\end{bmatrix}^\top \in \mathbb{C}^{n_2n_3}$ and $\mathbf{q}_{i,j} = \begin{bmatrix}q_{i,j,1} & \cdots & q_{i,j,n_3}\end{bmatrix}^\top \in \mathbb{C}^{n_3}$. Then, by the definition of T in (3.15),

Algorithm 2 FFT-based matrix-vector multiplication for $T^*\mathbf{p}$

Input: Any vector $\mathbf{p} = \begin{bmatrix}\mathbf{p}_1^\top & \cdots & \mathbf{p}_{n_3}^\top\end{bmatrix}^\top \in \mathbb{C}^n$ with $\mathbf{p}_k = \begin{bmatrix}\mathbf{p}_{1,k}^\top & \cdots & \mathbf{p}_{n_2,k}^\top\end{bmatrix}^\top$ and $\mathbf{p}_{j,k} \in \mathbb{C}^{n_1}$ for $j = 1,\dots,n_2$, $k = 1,\dots,n_3$.

Output: The vector $\mathbf{f} \equiv T^*\mathbf{p}$.

1: **for** $k = 1,\dots,n_3$ **do**
2: Compute $\xi_{i,k}$ with $\begin{bmatrix}\xi_{1,k} & \xi_{2,k} & \cdots & \xi_{n_1,k}\end{bmatrix} = (P_k^* E_{\mathbf{x}})\, U_{\mathbf{x}}$ in (5.7).
3: **end for**
4: **for** $i = 1,\dots,n_1$ **do**
5: Compute $\eta_{i,j}$ with $\begin{bmatrix}\eta_{i,1} & \cdots & \eta_{i,n_2}\end{bmatrix} = \left(\begin{bmatrix}\xi_{i,1} & \cdots & \xi_{i,n_3}\end{bmatrix}^\top E_{\mathbf{y},i}\right) U_{\mathbf{y}}$ in (5.8).
6: Compute Z_i with $Z_i = U_{\mathbf{z}}^* \begin{bmatrix}E_{\mathbf{z},i+1}^*\overline{\eta_{i,1}} & \cdots & E_{\mathbf{z},i+n_2}^*\overline{\eta_{i,n_2}}\end{bmatrix}$ in (5.10).
7: Set $\mathbf{f}((i-1)n_2n_3+1 : in_2n_3) = \frac{1}{\sqrt{n_1n_2n_3}}\mathrm{vec}(Z_i)$.
8: **end for**

and the results in (5.1c) and (5.2c), we have

$$\begin{aligned}
T\mathbf{q} =& \frac{1}{\sqrt{n_1n_2n_3}} \sum_{i=1}^{n_1}\sum_{j=1}^{n_2}\sum_{k=1}^{n_3} q_{i,j,k}\left(\mathbf{z}_{i,j,k}\otimes\mathbf{y}_{i,j}\otimes\mathbf{x}_i\right)\\
=& \frac{1}{\sqrt{n_1n_2n_3}} \sum_{i=1}^{n_1}\sum_{j=1}^{n_2} \left(\begin{bmatrix}\mathbf{z}_{i,j,1} & \cdots & \mathbf{z}_{i,j,n_3}\end{bmatrix}\mathbf{q}_{i,j}\right)\otimes\mathbf{y}_{i,j}\otimes\mathbf{x}_i\\
=& \frac{1}{\sqrt{n_1n_2n_3}} \sum_{i=1}^{n_1}\sum_{j=1}^{n_2} \left(E_{\mathbf{z},i+j}U_{\mathbf{z}}\mathbf{q}_{i,j}\right)\otimes\mathbf{y}_{i,j}\otimes\mathbf{x}_i\\
=& \frac{1}{\sqrt{n_1n_2n_3}} \sum_{i=1}^{n_1}\sum_{j=1}^{n_2} \mathrm{vec}\left(\left(\mathbf{y}_{i,j}\otimes\mathbf{x}_i\right)\left(E_{\mathbf{z},i+j}U_{\mathbf{z}}\mathbf{q}_{i,j}\right)^\top\right)\\
=& \frac{1}{\sqrt{n_1n_2n_3}} \sum_{i=1}^{n_1} \mathrm{vec}\left(\sum_{j=1}^{n_2}\left(\mathbf{y}_{i,j}\otimes\mathbf{x}_i\right)\left(E_{\mathbf{z},i+j}U_{\mathbf{z}}\mathbf{q}_{i,j}\right)^\top\right).
\end{aligned} \tag{5.12}$$

Let

$$Q_{\mathbf{z},i} \equiv \begin{bmatrix}E_{\mathbf{z},i+1}U_{\mathbf{z}}\mathbf{q}_{i,1} & E_{\mathbf{z},i+2}U_{\mathbf{z}}\mathbf{q}_{i,2} & \cdots & E_{\mathbf{z},i+n_2}U_{\mathbf{z}}\mathbf{q}_{i,n_2}\end{bmatrix}^\top \in \mathbb{C}^{n_2\times n_3} \tag{5.13}$$

for $i = 1,\dots,n_1$. Then Eq. (5.12) can be rewritten as

$$\begin{aligned}
T\mathbf{q} =& \frac{1}{\sqrt{n_1n_2n_3}} \sum_{i=1}^{n_1} \mathrm{vec}\left(\begin{bmatrix}\mathbf{y}_{i,1}\otimes\mathbf{x}_i & \cdots & \mathbf{y}_{i,n_2}\otimes\mathbf{x}_i\end{bmatrix} Q_{\mathbf{z},i}\right)\\
=& \frac{1}{\sqrt{n_1n_2n_3}} \sum_{i=1}^{n_1} \mathrm{vec}\left(\left(\begin{bmatrix}\mathbf{y}_{i,1} & \mathbf{y}_{i,2} & \cdots & \mathbf{y}_{i,n_2}\end{bmatrix} Q_{\mathbf{z},i}\right)\otimes\mathbf{x}_i\right)\\
=& \frac{1}{\sqrt{n_1n_2n_3}} \sum_{i=1}^{n_1} \mathrm{vec}\left(\left(E_{\mathbf{y},i}U_{\mathbf{y}}Q_{\mathbf{z},i}\right)\otimes\mathbf{x}_i\right).
\end{aligned} \tag{5.14}$$

Define

$$G_i \equiv \begin{bmatrix}\mathbf{g}_{i,1} & \mathbf{g}_{i,2} & \cdots & \mathbf{g}_{i,n_3}\end{bmatrix} \equiv E_{\mathbf{y},i}\left(U_{\mathbf{y}}Q_{\mathbf{z},i}\right) \in \mathbb{C}^{n_2\times n_3} \tag{5.15}$$

for $i = 1, \ldots, n_1$. Rewrite Eq. (5.14) as

$$
\begin{aligned}
T\mathbf{q} =& \frac{1}{\sqrt{n_1 n_2 n_3}} \sum_{i=1}^{n_1} \mathrm{vec}\left(\begin{bmatrix} \mathbf{g}_{i,1} & \mathbf{g}_{i,2} & \cdots & \mathbf{g}_{i,n_3} \end{bmatrix} \otimes \mathbf{x}_i \right) \\
=& \frac{1}{\sqrt{n_1 n_2 n_3}} \sum_{i=1}^{n_1} \mathrm{vec}\left(\begin{bmatrix} \mathbf{g}_{i,1} \otimes \mathbf{x}_i & \mathbf{g}_{i,2} \otimes \mathbf{x}_i & \cdots & \mathbf{g}_{i,n_3} \otimes \mathbf{x}_i \end{bmatrix} \right) \\
=& \frac{1}{\sqrt{n_1 n_2 n_3}} \mathrm{vec}\left(\begin{bmatrix} \mathrm{vec}\left(\sum_{i=1}^{n_1} \mathbf{x}_i \mathbf{g}_{i,1}^\top \right) & \cdots & \mathrm{vec}\left(\sum_{i=1}^{n_1} \mathbf{x}_i \mathbf{g}_{i,n_3}^\top \right) \end{bmatrix} \right).
\end{aligned}
$$

Since

$$
\begin{aligned}
\sum_{i=1}^{n_1} \mathbf{x}_i \mathbf{g}_{i,k}^\top &= \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_{n_1} \end{bmatrix} \begin{bmatrix} \mathbf{g}_{1,k} & \mathbf{g}_{2,k} & \cdots & \mathbf{g}_{n_1,k} \end{bmatrix}^\top \\
&= E_{\mathbf{x}} U_{\mathbf{x}} \begin{bmatrix} \mathbf{g}_{1,k} & \mathbf{g}_{2,k} & \cdots & \mathbf{g}_{n_1,k} \end{bmatrix}^\top
\end{aligned}
$$

for $k = 1, \ldots, n_3$, it implies that

$$
\begin{aligned}
&T\mathbf{q} = \frac{1}{\sqrt{n_1 n_2 n_3}} \times \\
&\mathrm{vec}\left(\begin{bmatrix} \mathrm{vec}\left(E_{\mathbf{x}} U_{\mathbf{x}} \begin{bmatrix} \mathbf{g}_{1,1}^\top \\ \mathbf{g}_{2,1}^\top \\ \vdots \\ \mathbf{g}_{n_1,1}^\top \end{bmatrix} \right) & \cdots & \mathrm{vec}\left(E_{\mathbf{x}} U_{\mathbf{x}} \begin{bmatrix} \mathbf{g}_{1,n_3}^\top \\ \mathbf{g}_{2,n_3}^\top \\ \vdots \\ \mathbf{g}_{n_1,n_3}^\top \end{bmatrix} \right) \end{bmatrix} \right).
\end{aligned} \tag{5.16}
$$

We summarize above processes for computing $T\mathbf{q}$ in Algorithm 3.

Algorithm 3 FFT-based matrix-vector multiplication for $T\mathbf{q}$

Input: Any vector $\mathbf{q} = \begin{bmatrix} \mathbf{q}_1^\top & \cdots & \mathbf{q}_{n_1}^\top \end{bmatrix}^\top \in \mathbb{C}^n$ with $\mathbf{q}_i = \begin{bmatrix} \mathbf{q}_{i,1}^\top & \cdots & \mathbf{q}_{i,n_2}^\top \end{bmatrix}^\top$ and $\mathbf{q}_{i,j} \in \mathbb{C}^{n_3}$ for $i = 1, \ldots, n_1, j = 1, \ldots, n_2$.

Output: The vector $\mathbf{g} \equiv T\mathbf{q}$.

1: **for** $i = 1, \ldots, n_1$ **do**

2: Compute $Q_{\mathbf{z},i}$ with $Q = U_{\mathbf{z}} \begin{bmatrix} \mathbf{q}_{i,1} & \mathbf{q}_{i,2} & \cdots & \mathbf{q}_{i,n_2} \end{bmatrix}$,
$Q_{\mathbf{z},i} = \begin{bmatrix} E_{\mathbf{z},i+1} Q(:,1) & E_{\mathbf{z},i+2} Q(:,2) & \cdots & E_{\mathbf{z},i+n_2} Q(:,n_2) \end{bmatrix}^\top$ in (5.13).

3: Compute $\mathbf{g}_{i,k}$ with $\begin{bmatrix} \mathbf{g}_{i,1} & \mathbf{g}_{i,2} & \cdots & \mathbf{g}_{i,n_3} \end{bmatrix} = E_{\mathbf{y},i} (U_{\mathbf{y}} Q_{\mathbf{z},i})$ in (5.15).

4: **end for**

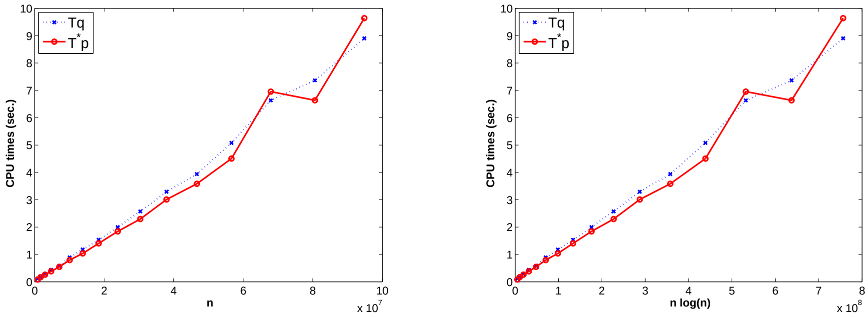
5: **for** $k = 1, \ldots, n_3$ **do**

6: Compute $Q = E_{\mathbf{x}} U_{\mathbf{x}} \begin{bmatrix} \mathbf{g}_{1,k} & \mathbf{g}_{2,k} & \cdots & \mathbf{g}_{n_1,k} \end{bmatrix}^\top$ in (5.16).

7: Set $\mathbf{g}((k-1)n_1 n_2 + 1 : k n_1 n_2) = \frac{1}{\sqrt{n_1 n_2 n_3}} \mathrm{vec}(Q)$.

8: **end for**

6. Numerical Results. We implement Algorithms 1, 2, and 3 by MATLAB to evaluate their timing performance. The matrices $[\xi_{i,k}]$, $[\eta_{i,j}]$, and Z_i in Lines 2, 5 and 6 of Algorithm 2 are computed by `fft`, which is the built-in discrete Fourier transform function in MATLAB. The matrices $Q_{\mathbf{z},i}$, $[\mathbf{g}_{i,k}]$, and Q in Lines 2, 3, and 6 of Algorithm 3 are computed by `ifft`, which is the built-in inverse discrete Fourier transform function in MATLAB. The functions `eigs` with symmetric option



(a) n (b) $n\log(n)$

FIG. 6.1. *CPU time for computing $T^*\mathbf{p}$ and $T\mathbf{q}$ with various n.*

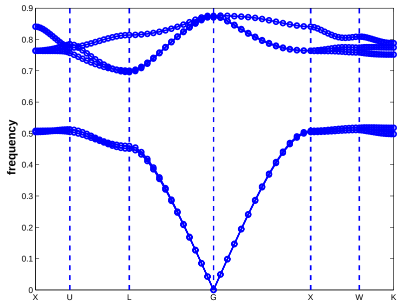
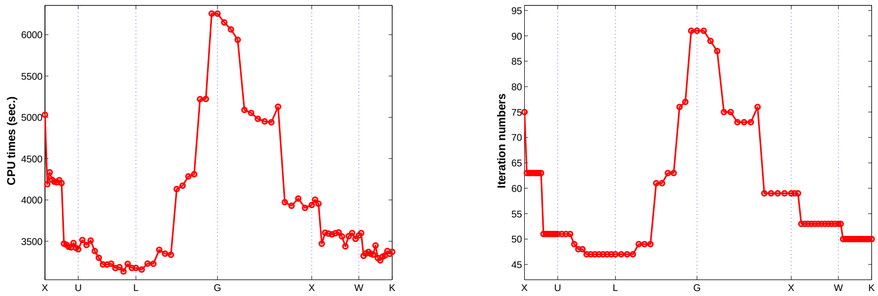


FIG. 6.2. *A computed band structure of the 3D photonic crystals with FCC lattice. The vectors $\mathbf{k}$ is traced along the boundary of the first Brillouin zone. The frequency $\omega = a\sqrt{\lambda}/(2\pi)$ is shown on the y-axis. The radius of the sphere is $r = 0.12a$ and the connecting spheroid has minor axis length $s = 0.11a$. The grid numbers $n_1 = n_2 = n_3 = 120$ and the dimension of the GEVP is $5,184,000$.*

and `pcg` in MATLAB are used for the IPL and CG methods, respectively. The stopping criteria for the eigensolver `eigs` and the linear system solver `pcg` are set to be $10^4 \times \epsilon/(2\sqrt{\delta_x^{-2} + \delta_y^{-2} + \delta_z^{-2}})$ and $\frac{\epsilon}{\delta_x^2} \times 10^{-3}$, respectively. The constant ϵ ($\approx 2^{-52}$) is the floating-point relative accuracy in MATLAB. In `eigs`, the maximal number of Lanczos vectors for the restart is 20 and the symmetric option is used. All computations are carried out on a workstation with two Intel Quad-Core Xeon X5687 3.6 GHz CPUs, 48 GB main memory, the RedHat Linux operation system, and IEEE double-precision floating-point arithmetic operations.

Figure 6.1(a) shows the timing results for computing $T^*\mathbf{p}$ and $T\mathbf{q}$ by Algorithm 2 and 3, respectively. The matrix size of T ranges from $884,736$ to $94,818,816$. In particular, the dimension of T is $\bar{n}_j^3$, where $\bar{n}_j = 96 + 24j = n_1 = n_2 = n_3$ for $j = 0, 1, \ldots, 15$. The average CPU time out of ten trials for each j is then plotted in the figure. We can see Algorithms 2 and 3 are extraordinarily efficient. They take less than 10 seconds to finish a $T^*\mathbf{p}$ or $T\mathbf{q}$ matrix-vector multiplication even for the matrix T whose dimension is as large as 95 million. Figure 6.1(b) shows that the complexity of $T^*\mathbf{p}$ and $T\mathbf{q}$ is $\mathcal{O}(n\log(n))$.

Being equipped with these fast $T^*\mathbf{p}$ or $T\mathbf{q}$ computational kernels, we evaluate



(a) CPU time (b) IPL iteration numbers

FIG. 6.3. *CPU time and iteration numbers of IPL method with various wave vector* $2\pi\mathbf{k}$.

n_1	90	120	150	180	210
λ_3	19.1144	19.1131	19.1190	19.1257	19.1251

TABLE 6.1
The third smallest positive eigenvalue for the wave vector $\mathbf{k} = L$ *with various* $n = n_1^3$.

how the IPL method (Algorithm 1) performs, in terms of CPU time and iteration numbers, to solve the eigenvalue problems for the band structure of the target photonic crystals. In the numerical experiments, we assume the piecewise constant and periodic dielectric diamond structure with face centered cubic lattice consists of dielectric spheres and connecting spheroid [8]. The radius of the spheres is $r = 0.12a$ and the connecting spheroid has minor axis length $s = 0.11a$ with $a = 1$. Inside the structure is the dielectric material with permittivity contrast $\varepsilon_i/\varepsilon_o = 13$. We solve the eigenvalue problems associated with the wave vector $2\pi\mathbf{k}$'s along the segments connecting X, U, L, G, X, W, and K in the first Brillouin zone. In each of the segments, fifteen uniformly distributed sampling wave vectors are chosen. For each wave vector, we compute the five smallest positive eigenvalues of the corresponding GEVP. The associated band structure is plotted in Figure 6.2, which shows that a band gap lies between the second and third smallest eigenvalue curves. In Table 6.1, we demonstrate the convergence of the third smallest positive eigenvalue λ_3 for the discrete eigenvalue problem with various mesh sizes for $\mathbf{k} = L$.

In the following numerical results, the dimension of the GEVP is $3\bar{n}_1^3 = 3 \times 120^3 = 5,184,000$ and the dimension of the SEVP we are actually solving is reduced to $2\bar{n}_1^3 = 2 \times 120^3 = 3,456,000$.

Computational results in CPU time of the IPL are shown in Figure 6.3(a). Out of all of the 90 test problems, the timing to solve each of the eigenvalue problems ranges from 50 to 104 minutes with average of 65 minutes. For the problems with dimension as large as 3.5 million, the timing results of the MATLAB codes are quite satisfactory. On average, the matrix $(Q_r^* B^{-1} Q_r)$ vector multiplications take about 77% of the total CPU time for solving the eigenvalue problem. In this matrix-vector multiplication, $T\mathbf{q}$ and $T^*\mathbf{q}$ require around 44% and 33% of CPU time, respectively. The discrete FFT MATLAB functions `ifft` and `fft` take about 68% and 64% of CPU times for computing $T\mathbf{q}$ and $T^*\mathbf{q}$, respectively. That is, `ifft` and `fft` take about $23\% (= 0.77 \times 0.44 \times 0.68)$ and $16\% (= 0.77 \times 0.33 \times 0.64)$ of the total CPU time for solving the eigenvalue problem.

In addition to the fast $T^*\mathbf{p}$ and $T\mathbf{q}$ multiplications, another factor contributing to the outstanding timing performance is the small number of iterations in the IPL. The total iteration numbers that the IPL takes to solve an eigenvalue problem for the five target eigenvalues are shown in Figure 6.3(b). Among the 90 cases we tested, the IPL takes 47 to 91 iterations (57 on average) to solve each of the eigenvalues. These small iteration numbers for such large problems are again remarkable.

Finally, to solve the linear systems within the IPL solver, the CG method takes around 40 iterations consistently for all of the test problems to fulfill the relative residual tolerance 6.40×10^{-15}. This fast convergence behavior is due to the well-conditioned coefficient matrix defined in (4.5) and can be justified by the following theoretical analysis. Convergence of the CG method for solving Eq. (4.5) depends on the ratio $\gamma = \frac{\sqrt{\kappa(Q_r^* B^{-1} Q_r)}-1}{\sqrt{\kappa(Q_r^* B^{-1} Q_r)}+1}$ as shown in [34]. In the numerical experiments, we have $\varepsilon_i/\varepsilon_o = 13$. Theorem 4.1 suggests that $\gamma \leq \gamma_B = \frac{\sqrt{13}-1}{\sqrt{13}+1} \approx 0.5657$. In other words, after 40 iterations, the residual is predicted to be less than $(\gamma_B)^{40} \approx 1.27 \times 10^{-10}$.

7. Conclusions. Aiming to solve the Maxwell equation that models the 3D photonic crystals with FCC lattice, we have derived an explicit eigendecomposition of the discrete double-curl operator and the orthogonal bases spanning the associated range and null spaces. Based on these results, we propose the inverse projective Lanczos method with the FFT-based matrix-vector multiplications that can solve the eigenvalue problems efficiently. This fast eigenvalue solver can significantly reduce the time needed to find the optimal shape of photonic crystals with larger band gap.

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Appendix A.

THEOREM A.1. *Let θ_i, $\theta_{i,j}$ and $\theta_{i,j,k}$ be defined in* (3.1), (3.3), *and* (3.8), *respectively, for $i = 1, \ldots, n_1$, $j = 1, \ldots, n_2$, $k = 1, \ldots, n_3$ and n_ℓ $(\ell = 1, 2, 3)$ be multiples of* 6. *Assume $\mathbf{k} = (\mathrm{k}_1, \mathrm{k}_2, \mathrm{k}_3) \neq 0$ with*

$$\underline{0 \leq \mathrm{k}_1 \leq \frac{\sqrt{2}}{a}, \; 0 \leq \mathrm{k}_2 < \frac{2\sqrt{2}}{\sqrt{3}a}, \; 0 \leq \mathrm{k}_3 < \frac{\sqrt{3}}{a}.} \tag{A.1}$$

Then $p_1 = \theta_i/(\imath 2\pi)$, $p_2 = \theta_{i,j}/(\imath 2\pi)$, and $p_3 = \theta_{i,j,k}/(\imath 2\pi)$ are integers if and only if $\mathbf{k} = \frac{\sqrt{2}}{a}(1, 1/\sqrt{3}, 1/\sqrt{6})^\top$.

Proof. From the definitions of θ_i, $\theta_{i,j}$, $\theta_{i,j,k}$, and the lattice vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ in (1.4), it follows that p_1, p_2, and p_3 are integers if and only if $\mathbf{k}$ satisfies that $\mathbf{k} \cdot \mathbf{a}_1 = n_1 p_1 - i$, $\mathbf{k} \cdot \mathbf{a}_2 = n_2 p_2 - j + \frac{1}{2} n_1 p_1$, and $\mathbf{k} \cdot \mathbf{a}_3 = n_3 p_3 - k + \frac{1}{2} n_1 p_1 + \frac{1}{3} n_2 p_2$. This is equivalent to $\mathrm{k}_1 = \frac{\sqrt{2}}{a}(n_1 p_1 - i)$, $\mathrm{k}_2 = \frac{2\sqrt{2}}{\sqrt{3}a}\left(n_2 p_2 + \frac{i}{2} - j\right)$ and $\mathrm{k}_3 = \frac{\sqrt{3}}{a}\left(n_3 p_3 - k + \frac{1}{3}(i + j)\right)$. By assumption in (A.1), it implies that

$$0 \leq n_1 p_1 - i \leq 1, \tag{A.2}$$

$$0 \leq n_2 p_2 + \frac{i}{2} - j < 1, \text{ and} \tag{A.3}$$

$$0 \leq n_3 p_3 - k + \frac{1}{3}(i + j) < 1. \tag{A.4}$$

Since $1 \le i \le n_1$, from (A.2), it holds that $p_1 = 1$ and $i = n_1$ or $i = n_1 - 1$.
Case 1. $i = n_1$ (which implies $\mathrm{k}_1 = 0$). From (A.3), even n_1 and $1 \le j \le n_2$, we have $j = \frac{n_1}{2}$, $p_2 = 0$, and $\mathrm{k}_2 = 0$. Then Eq. (A.4) becomes $0 \le n_3 p_3 - k + \frac{1}{2} n_1 < 1$. Since $\frac{1}{2} n_1$ is an integer, we have $n_3 p_3 - k + \frac{1}{2} n_1 = 0$ or $\mathrm{k}_3 = 0$, which contradicts $\mathbf{k} \neq 0$.
Case 2. $i = n_1 - 1$ (which implies $\mathrm{k}_1 = \frac{\sqrt{2}}{a}$). From (A.3), it follows that $0 < \frac{n_1 - 1}{2} - j < 1$ and $p_2 = 0$. The fact implies that $j = \frac{n_1 - 2}{2}$ and therefore $\mathrm{k}_2 = \frac{\sqrt{2}}{\sqrt{3}a}$. Consequently, from (A.4), it holds that $0 \le -k + \frac{1}{2} n_1 - \frac{2}{3} < 1$ and $p_3 = 0$, which implies that $k = \frac{1}{2} n_1 - 1$, and therefore $\mathrm{k}_3 = \frac{\sqrt{2}}{\sqrt{6}a}$ or $\mathbf{k} = \frac{\sqrt{2}}{a}(1, 1/\sqrt{3}, 1/\sqrt{6})^\top$. $\square$

The following theorem asserts that C_1, C_2, and C_3 are normal and commute with each other.

THEOREM A.2. *For C_1, C_2, and C_3 defined in* (2.3a), *it holds that $C_i^* C_j = C_j C_i^*$ and $C_i C_j = C_j C_i$ for $i, j = 1, 2, 3$.*

Proof. First, by definitions of K_i and J_i in (2.4), (2.5a), and (2.5b), it holds that $J_2^* J_2 = I_{n_1}$, $J_3^* J_3 = I_{n_1 n_2}$ as well as $K_1^* K_1 = I_{n_1}$, $K_2^* K_2 = I_{n_1 n_2}$, and $K_3^* K_3 = I_n$. We then have $C_j^* C_j = C_j C_j^*$ for $j = 1, 2, 3$. Furthermore, it is easy to check that $K_1 J_2^* = J_2^* K_1$, $K_1^* J_2 = J_2 K_1^*$, and $K_1 J_2 = J_2 K_1$. Therefore, we have $C_1^* C_2 = C_2 C_1^*$, $C_1 C_2^* = C_2^* C_1$, and $C_1 C_2 = C_2 C_1$.

Second, we partition K_2 as

$$K_2 = \begin{bmatrix} K_{22} & (\mathbf{e}_m \mathbf{e}_1^\top) \otimes I_{n_1} & 0 \\ 0 & K_{22} & (\mathbf{e}_m \mathbf{e}_1^\top) \otimes I_{n_1} \\ e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_2} (\mathbf{e}_m \mathbf{e}_1^\top) \otimes J_2 & 0 & K_{22} \end{bmatrix},$$

where $m = n_2/3$, $K_{22} = \begin{bmatrix} -1 & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & -1 \end{bmatrix} \otimes I_{n_1} \in \mathbb{C}^{\frac{n_1 n_2}{3} \times \frac{n_1 n_2}{3}}$, and $\mathbf{e}_j$ is the jth column of I_m. Consequently,

$$K_2 J_3^* = \begin{bmatrix} 0 & K_{22}(I_m \otimes J_2^*) & (\mathbf{e}_m \mathbf{e}_1^\top) \otimes J_2^* \\ e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_2} (\mathbf{e}_m \mathbf{e}_1^\top) \otimes I_{n_1} & 0 & K_{22}(I_m \otimes J_2^*) \\ e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_2} K_{22} & e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_2} ((\mathbf{e}_m \mathbf{e}_1^\top) \otimes I_{n_1}) & 0 \end{bmatrix}$$

and

$$J_3^* K_2 = \begin{bmatrix} 0 & (I_m \otimes J_2^*) K_{22} & (\mathbf{e}_m \mathbf{e}_1^\top) \otimes J_2^* \\ e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_2} (\mathbf{e}_m \mathbf{e}_1^\top) \otimes I_{n_1} & 0 & (I_m \otimes J_2^*) K_{22} \\ e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_2} K_{22} & e^{\imath 2\pi \mathbf{k}\cdot\mathbf{a}_2} ((\mathbf{e}_m \mathbf{e}_1^\top) \otimes I_{n_1}) & 0 \end{bmatrix}.$$

Since $K_{22}(I_m \otimes J_2^*) = (I_m \otimes J_2^*) K_{22}$, it follows that $K_2 J_3^* = J_3^* K_2$. Similarly, $K_2^* J_3 = J_3 K_2^*$ and $K_2 J_3 = J_3 K_2$. We have $C_2^* C_3 = C_3 C_2^*$, $C_2 C_3^* = C_3^* C_2$ and $C_2 C_3 = C_3 C_2$.

Finally, by the definitions of C_1 and C_3 in (2.3a), it is easy to check that $C_1^* C_3 = C_3 C_1^*$, $C_1 C_3^* = C_3^* C_1$, and $C_1 C_3 = C_3 C_1$. $\square$

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