Bifurcation Analysis of the Eigenstructure of the Discrete Single-curl Operator in Three-dimensional Maxwell's Equations with Pasteur Media

Xin Liang* Zhen-Chen Guo† Tsung-Ming Huang‡ Tiexiang Li§
Wen-Wei Lin¶

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Abstract

This paper focuses on studying the bifurcation analysis of the eigenstructure of the γ-parameterized generalized eigenvalue problem (γ-GEP) arising in three-dimensional (3D) source-free Maxwell's equations with Pasteur media, where γ is the magnetoelectric chirality parameter. For the weakly coupled case, namely, $\gamma < \gamma_* \equiv$ critical value, the γ-GEP is positive definite, which has been well-studied by Chern et. al, 2015. For the strongly coupled case, namely, $\gamma > \gamma_*$, the γ-GEP is no longer positive definite, introducing a totally different and complicated structure. For the critical strongly coupled case, numerical computations for electromagnetic fields have been presented by Huang et. al, 2018. In this paper, we build several theoretical results on the eigenstructure behavior of the γ-GEPs. We prove that the γ-GEP is regular for any $\gamma > 0$, and the γ-GEP has 2×2 Jordan blocks of infinite eigenvalues at the critical value γ_*. Then, we show that the 2×2 Jordan block will split into a complex conjugate eigenvalue pair that rapidly goes down and up and then collides at some real point near the origin. Next, it will bifurcate into two real eigenvalues, with one moving toward the left and the other to the right along the real axis as γ increases. A newly formed state whose energy is smaller than the ground state can be created as γ is larger than the critical value. This stunning feature of the physical phenomenon would be very helpful in practical applications. Therefore, the purpose of this paper is to clarify the corresponding theoretical eigenstructure of 3D Maxwell's equations with Pasteur media.

Key words. Bifurcation analysis, Eigenstructure, Maxwell's equations, Pasteur media, Jordan block, Regular matrix pair.

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1 Introduction

The eigenstructure of the discrete single-curl operator $\nabla\times$ is fundamental and vital for efficient numerical simulations of complex materials. Here, complex materials, or physically, complex media,

*Yau Mathematical Sciences Center, Tsinghua University, Beijing 100084, China. E-mail: liangxinslm@tsinghua.edu.cn. Supported in part by the MOST.

†Department of Mathematics, Nanjing University, Nanjing 210093, Jiangsu, China. E-mail: guozhenchen@nju.edu.cn. Supported in part by the MOST.

‡Department of Mathematics, National Taiwan Normal University, Taipei 116, Taiwan. E-mail: min@ntnu.edu.tw. Supported in part by the Ministry of Science and Technology (MOST) 108-2115-M-003-012-MY2 and the National Center for Theoretical Sciences (NCTS) in Taiwan.

§School of Mathematics, Southeast University, Nanjing 211189, Jiangsu, China. E-mail: txli@seu.edu.cn. Supported by the National Natural Science Foundation of China (NSFC) 11971105 and the Shing-Tung Yau Center of Southeast University.

¶Department of Applied Mathematics, National Chiao Tung University, Hsinchu 300, Taiwan. E-mail: wwlin@am.nctu.edu.tw. Supported in part by the MOST 106-2628-M-009-004-, the NCTS, and the ST Yau Centre at the National Chiao Tung University.

imply coupling effects between electric and magnetic fields. Bianisotropic material is an important class of complex media (see, e.g., [12, Section 5.3]), of which the coupling effects between electric and magnetic fields can be described by the Tellegen representation of the constitutive relations

$$\boldsymbol{B} = \boldsymbol{\mu}\boldsymbol{H} + \boldsymbol{\zeta}\boldsymbol{E}, \qquad \boldsymbol{D} = \boldsymbol{\varepsilon}\boldsymbol{E} + \boldsymbol{\xi}\boldsymbol{H},$$

where $\boldsymbol{E}, \boldsymbol{H}, \boldsymbol{D}, \boldsymbol{B}$ are the electric, the magnetic fields, the dielectric displacement, and the magnetic induction at the position $\boldsymbol{x}$, respectively, $\boldsymbol{\mu}$ is the permeability, $\boldsymbol{\varepsilon}$ is the permittivity, and $\boldsymbol{\zeta}, \boldsymbol{\xi}$ are magnetoelectric parameters. Usually, $\boldsymbol{\mu}, \boldsymbol{\varepsilon}, \boldsymbol{\zeta}, \boldsymbol{\xi}$ are dyadics (a.k.a. second-order tensors) of dimension three. In particular, a bianisotropic medium is also called a biisotropic medium, if $\boldsymbol{\mu}, \boldsymbol{\varepsilon}, \boldsymbol{\zeta}, \boldsymbol{\xi}$ are scalar dyadics, or equivalently,

$$\boldsymbol{\mu} = \mu\boldsymbol{I}, \quad \boldsymbol{\varepsilon} = \varepsilon\boldsymbol{I}, \quad \boldsymbol{\zeta} = \zeta\boldsymbol{I}, \quad \boldsymbol{\xi} = \xi\boldsymbol{I},$$

where $\boldsymbol{I}$ represents the identity dyadics. Specifically, a Pasteur medium (a.k.a. the reciprocal chiral medium) is a type of biisotropic media, where

$$\xi = \imath\gamma, \qquad \zeta = -\imath\gamma, \qquad \gamma \geq 0. \tag{1}$$

Mathematically, the propagation of electromagnetic waves in bianisotropic media is modeled by the three-dimensional (3D) frequency domain source-free Maxwell's equations with the constitutive relations

$$\begin{aligned} \nabla \times \boldsymbol{E} &= \imath\omega\boldsymbol{B}, \qquad \nabla \cdot \boldsymbol{B} = 0, \\ \nabla \times \boldsymbol{H} &= -\imath\omega\boldsymbol{D}, \qquad \nabla \cdot \boldsymbol{D} = 0, \end{aligned}$$

or equivalently,

$$\begin{bmatrix} \nabla\times & 0 \\ 0 & \nabla\times \end{bmatrix} \begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{bmatrix} = \imath\omega \begin{bmatrix} \boldsymbol{\zeta} & \boldsymbol{\mu} \\ -\boldsymbol{\varepsilon} & -\boldsymbol{\xi} \end{bmatrix} \begin{bmatrix} \boldsymbol{E} \\ \boldsymbol{H} \end{bmatrix}, \qquad \begin{bmatrix} \nabla\cdot & 0 \\ 0 & \nabla\cdot \end{bmatrix} \begin{bmatrix} \boldsymbol{D} \\ \boldsymbol{B} \end{bmatrix} = 0,$$

where ω is the frequency. The Bloch theorem, from the theorem named after F. Bloch (see, e.g., [10, p. 167]), implies that the solutions of the Schrödinger equation for a periodic potential must be of a quasi-periodic form, stating that

> The eigenfunctions of the wave equation for a periodic potential are the product of a plane wave $\exp(\imath 2\pi \boldsymbol{k} \cdot \boldsymbol{x})$ times a function $u_{\boldsymbol{k}}(\boldsymbol{x})$ with the periodicity of the crystal lattice.

Based on the Bloch theorem, the Bloch eigenvectors $\boldsymbol{E}$ and $\boldsymbol{H}$ on any crystal lattice, satisfying the quasi-periodic conditions

$$\boldsymbol{E}(\boldsymbol{x} + \boldsymbol{a}_\ell) = \boldsymbol{E}(\boldsymbol{x}) \exp(\imath 2\pi \boldsymbol{k} \cdot \boldsymbol{a}_\ell), \qquad \boldsymbol{H}(\boldsymbol{x} + \boldsymbol{a}_\ell) = \boldsymbol{H}(\boldsymbol{x}) \exp(\imath 2\pi \boldsymbol{k} \cdot \boldsymbol{a}_\ell)$$

are of interest, where $2\pi\boldsymbol{k}$ is the Bloch wave vector in the first Brillouin zone $\mathcal{B}$, and $\boldsymbol{a}_\ell, \ell = 1, 2, 3$ are the lattice translation vectors (see, e.g., [9, p. 34]).

Using Yee's scheme [13], a finite difference discretization that satisfies the source-free conditions and the quasi-periodicity conditions naturally, the discretized Maxwell's equations are

$$\begin{bmatrix} C & 0 \\ 0 & C^{\mathrm{H}} \end{bmatrix} \begin{bmatrix} \boldsymbol{e} \\ \boldsymbol{h} \end{bmatrix} = \imath\omega \begin{bmatrix} \zeta_d & \mu_d \\ -\varepsilon_d & -\xi_d \end{bmatrix} \begin{bmatrix} \boldsymbol{e} \\ \boldsymbol{h} \end{bmatrix}, \tag{2}$$

where μ_d, ε_d, ξ_d and ζ_d are diagonal matrices, and C is special structured, facilitating the introduction of the fast Fourier transform (FFT) to accelerate numerical simulations [3, 6, 8] (see eq. (3)-eq. (6) below, for details).

For the Pasteur media, the matrix pair in eq. (2) is positive definite when the parameter γ in eq. (1) is small, but it becomes an indefinite pair as γ becomes larger (see below). The weakly coupled case, namely, the case in which the matrix pair is positive definite, has been analyzed by

Chern et al. [3] in 2015. For the strongly coupled case, the matrix pair is no longer a positive-definite matrix pair, introducing a totally different and complicated structure. For the critical strongly coupled case, numerical computations for the electromagnetic fields $\boldsymbol{E}$ and $\boldsymbol{H}$ have been studied by Huang et. al. [7], but lack of theory makes it difficult to guarantee that the numerical results are valid and reliable.

In this paper, we build several theoretical results on the eigenstructure behavior of the discrete single-curl operator in 3D Maxwell's equations for Pasteur media:

(a) The matrix pair in eq. (2) is always regular regardless of how large γ is;

(b) The matrix pair eq. (2) has 2×2 Jordan blocks of the infinite eigenvalues at the critical value $\gamma = \gamma_*$. Then, the 2×2 Jordan block will split into a pair of complex conjugate eigenvalues that move rapidly down and up and collide at some real point near the origin to form an associated 2×2 Jordan block of a real eigenvalue;

(c) This 2×2 Jordan block will bifurcate into two real eigenvalues such that one moves toward the left and the other to the right along the real axis;

(d) A newly formed state whose energy is smaller than the ground state can be created as γ is larger than the critical value γ_*.

The feature exhibited by the physical phenomenon derived from the above three points (b)-(d) is an astonishing finding. This discovery would be very useful in practical applications. However, the corresponding theoretical eigenstructure behavior should first be clarified.

Notation. $\iota = \sqrt{-1}$ is the imaginary unit; $\mathrm{e} = \exp(1)$ is Euler's number. For any $n \in \mathbb{N}$, $\eta_n = \mathrm{e}^{\frac{2\pi\iota}{n}}$ is an nth root of unity. For any index set $\mathcal{I}$, $I^{\mathcal{I}}$ denotes the diagonal matrix whose ith diagonal entry is 1 for all $i \in \mathcal{I}$ and 0 otherwise; $I^{\mathcal{I}}_{\sigma}$ denotes the matrix consisting of all nonzero columns of $I^{\mathcal{I}}$; and $|\mathcal{I}|$ denotes the number of its elements. I_n is the identity matrix of size n; in particular, I_0 is an empty matrix; e_i is the ith column of I_n. For a matrix X, X^{T} and X^{H} are its transpose and conjugate transpose, respectively; $\mathcal{N}(X) = \{v : Xv = 0\}$ is the kernel of X. For matrices X, Y, $X \otimes Y$ is their Kronecker product; $X \succeq Y$ means that $X - Y$ is positive semidefinite, similarly for "$\succ$", "$\preceq$", and "$\prec$". For $m \in \mathbb{N}$, $\alpha \in \mathbb{C}$ and $X \in \mathbb{C}^{n\times n}$, write

$$V_{m\times n}(\alpha) := \begin{bmatrix} 1 & 1 & \cdots & 1 \\ \alpha & \alpha^2 & \cdots & \alpha^n \\ \vdots & \vdots & & \vdots \\ \alpha^{m-1} & \alpha^{2(m-1)} & \cdots & \alpha^{n(m-1)} \end{bmatrix}, \quad K_m(X) := \begin{bmatrix} & I_n & & \\ & & \ddots & \\ & & & I_n \\ X & & & \end{bmatrix}_{mn\times mn}.$$

In particular, write $V_m(\alpha) = V_{m\times 1}(\alpha)$, $D_m(\alpha) = \alpha \operatorname{diag}(V_m(\alpha))$.

2 Preliminaries

2.1 Discretization

It is well known from crystallography that crystal structures can be classified into 14 Bravais lattices [1, 2]. Because of various lattices, the discretized single-curl operators C and C^{H} in eq. (2) on the electric and magnetic fields, respectively, may have different forms. In the discretization process, $\mathcal{D}_i$ and $\mathcal{D}_o$ denote the sets including the indices of all vertices inside and outside, respectively, the medium (usually the domain would be of vacuum or air but could be of another medium). Then, $\mathcal{D} = \mathcal{D}_i \cup \mathcal{D}_o$ is the discretization grid. Moreover, n_1, n_2, n_3 denote the numbers of grid vertices in the x, y, z directions, respectively, and $\delta_1, \delta_2, \delta_3$ for the associated mesh lengths. Write $n = n_1n_2n_3$.

The discretized Maxwell's equations are eq. (2), in which ζ_d, μ_d, ε_d, ξ_d are decided by the shape of the medium, and C is given by Yee's scheme. For the former, ζ_d, μ_d, ε_d, ξ_d may not have the same value in three directions of some boundary points. However, for convenience of notation, in this paper, we consider the case that

$$\mu_d = \mu_{io} I_3 \otimes I, \qquad \varepsilon_d = I_3 \otimes [\varepsilon_o I^{(o)} + \varepsilon_i I^{(i)}], \tag{3a}$$

$$\zeta_d = -\iota\gamma I_3 \otimes I^{(i)}, \qquad \xi_d = \iota\gamma I_3 \otimes I^{(i)}, \tag{3b}$$

where γ is the chirality, $\varepsilon_i, \varepsilon_o$ are the permittivities inside and outside the medium, respectively, and $\mu_{io} \equiv 1$ is the permeability. For simplicity, here we denote $I^{(i)} \equiv I^{\mathcal{D}_i}$ and $I^{(o)} \equiv I^{\mathcal{D}_o}$.

For the latter, we refer the readers to [8] in order to peruse the details of the whole discretization process. We provide some basic but important results to ensure this paper is self-contained. According to the type of the lattice, one of the 14 Bravais lattices, which represent all kinds of crystals, C, the discretized single-curl operator on the electric field by Yee's scheme, may have different forms which can be uniformly written as

$$C = \begin{bmatrix} 0 & -C_3 & C_2 \\ C_3 & 0 & -C_1 \\ -C_2 & C_1 & 0 \end{bmatrix}, \tag{4}$$

where

$$C_1 = \delta_1^{-1}[-I_n + I_{n_3} \otimes I_{n_2} \otimes K_{n_1}(\mathrm{e}^{\iota 2\pi \boldsymbol{k}\cdot\boldsymbol{a}_1})], \tag{5a}$$
$$C_2 = \delta_2^{-1}[-I_n + I_{n_3} \otimes K_{n_2}(\mathrm{e}^{\iota 2\pi \boldsymbol{k}\cdot\boldsymbol{a}_2} J_1)], \tag{5b}$$
$$C_3 = \delta_3^{-1}[-I_n + K_{n_3}(\mathrm{e}^{\iota 2\pi \boldsymbol{k}\cdot\boldsymbol{a}_3} J_2)], \tag{5c}$$

with $J_1 = J_{1,1}$ and

$$J_2 = \mathrm{e}^{\iota 2\pi \boldsymbol{k}\cdot\rho_2\boldsymbol{a}_2} \begin{bmatrix} & \mathrm{e}^{-\iota 2\pi \boldsymbol{k}\cdot\boldsymbol{a}_2} I_{m_2} \otimes J_{1,3} \\ I_{n_2-m_2} \otimes J_{1,2} & \end{bmatrix}, \tag{6a}$$
$$J_{1,\ell} = \mathrm{e}^{\iota 2\pi \boldsymbol{k}\cdot\rho_{1,\ell}\boldsymbol{a}_1} \begin{bmatrix} & \mathrm{e}^{-\iota 2\pi \boldsymbol{k}\cdot\boldsymbol{a}_1} I_{m_{1,\ell}} \\ I_{n_1-m_{1,\ell}} & \end{bmatrix}, \qquad \ell = 1,2,3. \tag{6b}$$

Here, $\rho_2, \rho_{1,1} \in \{0,1\}$, $\rho_{1,2}, \rho_{1,3} \in \{-1,0,1,2\}$ satisfying $\rho_{1,2} - \rho_{1,3} - \rho_{1,1} \in \{0,1\}$, and $m_2 \in [0, n_2] \cap \mathbb{N}$, $m_{1,\ell} \in [0, n_1] \cap \mathbb{N}$ for $\ell = 1,2,3$ satisfying $m_{1,2} - m_{1,3} - m_{1,1} \in \{0, n_1\}$. Write $m_1 := m_{1,1}$, $\rho_1 := \rho_{1,1}$, and $\widehat{\rho}_1 := \rho_2\rho_1 + \rho_2\rho_{1,2} + (1-\rho_2)\rho_{1,3}$.

C_1, C_2, C_3 are simultaneously diagonalizable by a unitary matrix, which is guaranteed by theorem 2.1.

Theorem 2.1 ([8]). *C_1, C_2, C_3 are simultaneously diagonalizable by the unitary matrix $T = [t_\ell]_{\ell=1,\ldots,n}$ in the forms*

$$\Lambda_1 := T^{\mathrm{H}} C_1 T = \delta_1^{-1}[-I_n + \eta_{n_1}^{\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_1} I_{n_3} \otimes I_{n_2} \otimes D_{n_1}(\eta_{n_1})], \tag{7a}$$
$$\Lambda_2 := T^{\mathrm{H}} C_2 T = \delta_2^{-1}[-I_n + \eta_{n_2}^{\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_2} I_{n_3} \otimes D_{n_2}(\eta_{n_2}) \otimes D_{n_1}(\eta_{n_1 n_2}^{-m_1})], \tag{7b}$$
$$\Lambda_3 := T^{\mathrm{H}} C_3 T = \delta_3^{-1}[-I_n + \eta_{n_3}^{\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_3} D_{n_3}(\eta_{n_3}) \otimes D_{n_2}(\eta_{n_3 n_2}^{-m_2}) \otimes D_{n_1}(\eta_{n_1 n_3}^{-\widehat{m}_1} \eta_{n_1 n_2 n_3}^{m_1 m_2})], \tag{7c}$$

where

$$t_{\langle i_1,i_2,i_3\rangle} = \tfrac{1}{\sqrt{n}} V_{n_3}(\eta_{n_3}^{\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_3+i_3} \eta_{n_2 n_3}^{-m_2 i_2} \eta_{n_1 n_3}^{-\widehat{m}_1 i_1} \eta_{n_1 n_2 n_3}^{m_1 m_2 i_1}) \otimes V_{n_2}(\eta_{n_2}^{\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_2+i_2} \eta_{n_1 n_2}^{-m_1 i_1}) \otimes V_{n_1}(\eta_{n_1}^{\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_1+i_1}) \tag{8}$$

for $i_1, i_2, i_3 \in \mathbb{Z}$, $\langle i_1, i_2, i_3\rangle$ is defined as

$$\langle i_1, i_2, i_3\rangle := (i_3' - 1)n_1 n_2 + (i_2' - 1)n_1 + i_1',$$

where $i_\ell' = i_\ell + t_\ell n_\ell, 1 \le i_\ell' \le n_\ell, t_\ell \in \mathbb{Z}, \ell = 1,2,3$, and

$$\begin{aligned}
\widehat{\boldsymbol{a}}_1 &= \boldsymbol{a}_1, \\
\widehat{\boldsymbol{a}}_2 &= \boldsymbol{a}_2 + (\rho_1 - \frac{m_1}{n_1})\widehat{\boldsymbol{a}}_1, \\
\widehat{\boldsymbol{a}}_3 &= \boldsymbol{a}_3 + (\rho_2 - \frac{m_2}{n_2})\widehat{\boldsymbol{a}}_2 + [\widehat{\rho}_1 - \frac{\widehat{m}_1}{n_1} - \rho_2(\rho_1 - \frac{m_1}{n_1})]\widehat{\boldsymbol{a}}_1, \\
\widehat{m}_1 &= \rho_2 m_1 + \rho_2 m_{1,2} + (1-\rho_2) m_{1,3}.
\end{aligned}$$

Note that

(a) $\widehat{\boldsymbol{a}}_1, \widehat{\boldsymbol{a}}_2, \widehat{\boldsymbol{a}}_3$ is an orthogonal basis of $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$, and $\|\widehat{\boldsymbol{a}}_\ell\|_2 = l_\ell = n_\ell \delta_\ell$ for $\ell = 1, 2, 3$.

(b) $2\pi \boldsymbol{k} \in \mathcal{B}$ implies

$$b_{l,\ell} \le \boldsymbol{k} \cdot \boldsymbol{a}_\ell \le b_{u,\ell}, \qquad \ell = 1, 2, 3, \tag{9}$$

where $b_{u,\ell} - b_{l,\ell} \le 1$, $b_{l,\ell} \in [-2/3, 0], b_{u,\ell} \in [0, 5/6]$.

As a result, the singular value decomposition of C can be calculated along the way in [3], which is shown in theorem 2.2.

Theorem 2.2 ([3, 8]). *If $\boldsymbol{k} \neq 0$, then:*

(a) $\Lambda_q := \Lambda_1^{\rm H}\Lambda_1 + \Lambda_2^{\rm H}\Lambda_2 + \Lambda_3^{\rm H}\Lambda_3 \succ 0$;

(b) $\Lambda_p := \left(\begin{bmatrix} 0 & -\tau_3 & \tau_2 \\ \tau_3 & 0 & -\tau_1 \\ -\tau_2 & \tau_1 & 0 \end{bmatrix} \otimes I_n \right) \begin{bmatrix} \Lambda_1^{\rm H} \\ \Lambda_2^{\rm H} \\ \Lambda_3^{\rm H} \end{bmatrix}$ *is of full column rank, provided $\tau_1\delta_1$, $\tau_2\delta_2$, $\tau_3\delta_3$ are distinct;*

(c) *the singular value decomposition (SVD) of C is*

$$\begin{aligned} C &= (I_3 \otimes T) \left[-\overline{\Pi_2}\, \overline{\Pi_1}\, \overline{\Pi_0} \right] \begin{bmatrix} \Lambda_q^{1/2} & & \\ & \Lambda_q^{1/2} & \\ & & 0 \end{bmatrix} \left[\Pi_1\, \Pi_2\, \Pi_0 \right]^{\rm H} (I_3 \otimes T^{\rm H}) \\ &\equiv \left[P_r\, P_0 \right] \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix} \left[Q_r\, Q_0 \right]^{\rm H} = P_r \Sigma Q_r^{\rm H}, \end{aligned} \tag{10}$$

where

$$\Pi_0 = \begin{bmatrix} \Lambda_1 \\ \Lambda_2 \\ \Lambda_3 \end{bmatrix} \Lambda_q^{-\frac{1}{2}}, \Pi_2 = \Lambda_p(\Lambda_p^{\rm H}\Lambda_p)^{-\frac{1}{2}}, \overline{\Pi_1} = \begin{bmatrix} 0 & -\Lambda_3 & \Lambda_2 \\ \Lambda_3 & 0 & -\Lambda_1 \\ -\Lambda_2 & \Lambda_1 & 0 \end{bmatrix} \Lambda_p(\Lambda_p^{\rm H}\Lambda_p\Lambda_q)^{-\frac{1}{2}}.$$

It is not difficult to observe that there is only one nonzero off-diagonal entry in each column or row of C_1, C_2, C_3. Physically, the entry represents the relation between a mesh node with its surroundings in the mesh grid, or equivalently, the neighbor in the lattice. The index of such an entry in C_1, C_2, C_3 is that of the neighbor of the node along $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$. For ease, these 6 neighbors of a node are called its *lattice neighbors*. Define

$$\mathcal{L}_\ell(i_1, i_2, i_3) := \{\langle i_1', i_2', i_3' \rangle : C_\ell(i_\ell, i_\ell') \neq 0 \text{ or } C_\ell(i_\ell', i_\ell) \neq 0\}, \qquad \ell = 1, 2, 3,$$

and $\mathcal{L}(i_1, i_2, i_3) := \mathcal{L}_1(i_1, i_2, i_3) \cup \mathcal{L}_2(i_1, i_2, i_3) \cup \mathcal{L}_3(i_1, i_2, i_3)$. Clearly, $\mathcal{L}(i_1, i_2, i_3)$ is the set of the node $\langle i_1, i_2, i_3 \rangle$ and its 6 lattice neighbors. Furthermore,

$$e_{\langle i_1, i_2, i_3 \rangle}^{\rm H} C_\ell I_\sigma^{\mathcal{D} \setminus \mathcal{L}(i_1, i_2, i_3)} = 0, \qquad e_{\langle i_1, i_2, i_3 \rangle}^{\rm H} C_\ell^{\rm H} I_\sigma^{\mathcal{D} \setminus \mathcal{L}(i_1, i_2, i_3)} = 0. \tag{11}$$

Moreover, we can define the boundary and interior of an index set $\mathcal{I}$:

$$\partial\mathcal{I} := \{\langle i_1, i_2, i_3 \rangle \in \mathcal{I} : \mathcal{L}(i_1, i_2, i_3) \setminus \mathcal{I} \neq \emptyset\}, \quad \mathcal{I}^\circ := \{\langle i_1, i_2, i_3 \rangle \in \mathcal{I} : \mathcal{L}(i_1, i_2, i_3) \subset \mathcal{I}\}.$$

2.2 Equivalence of generalized/quadratic eigenvalue problems (GEP /QEP)

It is easily seen that the GEP eq. (2) can be rewritten as

$$\iota \begin{bmatrix} I_{3n} & 0 \\ -\xi_d\mu_d^{-1} & -I_{3n} \end{bmatrix} \left(\begin{bmatrix} 0 & -\iota C \\ \iota C^{\rm H} & \iota\xi_d\mu_d^{-1}C - \iota C^{\rm H}\mu_d^{-1}\zeta_d \end{bmatrix} - \omega \begin{bmatrix} \mu_d & 0 \\ 0 & \varepsilon_d - \xi_d\mu_d^{-1}\zeta_d \end{bmatrix} \right)$$

$$\cdot \begin{bmatrix} I_{3n} & \mu_d^{-1}\zeta_d \\ 0 & I_{3n} \end{bmatrix} \begin{bmatrix} \boldsymbol{h} \\ \boldsymbol{e} \end{bmatrix} = 0.$$

Together with the choices of $\mu_d, \varepsilon_d, \zeta_d, \xi_d$, we can consider this matrix pair instead

$$\begin{bmatrix} 0 & -\iota C \\ \iota C^{\mathrm{H}} & -\gamma[(I_3 \otimes I^{(i)})C + C^{\mathrm{H}}(I_3 \otimes I^{(i)})] \end{bmatrix} - \omega \begin{bmatrix} I_3 \otimes I_n & 0 \\ 0 & I_3 \otimes [\varepsilon_o I^{(o)} + (\varepsilon_i - \gamma^2) I^{(i)}] \end{bmatrix} \tag{12}$$
$$:= A_\gamma - \omega B_\gamma,$$

also written as a matrix pair (A_γ, B_γ), which is equivalent to eq. (2) in the sense that

$$(\omega, \begin{bmatrix} \boldsymbol{h} - \iota\gamma(I_3 \otimes I^{(i)})\boldsymbol{e} \\ \boldsymbol{e} \end{bmatrix}) \text{ is an eigenpair of eq. (12)}$$
$$\Leftrightarrow \ (\omega, \begin{bmatrix} \boldsymbol{e} \\ \boldsymbol{h} \end{bmatrix}) \text{ is an eigenpair of eq. (2).}$$

Moreover, if $(\omega, \begin{bmatrix} \boldsymbol{e} \\ \boldsymbol{h} \end{bmatrix})$ is an eigenpair of eq. (2) with $\omega \neq 0$, then $\boldsymbol{h} = \iota(\gamma I_3 \otimes I^{(i)} - \omega^{-1} C)\boldsymbol{e}$. Note that A_γ, B_γ are Hermitian; (A_γ, B_γ) is regular if $\gamma \neq \gamma_* \equiv \sqrt{\varepsilon_i}$; $B_\gamma \succ 0$ if $\gamma < \gamma_*$; B_γ is indefinite if $\gamma > \gamma_*$. Thus, all eigenvalues of (A_γ, B_γ) are real if $\gamma < \gamma_*$.

The matrix pair (A_γ, B_γ) is also equivalent to a Hermitian quadratic matrix polynomial (a Hermitian QEP)

$$Q_\gamma(\omega) := C^{\mathrm{H}} C - \omega\gamma[(I_3 \otimes I^{(i)})C + C^{\mathrm{H}}(I_3 \otimes I^{(i)})] - \omega^2 I_3 \otimes [\varepsilon_o I^{(o)} + (\varepsilon_i - \gamma^2) I^{(i)}], \tag{13}$$

in the sense that for $\boldsymbol{e} \neq 0$,

$$(\omega, \boldsymbol{e}) \text{ is an eigenpair of eq. (13)} \Leftrightarrow (\omega, \begin{bmatrix} \boldsymbol{e} \\ \boldsymbol{h} \end{bmatrix}) \text{ is an eigenpair of eq. (2).}$$

Clearly, the eigenvalues of $Q_\gamma(\cdot)$ are real or appear in conjugate pairs if nonreal.

Suppose that ω is an eigenvalue of $Q_\gamma(\cdot)$ and $\boldsymbol{e}$ is its corresponding eigenvector. Then, $Q_\gamma(\omega)\boldsymbol{e} = 0$ gives

$$\boldsymbol{e}^{\mathrm{H}} Q_\gamma(\omega)\boldsymbol{e} = c(\boldsymbol{e}) - \omega\gamma b(\boldsymbol{e}) - \omega^2[\varepsilon_o a_o(\boldsymbol{e}) + (\varepsilon_i - \gamma^2) a_i(\boldsymbol{e})] = 0, \tag{14}$$

where

$$\begin{aligned} c(\boldsymbol{e}) &:= \boldsymbol{e}^{\mathrm{H}} C^{\mathrm{H}} C \boldsymbol{e} \geq 0, \\ b(\boldsymbol{e}) &:= \boldsymbol{e}^{\mathrm{H}}[(I_3 \otimes I^{(i)})C + C^{\mathrm{H}}(I_3 \otimes I^{(i)})]\boldsymbol{e} = 2\Re[\boldsymbol{e}^{\mathrm{H}}(I_3 \otimes I^{(i)})C\boldsymbol{e}] \in \mathbb{R}, \\ a_o(\boldsymbol{e}) &:= \boldsymbol{e}^{\mathrm{H}}[I_3 \otimes I^{(o)}]\boldsymbol{e} \geq 0, \\ a_i(\boldsymbol{e}) &:= \boldsymbol{e}^{\mathrm{H}}[I_3 \otimes I^{(i)}]\boldsymbol{e} \geq 0. \end{aligned}$$

Furthermore,

$$c(\boldsymbol{e}) = 0 \Leftrightarrow C\boldsymbol{e} = 0, \quad a_o(\boldsymbol{e}) = 0 \Leftrightarrow (I_3 \otimes I^{(o)})\boldsymbol{e} = 0, \quad a_i(\boldsymbol{e}) = 0 \Leftrightarrow (I_3 \otimes I^{(i)})\boldsymbol{e} = 0. \tag{15}$$

By eq. (14), ω is one of the roots of the scalar function

$$\omega_\pm(\boldsymbol{e}) = \frac{\gamma b(\boldsymbol{e}) \pm \Delta(\boldsymbol{e})^{1/2}}{-2[\varepsilon_o a_o(\boldsymbol{e}) + (\varepsilon_i - \gamma^2) a_i(\boldsymbol{e})]}, \tag{16a}$$

where

$$\Delta(\boldsymbol{e}) = \gamma^2 b(\boldsymbol{e})^2 + 4c(\boldsymbol{e})[\varepsilon_o a_o(\boldsymbol{e}) + (\varepsilon_i - \gamma^2) a_i(\boldsymbol{e})]. \tag{16b}$$

For $\gamma < \gamma_* = \sqrt{\varepsilon_i}$, eq. (2) and eq. (10) show that the matrix pair (A_γ, B_γ) has $2n$ semisimple zero eigenvalues. Furthermore, if $C\boldsymbol{e} \neq 0$, i.e., $c(\boldsymbol{e}) > 0$, then from eq. (16) it follows that (A_γ, B_γ) has $2n$ positive and $2n$ negative eigenvalues, respectively. Moreover, for $\gamma > \gamma_*$, if $\Im\omega \neq 0$, then $\bar{\omega}$ is the conjugate eigenvalue.

2.3 Null-space free GEP

Since the $6n \times 6n$ Hermitian matrix A_γ in eq. (12) has an extensive null space with nullity $2n$, from a computational viewpoint, this would affect and slow down the convergence of the desired smallest positive eigenvalues, and consequently a more compact form for the deflation of all zeros is necessary to be proposed. Fortunately, a $4n \times 4n$ null-space free GEP (NFGEP) has been derived in [3].

Theorem 2.3 ([3])**.** *If $\gamma \neq \gamma_* \equiv \sqrt{\varepsilon_i}$, then the GEP in eq. (2) can be reduced to a $4n \times 4n$ NFGEP*

$$\widehat{A}_r \boldsymbol{y}_r = \omega \left(\iota \begin{bmatrix} 0 & \Sigma_r^{-1} \\ -\Sigma_r^{-1} & 0 \end{bmatrix} \right) \boldsymbol{y}_r \equiv \omega \widehat{B}_r \boldsymbol{y}_r, \tag{17a}$$

and

$$\begin{bmatrix} \boldsymbol{h} \\ \boldsymbol{e} \end{bmatrix} = \iota \begin{bmatrix} -I_{3n} & -\zeta_d \\ \xi_d & \varepsilon_d \end{bmatrix}^{-1} \operatorname{diag}(P_r, Q_r)\, \boldsymbol{y}_r,$$

where

$$\widehat{A}_r := \widehat{A}_r(\gamma) \equiv \operatorname{diag}(P_r^{\mathrm{H}}, Q_r^{\mathrm{H}}) \begin{bmatrix} \zeta_d & -I_{3n} \\ I_{3n} & 0 \end{bmatrix} \begin{bmatrix} \Phi^{-1} & 0 \\ 0 & I_{3n} \end{bmatrix} \begin{bmatrix} \xi_d & I_{3n} \\ -I_{3n} & 0 \end{bmatrix} \operatorname{diag}(P_r, Q_r) \tag{17b}$$

with $\Phi := \Phi(\gamma) \equiv I_3 \otimes \left[\varepsilon_o I^{(o)} + (\varepsilon_i - \gamma^2) I^{(i)}\right]$ by eq. (3).

Theorem 2.4. *For $\gamma \lesssim \gamma_* \equiv \sqrt{\varepsilon_i}$, it holds generally that*

$$\begin{cases} \frac{d\omega(\gamma)}{d\gamma} \geq 0, & \text{if } \omega(\gamma) > 0, \\ \frac{d\omega(\gamma)}{d\gamma} \leq 0, & \text{if } \omega(\gamma) < 0, \end{cases}$$

i.e., all positive and negative eigenvalues of $(\widehat{A}_r, \widehat{B}_r)$ either move toward the right and the left, respectively, or stop motionless as γ becomes close to γ_*.

Proof. For $\gamma < \gamma_*$, $\widehat{A}_r$ in eq. (17b) is positive definite. There is an eigenvector $\boldsymbol{y}_r(\gamma)$ with $\boldsymbol{y}_r^{\mathrm{H}}(\gamma)\widehat{A}_r(\gamma)\boldsymbol{y}_r(\gamma) = 1$ such that

$$\frac{1}{\omega(\gamma)} = \boldsymbol{y}_r^{\mathrm{H}}(\gamma)\widehat{B}_r \boldsymbol{y}_r(\gamma). \tag{18a}$$

Because of $\boldsymbol{y}_r^{\mathrm{H}}(\gamma)\widehat{A}_r(\gamma)\boldsymbol{y}_r(\gamma) = 1$, we have

$$2\Re[(\boldsymbol{y}_r^{\mathrm{H}}(\gamma))'\widehat{A}_r(\gamma)\boldsymbol{y}_r(\gamma)] + \boldsymbol{y}_r^{\mathrm{H}}(\gamma)\widehat{A}_r'(\gamma)\boldsymbol{y}_r(\gamma) = 0. \tag{18b}$$

Taking the derivative of γ in eq. (18a), we have

$$\begin{aligned} -\frac{\omega'(\gamma)}{\omega(\gamma)^2} &= 2\Re[(\boldsymbol{y}_r^{\mathrm{H}}(\gamma))'\widehat{B}_r \boldsymbol{y}_r(\gamma)] \\ &= \frac{2}{\omega(\gamma)}\Re[(\boldsymbol{y}_r^{\mathrm{H}}(\gamma))'\widehat{A}_r(\gamma)\boldsymbol{y}_r(\gamma)] && \text{(by eq. (17a))} \\ &= -\frac{1}{\omega(\gamma)}\boldsymbol{y}_r^{\mathrm{H}}(\gamma)\widehat{A}_r'(\gamma)\boldsymbol{y}_r(\gamma) && \text{(by eq. (18b))} \\ &= -\frac{1}{\omega(\gamma)}\boldsymbol{z}_r^{\mathrm{H}}(\gamma)\left(I_3 \otimes \begin{bmatrix} \frac{2\gamma\varepsilon_i}{(\varepsilon_i-\gamma^2)^2} I^{(i)} & -\frac{\iota(\varepsilon_i+\gamma^2)}{(\varepsilon_i-\gamma^2)^2} I^{(i)} \\ \frac{\iota(\varepsilon_i+\gamma^2)}{(\varepsilon_i-\gamma^2)^2} I^{(i)} & \frac{2\gamma}{(\varepsilon_i-\gamma^2)^2} I^{(i)} \end{bmatrix} \right) \boldsymbol{z}_r(\gamma) && \text{(by eq. (17b))} \\ &\equiv -\frac{1}{\omega(\gamma)} d(\gamma), \end{aligned}$$

where $\boldsymbol{z}_r(\gamma) := \operatorname{diag}(P_r, Q_r)\boldsymbol{y}_r(\gamma)$. Since the matrix

$$W = \frac{1}{(\varepsilon_i - \gamma^2)^2} \begin{bmatrix} 2\gamma\varepsilon_i & -\iota(\varepsilon_i + \gamma^2) \\ \iota(\varepsilon_i + \gamma^2) & 2\gamma \end{bmatrix}$$

is orthogonally congruent to $\begin{bmatrix} 4\gamma(\varepsilon_i+1)(\varepsilon_i-\gamma^2)^{-2} & 0 \\ 0 & -[4\gamma(\varepsilon_i+1)]^{-1} \end{bmatrix}$, it holds generically that $d(\gamma) \geq 0$ as $\gamma \nearrow \gamma_*$. This implies that $\omega'(\gamma)$ has the same sign as $\omega(\gamma)$, for $d(\gamma) > 0$, and $\omega'(\gamma) = 0$ for $d(\gamma) = 0$. $\square$

3 Eigenstructure of the discrete single-curl operator

3.1 Regularity

Clearly, if $\gamma \neq \gamma_* = \sqrt{\varepsilon_i}$, since B_γ is nonsingular, the matrix (A_γ, B_γ) is regular. In the following, we will provide a condition to make (A_γ, B_γ) regular at $\gamma = \gamma_*$. For ease, in this subsection, we write $A = A_{\gamma_*}$, $B = B_{\gamma_*}$.

First, we locate the nullspace. It is easy to see that $\mathcal{N}(B) = \begin{bmatrix} 0 \\ I_3 \otimes I^{(i)} \end{bmatrix}$. By theorem 2.2, from the SVD of C, we know that $\mathcal{N}(C) = \mathcal{R}((I_3 \otimes T)\Pi_0)$ and $\mathcal{N}(C^{\mathrm{H}}) = \mathcal{R}((I_3 \otimes T)\overline{\Pi_0})$. Thus, $\mathcal{N}(A_\gamma) = \mathcal{R}(L_\gamma)$, where

$$L_\gamma = \begin{bmatrix} -\iota\gamma(I_3 \otimes I^{(i)})(I_3 \otimes T)\Pi_0 & (I_3 \otimes T)\overline{\Pi_0} \\ (I_3 \otimes T)\Pi_0 & 0 \end{bmatrix}.$$

Any column of L_γ is an eigenvector corresponding to the eigenvalue 0 of either the matrix A_γ or the matrix pair (A_γ, B_γ). In particular, for (A_γ, B_γ), we call these eigenvalues *trivial zero eigenvalues*.

Then, we try to find an equivalent condition such that (A, B) is regular. Hereafter, we use the notations $I_\sigma^{(i)}$ and $I_\sigma^{(o)}$ to denote the matrices consisting of the nonzero columns of $I^{(i)}$ and $I^{(o)}$, respectively.

Theorem 3.1. *For $\boldsymbol{z}_\ell \in \mathcal{N}(\Lambda_\ell^{\mathrm{H}}), \ell = 1, 2, 3$ satisfying*

$$I^{(o)}T\boldsymbol{z}_1 = I^{(o)}T\boldsymbol{z}_2 = I^{(o)}T\boldsymbol{z}_3, \tag{19}$$

$\mathcal{S}(\boldsymbol{z}_1, \boldsymbol{z}_2, \boldsymbol{z}_3)$ denotes the set of all nonzero $\boldsymbol{x}_1$ that satisfies

$$(I_n + \delta_1\Lambda_1)\boldsymbol{x}_1 - \boldsymbol{z}_1 = (I_n + \delta_2\Lambda_2)\boldsymbol{x}_1 - \boldsymbol{z}_2 = (I_n + \delta_3\Lambda_3)\boldsymbol{x}_1 - \boldsymbol{z}_3, \tag{20a}$$

$$I^{(o)}T\Lambda_1\boldsymbol{x}_1 = 0. \tag{20b}$$

Then, (A, B) is regular if and only if $\mathcal{S}(\boldsymbol{z}_1, \boldsymbol{z}_2, \boldsymbol{z}_3) = \{0\}$ for any proper $\boldsymbol{z}_\ell$.

Proof. Suppose that $\boldsymbol{x} \in \mathcal{N}(A) \cap \mathcal{N}(B)$. Since $\mathcal{N}(B) = \begin{bmatrix} 0 \\ I_3 \otimes I^{(i)} \end{bmatrix}$, $\boldsymbol{x}$ must be of the form $\begin{bmatrix} 0 \\ (I_3 \otimes I_\sigma^{(i)})\boldsymbol{e}_0 \end{bmatrix}$ with some suitable vector $\boldsymbol{e}_0$. Additionally, with some vectors $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$, $\boldsymbol{x}$ must be of the form

$$L_{\gamma_*}\begin{bmatrix} \boldsymbol{e}_1 \\ \iota\gamma_*\boldsymbol{e}_2 \end{bmatrix} = \begin{bmatrix} -\iota\gamma_*(I_3 \otimes I^{(i)})(I_3 \otimes T)\Pi_0\boldsymbol{e}_1 + \iota\gamma_*(I_3 \otimes T)\overline{\Pi_0}\boldsymbol{e}_2 \\ (I_3 \otimes T)\Pi_0\boldsymbol{e}_1 \end{bmatrix} = \begin{bmatrix} 0 \\ (I_3 \otimes I_\sigma^{(i)})\boldsymbol{e}_0 \end{bmatrix}. \tag{21}$$

From the second equation in eq. (21), the first equation implies that

$$(I_3 \otimes I^{(i)})(I_3 \otimes T)\Pi_0\boldsymbol{e}_1 = (I_3 \otimes I^{(i)})(I_3 \otimes I_\sigma^{(i)})\boldsymbol{e}_0 = (I_3 \otimes I_\sigma^{(i)})\boldsymbol{e}_0 = (I_3 \otimes T)\overline{\Pi_0}\boldsymbol{e}_2,$$

which yields that

$$(I_3 \otimes [T^{\mathrm{H}}I_\sigma^{(i)}])\boldsymbol{e}_0 = \Pi_0\boldsymbol{e}_1 = \overline{\Pi_0}\boldsymbol{e}_2, \tag{22}$$

with $\boldsymbol{e}_0 \neq 0$, and $\boldsymbol{e}_1$, $\boldsymbol{e}_2$ being not simultaneously zero. Let $\boldsymbol{x}_1 = \Lambda_q^{-1/2}\boldsymbol{e}_1$, $\boldsymbol{x}_2 = \Lambda_q^{-1/2}\boldsymbol{e}_2$ and $\boldsymbol{e}_0 = \begin{bmatrix} \boldsymbol{y}_1^{\mathrm{T}} & \boldsymbol{y}_2^{\mathrm{T}} & \boldsymbol{y}_3^{\mathrm{T}} \end{bmatrix}^{\mathrm{T}}$. The equations in eq. (22) are equivalent to

$$T^{\mathrm{H}}I_\sigma^{(i)}\boldsymbol{y}_1 = \Lambda_1\boldsymbol{x}_1 = \Lambda_1^{\mathrm{H}}\boldsymbol{x}_2, \quad T^{\mathrm{H}}I_\sigma^{(i)}\boldsymbol{y}_2 = \Lambda_2\boldsymbol{x}_1 = \Lambda_2^{\mathrm{H}}\boldsymbol{x}_2, \quad T^{\mathrm{H}}I_\sigma^{(i)}\boldsymbol{y}_3 = \Lambda_3\boldsymbol{x}_1 = \Lambda_3^{\mathrm{H}}\boldsymbol{x}_2. \tag{23}$$

Thus,

$$\boldsymbol{y}_1 = (I_\sigma^{(i)})^{\mathrm{H}} T \varLambda_1 \boldsymbol{x}_1, \quad \boldsymbol{y}_2 = (I_\sigma^{(i)})^{\mathrm{H}} T \varLambda_2 \boldsymbol{x}_1, \quad \boldsymbol{y}_3 = (I_\sigma^{(i)})^{\mathrm{H}} T \varLambda_3 \boldsymbol{x}_1.$$

Noticing that $\delta_i^{-1}(\mathrm{e}^{\iota\theta} - 1) = -\delta_i^{-1}(\mathrm{e}^{-\iota\theta} - 1)\mathrm{e}^{\iota\theta}$ for any $\theta \in \mathbb{R}$, we have $\varLambda_\ell = -\varLambda_\ell^{\mathrm{H}}(I_n + \delta_\ell \varLambda_\ell)$. By eq. (23), we have

$$-\boldsymbol{x}_2 = (I_n + \delta_1 \varLambda_1)\boldsymbol{x}_1 - \boldsymbol{z}_1 = (I_n + \delta_2 \varLambda_2)\boldsymbol{x}_1 - \boldsymbol{z}_2 = (I_n + \delta_3 \varLambda_3)\boldsymbol{x}_1 - \boldsymbol{z}_3, \tag{24}$$

namely, eq. (20a), where $\boldsymbol{z}_\ell \in \mathcal{N}(\varLambda_\ell^{\mathrm{H}})$. Left-multiplying $I^{(o)}T$ on the sides of eq. (23) and noticing that $I^{(o)}TT^{\mathrm{H}}I_\sigma^{(i)} = 0$, we have

$$I^{(o)}T\varLambda_1\boldsymbol{x}_1 = 0, \quad I^{(o)}T\varLambda_2\boldsymbol{x}_1 = 0, \quad I^{(o)}T\varLambda_3\boldsymbol{x}_1 = 0,$$

which is equivalent to eq. (20b) by the proper condition eq. (19). Therefore,

$$\mathcal{N}(A) \cap \mathcal{N}(B) = \left\{ \begin{bmatrix} 0 \\ (I_3 \otimes T)\varPi_0 \varLambda_q^{1/2} \boldsymbol{x}_1 \end{bmatrix} : \boldsymbol{x}_1 \in \mathcal{S} \right\}.$$

Noticing that

$$\begin{bmatrix} 0 \\ \varPi_0 \varLambda_q^{1/2} \boldsymbol{x}_1 \end{bmatrix} \neq 0 \;\Leftrightarrow\; \boldsymbol{x}_1^{\mathrm{H}} \varLambda_q^{1/2} \varPi_0^{\mathrm{H}} \varPi_0 \varLambda_q^{1/2} \boldsymbol{x}_1 = \boldsymbol{x}_1^{\mathrm{H}} \varLambda_q \boldsymbol{x}_1 \neq 0 \;\Leftrightarrow\; \boldsymbol{x}_1 \neq 0.$$

We have shown that $\mathcal{S}(\boldsymbol{z}_1, \boldsymbol{z}_2, \boldsymbol{z}_3) = \{0\}$ if and only if $\mathcal{N}(A) \cap \mathcal{N}(B) = \{0\}$. From Theorem 4.1 in [4], it follows that the regularity of (A, B) is equivalent to $\mathcal{S}(\boldsymbol{z}_1, \boldsymbol{z}_2, \boldsymbol{z}_3) = \{0\}$. □

At this point, we have an equivalence condition that (A, B) is regular. In practice, because the linear system in eq. (20) is overdetermined, the condition $\mathcal{S}(\boldsymbol{z}_1, \boldsymbol{z}_2, \boldsymbol{z}_3) = \{0\}$ is generically held, and therefore, $A - \omega B$ is always regular. A very lengthy and complex proof for showing the regularity of $A - \omega B$ can be found in the Appendix. From Theorem 4.1 of [4], it is possible that (A, B) has a defective infinite eigenvalue with a Jordan block of at most 2. Below we will give a very loose condition that (A, B) has this type of eigenvalue.

Theorem 3.2. *Suppose that (A, B) is regular. The matrix pair (A, B) has a defective infinite eigenvalue associated with a Jordan block of size two if and only if there exist $\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3$, not all zero vectors, such that*

$$(I_\sigma^{(i)})^{\mathrm{H}} M_2 I_\sigma^{(i)} \boldsymbol{x}_3 - (I_\sigma^{(i)})^{\mathrm{H}} M_3 I_\sigma^{(i)} \boldsymbol{x}_2 = 0, \tag{25a}$$

$$(I_\sigma^{(i)})^{\mathrm{H}} M_3 I_\sigma^{(i)} \boldsymbol{x}_1 - (I_\sigma^{(i)})^{\mathrm{H}} M_1 I_\sigma^{(i)} \boldsymbol{x}_3 = 0, \tag{25b}$$

$$(I_\sigma^{(i)})^{\mathrm{H}} M_1 I_\sigma^{(i)} \boldsymbol{x}_2 - (I_\sigma^{(i)})^{\mathrm{H}} M_2 I_\sigma^{(i)} \boldsymbol{x}_1 = 0, \tag{25c}$$

where $M_\ell = C_\ell - C_\ell^{\mathrm{H}}$.

Proof. Clearly, (A, B) has a defective infinite eigenvalue if and only if there exist nonzero vectors $\boldsymbol{x}, \boldsymbol{y}$ such that

$$B\boldsymbol{x} = 0, \quad B\boldsymbol{y} = A\boldsymbol{x}.$$

Thus, $\boldsymbol{x} \in \mathcal{N}(B), A\boldsymbol{x} \in \mathcal{R}(B)$. Since (A, B) is regular, $A\boldsymbol{x} \neq 0$. Noticing $\mathcal{N}(B) = \mathcal{R}(B)^\perp$, the equations are equivalent to

$$0 \neq \boldsymbol{x} \in \mathcal{N}(B), \quad \mathcal{N}(B)^{\mathrm{H}} A\boldsymbol{x} = 0,$$

namely,

$$\mathcal{N}\left(\mathrm{N}(B)^{\mathrm{H}} A \,\mathrm{N}(B)\right) \neq 0,$$

where $\mathrm{N}(B)$ is the basis matrix of $\mathcal{N}(B)$. Note that with $\gamma_* = \sqrt{\varepsilon_i}$, we have

$$\mathrm{N}(B)^{\mathrm{H}} A \,\mathrm{N}(B) = \begin{bmatrix} 0 \\ I_3 \otimes I_\sigma^{(i)} \end{bmatrix}^{\mathrm{H}} \begin{bmatrix} 0 & -\iota C \\ \iota C^{\mathrm{H}} & -\gamma_*[(I_3 \otimes I^{(i)})C + C^{\mathrm{H}}(I_3 \otimes I^{(i)})] \end{bmatrix} \begin{bmatrix} 0 \\ I_3 \otimes I_\sigma^{(i)} \end{bmatrix}$$

$$
\begin{aligned}
&= -\gamma_*(I_3 \otimes I_\sigma^{(i)})^{\mathrm{H}}[(I_3 \otimes I^{(i)})C + C^{\mathrm{H}}(I_3 \otimes I^{(i)})](I_3 \otimes I_\sigma^{(i)}) \\
&= -\gamma_*(I_3 \otimes I_\sigma^{(i)})^{\mathrm{H}}[C + C^{\mathrm{H}}](I_3 \otimes I_\sigma^{(i)}) \\
&= -\gamma_*(I_3 \otimes I_\sigma^{(i)})^{\mathrm{H}} \begin{bmatrix} 0 & -C_3 + C_3^{\mathrm{H}} & C_2 - C_2^{\mathrm{H}} \\ C_3 - C_3^{\mathrm{H}} & 0 & -C_1 + C_1^{\mathrm{H}} \\ -C_2 + C_2^{\mathrm{H}} & C_1 - C_1^{\mathrm{H}} & 0 \end{bmatrix} (I_3 \otimes I_\sigma^{(i)}) \\
&= -\gamma_*(I_3 \otimes I_\sigma^{(i)})^{\mathrm{H}} \begin{bmatrix} 0 & -M_3 & M_2 \\ M_3 & 0 & -M_1 \\ -M_2 & M_1 & 0 \end{bmatrix} (I_3 \otimes I_\sigma^{(i)}).
\end{aligned}
$$

Clearly, $\begin{bmatrix} \boldsymbol{x}_1^{\mathrm{T}} & \boldsymbol{x}_2^{\mathrm{T}} & \boldsymbol{x}_3^{\mathrm{T}} \end{bmatrix}^{\mathrm{T}} \in \mathcal{N}\left(\mathrm{N}(B)^{\mathrm{H}} A\, \mathrm{N}(B)\right)$ is equivalent to eq. (25). Finally, from Theorem 4.1 of [4], the defective infinite eigenvalue has a Jordan block of size two. □

Theorem 3.3. *Suppose that (A, B) is regular and $n_\ell > 2$. The matrix pair (A, B) has a defective infinite eigenvalue, as long as a mesh node with its 6 lattice neighbors (see section 2.1) are inside the medium, i.e., there exist some $i_\ell \in [1, n_\ell], \ell = 1, 2, 3,$ such that $\mathcal{L}(i_1, i_2, i_3) \subset \mathcal{D}_i$, or equivalently, $\langle i_1, i_2, i_3 \rangle \in \mathcal{D}_i^\circ$.*

As a result, (A, B) has a defective infinite eigenvalue, as long as n_ℓ is large enough.

Proof. First, we claim that under the assumption there exists a nonzero $\boldsymbol{y}$ such that

$$
(I_\sigma^{(o)})^{\mathrm{H}} M_\ell I_\sigma^{(i)} \boldsymbol{y} = 0, \quad \ell = 1, 2, 3; \qquad \sum_{\ell=1}^{3} \boldsymbol{y}^{\mathrm{H}} (I_\sigma^{(i)})^{\mathrm{H}} M_\ell^{\mathrm{H}} M_\ell I_\sigma^{(i)} \boldsymbol{y} \neq 0. \tag{26}
$$

Then, let $\boldsymbol{x}_\ell = (I_\sigma^{(i)})^{\mathrm{H}} M_\ell I_\sigma^{(i)} \boldsymbol{y}$. Note that $M_\ell = -M_\ell^{\mathrm{H}}$ and $M_\ell = T(\Lambda_\ell - \Lambda_\ell^{\mathrm{H}})T^{\mathrm{H}}$. We know M_1, M_2, M_3 are simultaneously diagonalizable by the unitary matrix T. Thus, by the orthogonality relations in the first equations of eq. (26), it holds that

$$
\begin{aligned}
&(I_\sigma^{(i)})^{\mathrm{H}} M_\ell I_\sigma^{(i)} \boldsymbol{x}_{\ell'} - (I_\sigma^{(i)})^{\mathrm{H}} M_{\ell'} I_\sigma^{(i)} \boldsymbol{x}_\ell \\
&= (I_\sigma^{(i)})^{\mathrm{H}} M_\ell I_\sigma^{(i)} (I_\sigma^{(i)})^{\mathrm{H}} M_{\ell'} I_\sigma^{(i)} \boldsymbol{y} - (I_\sigma^{(i)})^{\mathrm{H}} M_{\ell'} I_\sigma^{(i)} (I_\sigma^{(i)})^{\mathrm{H}} M_\ell I_\sigma^{(i)} \boldsymbol{y} \\
&= (I_\sigma^{(i)})^{\mathrm{H}} M_\ell [I - I_\sigma^{(o)} (I_\sigma^{(o)})^{\mathrm{H}}] M_{\ell'} I_\sigma^{(i)} \boldsymbol{y} - (I_\sigma^{(i)})^{\mathrm{H}} M_{\ell'} [I - I_\sigma^{(o)} (I_\sigma^{(o)})^{\mathrm{H}}] M_\ell I_\sigma^{(i)} \boldsymbol{y} \\
&= (I_\sigma^{(i)})^{\mathrm{H}} [M_\ell M_{\ell'} - M_{\ell'} M_\ell] I_\sigma^{(i)} \boldsymbol{y} = 0,
\end{aligned}
$$

or equivalently, $\boldsymbol{x}_\ell$ satisfy eq. (25). On the other hand,

$$
\begin{aligned}
\boldsymbol{x}_1^{\mathrm{H}} \boldsymbol{x}_1 + \boldsymbol{x}_2^{\mathrm{H}} \boldsymbol{x}_2 + \boldsymbol{x}_3^{\mathrm{H}} \boldsymbol{x}_3 &= \sum_\ell \boldsymbol{y}^{\mathrm{H}} (I_\sigma^{(i)})^{\mathrm{H}} M_\ell^{\mathrm{H}} I_\sigma^{(i)} (I_\sigma^{(i)})^{\mathrm{H}} M_\ell I_\sigma^{(i)} \boldsymbol{y} \\
&= \sum_\ell \boldsymbol{y}^{\mathrm{H}} (I_\sigma^{(i)})^{\mathrm{H}} M_\ell^{\mathrm{H}} [I - I_\sigma^{(o)} (I_\sigma^{(o)})^{\mathrm{H}}] M_\ell I_\sigma^{(i)} \boldsymbol{y} \\
&= \sum_\ell \boldsymbol{y}^{\mathrm{H}} (I_\sigma^{(i)})^{\mathrm{H}} M_\ell^{\mathrm{H}} M_\ell I_\sigma^{(i)} \boldsymbol{y} \neq 0,
\end{aligned}
$$

which means that $\boldsymbol{x}_\ell$ are not all zeros. Therefore, by theorem 3.2, we have the result.

Finally we prove the claim. Since $\mathcal{L}(i_1, i_2, i_3) \subset \mathcal{D}_i$, we know $\mathcal{D}_o \subset \mathcal{D} \setminus \mathcal{L}(i_1, i_2, i_3)$. By eq. (11),

$$
e_{\langle i_1, i_2, i_3 \rangle}^{\mathrm{H}} M_\ell I_\sigma^{(o)} = e_{\langle i_1, i_2, i_3 \rangle}^{\mathrm{H}} M_\ell^{\mathrm{H}} I_\sigma^{(o)} = 0.
$$

On the other hand, $M_\ell e_{\langle i_1, i_2, i_3 \rangle}$ is a column of M_ℓ and thus nonzero, as long as $n_\ell > 2$. Note that there exists $\boldsymbol{y}$ such that $e_{\langle i_1, i_2, i_3 \rangle} = I_\sigma^{(i)} \boldsymbol{y}$ because $e_{\langle i_1, i_2, i_3 \rangle} \in \mathcal{R}(I_\sigma^{(i)})$. Clearly, this $\boldsymbol{y}$ satisfies eq. (26). □

Remark 3.1. Write $M = \begin{bmatrix} M_1^{\mathrm{T}} & M_2^{\mathrm{T}} & M_3^{\mathrm{T}} \end{bmatrix}^{\mathrm{T}}$. From the proofs of theorems 3.2 and 3.3, we can see that $\begin{bmatrix} 0 \\ (I_3 \otimes [I_\sigma^{(i)} (I_\sigma^{(i)})^{\mathrm{H}}]) M e_{\langle i_1, i_2, i_3 \rangle} \end{bmatrix} = \begin{bmatrix} 0 \\ M e_{\langle i_1, i_2, i_3 \rangle} \end{bmatrix}$ is a corresponding eigenvector of the defective infinite eigenvalue.

3.2 The eigenvalue behavior when $\gamma \to \gamma_* + 0$

First, we observe the eigenvalues of $(A, B) = (A_{\gamma_*}, B_{\gamma_*})$. Write

$$G_m := \begin{bmatrix} & & 1 & 0 \\ & \iddots & \iddots & \\ 1 & \iddots & & \\ 0 & & & \end{bmatrix}_{m\times m}, \qquad F_m := \begin{bmatrix} & & 1 \\ & \iddots & \\ 1 & & \end{bmatrix}_{m\times m}.$$

By [5, Theorem 5.10.1] (also [11, Theorem 6.1]), any Hermitian regular matrix pair (A, B) is congruent to a Hermitian matrix pair which is a direct sum of the following types of blocks:

B-c. $(\begin{bmatrix} & \beta_j F_{k_j} + G_{k_j} \\ \overline{\beta_j} F_{k_j} + G_{k_j} & \end{bmatrix}, F_{2k_j})$, $\beta_j \in \mathbb{C} \setminus \mathbb{R}$, $j = 1, \dots, n_c$, with possible replacement of β_j by $\overline{\beta_j}$;

B-r. $\mu_j(\alpha_j F_{k_j} + G_{k_j}, F_{k_j})$, $\alpha_j \in \mathbb{R}, \mu_j \in \{1, -1\}$, $j = 1, \dots, n_r$;

B-∞. $\nu_j(F_{k_j}, G_{k_j})$, $\nu_j \in \{1, -1\}$, $j = 1, \dots, n_\infty$.

The form is uniquely determined by (A, B) up to a combination of permutations of those blocks. Furthermore, $\beta_j, \overline{\beta_j}$ are finite nonreal eigenvalues of (A, B); α_j is its real eigenvalue. Those k_j's corresponding to the same value α are called the *partial multiplicities* of α; all μ_j's and ν_j's are called the *sign characteristic* of (A, B). A real eigenvalue α_j with the corresponding $\mu_j = 1$ ($\mu_j = -1$) is called an eigenvalue of *positive type* (*negative type*).

First, as a consequence of the regularity and theorem 3.3, we have theorem 3.4.

Theorem 3.4. *The matrix pair (A, B) has at most $6|\mathcal{D}_i|$ infinite eigenvalues, each of which is either semisimple or of positive type and associated with a Jordan block of size 2, and at least $6n - 6|\mathcal{D}_i|$ semisimple eigenvalues of positive type.*

Proof. Note that $B \succeq 0$ with $\dim \mathcal{N}(B) = 3|\mathcal{D}_i|$ and (A, B) is regular. The result is a direct consequence of [4, Theorem 4.1] and theorem 3.3. □

Then, we provide a necessary condition of the existence of nonreal eigenvalues, or equivalently, a necessary condition that $Q_\gamma(\omega)$ has a nonreal eigenvalue.

Theorem 3.5. *For $\gamma \to \gamma_* + 0$, there exist purely imaginary eigenvalues. If $(\omega, \boldsymbol{e})$ is an eigenpair of $Q_\gamma(\cdot)$ with $\Im\omega \neq 0$, then:*

(a) $(I_3 \otimes I^{(o)})\boldsymbol{e} = 0$, $(I_3 \otimes I^{(i)})\boldsymbol{e} \neq 0$;

(b) $C\boldsymbol{e} \neq 0$, $\Re[\boldsymbol{e}^{\mathrm{H}}(I_3 \otimes I^{(i)})C\boldsymbol{e}] = 0$;

(c) *ω is pure imaginary, and* $\omega = \pm(\gamma^2 - \varepsilon_i)^{-1/2} \frac{\|C\boldsymbol{e}\|_2}{\|\boldsymbol{e}\|_2} \iota$.

(d) *$|\omega|$ becomes smaller as γ becomes larger.*

Proof. By theorems 3.3 and 3.4, $(A_{\gamma_*}, B_{\gamma_*})$ has a 2×2 Jordan block $W_{\gamma_*}(\lambda) \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ at infinity. Let $W_\gamma(\lambda) \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} - \lambda \begin{bmatrix} 1 & \eta \\ \eta & -\eta \end{bmatrix}$ be a small perturbation of $W_{\gamma_*}(\lambda)$ with $\eta \to 0^+$, as $\gamma \to \gamma_*^+$. Then, $W_\gamma(\lambda)$ has a complex eigenvalue ω of the form $\omega \equiv \frac{1}{1+\eta} + \iota \frac{1}{\sqrt{\eta}(1+\eta)}$ with $\Im\omega \neq 0$. By eq. (16), it implies that $\varDelta(\boldsymbol{e}) < 0$. Then, with $\gamma \to \gamma_*^+$, it forces that

$$b(\boldsymbol{e}) = 0, \quad c(\boldsymbol{e})a_o(\boldsymbol{e}) = 0, \quad c(\boldsymbol{e})a_i(\boldsymbol{e}) > 0,$$

which, together with eq. (15), implies the results of (a), (b) and (c). From eq. (14), item (d) holds because

$$\frac{\mathrm{d}(\iota\omega)}{\mathrm{d}\gamma} = \frac{2\gamma\omega^2 a_i(\boldsymbol{e})}{\pm|\varDelta(\boldsymbol{e})|^{1/2}} \quad \Rightarrow \quad \frac{\mathrm{d}|\omega|}{\mathrm{d}\gamma} = \frac{2\gamma\omega^2 a_i(\boldsymbol{e})}{|\varDelta(\boldsymbol{e})|^{1/2}} < 0.$$

□

3.3 Behavior of real eigenvalues

As we pointed out above, all the eigenvalues of the matrix pair (A_γ, B_γ) are real if $\gamma < \gamma_* \equiv \sqrt{\varepsilon_i}$. Now we begin to check the case $\gamma > \gamma_*$.

First, we build a relation between the change of inertia and the change of the number of real eigenvalues. For any Hermitian matrix X, denote by $p_+(X), p_-(X)$ the positive and negative indices of the inertia of X, respectively.

Theorem 3.6. *Let $C_\gamma(\omega) = A_\gamma - \omega B_\gamma$ with $\omega \in \mathbb{R}$, where A_γ, B_γ are defined as in eq. (12), and B_γ is nonsingular.*

(a) *if $p_+(C_{\gamma+0}(\omega)) - p_+(C_{\gamma-0}(\omega)) = t$ and $p_-(C_{\gamma+0}(\omega)) - p_-(C_{\gamma-0}(\omega)) = -t$, then ω is an eigenvalue associated with t Jordan blocks of odd size, of the matrix pair (A_γ, B_γ), which is either of positive type and monotonically increasing, or of negative type and monotonically decreasing;*

(b) *if $p_+(C_{\gamma+0}(\omega)) - p_+(C_{\gamma-0}(\omega)) = -t$ and $p_-(C_{\gamma+0}(\omega)) - p_-(C_{\gamma-0}(\omega)) = t$, then ω is an eigenvalue associated with t Jordan blocks of odd size, of the matrix pair (A_γ, B_γ), which is either of positive type and monotonically decreasing, or of negative type and monotonically increasing.*

Proof. First, we consider the inertia of the matrix $C_\gamma(\omega)$ for a fixed γ. Let us discuss the inertia of those blocks one after another, except **B-∞**. Note that from section 2.2, we know that both ω and $\bar{\omega}$ with $\Im\omega \neq 0$ are eigenvalues of (A_γ, B_γ).

(a) **B-c**: the corresponding matrix is

$$L = \begin{bmatrix} & (\beta_j - \omega)F_{m_j} + G_{m_j} \\ (\overline{\beta_j} - \omega)F_{m_j} + G_{m_j} & \end{bmatrix}$$

whose indices of inertia are $p_+(L) = m_j, p_-(L) = m_j$;

(b) **B-re**, **B-r** of even size $k_j = 2s$: the corresponding matrix is

$$L = \mu_j([\alpha_j - \omega]F_{k_j} + G_{k_j})$$

whose indices of inertia are $p_+(L) = s, p_-(L) = s$ if $\omega \neq \alpha_j$, or the same as $\mu_j F_{k_j-1}$, namely, $s - 1 + \frac{1+\mu_j}{2}$ and $s - 1 + \frac{1-\mu_j}{2}$, if $\omega = \alpha_j$;

(c) **B-ro**, **B-r** of odd size $k_j = 2s - 1$: the corresponding matrix is

$$L = \mu_j([\alpha_j - \omega]F_{k_j} + G_{k_j})$$

whose indices of inertia are $p_+(L) = s - 1 + \frac{1+\mu_j \operatorname{sign}(\alpha_j - \omega)}{2}, p_-(L) = s - 1 + \frac{1-\mu_j \operatorname{sign}(\alpha_j - \omega)}{2}$ if $\omega \neq \alpha_j$, or the same as $\mu_j F_{k_j-1}$, namely, $s - 1$ and $s - 1$ if $\omega = \alpha_j$.

Recall the form of $A_\gamma = C_\gamma(0)$. It can be seen that $p_+(A_\gamma) = p_-(A_\gamma)$ for any γ. Thus, counting the inertia of the blocks of different types, we have

$$\text{no. of } \mathbf{B\text{-}re}\binom{\mu=1}{\alpha=0} + \text{no. of } \mathbf{B\text{-}ro}\binom{\mu=1}{\alpha\neq 0} = \text{no. of } \mathbf{B\text{-}re}\binom{\mu=-1}{\alpha\neq 0} + \text{no. of } \mathbf{B\text{-}ro}\binom{\mu=-1}{\alpha=0}.$$

Note that the eigenvalues, as the functions of the entries of the matrix, are continuous. As γ goes from γ_1 to γ_2, the structure of the blocks may change in one or some combination of the ways below, provided ω is not an eigenvalue of either $(A_{\gamma_1}, B_{\gamma_1})$ or $(A_{\gamma_2}, B_{\gamma_2})$:

(a) **B-c** → **B-c**: the indices of inertia are the same;

(b) **B-re** → **B-c**: the indices of inertia are the same;

(c) **B-re** → **B-re**: the indices of inertia are the same;

(d) **B-ro**($\mu = 1$) $\to$ **B-ro**($\mu = 1$): the indices of inertia are the same if ω is not between $\alpha(\gamma_1)$ and $\alpha(\gamma_2)$, or the positive index decreases 1 and the negative index increases 1 if $\alpha(\gamma_2) < \omega < \alpha(\gamma_1)$, or the positive index increases 1 and the negative index decreases 1 if $\alpha(\gamma_2) > \omega > \alpha(\gamma_1)$;

(e) **B-ro**($\mu = 1$) $\to$ **B-ro**($\mu = -1$): the indices of inertia are the same if ω is between $\alpha(\gamma_1)$ and $\alpha(\gamma_2)$, or the positive index decreases 1 and the negative index increases 1 if $\omega < \alpha(\gamma_1), \omega < \alpha(\gamma_2)$, or the positive index increases 1 and the negative index decreases 1 if $\omega > \alpha(\gamma_1), \omega > \alpha(\gamma_2)$;

(f) **B-re** $\to$ **B-re** + **B-re**: the indices of inertia are the same;

(g) **B-ro**($\mu = 1$) $\to$ **B-re**($\mu = 1$) + **B-ro**($\mu = 1$): the indices of inertia are the same if ω is not between $\alpha(\gamma_1)$ and $\alpha(\gamma_2)$, or the positive index decreases 1 and the negative index increases 1 if $\alpha(\gamma_2) < \omega < \alpha(\gamma_1)$, or the positive index increases 1 and the negative index decreases 1 if $\alpha(\gamma_2) > \omega > \alpha(\gamma_1)$, noticing that $\alpha(\gamma_2)$ is the eigenvalue of **B-ro**;

(h) **B-re**($\mu = 1$) $\to$ **B-ro**($\mu = 1$) + **B-ro**($\mu = 1$): the indices of inertia are the same if ω is between $\alpha(\gamma_2)$ and $\alpha'(\gamma_2)$, or the positive index decreases 1 and the negative index increases 1 if $\omega < \alpha(\gamma_2), \omega < \alpha'(\gamma_2)$, or the positive index increases 1 and the negative index decreases 1 if $\omega > \alpha(\gamma_2), \omega > \alpha'(\gamma_2)$, noticing that $\alpha(\gamma_2), \alpha'(\gamma_2)$ are the eigenvalues of two **B-ro**'s;

(i) all the reverse (go from right to left) and all the opposite (change μ's sign).

For simplicity, we will not list all the cases. Some illustrations are given below.

(I) As we said before, any change of the structure of the blocks can be expressed as one or some combination of the cases listed above. For example, **B-c** $\to$ **B-ro**($\mu = 1$)+**B-ro**($\mu = -1$) can be treated as **B-c** $\to$ **B-re** $\to$ **B-ro**($\mu = 1$) + **B-ro**($\mu = 1$) $\to$ **B-ro**($\mu = 1$) + **B-ro**($\mu = -1$), namely, the combination of the reverse of item (b), item (h), and item (e). Note that we use a sequential form to represent it but it does not occur sequentially. However, representing the form sequentially does not affect counting the inertia.

(II) Noticing that $p_+(A_\gamma) = p_-(A_\gamma)$, item (e) or item (h) cannot happen singly. For example, for item (e), the case in which **B-ro**($\mu = 1$) $\to$ **B-ro**($\mu = -1$) happens on only one block and other blocks remain the same will break the equality that $p_+(A_\gamma) = p_-(A_\gamma)$.

(III) Item (e) may happen together with its reverse, namely, **B-ro**($\mu = 1$) $\to$ **B-ro**($\mu = -1$) and **B-ro**($\mu = -1$) $\to$ **B-ro**($\mu = 1$) happen simultaneously. However, if the involved eigenvalues are not the same, then ω cannot be both between $\alpha_1(\gamma_1), \alpha_1(\gamma_2)$ and between $\alpha_2(\gamma_1), \alpha_2(\gamma_2)$; otherwise, we can treat the case as item (d) that happens with its opposite, namely, **B-ro**($\mu = 1$) $\to$ **B-ro**($\mu = 1$) and **B-ro**($\mu = -1$) $\to$ **B-ro**($\mu = -1$) happen simultaneously.

(IV) If ω is between $\alpha(\gamma_1)$ and $\alpha(\gamma_2)$, then according to the continuity, ω must be an eigenvalue of $(A_{\gamma_*}, B_{\gamma_*})$ for some γ_* between γ_1, γ_2.

After a systematical check, we have the result as the summary. □

Theorem 3.7. *The case* **B-c** $\to$ **B-re** $\to$ **B-ro**($\mu = 1$) + **B-ro**($\mu = -1$) *occurs generically, i.e., if the complex conjugate eigenvalue curves* $\beta(\gamma)$ *and* $\bar{\beta}(\gamma)$ *collide at* $\alpha(\gamma_1) = \beta(\gamma_1) = \bar{\beta}(\gamma_1) \in \mathbb{R}$ *with* $\gamma = \gamma_1 > \gamma_*$*, then it would bifurcate into two real eigenvalues* $\alpha_\ell(\gamma_1^+)(\mu = 1)$ *and* $\alpha_r(\gamma_1^+)(\mu = -1)$.

Proof. theorems 3.4 and 3.5 show that $(A_{\gamma_*}, B_{\gamma_*})$ has a 2×2 Jordan block at infinity and a purely imaginary eigenpair $\{\pm \imath\omega(\gamma)\}$ is created for $\gamma \to \gamma_*^+$ with $\frac{d|\omega|}{d\gamma} < 0$. Then, from eq. (16), we denote the complex conjugate eigenvalue pair by $\{\beta(\gamma), \bar{\beta}(\gamma)\}$ with $\beta(\gamma_*^+) = \imath\omega(\gamma_*^+)$ and $\bar{\beta}(\gamma_*^+) = -\imath\omega(\gamma_*^+)$ which will collide at $\alpha_\ell(\gamma_1) = \alpha_r(\gamma_1) \in \mathbb{R}$ with $\gamma_1 > \gamma_*$. Consequently, it is sufficient to show that the tangent lines of $\beta(\gamma) \cup \bar{\beta}(\gamma)$ and $\alpha(\gamma) \equiv \alpha_\ell(\gamma) \cup \alpha_r(\gamma)$ at $\gamma = \gamma_1$ are orthogonal to the real x- and imaginary y-axes, respectively. Without loss of generality, we consider the following combinations with small perturbation $\eta \equiv \eta(\gamma) \to 0^+$ as $\gamma \to \gamma_1^\pm$.

(a) $\mathbf{B\text{-}c}(\gamma \to \gamma_1^-)$:

$$\left(\begin{bmatrix} 0 & \alpha(\gamma_1)+\sqrt{\eta}\iota \\ \alpha(\gamma_1)-\sqrt{\eta}\iota & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\right) \overset{\text{eq.}}{\sim} \left(\begin{bmatrix} 1 & \alpha(\gamma_1) \\ \alpha(\gamma_1) & -\eta \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\right)$$

Here and hereafter, "$\overset{\text{eq.}}{\sim}$" denotes the equivalence transformation between two matrix pairs.

(b) $\mathbf{B\text{-}re}(\gamma = \gamma_1)$:

$$\left(\begin{bmatrix} 1 & \alpha(\gamma_1) \\ \alpha(\gamma_1) & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\right)$$

(c) $\mathbf{B\text{-}ro}(\mu = 1) + \mathbf{B\text{-}ro}(\mu = -1)(\gamma \to \gamma_1^+)$:

$$\left(\begin{bmatrix} 1 & \alpha(\gamma_1) \\ \alpha(\gamma_1) & \eta \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\right) \overset{\text{eq.}}{\sim} \left(\begin{bmatrix} \alpha(\gamma_1)+\sqrt{\eta} & 0 \\ 0 & \alpha(\gamma_1)-\sqrt{\eta} \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right)$$

Note that here it holds that

$$\beta(\gamma_1^-) \equiv \alpha(\gamma_1) + \sqrt{\eta}\iota, \tag{27a}$$

$$\alpha_{\ell,r}(\gamma_1^+) \equiv \alpha(\gamma_1) \mp \sqrt{\eta}\ (\mu = \pm 1). \tag{27b}$$

In eq. (27a), by letting $y = \sqrt{\eta}$, we then have $\left.\frac{dy}{d\eta}\right|_{\eta=0} = \infty$ if and only if $\left.\frac{d\eta}{dy}\right|_{y=0\ (\gamma=\gamma_1)} = 0$. Similarly, letting $x = \sqrt{\eta}$, from eq. (27b) it follows that $\left.\frac{d\eta}{dx}\right|_{x=0\ (\gamma=\gamma_1)} = 0$. As a result, we have the theorem. □

From eq. (10), the SVD of C is written as

$$C = \begin{bmatrix} P_r & P_0 \end{bmatrix} \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} Q_r & Q_0 \end{bmatrix}^{\mathrm{H}} = P_r \Sigma Q_r^{\mathrm{H}} \quad \text{with} \quad \Sigma \succ 0.$$

We denote

$$U_0 := (I_3 \otimes I^{(o)})Q_0, \quad U_1 := P_r^{\mathrm{H}}(I_3 \otimes I^{(i)})Q_0, \quad U_2 := P_0^{\mathrm{H}}(I_3 \otimes I^{(i)})Q_0 \tag{28}$$

and use "$\sim$" to denote the congruence transformation that two Hermitian matrices have the same inertia. We have the following useful lemma.

Lemma 3.1. *Suppose $\boldsymbol{k} \neq 0$ and $n_\ell > 4$. Then, it holds that $U_2 \neq 0$ and*

$$A_\gamma - \alpha B_\gamma \sim C_\gamma(\alpha) \equiv \operatorname{diag}\left(-\alpha I_{3n}, \frac{1}{\alpha}\Sigma^2, -\alpha\left[\varepsilon_0 U_0^{\mathrm{H}} U_0 + \varepsilon_i U_1^{\mathrm{H}} U_1 + (\varepsilon_i - \gamma^2) U_2^{\mathrm{H}} U_2\right]\right) \tag{29}$$

as $\alpha \to 0$. Furthermore, $\alpha = 0^-$ and $\alpha = 0^+$ are, respectively, the eigenvalues of (A_γ, B_γ) with some $\gamma \equiv \gamma^- > \gamma_*$ and $\gamma \equiv \gamma^+ > \gamma_*$.

Proof. We consider the inertia of $A_\gamma - \alpha B_\gamma$ for a sufficiently small α.

$$\begin{aligned} & A_\gamma - \alpha B_\gamma \\ = & \begin{bmatrix} -\alpha I_{3n} & -\iota C \\ \iota C^{\mathrm{H}} & -\gamma[(I_3 \otimes I^{(i)})C + C^{\mathrm{H}}(I_3 \otimes I^{(i)})] - \alpha I_3 \otimes [\varepsilon_o I^{(o)} + (\varepsilon_i - \gamma^2) I^{(i)}] \end{bmatrix} \\ \sim & \begin{bmatrix} -\alpha I_{3n} & 0 \\ 0 & -\gamma[(I_3 \otimes I^{(i)})C + C^{\mathrm{H}}(I_3 \otimes I^{(i)})] - \alpha I_3 \otimes [\varepsilon_o I^{(o)} + (\varepsilon_i - \gamma^2) I^{(i)}] + \frac{1}{\alpha} C^{\mathrm{H}} C \end{bmatrix} \\ := & \begin{bmatrix} -\alpha I_{3n} & 0 \\ 0 & \frac{1}{\alpha} C^{\mathrm{H}} C - D \end{bmatrix}, \end{aligned}$$

where $D = \gamma[(I_3 \otimes I^{(i)})C + C^{\mathrm{H}}(I_3 \otimes I^{(i)})] + \alpha I_3 \otimes [\varepsilon_o I^{(o)} + (\varepsilon_i - \gamma^2) I^{(i)}]$. Thus, for $\widetilde{D} = \frac{1}{\alpha} C^{\mathrm{H}} C - D$, we have

$$\widetilde{D} \sim \begin{bmatrix} Q_r^{\mathrm{H}} \\ Q_0^{\mathrm{H}} \end{bmatrix} \widetilde{D} \begin{bmatrix} Q_r & Q_0 \end{bmatrix} = \begin{bmatrix} Q_r^{\mathrm{H}} \widetilde{D} Q_r & Q_r^{\mathrm{H}} \widetilde{D} Q_0 \\ Q_0^{\mathrm{H}} \widetilde{D} Q_r & Q_0^{\mathrm{H}} \widetilde{D} Q_0 \end{bmatrix}$$
$$\sim \begin{bmatrix} Q_r^{\mathrm{H}} \widetilde{D} Q_r & 0 \\ 0 & Q_0^{\mathrm{H}} \widetilde{D} Q_0 - Q_0^{\mathrm{H}} \widetilde{D} Q_r (Q_r^{\mathrm{H}} \widetilde{D} Q_r)^{-1} Q_r^{\mathrm{H}} \widetilde{D} Q_0 \end{bmatrix}.$$

Let us discuss the terms involved one by one.

(a) The term $Q_r^{\mathrm{H}} \widetilde{D} Q_r$: since

$$Q_r^{\mathrm{H}} \widetilde{D} Q_r = Q_r^{\mathrm{H}} \left(\frac{1}{\alpha} C^{\mathrm{H}} C - D \right) Q_r = \frac{1}{\alpha} \left(\Sigma^2 - \alpha Q_r^{\mathrm{H}} D Q_r \right),$$

we have

$$\begin{aligned} (Q_r^{\mathrm{H}} \widetilde{D} Q_r)^{-1} &= \alpha \left(\Sigma^2 - \alpha Q_r^{\mathrm{H}} D Q_r \right)^{-1} \\ &= \alpha \Sigma^{-1} \left(I - \alpha \Sigma^{-1} Q_r^{\mathrm{H}} D Q_r \Sigma^{-1} \right)^{-1} \Sigma^{-1} \\ &:= \alpha \Sigma^{-1} \left(I - \alpha D_1 \right)^{-1} \Sigma^{-1} \\ &= \alpha \Sigma^{-1} \left(I + \alpha D_1 \left[I - \alpha D_1 \right]^{-1} \right) \Sigma^{-1}, \end{aligned}$$

where $D_1 = \Sigma^{-1} Q_r^{\mathrm{H}} D Q_r \Sigma^{-1}$.

(b) The term $Q_0^{\mathrm{H}} \widetilde{D} Q_0$:

$$\begin{aligned} Q_0^{\mathrm{H}} \widetilde{D} Q_0 &= Q_0^{\mathrm{H}} \left(\frac{1}{\alpha} C^{\mathrm{H}} C - D \right) Q_0 = -Q_0^{\mathrm{H}} D Q_0 \\ &= -Q_0^{\mathrm{H}} \Big(\gamma[(I_3 \otimes I^{(i)})C + C^{\mathrm{H}}(I_3 \otimes I^{(i)})] \\ &\qquad + \alpha I_3 \otimes [\varepsilon_o I^{(o)} + (\varepsilon_i - \gamma^2) I^{(i)}] \Big) Q_0 \\ &= -\alpha Q_0^{\mathrm{H}} I_3 \otimes [\varepsilon_o I^{(o)} + (\varepsilon_i - \gamma^2) I^{(i)}] Q_0 \\ &= -\alpha [\varepsilon_o U_0^{\mathrm{H}} U_0 + (\varepsilon_i - \gamma^2)(U_1^{\mathrm{H}} U_1 + U_2^{\mathrm{H}} U_2)], \end{aligned}$$

where U_0, U_1 and U_2 are defined in eq. (28).

(c) The term $Q_0^{\mathrm{H}} \widetilde{D} Q_r$:

$$\begin{aligned} Q_0^{\mathrm{H}} \widetilde{D} Q_r &= Q_0^{\mathrm{H}} \left(\frac{1}{\alpha} C^{\mathrm{H}} C - D \right) Q_r = -Q_0^{\mathrm{H}} D Q_r \\ &= -Q_0^{\mathrm{H}} \Big(\gamma[(I_3 \otimes I^{(i)})C + C^{\mathrm{H}}(I_3 \otimes I^{(i)})] \\ &\qquad + \alpha I_3 \otimes [\varepsilon_o I^{(o)} + (\varepsilon_i - \gamma^2) I^{(i)}] \Big) Q_r \\ &= -\gamma Q_0^{\mathrm{H}} (I_3 \otimes I^{(i)}) P_r \Sigma - \alpha Q_0^{\mathrm{H}} I_3 \otimes [\varepsilon_o I^{(o)} + (\varepsilon_i - \gamma^2) I^{(i)}] Q_r \\ &= -\gamma U_1^{\mathrm{H}} \Sigma - \alpha Q_0^{\mathrm{H}} I_3 \otimes [\varepsilon_o I^{(o)} - (\varepsilon_i - \gamma^2)(I_n - I^{(o)})] Q_r \\ &= -\gamma U_1^{\mathrm{H}} \Sigma - \alpha (\varepsilon_o - \varepsilon_i + \gamma^2) U_0^{\mathrm{H}} Q_r - \alpha (\varepsilon_i - \gamma^2) Q_0^{\mathrm{H}} Q_r \\ &= -\gamma U_1^{\mathrm{H}} \Sigma - \alpha (\varepsilon_o - \varepsilon_i + \gamma^2) U_0^{\mathrm{H}} Q_r. \end{aligned}$$

Thus,

$$Q_0^{\mathrm{H}} \widetilde{D} Q_0 - Q_0^{\mathrm{H}} \widetilde{D} Q_r (Q_r^{\mathrm{H}} \widetilde{D} Q_r)^{-1} Q_r^{\mathrm{H}} \widetilde{D} Q_0$$

$$
\begin{aligned}
&= -\alpha[\varepsilon_o U_0^{\mathrm{H}} U_0 + (\varepsilon_i - \gamma^2)(U_1^{\mathrm{H}} U_1 + U_2^{\mathrm{H}} U_2)] \\
&\quad - [-\alpha(\varepsilon_o - \varepsilon_i + \gamma^2) U_0^{\mathrm{H}} Q_r - \gamma U_1^{\mathrm{H}} \Sigma] \alpha \Sigma^{-1} \left(I + \alpha D_1 \left[I - \alpha D_1 \right]^{-1} \right) \Sigma^{-1} \\
&\qquad\qquad \times [-\alpha(\varepsilon_o - \varepsilon_i + \gamma^2) U_0^{\mathrm{H}} Q_r - \gamma U_1^{\mathrm{H}} \Sigma]^{\mathrm{H}} \\
&= -\alpha[\varepsilon_o U_0^{\mathrm{H}} U_0 + (\varepsilon_i - \gamma^2)(U_1^{\mathrm{H}} U_1 + U_2^{\mathrm{H}} U_2)] - (-\gamma U_1^{\mathrm{H}} \Sigma) \alpha \Sigma^{-2} (-\gamma U_1^{\mathrm{H}} \Sigma)^{\mathrm{H}} + \mathrm{O}(\alpha^2) \\
&= -\alpha[\varepsilon_o U_0^{\mathrm{H}} U_0 + (\varepsilon_i - \gamma^2)(U_1^{\mathrm{H}} U_1 + U_2^{\mathrm{H}} U_2)] - \alpha \gamma^2 U_1^{\mathrm{H}} U_1 + \mathrm{O}(\alpha^2) \\
&:= -\alpha \left[\varepsilon_o U_0^{\mathrm{H}} U_0 + \varepsilon_i U_1^{\mathrm{H}} U_1 + (\varepsilon_i - \gamma^2) U_2^{\mathrm{H}} U_2 \right] + \mathrm{O}(\alpha^2).
\end{aligned}
$$

To summarize, for a sufficiently small α,

$$
\begin{aligned}
&A_\gamma - \alpha B_\gamma \\
&\sim \begin{bmatrix} -\alpha I_{3n} & & \\ & \frac{1}{\alpha}\Sigma^2 - Q_r^{\mathrm{H}} D Q_r & \\ & & -\alpha \left[\varepsilon_o U_0^{\mathrm{H}} U_0 + \varepsilon_i U_1^{\mathrm{H}} U_1 + (\varepsilon_i - \gamma^2) U_2^{\mathrm{H}} U_2 \right] + \mathrm{O}(\alpha^2) \end{bmatrix} \\
&\approx \begin{bmatrix} -\alpha I_{3n} & & \\ & \frac{1}{\alpha}\Sigma^2 & \\ & & -\alpha \left[\varepsilon_o U_0^{\mathrm{H}} U_0 + \varepsilon_i U_1^{\mathrm{H}} U_1 + (\varepsilon_i - \gamma^2) U_2^{\mathrm{H}} U_2 \right] \end{bmatrix} \qquad \text{as } \alpha \to 0.
\end{aligned}
$$

Now, we prove that $U_2 \neq 0$. Note that by theorem 2.2

$$
Q_0 = \begin{bmatrix} T\Lambda_1 \\ T\Lambda_2 \\ T\Lambda_3 \end{bmatrix} \Lambda_q^{-1/2}, \qquad P_0 = \begin{bmatrix} T\Lambda_1^{\mathrm{H}} \\ T\Lambda_2^{\mathrm{H}} \\ T\Lambda_3^{\mathrm{H}} \end{bmatrix} \Lambda_q^{-1/2}.
$$

Thus,

$$
\begin{aligned}
U_2 &= P_0^{\mathrm{H}} (I_3 \otimes I^{(i)}) Q_0 \\
&= \Lambda_q^{-1/2} \left(\Lambda_1 T^{\mathrm{H}} I^{(i)} T \Lambda_1 + \Lambda_2 T^{\mathrm{H}} I^{(i)} T \Lambda_2 + \Lambda_3 T^{\mathrm{H}} I^{(i)} T \Lambda_3 \right) \Lambda_q^{-1/2}.
\end{aligned}
$$

Consider $\Lambda_q^{1/2} e_{\langle n_1, m_1, \widehat{m}_1 \rangle} := \Lambda_q^{1/2} e_j$. Then,

$$
\begin{aligned}
&(\Lambda_q^{1/2} e_j)^{\mathrm{H}} U_2 \Lambda_q^{1/2} e_j \\
&= \left(\delta_1^{-2} (\eta_{n_1}^{\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_1} - 1)^2 + \delta_2^{-2} (\eta_{n_2}^{\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_2} - 1)^2 + \delta_3^{-2} (\eta_{n_3}^{\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_3} - 1)^2 \right) e_j^{\mathrm{H}} T^{\mathrm{H}} I^{(i)} T e_j.
\end{aligned}
$$

Since $Te_j = t_j$ of which each entry is nonzero by theorem 2.1, $t_j^{\mathrm{H}} I^{(i)} t_j > 0$. Note that

$$
\begin{aligned}
\Re \left(\sum_{\ell=1}^{3} \delta_\ell^{-2} (\eta_{n_\ell}^{\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_\ell} - 1)^2 \right) &= \Re \left(\sum_{\ell=1}^{3} \delta_\ell^{-2} (1 - 2\eta_{n_\ell}^{\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_\ell} + \eta_{n_\ell}^{2\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_\ell}) \right) \\
&= \sum_{\ell=1}^{3} \delta_\ell^{-2} \left(1 - 2\cos\frac{2\pi \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_\ell}{n_\ell} + \cos 2\frac{2\pi \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_\ell}{n_\ell} \right) \\
&= -2 \sum_{\ell=1}^{3} \delta_\ell^{-2} \cos\frac{2\pi \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_\ell}{n_\ell} (1 - \cos\frac{2\pi \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_\ell}{n_\ell}) < 0,
\end{aligned}
$$

in which the inequality holds because by theorem 2.1 and eq. (9), $|\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_\ell| \leq 1$, and when $n_\ell > 4$, $\cos\frac{2\pi \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_\ell}{n_\ell} > 0$; it is impossible that $\cos\frac{2\pi \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_1}{n_1} = \cos\frac{2\pi \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_2}{n_2} = \cos\frac{2\pi \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_3}{n_3} = 1$, contradicting $\boldsymbol{k} \neq 0$. As a result, $U_2 \neq 0$.

Finally, theorem 3.6 shows that α becomes an eigenvalue of the matrix pair $(A_{\gamma_*}, B_{\gamma_*})$ once the indices of the inertia of $A_\gamma - \alpha B_\gamma$ change by one whenever γ runs over γ_* increasingly or decreasingly. From eq. (29), it follows that for $\alpha = 0^-$ or 0^+, some diagonal entry of $C_\gamma(\alpha)$ must change sign as γ increases. Therefore, there exists $\gamma = \gamma^- > \gamma_*$ and $\gamma = \gamma^+ > \gamma_*$ such that $\alpha = 0^-$ and 0^+ are eigenvalues of (A_γ, B_γ), respectively. □

Theorem 3.8. *Suppose* $\boldsymbol{k} \neq 0$ *and* $n_\ell > 4$. *The number of positive/negative eigenvalues of* (A_γ, B_γ) *increases as* $\gamma > \gamma_* \equiv \sqrt{\varepsilon_i}$ *becomes larger; the new positive eigenvalue* $(\mu = -1)$ *and the new negative eigenvalue* $(\mu = 1)$ *associated with Jordan blocks of odd size appear in pairs, and they are initiated by a pair of complex conjugate eigenvalues. Moreover, this kind of pair can appear as many as* $\mathrm{rank}(\overline{\Pi_0}^{\mathrm{H}}(I_3 \otimes (T^{\mathrm{H}} I^{(i)} T))\Pi_0)$ *times.*

Proof. We first quote the following important results which have been proven above.

(a) Let $\alpha_1^{(-)}(\gamma)$ and $\alpha_1^{(+)}(\gamma)$ be the largest negative and smallest positive real eigenvalues of (A_γ, B_γ), for $\gamma < \gamma_*$. From theorem 2.4, it holds that $\frac{d\alpha_1^{(-)}(\gamma)}{d\gamma} < 0$ and $\frac{d\alpha_1^{(+)}(\gamma)}{d\gamma} > 0$ generically, i.e., $\alpha_1^{(-)}$ and $\alpha_1^{(+)}$ move toward the left and the right, respectively, when γ increases.

(b) theorems 3.4 and 3.5, respectively, show that $(A_{\gamma_*}, B_{\gamma_*})$ have defective infinite eigenvalues and $\frac{d|\omega(\gamma)|}{d\gamma} < 0$, where $\imath\omega(\gamma)$ is a purely imaginary eigenvalue of (A_γ, B_γ), for $\gamma \to \gamma_*^+$. theorem 3.7 shows that the tangent line of the complex conjugate eigenvalue curves $\beta(\gamma) \cup \bar{\beta}(\gamma)$ is orthogonal to the real axis at some $\gamma = \gamma_1$ and bifurcate into two real eigenvalues $\alpha_\ell(\gamma_1^+)(\mu = 1)$ and $\alpha_r(\gamma_1^+)(\mu = -1)$.

From lemma 3.1, we have that $\alpha = 0^-$ is an eigenvalue of $(A_{\gamma_2^-}, B_{\gamma_2^-})$ with $\gamma_2^- > \gamma_*$. From the continuity of eigenvalue curves and bifurcation theory, $\alpha = 0^-$ must have the following combination of cases listed in theorem 3.6.

$$\textbf{B-c} \to \textbf{B-re} \to \textbf{B-ro}(\mu = 1) + \textbf{B-ro}(\mu = -1).$$

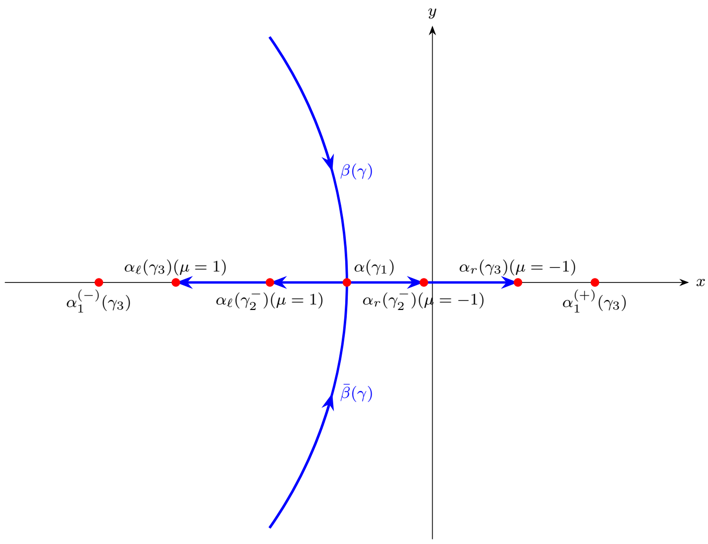


Figure 1: Scenario of bifurcation.

Scenario (see fig. 1 for details):

(i) Since $\alpha = 0^-$ is an eigenvalue of $(A_{\gamma_2^-}, B_{\gamma_2^-})$ and from the facts of (a) and (b), there is a complex conjugate eigenvalue pair $\{\beta(\gamma), \bar{\beta}(\gamma)\}$ of (A_γ, B_γ) for $\gamma_* < \gamma < \gamma_1$ such that they collide at $\gamma = \gamma_1$ with $\alpha_1^{(-)}(\gamma_1) < \alpha(\gamma_1) = \beta(\gamma_1) = \bar{\beta}(\gamma_1) < 0$ and bifurcate into two real eigenvalues $\alpha_\ell(\gamma_1^+)(\mu = 1)$ and $\alpha_r(\gamma_1^+)(\mu = -1)$ with $\alpha_\ell(\gamma_1^+)$ and $\alpha_r(\gamma_1^+)$ moving toward the left and the right, respectively.

(ii) Furthermore, there exist $\gamma_1 < \gamma_2^\pm < \gamma_3$ such that

$$\alpha_\ell(\gamma_2^\pm)(\mu = 1) < \alpha(\gamma_1) < \alpha_r(\gamma_2^\pm)(\mu = -1) \equiv 0^\pm \tag{30}$$

and

$$0 < \alpha_r(\gamma_3) < \alpha_1^{(+)}(\gamma_3) \tag{31}$$

which implies that a new smallest positive eigenvalue $\alpha_r(\gamma_3)$ is created at $\gamma = \gamma_3$.

We now show the following cases cannot happen.

(iii) If there is a complex conjugate eigenvalue pair $\{\hat{\beta}(\gamma), \bar{\hat{\beta}}(\gamma)\}$ of (A_γ, B_γ) that collides at $\gamma = \gamma_4 > \gamma_3$ with

$$0 < \alpha_r(\gamma_3) < \alpha_r(\gamma_4) < \hat{\alpha}_\ell(\gamma_4^+) \lesssim \hat{\alpha}(\gamma_4) = \hat{\beta}(\gamma_4) = \bar{\hat{\beta}}(\gamma_4) \lesssim \hat{\alpha}_r(\gamma_4^+), \tag{32}$$

(iv) then, $\alpha_r(\gamma_4)(\mu = -1)$ and $\hat{\alpha}_\ell(\gamma_4^+)$ will collide at $\alpha_r(\gamma_5)$ for $\gamma_4 \to \gamma_5$ increasingly, as the combination below.

$$\gamma = \gamma_5^- : \textbf{B-ro}(\mu = 1) + \textbf{B-ro}(\mu = -1) \\ \to \gamma = \gamma_5 : \textbf{B-re}(\mu = -1) \to \gamma = \gamma_5^+ : \textbf{B-c}. \tag{33}$$

(v) Then, from lemma 3.1, it follows that $p_+(C_{\gamma_5^-}(0^-)) < p_+(C_{\gamma_5^+}(0^-))$, which is a contradiction.

From eq. (29), lemma 3.1 and (ii), it follows that

$$p_-(C_{\gamma_2^-}(0^-)) < p_-(C_{\gamma_2^+}(0^-))$$

and

$$p_+(C_{\gamma_2^-}(0^+)) < p_+(C_{\gamma_2^+}(0^+)).$$

This implies that the new positive and negative eigenvalues $\alpha_r(\gamma_3)$ and $\alpha_\ell(\gamma_3)$ must be of negative $(\mu = -1)$ and positive $(\mu = 1)$ types, respectively.

On the other hand, another scenario in which the pair of eigenvalue curves $\{\beta(\gamma), \bar{\beta}(\gamma)\}$ for $\gamma_* < \gamma < \gamma_1$ collides at $\gamma = \gamma_1$ with

$$0 < \alpha(\gamma_1) = \beta(\gamma_1) = \bar{\beta}(\gamma_1) < \alpha_1^{(+)}(\gamma_1)$$

can also happen (see fig. 3(b) in section 4). A similar discussion as in (i)-(v) above is still held by replacing 0^- by 0^+ and considering all combinations symmetric to the purely imaginary axis. These two scenarios should be mutually exclusive.

Finally, the kind of pairs in (i) and (ii) can appear as many as

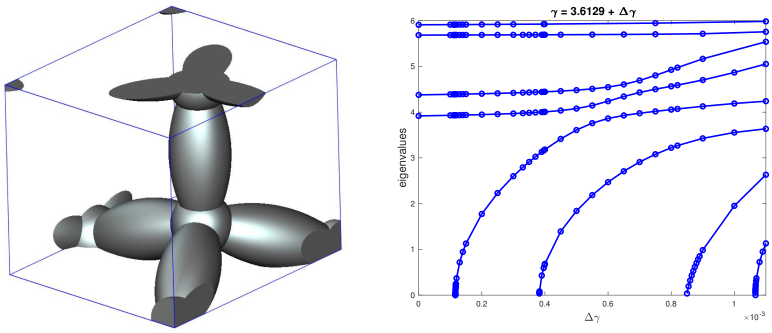
$$\operatorname{rank}(U_2) = \operatorname{rank}(\overline{\Pi_0}^{\mathrm{H}}(I_3 \otimes (T^{\mathrm{H}} I^{(i)} T))\Pi_0)$$

times because the matrix $(\varepsilon_i - \gamma^2)U_2^{\mathrm{H}} U_2$ in eq. (29) makes B_γ change signs $\operatorname{rank}(U_2)$ times, as $\gamma \to \infty$. □

4 Numerical results

To study numerical behaviors of the complex conjugate eigenvalue curves with $\gamma > \gamma_* \equiv \sqrt{\varepsilon_i}$, we consider the FCC lattice [7] which consists of dielectric spheres with connecting spheroids, as is shown in fig. 2(a). The mesh numbers n_1, n_2 and n_3 are taken as $n_1 = n_2 = n_3 = 96$, and the matrix dimension of $\widehat{A}_r$ in eq. (17b) is 3,538,944. Here, $\varepsilon_i = 13$.

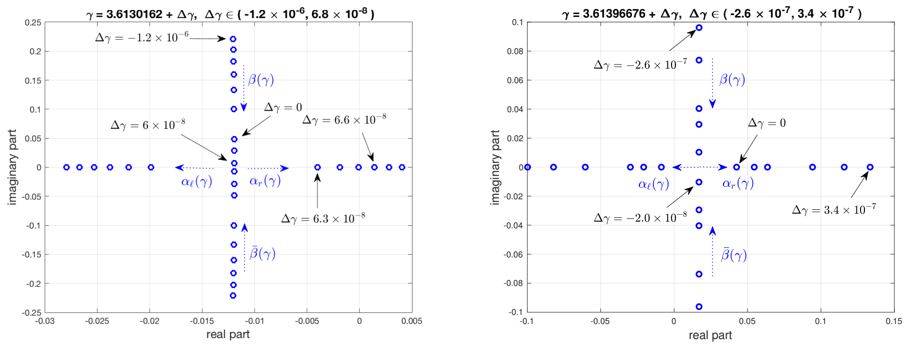
As shown by the numerical results shown in [7, Figure 4], there are four newly created smallest energies as γ increases from $\sqrt{\varepsilon_i} \approx 3.6056$ to 3.61397. The zoom-in view of the eigencurve-structure is shown in fig. 2(b). The results demonstrate that four newly created smallest energies are produced on the tiny increment $\Delta\gamma = 10^{-3}$ of γ. These energies emerge from lower frequencies and push the original eigenmodes to higher frequencies. These new smallest eigenvalues do not collide with the original eigenvalues so no bifurcation occurs again between these eigenvalues.



(a) Schema (b) Eigencurve-structure vs. various γ

Figure 2: A schema of 3D complex media with the FCC lattice and eigencurve-structure vs. various γ

In fig. 3, we demonstrate the local behavior of the complex conjugate eigenvalue curves which collide and bifurcate into two real eigenvalues at $\gamma = \gamma_1 \approx 3.6130162$ and $\gamma_4 \approx 3.61396676$. The results show that the tangent lines of $\beta(\gamma) \cup \bar{\beta}(\gamma)$ and $\alpha(\gamma) \equiv \alpha_\ell(\gamma) \cup \alpha_r(\gamma)$ at $\gamma = \gamma_1$ and γ_4 are orthogonal to the real x- and imaginary y-axes, respectively, as the proof of theorem 3.7. Moreover, the complex conjugate eigenvalue curves collide and bifurcate at $\alpha(\gamma_1) \approx -1.194 \times 10^{-2}$ and $\alpha(\gamma_4) \approx 1.693 \times 10^{-2}$, respectively. The negative and positive eigenvalues $\alpha(\gamma_1)$ and $\alpha(\gamma_4)$ instantly move toward the right and the left, respectively, to a new positive eigenvalue $\alpha_r(\gamma_1 + \varDelta\gamma_1)$ and a negative eigenvalue $\alpha_\ell(\gamma_4 + \varDelta\gamma_4)$ along the real axis, where $\varDelta\gamma_1 = 6 \times 10^{-9}$ and $\varDelta\gamma_4 = 2 \times 10^{-8}$.



(a) The first newly created smallest energy (b) The fourth newly created smallest energy

Figure 3: The local behavior of the complex conjugate eigenvalue curves which collide and bifurcate into two real eigenvalues at $\gamma \approx 3.6130162$ and 3.61396676.

5 Conclusions

In this paper, we prove a detailed bifurcation analysis of eigenstructures of the discrete single-curl operator in 3D Maxwell's equations with Pasteur media that depend on a chirality parameter γ as it varies. We compensate for the theoretical difficulties and guarantee that the numerical results are valid and reliable. These results can provide an important theoretical viewpoint on numerical computations, especially regarding the support of numerical results in [7] computed by the developed SIRA + MINRES for NFGEP. It is worth mentioning that in remark 3.1, we show that the associated electric field $\boldsymbol{e}$ of the defective infinite eigenvalue is zero outside the material. This provides a very good reason to explain that the electric field corresponding to the newly created smallest energy state is almost concentrated in the material such that only a small amount of the field leak into the background material.

In the future, it would be very challenging to compute the Bloch dispersion curves corresponding to a periodic array of plasmonic nanoparticles inside a chiral background medium.

A The regularity of $A - \omega B$

Theorem A.1. *$A - \omega B$ is always regular, as long as three line segments, parallel to the three mesh grid axes respectively, with end points lying on the boundary of the mesh grid are outside the medium, i.e., there exist some $i_1, i_1' \in [1, n_1], i_2, i_2' \in [1, n_2], i_3, i_3' \in [1, n_3]$, such that $\mathcal{G} \subset \mathcal{D}_o$, where $\mathcal{G} = \mathcal{G}_1 \cup \mathcal{G}_2 \cup \mathcal{G}_3$ with $\mathcal{G}_1 = \{\langle i, i_2, i_3' \rangle : i \in \mathbb{Z}\}$, $\mathcal{G}_2 = \{\langle i_1', i, i_3 \rangle : i \in \mathbb{Z}\}$, $\mathcal{G}_3 = \{\langle i_1, i_2', i \rangle : i \in \mathbb{Z}\}$.*

Proof. First, we will observe $\mathcal{S}$. To address it, we have to discuss several cases.

Case I. $\Lambda_\ell, \ell = 1, 2, 3$ are nonsingular. The only proper z_1, z_2, z_3 are all zero.

First, eq. (20a) has nontrivial solutions if and only if there exists $i_\ell \in [1, n_\ell], \ell = 1, 2, 3$, such that

$$\eta_{n_3}^{\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_3 + i_3} \eta_{n_2 n_3}^{-m_2 i_2} \eta_{n_1 n_3}^{-\widehat{m}_1 i_1} \eta_{n_1 n_2 n_3}^{m_1 m_2 i_1} = \eta_{n_2}^{\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_2 + i_2} \eta_{n_1 n_2}^{-m_1 i_1} = \eta_{n_1}^{\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_1 + i_1},$$

and in this case, the $\langle i_1, i_2, i_3 \rangle$-th entry of x_1 is nonzero. It is equivalent to

$$\begin{aligned} \frac{i_1 + \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_1}{n_1} - s_1 &= \frac{i_2 + \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_2 - \frac{m_1}{n_1} i_1}{n_2} - s_2 \\ &= \frac{i_3 + \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_3 - \frac{m_2}{n_2} i_2 - \frac{\widehat{m}_1}{n_1} i_1 + \frac{m_1 m_2}{n_1 n_2} i_1}{n_3} - s_3 =: \lambda \in [0, 1), \end{aligned}$$

for some $s_1, s_2, s_3 \in \mathbb{Z}$. In other words, $x_1 = I^{\mathcal{I}_0} x_1$, where

$$\mathcal{I}_0 := \{\langle \lambda\widehat{n}_1 - \kappa_1, \lambda\widehat{n}_2 - \kappa_2, \lambda\widehat{n}_3 - \kappa_3 \rangle : \lambda\widehat{n}_\ell - \kappa_\ell \in \mathbb{Z}, 0 < \lambda < 1\},$$

with

$$\begin{aligned} \widehat{n}_1 &= n_1, & \kappa_1 &= \boldsymbol{k}\cdot\boldsymbol{a}_1, \\ \widehat{n}_2 &= n_2 + m_1, & \kappa_2 &= \boldsymbol{k}\cdot(\boldsymbol{a}_2 + \rho_1\boldsymbol{a}_1) - m_1 s_1, \\ \widehat{n}_3 &= n_3 + m_2 + \widehat{m}_1, & \kappa_3 &= \boldsymbol{k}\cdot(\boldsymbol{a}_3 + \rho_2\boldsymbol{a}_2 + \widehat{\rho}_1\boldsymbol{a}_1) - m_2 s_2 - \widehat{m}_1 s_1. \end{aligned}$$

Clearly, $x_1 \neq 0$ is equivalent to $(I_\sigma^{\mathcal{I}_0})^{\mathrm{T}} x_1 \neq 0$. Moreover, if $\mathcal{I}_0 \neq \emptyset$, then it can be shown that[1]

$$\mathcal{I}_0 = \{\langle \lambda\widehat{n}_1 - \kappa_1, \lambda\widehat{n}_2 - \kappa_2, \lambda\widehat{n}_3 - \kappa_3 \rangle : \lambda = \lambda_0 + \frac{p}{\widehat{n}_{123}}, p \in [0, \widehat{n}_{123}) \cap \mathbb{Z}\},$$

with $\lambda_0 \in [0, \frac{1}{\widehat{n}_{123}})$ satisfying $\lambda_0\widehat{n}_\ell - \kappa_\ell \in \mathbb{Z}$, and $\widehat{n}_{123} = \gcd(\widehat{n}_1, \widehat{n}_2, \widehat{n}_3)$, the greatest common divisor of $\widehat{n}_1$, $\widehat{n}_2$ and $\widehat{n}_3$. Note that λ_0 here is unique, and $|\mathcal{I}_0| = \widehat{n}_{123}$.

Then, consider eq. (20b), namely, solving $I^{(o)} T \Lambda_1 x_1 = 0$. For ease, we mainly discuss the case that the related index sets are nonempty. Inserting the solution of eq. (20a) into eq. (20b), we have

$$0 = I^{(o)} T \Lambda_1 x_1 = I^{(o)} T \Lambda_1 I^{\mathcal{I}_0} x_1 = I^{(o)} T I^{\mathcal{I}_0} \Lambda_1 x_1 = I^{(o)} T I_\sigma^{\mathcal{I}_0} [(I_\sigma^{\mathcal{I}_0})^{\mathrm{T}} \Lambda_1 x_1].$$

Recall the form of $T = [t_\ell]$ in eq. (8). Write

$$U_{\widehat{n}_{123}} = [u_{\widehat{n}_{123}, p}]_{p=1,\dots,\widehat{n}_{123}}, \qquad u_{\widehat{n}_{123}, p} := V_{n_3}(\eta_{\widehat{n}_{123}}^p) \otimes V_{n_2}(\eta_{\widehat{n}_{123}}^p) \otimes V_{n_1}(\eta_{\widehat{n}_{123}}^p).$$

and $t_0 = t_{\langle \lambda_0\widehat{n}_1 - \kappa_1, \lambda_0\widehat{n}_2 - \kappa_2, \lambda_0\widehat{n}_3 - \kappa_3 \rangle}$. It can be seen that

$$t_{\langle (\lambda_0 + \frac{p}{\widehat{n}_{123}})\widehat{n}_1 - \kappa_1, (\lambda_0 + \frac{p}{\widehat{n}_{123}})\widehat{n}_2 - \kappa_2, (\lambda_0 + \frac{p}{\widehat{n}_{123}})\widehat{n}_3 - \kappa_3 \rangle} = \mathrm{diag}(u_{\widehat{n}_{123}, p}) t_0 = \mathrm{diag}(t_0) u_{\widehat{n}_{123}, p},$$

[1] if $\langle \lambda\widehat{n}_1 - \kappa_1, \lambda\widehat{n}_2 - \kappa_2, \lambda\widehat{n}_3 - \kappa_3 \rangle \in \mathcal{I}_0$, then $\langle \lambda'\widehat{n}_1 - \kappa_1, \lambda'\widehat{n}_2 - \kappa_2, \lambda'\widehat{n}_3 - \kappa_3 \rangle \in \mathcal{I}_0$ for $\lambda' = \lambda + \frac{p}{\gcd(\widehat{n}_1, \widehat{n}_2, \widehat{n}_3)}$ with $p \in \mathbb{Z}$. On the other hand, if $\langle \lambda\widehat{n}_1 - \kappa_1, \lambda\widehat{n}_2 - \kappa_2, \lambda\widehat{n}_3 - \kappa_3 \rangle \in \mathcal{I}_0$ and $\langle \lambda'\widehat{n}_1 - \kappa_1, \lambda'\widehat{n}_2 - \kappa_2, \lambda'\widehat{n}_3 - \kappa_3 \rangle \in \mathcal{I}_0$, then $(\lambda - \lambda')\widehat{n}_\ell \in \mathbb{Z}$, which infers $(\lambda - \lambda') \gcd(\widehat{n}_1, \widehat{n}_2, \widehat{n}_3) \in \mathbb{Z}$ by Bézout's identity.

and then $TI_\sigma^{\mathcal{I}_0} = \operatorname{diag}(t_0)U_{\widehat{n}_{123}}$. Thus,

$$\begin{aligned} 0 &= I^{(o)}TI_\sigma^{\mathcal{I}_0}[(I_\sigma^{\mathcal{I}_0})^{\mathrm{T}}\Lambda_1 x_1] \\ &= I^{(o)}\operatorname{diag}(t_0)U_{\widehat{n}_{123}}[(I_\sigma^{\mathcal{I}_0})^{\mathrm{T}}\Lambda_1 x_1] \\ &= \operatorname{diag}(t_0)I^{(o)}U_{\widehat{n}_{123}}[(I_\sigma^{\mathcal{I}_0})^{\mathrm{T}}\Lambda_1 I_\sigma^{\mathcal{I}_0}][(I_\sigma^{\mathcal{I}_0})^{\mathrm{T}}x_1]. \end{aligned}$$

Noticing that each entry of t_0 is nonzero, and $(I_\sigma^{\mathcal{I}_0})^{\mathrm{T}}\Lambda_1 I_\sigma^{\mathcal{I}_0}$ is nonsingular, $\mathcal{S} = \{0\}$ is equivalent to $I^{(o)}U_{\widehat{n}_{123}}x = 0$ has only trivial solutions, namely, $I^{(o)}U_{\widehat{n}_{123}}$ is of full column rank.

Case II-1. $\Lambda_\ell, \ell = 2, 3$ are nonsingular, but Λ_1 is singular. By the form of Λ_1 in eq. (7),

$$\Lambda_1 \text{ is singular} \Leftrightarrow \frac{i_1 + \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_1}{n_1} \in \mathbb{Z} \text{ for some } i_1 \Leftrightarrow \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_1 = 0,$$

and for the case $i_1 = n_1$. The only proper z_2, z_3 are both zero.

First, eq. (20a) has nontrivial solutions, if and only if:

(1) there exists $i_\ell \in [1, n_\ell], \ell = 1, 2, 3,\ i_1 \neq n_1$, such that

$$\begin{aligned} \frac{i_1 + \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_1}{n_1} - s_1 &= \frac{i_2 + \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_2 - \frac{m_1}{n_1}i_1}{n_2} - s_2 \\ &= \frac{i_3 + \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_3 - \frac{m_2}{n_2}i_2 - \frac{\widehat{m}_1}{n_1}i_1 + \frac{m_1 m_2}{n_1 n_2}i_1}{n_3} - s_3 =: \lambda \in [0, 1), \end{aligned}$$

for some $s_1, s_2, s_3 \in \mathbb{Z}$. For the case, the $\langle i_1, i_2, i_3\rangle$-th entry of x_1 is nonzero.

(2) there exists $i_\ell \in [1, n_\ell], \ell = 2, 3$, such that

$$\begin{aligned} &\frac{i_2 + \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_2 - \frac{m_1}{n_1}n_1}{n_2} - s_2 \\ &\qquad = \frac{i_3 + \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_3 - \frac{m_2}{n_2}i_2 - \frac{\widehat{m}_1}{n_1}n_1 + \frac{m_1 m_2}{n_1 n_2}n_1}{n_3} - s_3 =: \lambda \in [0, 1), \end{aligned}$$

for some $s_1, s_2, s_3 \in \mathbb{Z}$. For the case, the $\langle n_1, i_2, i_3\rangle$-th entry of x_1 is decided by z_1, where $z_1 \in \mathcal{R}(I_\sigma^{\mathcal{I}_1})$, and

$$\begin{aligned} \mathcal{I}_1 &:= \{\langle n_1, \lambda\widehat{n}_2 - \kappa_2, \lambda\widehat{n}_3 - \kappa_3\rangle : \lambda\widehat{n}_\ell - \kappa_\ell \in \mathbb{Z}, 0 < \lambda < 1\} \\ &= \{\langle n_1, \lambda\widehat{n}_2 - \kappa_2, \lambda\widehat{n}_3 - \kappa_3\rangle : \lambda = \lambda_1 + \frac{p}{\widehat{n}_{23}}, p \in [0, \widehat{n}_{23}) \cap \mathbb{Z}\}, \end{aligned}$$

and

$$\begin{aligned} \widehat{n}_2 &= n_2, & \kappa_2 &= \boldsymbol{k}\cdot(\boldsymbol{a}_2 + \rho_1\boldsymbol{a}_1) - m_1, \\ \widehat{n}_3 &= n_3 + m_2, & \kappa_3 &= \boldsymbol{k}\cdot(\boldsymbol{a}_3 + \rho_2\boldsymbol{a}_2 + \widehat{\rho}_1\boldsymbol{a}_1) - m_2 s_2 - \widehat{m}_1. \end{aligned}$$

In detail, $(I_\sigma^{\mathcal{I}_1})^{\mathrm{H}}x_1 = -\delta_2[(I_\sigma^{\mathcal{I}_1})^{\mathrm{H}}\Lambda_2 I_\sigma^{\mathcal{I}_1}]^{-1}(I_\sigma^{\mathcal{I}_1})^{\mathrm{H}}z_1$.

In other words, $x_1 = I^{\mathcal{I}_0\cup\mathcal{I}_1}x_1$. Moreover, if $\mathcal{I}_1 \neq \emptyset$, with $\lambda_1 \in [0, \frac{1}{\widehat{n}_{23}})$ satisfying $\lambda_0\widehat{n}_\ell - \kappa_\ell \in \mathbb{Z}$, and $\widehat{n}_{23} = \gcd(\widehat{n}_2, \widehat{n}_3)$. Note that λ_1 here is unique, and $|\mathcal{I}_1| = \widehat{n}_{23}$. Clearly, $x_1 \neq 0$ is equivalent to $(I_\sigma^{\mathcal{I}_0\cup\mathcal{I}_1})^{\mathrm{T}}x_1 \neq 0$.

Then, consider eqs. (19) and (20b), namely, solving $I^{(o)}T\Lambda_1 x_1 = 0, I^{(o)}Tz_1 = 0$. For ease, we mainly discuss the case in which the related index sets are nonempty. Inserting the solution of eq. (20a) into eq. (20b), we have

$$0 = \begin{bmatrix} I^{(o)}T\Lambda_1 x_1 \\ I^{(o)}Tz_1 \end{bmatrix} = \begin{bmatrix} I^{(o)}T\Lambda_1 I^{\mathcal{I}_0}x_1 \\ I^{(o)}TI^{\mathcal{I}_1}z_1 \end{bmatrix} = \begin{bmatrix} I^{(o)}TI_\sigma^{\mathcal{I}_0}[(I_\sigma^{\mathcal{I}_0})^{\mathrm{T}}\Lambda_1 x_1] \\ I^{(o)}TI_\sigma^{\mathcal{I}_1}[(I_\sigma^{\mathcal{I}_1})^{\mathrm{T}}z_1] \end{bmatrix}$$

$$= \begin{bmatrix} I^{(o)} T I_\sigma^{\mathcal{I}_0} & \\ & I^{(o)} T I_\sigma^{\mathcal{I}_1} \end{bmatrix} \begin{bmatrix} (I_\sigma^{\mathcal{I}_0})^{\mathrm{T}} \Lambda_1 x_1 \\ (I_\sigma^{\mathcal{I}_1})^{\mathrm{T}} z_1 \end{bmatrix}.$$

Similarly, $\mathcal{S} = \{0\}$ is equivalent to $\begin{bmatrix} I^{(o)} U_{\widehat{n}_{123}} & \\ & I^{(o)} U_{\widehat{n}_{23}} \end{bmatrix}$ is of full column rank, where

$$U_{\widehat{n}_{23}} = [u_{\widehat{n}_{23},p}]_{p=1,\dots,\widehat{n}_{23}}, \qquad u_{\widehat{n}_{13},p} := V_{n_3}(\eta^p_{\widehat{n}_{23}}) \otimes V_{n_2}(\eta^p_{\widehat{n}_{13}}) \otimes V_{n_1}(1).$$

Case II-2. $\Lambda_\ell, \ell = 1, 3$ are nonsingular, but Λ_2 is singular. By the form of Λ_2 in eq. (7), we have:

(1) $m_1 = 0$:

$$\Lambda_2 \text{ is singular} \Leftrightarrow \frac{i_2 + \boldsymbol{k} \cdot \widehat{\boldsymbol{a}}_2}{n_2} \in \mathbb{Z} \text{ for some } i_2 \Leftrightarrow \boldsymbol{k} \cdot \widehat{\boldsymbol{a}}_2 = 0,$$

and everything is similar to **Case II-1**. $\mathcal{S} = \{0\}$ is equivalent to the matrix $\begin{bmatrix} I^{(o)} U_{\widehat{n}_{123}} & \\ & I^{(o)} U_{\widehat{n}_{13}} \end{bmatrix}$ is of full column rank, where

$$U_{\widehat{n}_{13}} = [u_{\widehat{n}_{13},p}]_{p=1,\dots,\widehat{n}_{13}}, \qquad u_{\widehat{n}_{13},p} := V_{n_3}(\eta^p_{\widehat{n}_{13}}) \otimes V_{n_2}(1) \otimes V_{n_1}(\eta^p_{\widehat{n}_{13}}).$$

(2) $m_1 \neq 0$:

$$\Lambda_2 \text{ is singular} \Leftrightarrow \frac{i_2 + \boldsymbol{k} \cdot \widehat{\boldsymbol{a}}_2 - \frac{m_1}{n_1} i_1}{n_2} \in \mathbb{Z} \text{ for some } i_1, i_2$$
$$\Leftrightarrow \widetilde{n}_2 := \frac{n_1}{m_1} \boldsymbol{k} \cdot \widehat{\boldsymbol{a}}_2 \in \mathbb{Z},$$

and for the case $i_1 = \widetilde{n}_2, i_2 = n_2$. The only proper z_1, z_3 are both zero.

First, eq. (20a) has nontrivial solutions, if and only if:

(a) there exists $i_\ell \in [1, n_\ell], \ell = 1, 2, 3$, $(i_1, i_2) \neq (\widetilde{n}_2, n_2)$, such that

$$\frac{i_1 + \boldsymbol{k} \cdot \widehat{\boldsymbol{a}}_1}{n_1} - s_1 = \frac{i_2 + \boldsymbol{k} \cdot \widehat{\boldsymbol{a}}_2 - \frac{m_1}{n_1} i_1}{n_2} - s_2$$
$$= \frac{i_3 + \boldsymbol{k} \cdot \widehat{\boldsymbol{a}}_3 - \frac{m_2}{n_2} i_2 - \frac{\widehat{m}_1}{n_1} i_1 + \frac{m_1 m_2}{n_1 n_2} i_1}{n_3} - s_3 =: \lambda \in [0, 1),$$

for some $s_1, s_2, s_3 \in \mathbb{Z}$. For the case, the $\langle i_1, i_2, i_3 \rangle$-th entry of x_1 is nonzero.

(b) $(i_1, i_2) = (\widetilde{n}_2, n_2)$. For the case, the $\langle \widetilde{n}_2, n_2, i_3 \rangle$-th entry of x_1 is decided by z_2, where $z_2 \in \mathcal{R}(I_\sigma^{\mathcal{I}_2^m})$, and

$$\mathcal{I}_2^m := \{\langle \widetilde{n}_2, n_2, i_3 \rangle\}.$$

In detail, $(I_\sigma^{\mathcal{I}_2^m})^{\mathrm{H}} x_1 = -\delta_3 [(I_\sigma^{\mathcal{I}_2^m})^{\mathrm{H}} \Lambda_3 I_\sigma^{\mathcal{I}_2^m}]^{-1} (I_\sigma^{\mathcal{I}_2^m})^{\mathrm{H}} z_2$.

In other words, $x_1 = I^{\mathcal{I}_0 \cup \mathcal{I}_2^m} x_1$. Note that $|\mathcal{I}_2^m| = n_3$. Clearly, $x_1 \neq 0$ is equivalent to $(I_\sigma^{\mathcal{I}_0 \cup \mathcal{I}_2^m})^{\mathrm{T}} x_1 \neq 0$.

Then, consider eqs. (19) and (20b), namely, solving $I^{(o)} T \Lambda_1 x_1 = 0, I^{(o)} T z_2 = 0$. The steps proceed similarly to **Case II-1**. $\mathcal{S} = \{0\}$ is equivalent to $\begin{bmatrix} I^{(o)} U_{\widehat{n}_{123}} & \\ & I^{(o)} U_{n_3} \end{bmatrix}$ is of full column rank, where

$$U_{n_3} = [u_{n_3,p}]_{p=1,\dots,n_3}, \qquad u_{n_3,p} := V_{n_3}(\eta^p_{n_3}) \otimes V_{n_2}(1) \otimes V_{n_1}(1).$$

Case II-3. $\Lambda_\ell, \ell = 1, 2$ are nonsingular, but Λ_3 is singular. By the form of Λ_3 in eq. (7), we have:

(1) $\widehat{m}_1 = 0, m_2 = 0$:

$$\begin{aligned} \Lambda_3 \text{ is singular} &\Leftrightarrow \frac{i_3 + \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_3}{n_2} \in \mathbb{Z} \text{ for some } i_3 \\ &\Leftrightarrow \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_3 = 0, \end{aligned}$$

and everything is similar to **Case II-1**. $\mathcal{S} = \{0\}$ is equivalent to the matrix $\begin{bmatrix} I^{(o)}U_{\widehat{n}_{123}} & \\ & I^{(o)}U_{\widehat{n}_{12}} \end{bmatrix}$ is of full column rank, where

$$U_{\widehat{n}_{12}} = [u_{\widehat{n}_{12},p}]_{p=1,\ldots,\widehat{n}_{12}}, \qquad u_{\widehat{n}_{12},p} := V_{n_3}(1) \otimes V_{n_2}(\eta^p_{\widehat{n}_{12}}) \otimes V_{n_1}(\eta^p_{\widehat{n}_{12}}).$$

(2) $\widehat{m}_1 \neq 0, m_2 = 0$:

$$\begin{aligned} \Lambda_3 \text{ is singular} &\Leftrightarrow \frac{i_3 + \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_3 - \frac{\widehat{m}_1}{n_1} i_1}{n_3} \in \mathbb{Z} \text{ for some } i_1, i_3 \\ &\Leftrightarrow \widetilde{n}_{3,1} := \frac{n_1}{\widehat{m}_1}\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_3 \in \mathbb{Z}, \end{aligned}$$

and everything is similar to **Case II-2**(2). $\mathcal{S} = \{0\}$ is equivalent to the matrix $\begin{bmatrix} I^{(o)}U_{\widehat{n}_{123}} & \\ & I^{(o)}U_{n_2} \end{bmatrix}$ is of full column rank, where

$$U_{n_2} = [u_{n_2,p}]_{p=1,\ldots,n_2}, \qquad u_{n_2,p} := V_{n_3}(1) \otimes V_{n_2}(\eta^p_{n_2}) \otimes V_{n_1}(1).$$

(3) $m_2 \neq 0, \widehat{m}_1 = 0, m_1 = 0$:

$$\begin{aligned} \Lambda_3 \text{ is singular } &\Leftrightarrow \frac{i_3 + \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_3 - \frac{m_2}{n_2} i_2}{n_3} \in \mathbb{Z} \text{ for some } i_2, i_3 \\ &\Leftrightarrow \widetilde{n}_{3,2} := \frac{n_1}{\widehat{m}_1}\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_3 \in \mathbb{Z}, \end{aligned}$$

and everything is similar to **Case II-2**(2). $\mathcal{S} = \{0\}$ is equivalent to the matrix $\begin{bmatrix} I^{(o)}U_{\widehat{n}_{123}} & \\ & I^{(o)}U_{\widehat{n}_{1}} \end{bmatrix}$ is of full column rank, where

$$U_{n_1} = [u_{n_1,p}]_{p=1,\ldots,n_1}, \qquad u_{n_1,p} := V_{n_3}(1) \otimes V_{n_2}(1) \otimes V_{n_1}(\eta^p_{n_1}).$$

(4) $m_2 \neq 0$, $\widehat{m}_1, m_1$ not both zero:

$$\Lambda_3 \text{ is singular } \Leftrightarrow \frac{i_3 + \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_3 - \frac{m_2}{n_2} i_2 - \frac{\widehat{m}_1}{n_1} i_1 + \frac{m_1 m_2}{n_1 n_2} i_1}{n_3} \in \mathbb{Z} \text{ for some } i_1, i_2, i_3,$$

and for the case where there is only one choice (i_1, i_2, i_3). Write the single-element set as $\mathcal{I}_3^m$. The only proper z_1, z_2 are both zero.

First, eq. (20a) has nontrivial solutions, if and only if:

(a) there exists $i_\ell \in [1, n_\ell], \ell = 1, 2, 3$, $(i_1, i_2, i_3) \notin \mathcal{I}_3^m$, such that

$$\begin{aligned} \frac{i_1 + \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_1}{n_1} - s_1 &= \frac{i_2 + \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_2 - \frac{m_1}{n_1} i_1}{n_2} - s_2 \\ &= \frac{i_3 + \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_3 - \frac{m_2}{n_2} i_2 - \frac{\widehat{m}_1}{n_1} i_1 + \frac{m_1 m_2}{n_1 n_2} i_1}{n_3} - s_3 =: \lambda \in [0, 1), \end{aligned}$$

for some $s_1, s_2, s_3 \in \mathbb{Z}$. For the case, the $\langle i_1, i_2, i_3 \rangle$-th entry of x_1 is nonzero.

(b) $(i_1,i_2,i_3)\in\mathcal{I}_3^m$. For the case, the $\langle\widetilde{n}_2,n_2,i_3\rangle$-th entry of x_1 is decided by z_3, where $z_2\in\mathcal{R}(I_\sigma^{\mathcal{I}_3^m})$. In detail,

$$(I_\sigma^{\mathcal{I}_3^m})^{\mathrm{H}}x_1=-\delta_3[(I_\sigma^{\mathcal{I}_3^m})^{\mathrm{H}}\mathit{\Lambda}_3 I_\sigma^{\mathcal{I}_3^m}]^{-1}(I_\sigma^{\mathcal{I}_3^m})^{\mathrm{H}}z_3.$$

In other words, $x_1=I^{\mathcal{I}_0\cup\mathcal{I}_3^m}x_1$. Note that $|\mathcal{I}_3^m|=n_1$. Clearly, $x_1\neq 0$ is equivalent to $(I_\sigma^{\mathcal{I}_0\cup\mathcal{I}_3^m})^{\mathrm{T}}x_1\neq 0$.

Then, consider eqs. (19) and (20b), namely, solving $I^{(o)}T\mathit{\Lambda}_1x_1=0, I^{(o)}Tz_3=0$. The steps proceed similarly to **Case II-1**. $\mathcal{S}=\{0\}$ is equivalent to $\begin{bmatrix}I^{(o)}U_{\widehat{n}_{123}} & \\ & I^{(o)}U_1\end{bmatrix}$ is of full column rank, where

$$U_1=[u_{1,1}],\qquad u_{1,1}:=V_{n_3}(1)\otimes V_{n_2}(1)\otimes V_{n_1}(1).$$

Case III-3. $\mathit{\Lambda}_\ell,\ell=1,2$ are singular, but $\mathit{\Lambda}_3$ is nonsingular. The only proper $z_3=0$. By the form of $\mathit{\Lambda}_1,\mathit{\Lambda}_2$ in eq. (7), we have:

(1) $m_1=0$: it is similar to the combination of **Case II-1** and **Case II-2**(1).

$$\mathit{\Lambda}_1 \text{ is singular} \Leftrightarrow \frac{i_1+\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_1}{n_1}\in\mathbb{Z}\text{ for some } i_1 \Leftrightarrow \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_1=0,$$

$$\mathit{\Lambda}_2 \text{ is singular} \Leftrightarrow \frac{i_2+\boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_2}{n_2}\in\mathbb{Z}\text{ for some } i_2 \Leftrightarrow \boldsymbol{k}\cdot\widehat{\boldsymbol{a}}_2=0.$$

In detail,

$$(I_\sigma^{\mathcal{I}_1})^{\mathrm{H}}x_1=-\delta_3[(I_\sigma^{\mathcal{I}_1})^{\mathrm{H}}\mathit{\Lambda}_3I_\sigma^{\mathcal{I}_1}]^{-1}(I_\sigma^{\mathcal{I}_1})^{\mathrm{H}}z_1,$$

and

$$(I_\sigma^{\mathcal{I}_2})^{\mathrm{H}}x_1=-\delta_3[(I_\sigma^{\mathcal{I}_2})^{\mathrm{H}}\mathit{\Lambda}_3I_\sigma^{\mathcal{I}_2}]^{-1}(I_\sigma^{\mathcal{I}_2})^{\mathrm{H}}z_2.$$

This forces $(I_\sigma^{\mathcal{I}_1\cap\mathcal{I}_2})^{\mathrm{H}}z_1=(I_\sigma^{\mathcal{I}_1\cap\mathcal{I}_2})^{\mathrm{H}}z_2$.

Then, consider eqs. (19) and (20b), namely, solving $I^{(o)}T\mathit{\Lambda}_1x_1=0, I^{(o)}Tz_1=0, I^{(o)}Tz_2=0$. For ease, we mainly discuss the case in which the related index sets are nonempty. Inserting the solution of eq. (20a) into eq. (20b), we have

$$0=\begin{bmatrix}I^{(o)}T\mathit{\Lambda}_1x_1\\ I^{(o)}Tz_1\\ I^{(o)}Tz_2\\ (I_\sigma^{\mathcal{I}_1\cap\mathcal{I}_2})^{\mathrm{H}}(z_1-z_2)\end{bmatrix}=\begin{bmatrix}I^{(o)}TI_\sigma^{\mathcal{I}_0}[(I_\sigma^{\mathcal{I}_0})^{\mathrm{T}}\mathit{\Lambda}_1x_1]\\ I^{(o)}TI_\sigma^{\mathcal{I}_1}[(I_\sigma^{\mathcal{I}_1})^{\mathrm{T}}z_1]\\ I^{(o)}TI_\sigma^{\mathcal{I}_2}[(I_\sigma^{\mathcal{I}_2})^{\mathrm{T}}z_2]\\ (I_\sigma^{\mathcal{I}_1\cap\mathcal{I}_2})^{\mathrm{H}}(z_1-z_2)\end{bmatrix}=\widetilde{T}\begin{bmatrix}(I_\sigma^{\mathcal{I}_0})^{\mathrm{T}}\mathit{\Lambda}_1x_1\\ (I_\sigma^{\mathcal{I}_1\setminus\mathcal{I}_2})^{\mathrm{T}}z_1\\ (I_\sigma^{\mathcal{I}_1\cap\mathcal{I}_2})^{\mathrm{T}}z_1\\ (I_\sigma^{\mathcal{I}_2\setminus\mathcal{I}_1})^{\mathrm{T}}z_2\\ (I_\sigma^{\mathcal{I}_1\cap\mathcal{I}_2})^{\mathrm{T}}z_2\end{bmatrix},$$

where $\widetilde{T}=\begin{bmatrix}I^{(o)}TI_\sigma^{\mathcal{I}_0} & & & & \\ & I^{(o)}TI_\sigma^{\mathcal{I}_1\setminus\mathcal{I}_2} & I^{(o)}TI_\sigma^{\mathcal{I}_1\cap\mathcal{I}_2} & & \\ & & & I^{(o)}TI_\sigma^{\mathcal{I}_2\setminus\mathcal{I}_1} & I^{(o)}TI_\sigma^{\mathcal{I}_1\cap\mathcal{I}_2}\\ & & I & & -I\end{bmatrix}$. This equation has only trivial solutions, as long as $\begin{bmatrix}I^{(o)}TI_\sigma^{\mathcal{I}_0} & & \\ & I^{(o)}TI_\sigma^{\mathcal{I}_1} & \\ & & I^{(o)}TI_\sigma^{\mathcal{I}_2}\end{bmatrix}$ is of full column rank. Thus $\mathcal{S}=\{0\}$, as long as $\begin{bmatrix}I^{(o)}U_{\widehat{n}_{123}} & & \\ & I^{(o)}U_{\widehat{n}_{23}} & \\ & & I^{(o)}U_{\widehat{n}_{13}}\end{bmatrix}$ is of full column rank.

(2) $m_1\neq 0$: it is similar to **Case III-3**(1), considering the combination of **Case II-1** and **Case II-2**(2). Thus $\mathcal{S}=\{0\}$, as long as $\begin{bmatrix}I^{(o)}U_{\widehat{n}_{123}} & & \\ & I^{(o)}U_{\widehat{n}_{23}} & \\ & & I^{(o)}U_{\widehat{n}_{3}}\end{bmatrix}$ is of full column rank.

Case III-2. $\Lambda_\ell, \ell = 1,3$ are singular, but Λ_2 is nonsingular. It is similar to **Case III-1**, considering the combination of **Case II-1** and **Case II-3**,

Case III-1.. $\Lambda_\ell, \ell = 2,3$ are singular, but Λ_1 is nonsingular. It is similar to **Case III-1**, considering the combination of **Case II-2** and **Case II-3**.

Case IV. $\Lambda_\ell, \ell = 1,2,3$ are all singular.

(1) $m_1 = 0, \widehat{m}_1 = 0, m_2 = 0$: it is similar to **Case III-1**(1), considering the combination of **Case II-1**, **Case II-2** and **Case II-3**. Since $\Lambda_q = \Lambda_1^{\mathrm{H}}\Lambda_1 + \Lambda_2^{\mathrm{H}}\Lambda_2 + \Lambda_3^{\mathrm{H}}\Lambda_3 \succ 0$, we know $\mathcal{I}_1 \cap \mathcal{I}_2 \cap \mathcal{I}_3 = \emptyset$. Note that $(I_\sigma^{\mathcal{I}_1\cap\mathcal{I}_2})^{\mathrm{H}} z_1 = (I_\sigma^{\mathcal{I}_1\cap\mathcal{I}_2})^{\mathrm{H}} z_2$, $(I_\sigma^{\mathcal{I}_1\cap\mathcal{I}_3})^{\mathrm{H}} z_1 = (I_\sigma^{\mathcal{I}_1\cap\mathcal{I}_3})^{\mathrm{H}} z_3$, and $(I_\sigma^{\mathcal{I}_3\cap\mathcal{I}_2})^{\mathrm{H}} z_3 = (I_\sigma^{\mathcal{I}_3\cap\mathcal{I}_2})^{\mathrm{H}} z_2$. Thus, $\mathcal{S} = \{0\}$, as long as $\begin{bmatrix} I^{(o)}U_{\widehat{n}_{123}} & & & \\ & I^{(o)}U_{\widehat{n}_{23}} & & \\ & & I^{(o)}U_{\widehat{n}_{13}} & \\ & & & I^{(o)}U_{\widehat{n}_{12}} \end{bmatrix}$ is of full column rank.

(2) other cases: everything is similar.

To summarize, $\mathcal{S} = \{0\}$, as long as all the matrices below are of full column rank:

$$I^{(o)}U_{\widehat{n}_{123}}, I^{(o)}U_{\widehat{n}_{12}}, I^{(o)}U_{\widehat{n}_{23}}, I^{(o)}U_{\widehat{n}_{13}}, I^{(o)}U_{n_1}, I^{(o)}U_{n_2}, I^{(o)}U_{n_3}, I^{(o)}U_1.$$

Under the condition,

(1) $I^{(o)}U_1$ is of full rank because there is only one column, and each entry is 1.

(2) if $\mathcal{G}_1 = \{\langle i_1, i_2, i_3\rangle : i_1 \in \mathbb{Z}\} \subset \mathcal{D}_o$:
then $(I_\sigma^{\mathcal{G}})^{\mathrm{T}} I^{(o)}U_{\widehat{n}_{123}} = \eta_{\widehat{n}_{123}}^{i_2+i_3-2} V_{n_1\times\widehat{n}_{123}}(\eta_{\widehat{n}_{123}})$. Since $|\eta_{\widehat{n}_{123}}| = 1$ and the upper square block of $V_{n_1\times\widehat{n}_{123}}(\eta_{\widehat{n}_{123}})$ is $V_{\widehat{n}_{123}\times\widehat{n}_{123}}(\eta_{\widehat{n}_{123}})$, the DFT matrix of size $\widehat{n}_{123}$ that is nonsingular, we know $(I_\sigma^{\mathcal{G}})^{\mathrm{T}} I^{(o)}U_{\widehat{n}_{123}}$ is of full column rank, and so is $I^{(o)}U_{\widehat{n}_{123}}$. Similarly, $I^{(o)}U_{\widehat{n}_{12}}, I^{(o)}U_{\widehat{n}_{13}}, I^{(o)}U_{n_1}$ are of full column rank.

(3) if $\mathcal{G}_2 = \{\langle i_1, i_2, i_3\rangle : i_2 \in \mathbb{Z}\} \subset \mathcal{D}_o$:
then similarly $I^{(o)}U_{\widehat{n}_{123}}, I^{(o)}U_{\widehat{n}_{12}}, I^{(o)}U_{\widehat{n}_{23}}, I^{(o)}U_{n_2}$ are of full column rank.

(4) if $\mathcal{G}_3 = \{\langle i_1, i_2, i_3\rangle : i_3 \in \mathbb{Z}\} \subset \mathcal{D}_o$:
then similarly $I^{(o)}U_{\widehat{n}_{123}}, I^{(o)}U_{\widehat{n}_{13}}, I^{(o)}U_{\widehat{n}_{23}}, I^{(o)}U_{n_3}$ are of full column rank.

As a result, we have the lemma. □

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