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

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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, γ < γ∗ ≡ critical value, the γ-GEP is positive definite, which has been well-studied by Chern et. al, 2015. For the strongly coupled case, namely, γ > γ∗, 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 γ > 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 ∇× is fundamental and vital for efficient numerical simulations of complex materials. Here, complex materials, or physically, complex media,
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

\[ B = \mu H + \zeta E, \quad D = \varepsilon E + \xi H, \]

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

\[ \mu = \mu I, \quad \varepsilon = \varepsilon I, \quad \zeta = \zeta I, \quad \xi = \xi I, \]

where \( I \) represents the identity dyadics. Specifically, a Pasteur medium (a.k.a. the reciprocal chiral medium) is a type of biisotropic media, where \( \xi = \iota \gamma, \quad \zeta = -\iota \gamma, \quad \gamma \geq 0 \).

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

\[ \nabla \times E = \iota \omega B, \quad \nabla \cdot B = 0, \]
\[ \nabla \times H = -\iota \omega D, \quad \nabla \cdot D = 0, \]

or equivalently,

\[ \begin{bmatrix} \nabla \times & 0 \\ 0 & \nabla \times \end{bmatrix} \begin{bmatrix} E \\ H \end{bmatrix} = \iota \omega \begin{bmatrix} \zeta & \mu \\ -\varepsilon & -\xi \end{bmatrix} \begin{bmatrix} E \\ H \end{bmatrix}, \quad \begin{bmatrix} \nabla \cdot & 0 \\ 0 & \nabla \cdot \end{bmatrix} \begin{bmatrix} D \\ B \end{bmatrix} = 0, \]

where \( \omega \) 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 \( \exp(i2\pi k \cdot x) \) times a function \( u_k(x) \) with the periodicity of the crystal lattice.

Based on the Bloch theorem, the Bloch eigenvectors \( E \) and \( H \) on any crystal lattice, satisfying the quasi-periodic conditions

\[ E(x + a_\ell) = E(x) \exp(i2\pi k \cdot a_\ell), \quad H(x + a_\ell) = H(x) \exp(i2\pi k \cdot a_\ell) \]

are of interest, where \( 2\pi k \) is the Bloch wave vector in the first Brillouin zone \( B \), and \( a_\ell, \ell = 1, 2, 3 \) 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

\[ \begin{bmatrix} C & 0 \\ 0 & C^H \end{bmatrix} \begin{bmatrix} e \\ h \end{bmatrix} = \iota \omega \begin{bmatrix} \zeta_d & \mu_d \\ -\varepsilon_d & -\xi_d \end{bmatrix} \begin{bmatrix} e \\ h \end{bmatrix}, \]

where \( \mu_d, \varepsilon_d, \zeta_d \) and \( \xi_d \) 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 (2.1)-(2.4) below, for details).

For the Pasteur media, the matrix pair in (1.2) is positive definite when the parameter \( \gamma \) in (1.1) is small, but it becomes an indefinite pair as \( \gamma \) 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 $E$ and $H$ 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 (1.2) is always regular regardless of how large $\gamma$ is;

(b) The matrix pair (1.2) has $2 \times 2$ Jordan blocks of the infinite eigenvalues at the critical value $\gamma = \gamma_*$. Then, the $2 \times 2$ 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 $2 \times 2$ Jordan block of a real eigenvalue;

(c) This $2 \times 2$ 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 $\gamma$ is larger than the critical value $\gamma_*$. 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.** $i = \sqrt{-1}$ is the imaginary unit; $e = \exp(1)$ is Euler’s number. For any $n \in \mathbb{N}$, $\eta_n = e^{\frac{2\pi i}{n}}$ is an $n$th root of unity. For any index set $\mathcal{I}$, $I^\mathcal{I}$ denotes the diagonal matrix whose $i$th diagonal entry is 1 for all $i \in \mathcal{I}$ and 0 otherwise; $I^\mathcal{I}_2$ denotes the matrix consisting of all nonzero columns of $I^\mathcal{I}_2$; 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 $i$th 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 “$\prec$”, “$\preceq$”, and “$\succ$”. For $m \in \mathbb{N}, \alpha \in \mathbb{C}$ and $X \in \mathbb{C}^{m \times n}$, write

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

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

## 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 (1.2) 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 (1.2), in which $\zeta_d, \mu_d, \varepsilon_d, \xi_d$ are decided by the shape of the medium, and $C$ is given by Yee’s scheme. For the former, $\zeta_d, \mu_d, \varepsilon_d, \xi_d$ 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

$$\mu_d = \mu_o I_3 \otimes I, \quad \varepsilon_d = I_3 \otimes [\varepsilon_o I^{(o)} + \varepsilon_i I^{(i)}],$$

(2.1a)
\[ \zeta_d = -\ell \gamma I_3 \otimes I^{(i)}, \quad \zeta_d = \ell \gamma I_3 \otimes I^{(i)}, \] (2.1b) where \( \gamma \) is the chirality, \( \varepsilon_1, \varepsilon_2 \) are the permittivities inside and outside the medium, respectively, and \( \mu_{\infty} \equiv 1 \) is the permeability. For simplicity, here we denote \( I^{(i)} \equiv I^{D_i} \) and \( I^{(o)} \equiv I^{D_o} \).

For the latter, we refer the readers to [8] in order to pursue 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

\[ C = \begin{bmatrix} 0 & -C_3 & C_2 \\ C_3 & 0 & -C_1 \\ -C_2 & C_1 & 0 \end{bmatrix}, \] (2.2)

where

\[ C_1 = \delta_1^{-1} [-I_n + I_{m_3} \otimes I_{n_2} \otimes K_{n_1}(e^{2\pi k a_1})], \] (2.3a)
\[ C_2 = \delta_2^{-1} [-I_n + I_{m_3} \otimes K_{n_2}(e^{2\pi k a_2} J_1)], \] (2.3b)
\[ C_3 = \delta_3^{-1} [-I_n + K_{n_3}(e^{2\pi k a_3} J_2)], \] (2.3c)

with \( J_1 = J_{1,1} \) and

\[ J_2 = e^{2\pi k \rho_2 a_2} \left[ I_{n_2-m_2} \otimes J_{1,2} \right], \]
\[ J_1, \ell = e^{2\pi k \rho_1 \tau_{1,\ell}} \left[ I_{n_2-m_2} \right] e^{2\pi k \rho_2 a_2} J_{1,\ell}, \] \[ \ell = 1, 2, 3. \] (2.4a)

Here, \( \rho_2, \rho_1, 1, 2 \in \{0, 1\}, \rho_1, 2, 1, 3, 1 \in \{-1, 0, 1, 2\} \) satisfying \( \rho_{1,2} - \rho_{1,3} - m_{1,1} \in \{0, 1\}, \) 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 \( m_1 := m_{1,1}, m_1 := m_{1,1}, \) and \( m_1 := \rho_2 \rho_1 + \rho_2 \rho_1 + (1 - \rho_2) m_{1,3} \).

\( C_1, C_2, C_3 \) 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 \( T = [t_{\ell}]_{\ell=1,...,n} \) in the forms

\[ A_1 := T^H C_1 T = \delta_1^{-1} [-I_n + \eta_{m_1} \bar{a}_1 I_{n_2} \otimes D_{n_1}({\eta_{m_1}})], \] (2.5a)
\[ A_2 := T^H C_2 T = \delta_2^{-1} [-I_n + \eta_{m_2} \bar{a}_2 I_{n_2} \otimes D_{n_1}({\eta_{m_1}})], \] (2.5b)
\[ A_3 := T^H C_3 T = \delta_3^{-1} [-I_n + \eta_{m_2} \bar{a}_3 D_{n_2}({\eta_{m_3}}) \otimes D_{n_1}({\eta_{m_1}})], \] (2.5c)

where

\[ t_{i_1 i_2 i_3} = \frac{1}{\sqrt{\ell}} V_n (\eta_{\tilde{n}_n} \eta_{\bar{a}_3 + i_1} \eta_{\tilde{n}_n} \eta_{\bar{a}_2 + i_3} \eta_{\tilde{n}_n} \eta_{\bar{a}_1 + i_2}) \otimes V_n (\eta_{\tilde{n}_n} \eta_{\bar{a}_2 + i_3} \eta_{\tilde{n}_n} \eta_{\bar{a}_1 + i_2}) \otimes V_n (\eta_{\tilde{n}_n} \eta_{\bar{a}_1 + i_2}) \] (2.6)

for \( i_1, i_2, i_3 \in \mathbb{Z}, \{i_1, i_2, i_3\} \) is defined as

\[ (i_1, i_2, i_3) := (i_1', i_2', i_3') := (i_1' - 1)n_1n_2 + (i_2' - 1)n_1 + i_1', \]

where \( i_1' = i_1 + \ell n_1, 1 \leq i_1' \leq n_1, \ell \in \mathbb{Z}, \ell = 1, 2, 3, \) and

\[ \tilde{a}_1 = a_1, \]
\[ \tilde{a}_2 = a_2 + (\rho_1 - m_1 n_1) \tilde{a}_1, \]
\[ \tilde{a}_3 = a_3 + (\rho_2 - m_2 n_2) \tilde{a}_2 + [\tilde{m}_1 - m_1 n_1] - \rho_2 (\rho_1 - m_1 n_1) \tilde{a}_1, \]
\[ \tilde{m}_1 = \rho_2 m_1 + \rho_2 m_1 + (1 - \rho_2) m_{1,3}. \]
Note that
(a) \( \tilde{a}_1, \tilde{a}_2, \tilde{a}_3 \) is an orthogonal basis of \( a_1, a_2, a_3 \), and \( \| \tilde{a}_\ell \|_2 = l_\ell = n_\ell \delta_\ell \) for \( \ell = 1, 2, 3 \).

(b) \( 2\pi k \in \mathcal{B} \) implies
\[
| b_{\ell, \ell} | \leq k \cdot a_\ell \leq b_{\ell, \ell}, \quad \ell = 1, 2, 3,
\]
where \( b_{\ell, \ell} - b_{\ell, \ell} \leq 1, b_{\ell, \ell} \in [-2/3, 0], b_{\ell, \ell} \in [0, 5/6] \).

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 \( k \neq 0 \), then:

(a) \( A_q := A_1^H A_1 + A_2^H A_2 + A_3^H A_3 \succ 0 \);

(b) \( A_p := \begin{bmatrix} 0 & -\tau_3 & \tau_2 \\ \tau_3 & 0 & -\tau_1 \\ -\tau_2 & \tau_1 & 0 \end{bmatrix} \otimes I_n \) 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
\[
C = (I_3 \otimes T) \begin{bmatrix} A_q^{1/2} \\ A_q^{-1/2} \end{bmatrix} \begin{bmatrix} \Pi_1 \Pi_2 \Pi_0 \end{bmatrix}^{H} (I_3 \otimes T^H) = [P_r, P_0] \begin{bmatrix} \Sigma 0 \\ 0 0 \end{bmatrix} [Q_r, Q_0]^H = P_r \Sigma Q_r^H,
\]
where
\[
\Pi_0 = \begin{bmatrix} A_1 \\ A_2 \\ A_3 \end{bmatrix} \begin{bmatrix} A_q^{-1/2} \\ \Pi_1 \end{bmatrix} A_p (A_p^H A_p)^{-1/2} \Pi_1 = \begin{bmatrix} 0 & -A_3 & A_2 \\ A_3 & 0 & -A_1 \\ -A_2 & A_1 & 0 \end{bmatrix} A_p (A_p^H A_p)^{-1/2}.
\]

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 \( a_1, a_2, a_3 \). For ease, these 6 neighbors of a node are called its **lattice neighbors**. Define
\[
\mathcal{L}_\ell(i_1, i_2, i_3) := \{ (i'_1, i'_2, i'_3) : C_\ell(i_1', i_2', i_3') \neq 0 \text{ or } C_\ell(i_1', i_2') \neq 0 \}, \quad \ell = 1, 2, 3,
\]
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 \( \{i_1, i_2, i_3\} \) and its 6 lattice neighbors. Furthermore,
\[
\mathcal{L}(i_1, i_2, i_3) C_\ell \mathcal{L}(i_1, i_2, i_3) = 0, \quad \mathcal{L}(i_1, i_2, i_3) C_\ell \mathcal{L}(i_1, i_2, i_3) = 0.
\]

Moreover, we can define the boundary and interior of an index set \( \mathcal{I} \):
\[
\partial \mathcal{I} := \{ (i_1, i_2, i_3) \in \mathcal{I} : \mathcal{L}(i_1, i_2, i_3) \setminus \mathcal{I} \neq \emptyset \}, \quad \mathcal{I}^0 := \{ (i_1, i_2, i_3) \in \mathcal{I} : \mathcal{L}(i_1, i_2, i_3) \subset \mathcal{I} \}.
\]

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

It is easily seen that the GEP (1.2) can be rewritten as
\[
\begin{bmatrix} I_{3n}^{-1} & 0 \\ -\xi_d \mu_d^{-1} & -I_{3n} \end{bmatrix} \begin{bmatrix} 0 & -\tau C \\ i C^H \xi_d \mu_d^{-1} C & -\tau C \end{bmatrix} \begin{bmatrix} \mu_d \\ 0 \end{bmatrix} - \omega \begin{bmatrix} \mu_d \\ 0 \end{bmatrix} - \xi_d \mu_d^{-1} \zeta_d = 0,
\]
Together with the choices of \( \mu_d, \varepsilon_d, \zeta_d, \xi_d \), we can consider this matrix pair instead

\[
\begin{bmatrix}
0 & -iC \\
\i C^H - \gamma [(I_N \otimes I^{(i)})C + C^H(I_N \otimes I^{(i)})] & -\omega [I_N \otimes I_N - \i e_o I^{(o)} + (\varepsilon_i - \gamma^2)I^{(i)}]
\end{bmatrix}
\]

\[
:= A_{\gamma} - \omega B_{\gamma},
\]

also written as a matrix pair \((A_{\gamma}, B_{\gamma})\), which is equivalent to (1.2) in the sense that

\[
\begin{bmatrix}
h \\
e
\end{bmatrix} = 0.
\]

Moreover, if \((\omega, \begin{bmatrix} e \\ h \end{bmatrix})\) is an eigenpair of (1.2) with \( \omega \neq 0 \), then \( h = i(\gamma I_3 \otimes I^{(i)} - \omega^{-1} C)e \). Note

that \((A_{\gamma}, B_{\gamma})\) are Hermitian: \((A_{\gamma}, B_{\gamma})\) is regular if \( \gamma \neq \gamma_* \equiv \sqrt{\varepsilon} \); \( B_{\gamma} \) is indefinite if \( \gamma > \gamma_* \). Thus, all eigenvalues of \((A_{\gamma}, B_{\gamma})\) are real if \( \gamma < \gamma_* \).

The matrix pair \((A_{\gamma}, B_{\gamma})\) is also equivalent to a Hermitian quadratic matrix polynomial (a Hermitian QEP)

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

in the sense that for \( e \neq 0 \),

\[
(\omega, e) \text{ is an eigenpair of } (2.11) \Leftrightarrow (\omega, \begin{bmatrix} e \\ h \end{bmatrix}) \text{ is an eigenpair of } (1.2).
\]

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

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

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

where

\[
c(e) := e^H C^H Ce \geq 0,
\]

\[
b(e) := e^H [(I_N \otimes I^{(i)}) C + C^H (I_N \otimes I^{(i)})] e - 2\Re[e^H (I_N \otimes I^{(i)}) Ce] \in \mathbb{R},
\]

\[
a_o(e) := e^H I_N \otimes I^{(o)} e \geq 0,
\]

\[
a_i(e) := e^H (I_N \otimes I^{(o)}) e \geq 0.
\]

Furthermore,

\[
c(e) = 0 \Leftrightarrow Ce = 0, \quad a_o(e) = 0 \Leftrightarrow (I_N \otimes I^{(o)}) e = 0, \quad a_i(e) = 0 \Leftrightarrow (I_N \otimes I^{(i)}) e = 0.
\]

By (2.12), \( \omega \) is one of the roots of the scalar function

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

where

\[
\Delta(e) = \gamma^2 b(e)^2 + 4c(e)[\varepsilon_o a_o(e) + (\varepsilon_i - \gamma^2) a_i(e)].
\]
2.3 Null-space free GEP

Since the $6n \times 6n$ Hermitian matrix $A$ in (2.10) 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 (1.2) can be reduced to a $4n \times 4n$ NFGEP

$$\hat{A}_r y_r = \omega \left( \begin{bmatrix} 0 & \Sigma_r^{-1} \\ -\Sigma_r^{-1} & 0 \end{bmatrix} \right) y_r \equiv \omega \hat{B}_r y_r, \tag{2.15a}$$

and

$$[h \ e] = \omega \left[ \begin{bmatrix} -I_{3n} & -\xi_d \\ \xi_d & \varepsilon_d \end{bmatrix} \right]^{-1} \text{diag} \left( P_r, Q_r \right) y_r,$$

where

$$\hat{A}_r := \hat{A}_r(\gamma) \equiv \text{diag}(P_r^H, Q_r^H) \left[ \begin{bmatrix} \xi_d & -I_{3n} \\ I_{3n} & 0 \end{bmatrix} \right] \left[ \begin{bmatrix} \Phi & 0 \\ 0 & I_{3n} \end{bmatrix} \right] \left[ \begin{bmatrix} \xi_d & I_{3n} \\ -I_{3n} & 0 \end{bmatrix} \right] \text{diag}(P_r, Q_r) \tag{2.15b}$$

with $\Phi := \Phi(\gamma) \equiv I_3 \otimes (\varepsilon_i \varepsilon_d + (\varepsilon_i - \gamma^2) I(i))$ by (2.1).

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

$$\left\{ \begin{array}{l} \frac{d \omega(\gamma)}{d \gamma} \geq 0, \quad \text{if } \omega(\gamma) > 0, \\ \frac{d \omega(\gamma)}{d \gamma} \leq 0, \quad \text{if } \omega(\gamma) < 0, \end{array} \right.$$ 

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

Proof. For $\gamma < \gamma_*$, $\hat{A}_r$ in (2.15b) is positive definite. There is an eigenvector $y_r(\gamma)$ with $y_r^H(\gamma) \hat{A}_r(\gamma) y_r(\gamma) = 1$ such that

$$\frac{1}{\omega(\gamma)} = y_r^H(\gamma) \hat{B}_r y_r(\gamma). \tag{2.16a}$$

Because of $y_r^H(\gamma) \hat{A}_r(\gamma) y_r(\gamma) = 1$, we have

$$2R[(y_r^H(\gamma))^T \hat{A}_r(\gamma) y_r(\gamma)] + y_r^H(\gamma) \hat{A}_r(\gamma) y_r(\gamma) = 0. \tag{2.16b}$$

Taking the derivative of $\gamma$ in (2.16a), we have

$$-\frac{\omega'(\gamma)}{\omega(\gamma)^2} = 2\Re[(y_r^H(\gamma))^T \hat{B}_r y_r(\gamma)]$$

$$= \frac{2}{\omega(\gamma)} \Re[(y_r^H(\gamma))^T \hat{A}_r(\gamma) y_r(\gamma)] \tag{by (2.15a)}$$

$$= -\frac{1}{\omega(\gamma)} y_r^H(\gamma) \hat{A}_r(\gamma) y_r(\gamma) \tag{by (2.16b)}$$

$$= -\frac{1}{\omega(\gamma)} z_r^H(\gamma) \left( I_3 \otimes \left[ \frac{2\varepsilon_i}{2\varepsilon_i + \gamma^2} \frac{f(i)}{f(i)} \right] \right) z_r(\gamma) \tag{by (2.15b)}$$

$$= -\frac{1}{\omega(\gamma)} d(\gamma),$$

where $z_r(\gamma) := \text{diag}(P_r, Q_r) y_r(\gamma)$. Since the matrix

$$W = \frac{1}{(\varepsilon_i - \gamma^2)^2} \left[ \begin{bmatrix} 2\gamma \varepsilon_i & -\varepsilon_i^2 \gamma^2 \\ \varepsilon_i^2 \gamma^2 & 2\gamma \end{bmatrix} \right]$$

is orthogonally congruent to $\left[ \begin{bmatrix} 4\gamma(\varepsilon_i + 1)(\varepsilon_i - \gamma^2)^{-2} & 0 \\ 0 & -[4\gamma(\varepsilon_i + 1)]^{-2} \end{bmatrix} \right]$, 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 $d(\gamma) = 0$. \hfill $\square$
3 Eigenstructure of the discrete single-curl operator

3.1 Regularity

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

First, we locate the nullspace. It is easy to see that $\mathcal{N}(B) = \left[ \begin{array}{c} 0 \\ I_{3} \otimes I^{(i)} \end{array} \right]$. By theorem 2.2, from the SVD of $C$, we know that $\mathcal{N}(C) = \mathcal{R}((I_{3} \otimes T)H_{0})$ and $\mathcal{N}(C^{0}) = \mathcal{R}((I_{3} \otimes T)\Pi_{0})$. Thus, $\mathcal{N}(A_{\gamma}) = \mathcal{R}(L_{\gamma})$, where

$$L_{\gamma} = \left[ -i\gamma(I_{3} \otimes I^{(i)})(I_{3} \otimes T)H_{0} \\ (I_{3} \otimes T)\Pi_{0} \right].$$

Any column of $L_{\gamma}$ is an eigenvector corresponding to the eigenvalue 0 of either the matrix $A_{\gamma}$ or the matrix pair $(A_{\gamma}, B_{\gamma})$. In particular, for $(A_{\gamma}, B_{\gamma})$, 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 $I\prime_{s}^{(i)}$ and $I\prime_{s}^{(0)}$ to denote the matrices consisting of the nonzero columns of $I^{(i)}$ and $I^{(0)}$, respectively.

**Theorem 3.1.** For $z_{\ell} \in \mathcal{N}(A_{s}^{H}), \ell = 1, 2, 3$ satisfying

$$I^{(0)}Tz_{1} = I^{(0)}Tz_{2} = I^{(0)}Tz_{3}, \quad (3.1)$$

$S(z_{1}, z_{2}, z_{3})$ denotes the set of all nonzero $x_{1}$ that satisfies

$$(I_{n} + \delta_{1}A_{1})x_{1} - z_{1} = (I_{n} + \delta_{2}A_{2})x_{1} - z_{2} = (I_{n} + \delta_{3}A_{3})x_{1} - z_{3}, \quad (3.2a)$$

$$I^{(0)}TA_{1}x_{1} = 0. \quad (3.2b)$$

Then, $(A, B)$ is regular if and only if $S(z_{1}, z_{2}, z_{3}) = \{0\}$ for any proper $z_{\ell}$.

**Proof.** Suppose that $x \in \mathcal{N}(A) \cap \mathcal{N}(B)$. Since $\mathcal{N}(B) = \left[ \begin{array}{c} 0 \\ I_{3} \otimes I^{(i)} \end{array} \right]$, $x$ must be of the form

$$\left[ \begin{array}{c} 0 \\ (I_{3} \otimes I_{s}^{(i)})e_{0} \end{array} \right]$$

with some suitable vector $e_{0}$. Additionally, with some vectors $e_{1}$ and $e_{2}, x$ must be of the form

$$L_{\gamma_{\ast}} \left[ \begin{array}{c} e_{1} \\ \gamma_{\ast}e_{2} \end{array} \right] = \left[ \begin{array}{c} -i\gamma_{\ast}(I_{3} \otimes I^{(i)})(I_{3} \otimes T)H_{0}e_{1} + i\gamma_{\ast}(I_{3} \otimes T)\Pi_{0}e_{2} \\ (I_{3} \otimes T)H_{0}e_{1} \end{array} \right] = \left[ \begin{array}{c} 0 \\ (I_{3} \otimes I_{s}^{(i)})e_{0} \end{array} \right]. \quad (3.3)$$

From the second equation in (3.3), the first equation implies that

$$(I_{3} \otimes I^{(i)})(I_{3} \otimes T)H_{0}e_{1} = (I_{3} \otimes I^{(i)})(I_{3} \otimes I_{s}^{(i)})e_{0} = (I_{3} \otimes I_{s}^{(i)})e_{0} = (I_{3} \otimes T)\Pi_{0}e_{2},$$

which yields that

$$(I_{3} \otimes [T^{H}I\prime_{s}^{(i)}])e_{0} = H_{0}e_{1} = \Pi_{0}e_{2}, \quad (3.4)$$

with $e_{0} \neq 0$, and $e_{1}, e_{2}$ being not simultaneously zero. Let $x_{1} = A_{q}^{-1/2}e_{1}, x_{2} = A_{q}^{-1/2}e_{2}$ and $e_{0} = [y_{1}^{T} \ y_{2}^{T} \ y_{3}^{T}]^{T}$. The equations in (3.4) are equivalent to

$$T^{H}I\prime_{s}^{(i)}y_{1} = A_{1}x_{1} = A_{1}^{H}x_{1}, \quad T^{H}I\prime_{s}^{(i)}y_{2} = A_{2}x_{1} = A_{2}^{H}x_{2}, \quad T^{H}I\prime_{s}^{(i)}y_{3} = A_{3}x_{1} = A_{3}^{H}x_{3}. \quad (3.5)$$

Thus,

$$y_{1} = (I\prime_{s}^{(i)})^{H}TA_{1}x_{1}, \quad y_{2} = (I\prime_{s}^{(i)})^{HT}A_{2}x_{1}, \quad y_{3} = (I\prime_{s}^{(i)})^{HT}A_{3}x_{1}.$$

Noticing that $\delta_{s}^{-1}(e^{\theta} - 1) = -\delta_{s}^{-1}(e^{-\theta} - 1)e^{\theta}$ for any $\theta \in \mathbb{R}$, we have $A_{s} = -A_{s}^{H}(I_{n} + \delta_{s}A_{s})$. By (3.5), we have

$$-x_{2} = (I_{n} + \delta_{1}A_{1})x_{1} - z_{1} = (I_{n} + \delta_{2}A_{2})x_{1} - z_{2} = (I_{n} + \delta_{3}A_{3})x_{1} - z_{3}, \quad (3.6)$$

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namely, (3.2a), where $z_t \in \mathcal{N}(A_t^H)$. Left-multiplying $I^{(o)}T$ on the sides of (3.5) and noticing that $I^{(o)}T T^H I_t^{(o)} = 0$, we have

$$I^{(o)}T A_1 x_1 = 0, \quad I^{(o)}T A_2 x_1 = 0, \quad I^{(o)}T A_3 x_1 = 0,$$

which is equivalent to (3.2b) by the proper condition (3.1). Therefore,

$$\mathcal{N}(A) \cap \mathcal{N}(B) = \left\{ \begin{bmatrix} 0 \\ (I_3 \otimes T) I_0 A_q^{1/2} x_1 \end{bmatrix} : x_1 \in \mathbb{S} \right\}.$$  

Noticing that

$$\begin{bmatrix} 0 \\ I_0 A_q^{1/2} x_1 \end{bmatrix} \neq 0 \iff x_1^H A_q^{1/2} I_0^H I_0 A_q^{1/2} x_1 = x_1^H A_q x_1 \neq 0 \iff x_1 \neq 0.$$  

We have shown that $\mathcal{S}(z_1, z_2, z_3) = \{0\}$ 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 $\mathcal{S}(z_1, z_2, z_3) = \{0\}$.  

At this point, we have an equivalence condition that $(A, B)$ is regular. In practice, because the linear system in (3.2) is overdetermined, the condition $\mathcal{S}(z_1, z_2, z_3) = \{0\}$ 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 $x_1, x_2, x_3$, not all zero vectors, such that

$$(I^{(i)})^H M_2 I^{(i)} x_3 - (I^{(i)})^H M_3 I^{(i)} x_2 = 0,$$

$$(I^{(i)})^H M_3 I^{(i)} x_1 - (I^{(i)})^H M_1 I^{(i)} x_3 = 0,$$

$$(I^{(i)})^H M_1 I^{(i)} x_2 - (I^{(i)})^H M_2 I^{(i)} x_1 = 0,$$

where $M_t = C_t - C_t^H$.

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

$$B x = 0, \quad B y = A x.$$  

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

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

namely,

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

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

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

$$= -\gamma_* (I_3 \otimes I^{(i)}_\sigma)^H [(I_3 \otimes I^{(i)}) C + C^H (I_3 \otimes I^{(i)})] (I_3 \otimes I^{(i)}_\sigma)$$

$$= -\gamma_* (I_3 \otimes I^{(i)}_\sigma)^H (C^3 - C_3^H - C_2 + C_2^H) (I_3 \otimes I^{(i)}_\sigma)$$

$$= \begin{bmatrix} 0 & C_2 - C_2^H & C_1 - C_1^H & 0 \\ C_3 - C_3^H & 0 & -C_1 + C_1^H & 0 \\ -C_2 + C_2^H & C_1 - C_1^H & 0 & -C_3 + C_3^H \\ -C_3 + C_3^H & 0 & -C_1 + C_1^H & 0 \end{bmatrix} (I_3 \otimes I^{(i)}_\sigma)$$

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Clearly, \([x_1^T \ x_2^T \ x_3^T]^T \in N((B^H A N(B))^2)\) is equivalent to (3.7). 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 \(n_t > 2\). 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 \(i_\ell \in [1, n_t], \ell = 1, 2, 3, \) such that \(\mathcal{L}(i_1, i_2, i_3) \subset D_o\), or equivalently, \((i_1, i_2, i_3) \in D^o_0\).

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

**Proof.** First, we claim that under the assumption there exists a nonzero \(y\) such that

\[
(I^{(i)}_{\sigma})^H M_\ell I^{(i)}_{\sigma} y = 0, \quad \ell = 1, 2, 3; \quad \sum_{\ell=1}^3 y^H (I^{(i)}_{\sigma})^H M_\ell I^{(i)}_{\sigma} y \neq 0. \tag{3.8}
\]

Then, let \(x_\ell = (I^{(i)}_{\sigma})^H M_\ell I^{(i)}_{\sigma} y\). Note that \(M_\ell = -M_\ell^H\) and \(M_\ell = T(A_\ell - A_\ell^H)^T\). 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 (3.8), it holds that

\[
(I^{(i)}_{\sigma})^H M_\ell I^{(i)}_{\sigma} x_\ell - (I^{(i)}_{\sigma})^H M_\ell I^{(i)}_{\sigma} x_\ell = (I^{(i)}_{\sigma})^H M_\ell I^{(i)}_{\sigma} y - (I^{(i)}_{\sigma})^H M_\ell I^{(i)}_{\sigma} y = (I^{(i)}_{\sigma})^H M_\ell (I - I^{(i)}_{\sigma})^H M_\ell y - (I^{(i)}_{\sigma})^H M_\ell (I - I^{(i)}_{\sigma})^H M_\ell y = (I^{(i)}_{\sigma})^H M_\ell M_\ell - M_\ell M_\ell I^{(i)}_{\sigma} y = 0,
\]

or equivalently, \(x_\ell\) satisfy (3.7). On the other hand,

\[
x_1^H x_1 + x_2^H x_2 + x_3^H x_3 = \sum_{\ell} y^H (I^{(i)}_{\sigma})^H M_\ell^H (I^{(i)}_{\sigma})^H M_\ell I^{(i)}_{\sigma} y = \sum_{\ell} y^H (I^{(i)}_{\sigma})^H M_\ell^H (I^{(i)}_{\sigma})^H M_\ell I^{(i)}_{\sigma} y = \sum_{\ell} y^H (I^{(i)}_{\sigma})^H M_\ell^H M_\ell I^{(i)}_{\sigma} y \neq 0,
\]

which means that \(x_\ell\) are not all zeros. Therefore, by theorem 3.2, we have the result.

Finally we prove the claim. Since \(\mathcal{L}(i_1, i_2, i_3) \subset D_o\), we know \(D_o \subset D \setminus \mathcal{L}(i_1, i_2, i_3)\). By (2.9),

\[
epsilon^{H}_{(i_1, i_2, i_3)} M_\ell I^{(i)}_{\sigma} = \epsilon^{H}_{(i_1, i_2, i_3)} M_\ell I^{(i)}_{\sigma} = 0.
\]

On the other hand, \(M_\ell e_{(i_1, i_2, i_3)}\) is a column of \(M_\ell\) and thus nonzero, as long as \(n_t > 2\). Note that there exists \(y\) such that \(\epsilon_{(i_1, i_2, i_3)} = I^{(i)}_{\sigma}\) because \(\epsilon_{(i_1, i_2, i_3)} \in \mathcal{R}(I^{(i)}_{\sigma})\). Clearly, this \(y\) satisfies (3.8).

**Remark 3.1.** Write \(M = [M_1^T \ M_2^T \ M_3^T]^T\). From the proofs of theorems 3.2 and 3.3, we can see that

\[
\begin{bmatrix}
(I_3 \otimes (I^{(i)}_{\sigma} I^{(i)}_{\sigma})) M_\ell e_{(i_1, i_2, i_3)}
\end{bmatrix}
= \begin{bmatrix}
0 \\
M_\ell e_{(i_1, i_2, i_3)}
\end{bmatrix}
\]

is a corresponding eigenvector of the defective infinite eigenvalue.
3.2 The eigenvalue behavior when \( \gamma \rightarrow \gamma_* + 0 \)

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

\[
G_m := \begin{bmatrix} 1 & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 1 \end{bmatrix}_{m \times m}, \quad F_m := \begin{bmatrix} 1 \\ \vdots \\ 0 \end{bmatrix}_{m \times m}.
\]

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:

\( \text{B-c.} \ (\beta_j F_{kj} + G_{kj}, F_{2kj}), \ \beta_j \in \mathbb{C} \setminus \mathbb{R}, \ j = 1, \ldots, n_c, \) with possible replacement of \( \beta_j \) by \( \overline{\beta_j} \);

\( \text{B-r.} \ \mu_j (\alpha_j F_{kj} + G_{kj}), \ \alpha_j \in \mathbb{R}, \mu_j \in \{1, -1\}, \ j = 1, \ldots, n_r; \)

\( \text{B-\infty.} \ \nu_j (F_{kj} + G_{kj}), \ \nu_j \in \{1, -1\}, \ j = 1, \ldots, n_\infty. \)

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 \((A, B)\); \( \alpha_j \) is its real eigenvalue. Those \( k_j \)'s corresponding to the same value \( \alpha \) are called the \textit{partial multiplicities} of \( \alpha \); all \( \mu_j \)'s and \( \nu_j \)'s are called the \textit{sign characteristic} of \((A, B)\). A real eigenvalue \( \alpha_j \) with the corresponding \( \mu_j = 1 \) \( (\mu_j = -1) \) is called an eigenvalue of \textit{positive type} (\textit{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 \(6|\mathcal{D}_1|\) infinite eigenvalues, each of which is either semisimple or of positive type and associated with a Jordan block of size 2, and at least \(6n - 6|\mathcal{D}_1|\) semisimple eigenvalues of positive type.

**Proof.** Note that \( B \succeq 0 \) with \( \dim \mathcal{N}(B) = 3|\mathcal{D}_1| \) 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 \( \gamma \rightarrow \gamma_* + 0 \), there exist purely imaginary eigenvalues. If \((\omega, e)\) is an eigenpair of \( Q_\gamma(\omega) \) with \( \Im \omega \neq 0 \), then:

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

\( \text{(b)} \) \( Ce \neq 0, \Re[e^{\omega^*}(I_3 \otimes I^{(i)})Ce] = 0; \)

\( \text{(c)} \) \( \omega \) is pure imaginary, and \( \omega = \pm(\gamma^2 - \varepsilon_i)^{-1/2} \frac{\|Ce\|}{\|\omega\|}; \)

\( \text{(d)} \) \( |\omega| \) becomes smaller as \( \gamma \) becomes larger.

**Proof.** By theorems 3.3 and 3.4, \((A_{\gamma_*}, B_{\gamma_*})\) has a \(2 \times 2\) Jordan block \( W_\gamma(\lambda) \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} - \lambda \begin{bmatrix} 1 & \eta \\ \eta & -\eta \end{bmatrix} \) be a small perturbation of \( W_\gamma(\lambda) \) with \( \eta \rightarrow 0^+, \) as \( \gamma \rightarrow \gamma_*^+. \) Then, \( W_\gamma(\lambda) \) has a complex eigenvalue \( \omega \) of the form \( \omega \equiv \frac{1}{1+\eta} + i \frac{1}{\sqrt{\eta(1+\eta)}} \) with \( \Im \omega \neq 0. \) By (2.14), it implies that \( \Delta(e) < 0. \) Then, with \( \gamma \rightarrow \gamma_*^+, \) it forces that

\[
b(e) = 0, \quad c(e)a_\omega(e) = 0, \quad c(e)a_\omega(e) > 0,
\]

which, together with (2.13), implies the results of (a), (b) and (c). From (2.12), item (d) holds because

\[
\frac{d(|\omega|)}{d\gamma} = \frac{2\gamma\omega^2 a_\omega(e)}{|\Delta(e)|^{1/2}} \Rightarrow \frac{d(|\omega|)}{d\gamma} = \frac{2\gamma\omega^2 a_\omega(e)}{|\Delta(e)|^{1/2}} < 0.
\]

\[\square\]
3.3 Behavior of real eigenvalues

As we pointed out above, all the eigenvalues of the matrix pair \((A_\gamma, B_\gamma)\) are real if \(\gamma < \gamma_* \equiv \sqrt{\varepsilon}\). 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 \(A_\gamma, B_\gamma\) are defined as in (2.10), and \(B_\gamma\) 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 \(\omega\) is an eigenvalue associated with \(t\) Jordan blocks of odd size, of the matrix pair \((A_\gamma, B_\gamma)\), 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 \(\omega\) is an eigenvalue associated with \(t\) Jordan blocks of odd size, of the matrix pair \((A_\gamma, B_\gamma)\), 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 \(\gamma\). Let us discuss the inertia of those blocks one after another, except \(B-\infty\). Note that from section 2.2, we know that both \(\omega\) and \(\bar{\omega}\) with \(3\omega \neq 0\) are eigenvalues of \((A_\gamma, B_\gamma)\).

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

\[
L = \left[ (\beta_j - \omega)F_{m_j} + G_{m_j} \right]
\]

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 \(p_+(L) = s - 1 + \frac{1+\mu_j \text{ sign}(\alpha_j - \omega)}{2}, p_-(L) = s - 1 + \frac{1-\mu_j \text{ sign}(\alpha_j - \omega)}{2}\)

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 \(\gamma\). Thus, counting the inertia of the blocks of different types, we have

\[
\text{no. of } B-re(\mu=1) + \text{no. of } B-ro(\alpha=1) = \text{no. of } B-re(\mu=-1) + \text{no. of } B-ro(\alpha=-1).
\]

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

(a) \(B-c \rightarrow B-c\): the indices of inertia are the same;

(b) \(B-re \rightarrow B-c\): the indices of inertia are the same;

(c) \(B-re \rightarrow B-re\): the indices of inertia are the same;
After a systematical check, we have the result as the summary.

Theorem 3.7. which will collide at \(\beta\) the tangent lines of \(\eta\) with small perturbation \(y\) B-ro

(I) As we said before, any change of the structure of the blocks can be expressed as one or some all the reverse (go from right to left) and all the opposite (change \(\mu\)'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, \(\text{B-ro}(\mu = 1) = \text{B-ro}(\mu = 1) + \text{B-ro}(\mu = 1)\) can be treated as \(\text{B-c} \rightarrow \text{B-re} \rightarrow \text{B-ro}(\mu = 1) \rightarrow \text{B-ro}(\mu = 1) + \text{B-ro}(\mu = 1)\), 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 \(\text{B-ro}(\mu = 1) \rightarrow \text{B-ro}(\mu = 1)\) and \(\text{B-ro}(\mu = 1) \rightarrow \text{B-ro}(\mu = 1)\) happen simultaneously. However, if the involved eigenvalues are not the same, then \(\omega\) cannot be both between \(\alpha(\gamma_2)\) and \(\alpha(\gamma_2)\), or the positive index decreases 1 and the negative index increases 1 if \(\omega > \alpha(\gamma_2), \omega > \alpha(\gamma_2)\), 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 \(\mu\)'s sign).

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

Theorem 3.7. The case \(\text{B-c} \rightarrow \text{B-re} \rightarrow \text{B-ro}(\mu = 1) + \text{B-ro}(\mu = 1)\) 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 \(\gamma = \gamma > \gamma_*\), then it would bifurcate into two real eigenvalues \(\alpha(\gamma_1^\pm)(\mu = 1)\) and \(\alpha(\gamma_2^\pm)(\mu = 1)\).

Proof. theorems 3.4 and 3.5 show that \((A_{3\gamma}, B_{3\gamma})\) has a \(2 \times 2\) Jordan block at infinity and a purely imaginary eigenpair \(\pm \omega(\gamma)\) is created for \(\gamma \to \gamma_*^+\) with \(\frac{d\omega(\gamma)}{d\gamma} < 0\). Then, from (2.14), we denote the complex conjugate eigenvalue pair by \(\{\beta(\gamma), \bar{\beta}(\gamma)\}\) with \(\beta(\gamma^*) = \omega(\gamma^*)\) and \(\bar{\beta}(\gamma^*) = -\omega(\gamma^*)\) which will collide at \(\alpha(\gamma_1) = \alpha(\gamma_2) \in \mathbb{R}\) with \(\gamma > \gamma_*\). Consequently, it is sufficient to show that the tangent lines of \(\beta(\gamma)\) \(\cup \bar{\beta}(\gamma)\) and \(\alpha(\gamma) \equiv \alpha(\gamma) \cup \alpha(\gamma)\) 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 \(\gamma \to \gamma_*^+\).
We denote \( \text{Lemma 3.1.} \)
inertia. We have the following useful lemma.

**Proof.** We consider the inertia of \( B \). For a sufficiently small \( \alpha \),

\[
\begin{align*}
\left[ \begin{array}{cc}
0 & \alpha(\gamma_1) + \sqrt{\gamma} \\
\alpha(\gamma_1) - \sqrt{\gamma} & 0
\end{array} \right] &= \left[ \begin{array}{cc}
0 & 1 \\
1 & 0
\end{array} \right]
\end{align*}
\]

Here and hereafter, \( \sim^{eq.} \) denotes the equivalence transformation between two matrix pairs.

**Proof.** We consider the inertia of \( B \).

\[
\begin{align*}
\left[ \begin{array}{cc}
1 & \alpha(\gamma_1) \\
\alpha(\gamma_1) & 0
\end{array} \right]
\end{align*}
\]

\[
\left[ \begin{array}{cc}
0 & 1 \\
1 & 0
\end{array} \right]
\]

**Proof.** We consider the inertia of \( B \). For a sufficiently small \( \alpha \),

\[
\begin{align*}
\left[ \begin{array}{cc}
0 & \alpha(\gamma_1) + \sqrt{\gamma} \\
\alpha(\gamma_1) - \sqrt{\gamma} & 0
\end{array} \right] &= \left[ \begin{array}{cc}
0 & 1 \\
1 & 0
\end{array} \right]
\end{align*}
\]

Note that here it holds that

\[
\beta(\gamma_1) = \alpha(\gamma_1) + \sqrt{\gamma}, \quad (3.9a)
\]

\[
\alpha_{\epsilon, \gamma}(\gamma^+) = \alpha(\gamma_1) + \sqrt{\gamma} (\mu = \pm 1). \quad (3.9b)
\]

In (3.9a), by letting \( y = \sqrt{\gamma} \), we then have \( \frac{dy}{dy}_{y=0} = \infty \) if and only if \( \frac{dy}{dy}_{y=0} (\gamma=\gamma_1) = 0 \). Similarly, letting \( x = \sqrt{\gamma} \), from (3.9b) it follows that \( \frac{dy}{dy}_{y=0} (\gamma=\gamma_1) = 0 \). As a result, we have the theorem. \( \square \)

From (2.8), the SVD of \( C \) is written as

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

We denote

\[
U_0 := (I_3 \otimes I^{(i)}) Q_0, \quad U_1 := P_r^H (I_3 \otimes I^{(i)}) Q_0, \quad U_2 := P_0^H (I_3 \otimes I^{(i)}) Q_0
\]

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 \( k \neq 0 \) and \( n_\ell > 4 \). Then, it holds that \( U_2 \neq 0 \) and

\[
A_\gamma - \alpha B_\gamma \sim C_\gamma(\alpha) \equiv \begin{bmatrix} -\alpha I_{3n} & \frac{1}{\alpha} \Sigma^2 - \alpha \left[ \varepsilon U_0^H U_0 + \varepsilon_1 U_1^H U_1 + (\varepsilon_1 - \gamma^2) U_2^H U_2 \right] \end{bmatrix}
\]

as \( \alpha \to 0 \). Furthermore, \( \alpha = 0^- \) and \( \alpha = 0^+ \) are, respectively, the eigenvalues of \( (A_\gamma, B_\gamma) \) 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 \( \alpha \).

\[
A_\gamma - \alpha B_\gamma
\]

\[
= \begin{bmatrix} -\alpha I_{3n} & \frac{1}{\alpha} \Sigma^2 - \alpha \left[ \varepsilon U_0^H U_0 + \varepsilon_1 U_1^H U_1 + (\varepsilon_1 - \gamma^2) U_2^H U_2 \right] \\
\frac{1}{\alpha} \Sigma^2 - \alpha \left[ \varepsilon U_0^H U_0 + \varepsilon_1 U_1^H U_1 + (\varepsilon_1 - \gamma^2) U_2^H U_2 \right] & 0
\end{bmatrix}
\]

\[
\sim \begin{bmatrix} -\alpha I_{3n} & 0 \\
0 & 0
\end{bmatrix}
\]

\[
:= \begin{bmatrix} -\alpha I_{3n} & 0 \\
0 & \frac{1}{\alpha} \Sigma^2 - \alpha \left[ \varepsilon U_0^H U_0 + \varepsilon_1 U_1^H U_1 + (\varepsilon_1 - \gamma^2) U_2^H U_2 \right]
\end{bmatrix}
\]

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

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

Let us discuss the terms involved one by one.

(a) The term $Q^H \tilde{D}Q_r$: since

$$
Q^H \tilde{D}Q_r = Q^H \left(\frac{1}{\alpha}C^HC - D\right)Q_r = \frac{1}{\alpha}(\Sigma^2 - \alpha Q^HrDQ_r),
$$

we have

$$(Q^H \tilde{D}Q_r)^{-1} = \alpha(\Sigma^2 - \alpha Q^HrDQ_r)^{-1}
= \alpha\Sigma^{-1} (I - \alpha\Sigma^{-1}Q^HrDQ_r\Sigma^{-1})^{-1} \Sigma^{-1}
= \alpha\Sigma^{-1} (I - \alpha D_1)^{-1} \Sigma^{-1}
= \alpha\Sigma^{-1} (I + \alpha D_1 I - \alpha D_1)^{-1} \Sigma^{-1},
$$

where $D_1 = \Sigma^{-1}Q^HrDQ_r\Sigma^{-1}$.

(b) The term $Q^H \tilde{D}Q_0$:

$$
Q^H \tilde{D}Q_0 = Q^H \left(\frac{1}{\alpha}C^HC - D\right)Q_0 = -Q^HrDQ_0
= -Q^H \left(\gamma[I_3 \otimes I^{(i)}]C + C^H[I_3 \otimes I^{(i)}] \right)
+ \alpha I_3 \otimes [\varepsilon_o I^{(o)} + (\varepsilon_i - \gamma^2)I^{(i)}]Q_0
= -\alpha Q^HrI_3 \otimes [\varepsilon_o I^{(o)} + (\varepsilon_i - \gamma^2)I^{(i)}]Q_0
= -\alpha[\varepsilon_o U^H_0U_0 + (\varepsilon_i - \gamma^2)(U^H_1U_1 + U^H_2U_2)],
$$

where $U_0$, $U_1$ and $U_2$ are defined in (3.10).

(c) The term $Q^H_0 \tilde{D}Q_r$:

$$
Q^H_0 \tilde{D}Q_r = Q^H_0 \left(\frac{1}{\alpha}C^HC - D\right)Q_r = -Q^H_0rDQ_r,
= -Q^H_0 \left(\gamma[I_3 \otimes I^{(i)}]C + C^H[I_3 \otimes I^{(i)}] \right)
+ \alpha I_3 \otimes [\varepsilon_o I^{(o)} + (\varepsilon_i - \gamma^2)I^{(i)}]Q_r
= -\gamma Q^H_0[I_3 \otimes I^{(i)}]P_r \Sigma - \alpha Q^H_0I_3 \otimes [\varepsilon_o I^{(o)} + (\varepsilon_i - \gamma^2)I^{(i)}]Q_r
= -\gamma U^H_0 \Sigma - \alpha Q^H_0I_3 \otimes [\varepsilon_o I^{(o)} + (\varepsilon_i - \gamma^2)(I_n - I^{(i)})]Q_r
= -\gamma U^H_1 \Sigma - \alpha (\varepsilon_o - \varepsilon_i + \gamma^2)U^H_0Q_r - \alpha (\varepsilon_i - \gamma^2)Q^H_0Q_r
= -\gamma U^H_1 \Sigma - \alpha (\varepsilon_o - \varepsilon_i + \gamma^2)U^H_0Q_r.
$$

Thus,

$$
Q^H_0 \tilde{D}Q_0 = -Q^H_0 \tilde{D}Q_r(Q^H \tilde{D}Q_r)^{-1}Q^H_r \tilde{D}Q_0
$$
To summarize, for a sufficiently small $\alpha$, the indices of the inertia of $A$

\[
\text{As a result, in which the inequality holds because by theorem 2.1 and (2.7),}
\]

\[
\text{decreasingly. From (3.11), it follows that for } \alpha
\]

\[
\text{Thus,}
\]

\[
\text{Consider}
\]

\[
\text{Since}
\]

\[
\text{Finally, theorem 3.6 shows that $\alpha$ becomes an eigenvalue of the matrix pair $(A_\gamma, B_\gamma)$ once}
\]

\[
\text{the indices of the inertia of $A_\gamma - \alpha B_\gamma$ change by one whenever $\gamma$ runs over $\gamma_*$ increasingly or}
\]

\[
\text{decreasingly. From (3.11), it follows that for $\alpha = 0^-$ or $0^+$, some diagonal entry of $C_\gamma(\alpha)$ must}
\]

\[
\text{change sign as $\gamma$ increases. Therefore, there exists $\gamma = \gamma^- > \gamma_*$ and $\gamma = \gamma^+ > \gamma_*$ such that $\alpha = 0^-$}
\]

\[
\text{and $0^+$ are eigenvalues of $(A_\gamma, B_\gamma)$, respectively.}
\]
**Theorem 3.8.** Suppose \( k \neq 0 \) and \( n_\ell > 4 \). The number of positive/negative eigenvalues of \((A_\gamma, B_\gamma)\) increases as \( \gamma > \gamma_* \equiv \sqrt{\epsilon} \) 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 \( \text{rank}(\Pi B_\ell (I_3 \otimes (T^H I^0 T)) B_\ell) \) 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 \((A_\gamma, B_\gamma)\), 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 \( \gamma \) 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 \( \omega(\gamma) \) is a purely imaginary eigenvalue of \((A_\gamma, B_\gamma)\), for \( \gamma \to \gamma_*^+ \). Theorem 3.7 shows that the tangent line of the complex conjugate eigenvalue curves \( \beta(\gamma) \) is orthogonal to the real axis at some \( \gamma = \gamma_1 \) and bifurcate into two real eigenvalues \( \alpha(\gamma_1^+)(\mu = 1) \) and \( \alpha(\gamma_1^-)(\mu = -1) \).

From Lemma 3.1, we have that \( \alpha = 0^- \) is an eigenvalue of \((A_\gamma, B_\gamma)\) 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.

\[
B \cdot c \to B \cdot r \to B \cdot ro(\mu = 1) + B \cdot ro(\mu = -1).
\]

![Figure 3.1: Scenario of bifurcation.](image)

Scenario (see Figure 3.1 for details):

(i) Since \( \alpha = 0^- \) is an eigenvalue of \((A_\gamma, B_\gamma)\) and from the facts of (a) and (b), there is a complex conjugate eigenvalue pair \( \{\beta(\gamma), \bar{\beta}(\gamma)\} \) of \((A_\gamma, B_\gamma)\) 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 \( \alpha(\gamma_1^+)(\mu = 1) \) and \( \alpha(\gamma_1^-)(\mu = -1) \) with \( \alpha(\gamma_1^+)(\mu = 1) \) and \( \alpha(\gamma_1^-)(\mu = -1) \) moving toward the left and the right, respectively.

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

\[
\alpha_1(\gamma_2^+)(\mu = 1) < \alpha(\gamma_1) < \alpha(\gamma_2^+)(\mu = -1) \equiv 0^+ \tag{3.12}
\]
\[ 0 < \alpha_r(\gamma_3) < \alpha_1(\gamma_3) \]  

(3.13)

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 \( \{\tilde{\beta}(\gamma), \bar{\beta}(\gamma)\} \) of \((A_1, B_1)\) that collides at \( \gamma = \gamma_4 > \gamma_3 \) with

\[ 0 < \alpha_r(\gamma_3) < \alpha_r(\gamma_4) < \tilde{\alpha}_r(\gamma_4) \leq \hat{\alpha}(\gamma_4) = \tilde{\beta}(\gamma_4) \leq \hat{\alpha}(\gamma_4^+) \]  

(3.14)

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

\[ \gamma = \gamma_5^0 : B-ro(\mu = 1) + B-ro(\mu = -1) \]

\[ \to \gamma = \gamma_5 : B-re(\mu = -1) \to \gamma = \gamma_5^+ : B-re. \]  

(3.15)

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

From (3.11), 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 \( \{\tilde{\beta}(\gamma), \bar{\beta}(\gamma)\} \) 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 figure 2(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

\[ \text{rank}(U_2) = \text{rank}(\Pi_0^H(I_3 \otimes (T^H I(1))T))\Pi_0) \]

times because the matrix \((\varepsilon_i - \gamma^2)U_2^H U_2 \) in (3.11) makes \( B_\gamma \) change signs \( \text{rank}(U_2) \) times, as \( \gamma \to \infty \).

\[ \square \]

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 figure 1(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 \( \hat{A}_r \) in (2.15b) 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 \( \gamma \) increases from \( \sqrt{\varepsilon_i} \approx 3.6056 \) to 3.61397. The zoom-in view of the eigencurve-structure is shown in figure 1(b). The results demonstrate that four newly created smallest energies are produced on the tiny increment \( \Delta \gamma = 10^{-3} \) of \( \gamma \). 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.
In figure 4.2, 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 \( \alpha(\gamma) \equiv \alpha_r(\gamma) \cup \alpha_l(\gamma) \) at \( \gamma = \gamma_1 \) and \( \gamma_4 \) 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 \( \alpha_r(\gamma_1 + \Delta \gamma_1) \) and a negative eigenvalue \( \alpha_l(\gamma_4 + \Delta \gamma_4) \) along the real axis, where \( \Delta \gamma_1 = 6 \times 10^{-9} \) and \( \Delta \gamma_4 = 2 \times 10^{-8} \).

Figure 4.2: 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 \( \gamma \) 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 \( \mathbf{e} \) 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 \( G = G_1 \cup G_2 \cup G_3 \) with \( G_1 = \{ (i, i_2, i_3') : i \in \mathbb{Z} \}, G_2 = \{ (i'_1, i, i_3) : i \in \mathbb{Z} \}, G_3 = \{ (i_1, i'_2, i) : i \in \mathbb{Z} \}. \)

**Proof.** First, we will observe \( S \). To address it, we have to discuss several cases.

**Case I.** \( A_\ell, \ell = 1, 2, 3 \) are nonsingular. The only proper \( z_1, z_2, z_3 \) are all zero.

First, (3.2a) has nontrivial solutions if and only if there exists \( i_\ell \in [1, n_\ell], \ell = 1, 2, 3, \) such that

\[
\eta_{n_\ell}^k \hat{\lambda}_3 + i_\ell \eta_{n_\ell}^{-m} \hat{\lambda}_3 m_{n_\ell} = \eta_{n_\ell}^k \hat{\lambda}_2 + i_\ell \eta_{n_\ell}^{-m} \hat{\lambda}_2 m_{n_\ell} = \eta_{n_\ell}^k \hat{\lambda}_1 + i_\ell \eta_{n_\ell}^{-m} \hat{\lambda}_1 m_{n_\ell},
\]

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

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

for some \( s_1, s_2, s_3 \in \mathbb{Z} \). In other words, \( x_1 = I_T^0 x_1 \), where

\[
I_0 := \{ \langle \hat{\lambda} n_1 - \kappa_1, \hat{\lambda} n_2 - \kappa_2, \hat{\lambda} n_3 - \kappa_3 \rangle : \lambda \hat{\lambda} \in [0, 1), \}
\]

with

\[
\hat{\lambda} n_1 = n_1, \quad \kappa_1 = k \cdot a_1, \\
\hat{\lambda} n_2 = n_2 + m_1, \quad \kappa_2 = k \cdot (a_2 + p_1 a_1) - m_1 s_1, \\
\hat{\lambda} n_3 = n_3 + m_2 + \hat{m}_1, \quad \kappa_3 = k \cdot (a_3 + p_2 a_2 + \hat{m}_1 a_1) - m_2 s_2 - \hat{m}_1 s_1.
\]

Clearly, \( x_1 \neq 0 \) is equivalent to \( (I_T^0)^* T^0 x_1 \neq 0 \). Moreover, if \( I_0 \neq \emptyset \), then it can be shown that

\[
I_0 = \{ \langle \hat{\lambda} n_1 - \kappa_1, \hat{\lambda} n_2 - \kappa_2, \hat{\lambda} n_3 - \kappa_3 \rangle : \lambda = \lambda_0 + \frac{p}{n_1}, p \in [0, n_1) \cap \mathbb{Z}, \}
\]

with \( \lambda_0 \in [0, \frac{1}{n_1}) \) satisfying \( \lambda_0 \hat{\lambda} n_1 - \kappa_1 \in \mathbb{Z} \), and \( \hat{n}_1 = \text{gcd}(\hat{n}_1, \hat{n}_2, \hat{n}_3) \), the greatest common divisor of \( \hat{n}_1, \hat{n}_2 \) and \( \hat{n}_3 \). Note that \( \lambda_0 \) here is unique, and \( |I_0| = \hat{n}_1 = n_1. \)

Then, consider (3.2b), namely, solving \( I_T^0 T A_1 x_1 = 0 \). For ease, we mainly discuss the case that the related index sets are nonempty. Inserting the solution of (3.2a) into (3.2b), we have

\[
0 = I_T^0 T A_1 x_1 = I_T^0 T T I_T^0 A_1 x_1 = I_T^0 T T I_T^0 A_1 |x_1|. \]

Recall the form of \( T = |t_\ell| \) in (2.6). Write

\[
U_{n_1} = [u_{n_1}^\alpha | p = 1, \ldots, n_1], \quad u_{n_1}^\alpha := V_{n_3}(\beta_{n_1}^\alpha) \otimes V_{n_2}(\gamma_{n_1}^\beta) \otimes V_{n_1}(\delta^\gamma_{n_1}^\alpha),
\]

and \( t_0 = t(\lambda n_1 - \kappa_1, \lambda n_2 - \kappa_2, \lambda n_3 - \kappa_3) \). It can be seen that

\[
t((\lambda + \frac{p}{n_1} n_1 - \kappa_1, (\lambda + \frac{p}{n_1} n_2 - \kappa_2, (\lambda + \frac{p}{n_1} n_3 - \kappa_3)) = \text{diag}(u_{n_1}) t_0 = \text{diag}(t_0) u_{n_1},
\]

with \( p \in \mathbb{Z} \). On the other hand, if \( \lambda \hat{n}_1 - \kappa_1, \lambda \hat{n}_2 - \kappa_2, \lambda \hat{n}_3 - \kappa_3 \) is \( I_0 \), then \( (\lambda \hat{n}_1 - \kappa_1, \lambda \hat{n}_2 - \kappa_2, \lambda \hat{n}_3 - \kappa_3) \) is \( I_0 \). and \( \lambda \hat{n}_1 - \kappa_1, \lambda \hat{n}_2 - \kappa_2, \lambda \hat{n}_3 - \kappa_3 \) is \( I_0 \), then \( \lambda - \lambda' \hat{n}_1 = 0 \) in \( \mathbb{Z} \), which infers \( \lambda - \lambda' \text{gcd}(\hat{n}_1, \hat{n}_2, \hat{n}_3) \in \mathbb{Z} \) by Bézout’s identity.
and then $TI_σ^T = \text{diag}(t_0)U_{\tilde{n}_{123}}$. Thus,
\[
0 = I^{(o)}TI_σ^T[(I_σ^0)^TA_1x_1]
= I^{(o)}\text{diag}(t_0)U_{\tilde{n}_{123}}[(I_σ^0)^TA_1x_1]
= \text{diag}(t_0)I^{(o)}U_{\tilde{n}_{123}}[(I_σ^0)^TA_1I_σ^0][(I_σ^0)^T x_1].
\]
Noticing that each entry of $t_0$ is nonzero, and $(I_σ^0)^TA_1I_σ^0$ is nonsingular, $S = \{0\}$ is equivalent to $I^{(o)}U_{\tilde{n}_{123}} x = 0$ has only trivial solutions, namely, $I^{(o)}U_{\tilde{n}_{123}}$ is of full column rank.

**Case II-1.** $A_\ell, \ell = 2, 3$ are nonsingular, but $A_1$ is singular. By the form of $A_1$ in \eqref{2.5},
\[
A_1 \text{ is singular } \iff i_1 + k \cdot \hat{a}_1 \equiv \frac{n_1}{n_1} \in \mathbb{Z} \text{ for some } i_1 \iff k \cdot \hat{a}_1 = 0,
\]
and for the case $i_1 = n_1$. The only proper $z_2, z_3$ are both zero.

First, \eqref{3.2a} has nontrivial solutions, if and only if:

1. there exists $i_\ell \in [1, n_\ell], \ell = 1, 2, 3, i_\ell \neq n_\ell$, such that
\[
\frac{i_1 + k \cdot \hat{a}_1}{n_1} - s_1 = \frac{i_2 + k \cdot \hat{a}_2 - \frac{m_1 n_1}{n_1}}{n_2} - s_2
\]
\[
= \frac{i_3 + k \cdot \hat{a}_3 - \frac{m_2 n_2}{n_1 n_2} - \frac{m_3 n_3}{n_1} + \frac{m_3 n_2}{n_1 n_2} n_1}{n_3} - s_3 =: \lambda \in [0, 1),
\]

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

2. there exists $i_\ell \in [1, n_\ell], \ell = 2, 3$, such that
\[
\frac{i_2 + k \cdot \hat{a}_2 - \frac{m_1}{n_1}}{n_2} - s_2
\]
\[
= \frac{i_3 + k \cdot \hat{a}_3 - \frac{m_2}{n_2} i_2 - \frac{m_3}{n_1} n_1 + \frac{m_3}{n_1 n_2} n_1}{n_3} - s_3 =: \lambda \in [0, 1),
\]

for some $s_1, s_2, s_3 \in \mathbb{Z}$. For the case, the $(n_1, i_1, i_2, i_3)$-th entry of $x_1$ is decided by $z_1$, where $z_1 \in R(I_σ^z)$, and

$$
\mathcal{I}_1 := \{(n_1, \lambda \tilde{n}_2 - \kappa_2, \lambda \tilde{n}_3 - \kappa_3) : \lambda \tilde{n}_1 - \kappa_\ell \in \mathbb{Z}, 0 < \lambda < 1\}
= \{(n_1, \lambda \tilde{n}_2 - \kappa_2, \lambda \tilde{n}_3 - \kappa_3) : \lambda = \lambda_1 + \frac{\rho}{\tilde{n}_2}, \rho \in [0, \tilde{n}_2) \cap \mathbb{Z}\},
$$

and
\[
\tilde{n}_2 = n_2, \quad \kappa_2 = k \cdot (a_2 + \rho_1 a_1) - m_1,
\]
\[
\tilde{n}_3 = n_3 + m_2, \quad \kappa_3 = k \cdot (a_3 + \rho_2 a_2 + \hat{\rho}_1 a_1) - m_2 - s_2 - \hat{m}_1.
\]

In detail, $(I_σ^z)^{\text{H}} x_1 = -\delta_2[(I_σ^z)^{\text{H}} A_2 I_σ^z]^{-1} (I_σ^z)^{\text{H}} z_1$.

In other words, $x_1 = I_{\tilde{n}_2, \tilde{n}_3} x_1$. Moreover, if $\mathcal{I}_1 \neq \emptyset$, with $\lambda_1 \in [0, \frac{\tilde{n}_2}{\tilde{n}_2})$ satisfying $\lambda \tilde{n}_1 - \kappa_\ell \in \mathbb{Z}$, and $\tilde{n}_2 = \text{gcd}(\tilde{n}_2, \tilde{n}_3)$. Note that $\lambda_1$ here is unique, and $|\mathcal{I}_1| = \tilde{n}_2$. Clearly, $x_1 \neq 0$ is equivalent to $(I_σ^z)^{\text{H}} x_1 \neq 0$.

Then, consider \eqref{3.2b} and \eqref{3.1}, namely, solving $I^{(o)}TA_1x_1 = 0, I^{(o)}Tz_1 = 0$. For ease, we mainly discuss the case in which the related index sets are nonempty. Inserting the solution of \eqref{3.2a} into \eqref{3.2b}, we have
\[
0 = \begin{bmatrix} I^{(o)}TA_1x_1 \\ I^{(o)}Tz_1 \end{bmatrix} = \begin{bmatrix} I^{(o)}TA_1I_{\tilde{n}_2}x_1 \\ I^{(o)}Tz_1 \end{bmatrix} = \begin{bmatrix} I^{(o)}TTI_σ^T[(I_σ^0)^TA_1x_1] \\ I^{(o)}TTI_σ^Tz_1 \end{bmatrix}.
Similarly, \( S = \{0\} \) is equivalent to \[
\begin{bmatrix}
(I^{(o)}TI_2^{(o)})
\end{bmatrix}
\]
is of full column rank, where
\[
U_{\tilde{n}_{23}} = [u_{\tilde{n}_{23},p}]_{p=1,...,\tilde{n}_{23}}, \quad u_{\tilde{n}_{13},p} := V_{n_3}(\eta_{\tilde{n}_{23}}^p) \otimes V_{n_2}(\eta_{\tilde{n}_{13}}^p) \otimes V_{n_1}(1).
\]

**Case II-2.** \( \alpha, \ell = 1,3 \) are nonsingular, but \( A_2 \) is singular. By the form of \( A_2 \) in (2.5), we have:

1. \( m_1 = 0 \):
   
   \( A_2 \) is singular \( \Leftrightarrow \frac{i_2 + k \cdot \hat{a}_2}{n_2} \in \mathbb{Z} \) for some \( i_1, i_2 \)

   and everything is similar to **Case II-1.** \( S = \{0\} \) is equivalent to the matrix \[
\begin{bmatrix}
(I^{(o)}U_{\tilde{n}_{123}})
\end{bmatrix}
\]
is of full column rank, where
\[
U_{\tilde{n}_{13}} = [u_{\tilde{n}_{13},p}]_{p=1,...,\tilde{n}_{13}}, \quad u_{\tilde{n}_{13},p} := V_{n_3}(\eta_{\tilde{n}_{13}}^p) \otimes V_{n_2}(1) \otimes V_{n_1}(\eta_{\tilde{n}_{13}}^p).
\]

2. \( m_1 \neq 0 \):
   
   \( A_2 \) is singular \( \Leftrightarrow \frac{i_2 + k \cdot \hat{a}_2 - \frac{m_1 i_1}{n_1}}{n_3} \in \mathbb{Z} \) for some \( i_1, i_2 \)

   and for the case \( i_1 = \tilde{n}_2, i_2 = n_2 \). The only proper \( z_1, z_2, z_3 \) are both zero.

First, (3.2a) has nontrivial solutions, if and only if:

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

\[
\frac{i_1 + k \cdot \hat{a}_1}{n_1} = s_1 = \frac{i_2 + k \cdot \hat{a}_2 - \frac{m_1 i_1}{n_1}}{n_2} = s_2
\]

\[
\frac{i_3 + k \cdot \hat{a}_3 - \frac{m_2 i_2}{n_2} - \frac{\tilde{a}_1 i_1}{n_1} + \frac{m_1 m_2 i_1}{n_1 n_2}}{n_3} = s_3 =: \lambda \in [0, 1),
\]

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

(b) \((i_1, i_2) = (\tilde{n}_2, n_2) \). For the case, the \((\tilde{n}_2, n_2, i_3)\)-th entry of \( x_1 \) is decided by \( z_2 \), where
\[
z_2 \in \mathcal{R}(I_2^{(m)}) \}
\]

\( I_2^{(m)} := \{ (\tilde{n}_2, n_2, i_3) \} \).

In detail, \((I_2^{(m)})^HX_1 = -\delta_3[(I_2^{(m)})^HA_2I_2^{(m)}]^{-1}(I_2^{(m)})^H2_2 \).

In other words, \( x_1 = I_2^{(m)}x_1 \). Note that \( I_2^{(m)} = n_3 \). Clearly, \( x_1 \neq 0 \) is equivalent to \((I_2^{(m)})^HT_x \neq 0 \).

Then, consider (3.2b) and (3.1), namely, solving \( I^{(o)}TA_1x_1 = 0, I^{(o)}Tz_2 \). The steps proceed similarly to **Case II-1.** \( S = \{0\} \) is equivalent to \[
\begin{bmatrix}
(I^{(o)}U_{\tilde{n}_{123}})
\end{bmatrix}
\]
is of full column rank, where
\[
U_{n_3} = [u_{n_3,p}]_{p=1,...,n_3}, \quad u_{n_3,p} := V_{n_3}(\eta_{n_3}^p) \otimes V_{n_2}(1) \otimes V_{n_1}(1).
\]

**Case II-3.** \( \alpha, \ell = 1,2 \) are nonsingular, but \( A_3 \) is singular. By the form of \( A_3 \) in (2.5), we have:
(1) $\hat{m}_1 = 0, m_2 = 0$:

\[ A_3 \text{ is singular} \iff \frac{i_3 + k \cdot \hat{a}_3}{m_2} \in \mathbb{Z} \text{ for some } i_3 \]
\[ \iff k \cdot \hat{a}_3 = 0, \]

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

\[ U_{n_{12}} = [u_{n_{12},p}]_{p=1,\ldots,n_{12}}, \quad u_{n_{12},p} := V_{n_3}(1) \otimes V_{n_2}(\eta_{n_{12}}^p) \otimes V_{n_1}(\eta_{n_{12}}^p). \]

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

\[ A_3 \text{ is singular} \iff \frac{i_3 + k \cdot \hat{a}_3 - \frac{m_1}{m_2} i_1}{n_3} \in \mathbb{Z} \text{ for some } i_1, i_3 \]
\[ \iff \tilde{n}_{3,1} := \frac{n_1}{m_1} k \cdot \hat{a}_3 \in \mathbb{Z}, \]

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

\[ U_{n_2} = [u_{n_2,p}]_{p=1,\ldots,n_2}, \quad u_{n_2,p} := V_{n_3}(1) \otimes V_{n_2}(\eta_{n_2}^p) \otimes V_{n_1}(1). \]

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

\[ A_3 \text{ is singular} \iff \frac{i_3 + k \cdot \hat{a}_3 - \frac{m_2}{m_1} i_2}{n_3} \in \mathbb{Z} \text{ for some } i_2, i_3 \]
\[ \iff \tilde{n}_{3,2} := \frac{n_1}{m_1} k \cdot \hat{a}_3 \in \mathbb{Z}, \]

and everything is similar to Case II-2(2). $\mathcal{S} = \{0\}$ is equivalent to the matrix \[ \begin{bmatrix} I^{(o)} U_{n_{123}} \\ I^{(o)} U_{n_1} \end{bmatrix} \]
is of full column rank, where

\[ U_{n_1} = [u_{n_1,p}]_{p=1,\ldots,n_1}, \quad u_{n_1,p} := V_{n_3}(1) \otimes V_{n_2}(1) \otimes V_{n_1}(\eta_{n_1}^p). \]

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

\[ A_3 \text{ is singular} \iff \frac{i_3 + k \cdot \hat{a}_3 - \frac{m_2}{n_2} i_2 - \frac{m_1}{n_1} i_1 + \frac{m_1 m_2}{n_1 n_2} i_1}{n_3} \in \mathbb{Z} \text{ for some } i_1, i_2, i_3, \]

and for the case where there is only one choice $(i_1, i_2, i_3)$. Write the single-element set as $I_3^m$. The only proper $z_1, z_2$ are both zero.

First, (3.2a) has nontrivial solutions, if and only if:

(a) there exists $i \in [1, n]$, $\ell = 1, 2, 3$, $(i_1, i_2, i_3) \notin X_3^m$, such that

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

for some $s_1, s_2, s_3 \in \mathbb{Z}$. For the case, the $(i_1, i_2, i_3)$-th entry of $x_1$ is nonzero.
(b) \((i_1, i_2, i_3) \in I_3^m\). For the case, the \((\tilde{n}_2, n_2, i_3)\)-th entry of \(x_1\) is decided by \(z_3\), where \(z_2 \in \mathcal{R}(I^{n_3}_{3})\). In detail,

\[
(I^{n_3}_{3})^H x_1 = -\delta_3[[I^{n_3}_{3}]^H A_3 I^{n_3}_{3}]^{-1} (I^{n_3}_{3})^H z_3.
\]

In other words, \(x_1 = I_3^m \cup I_3^{n_3} x_1\). Note that \(|I^{n_3}_{3}| = n_1\). Clearly, \(x_1 \neq 0\) is equivalent to \((I^{n_3}_{3})^T x_1 \neq 0\).

Then, consider (3.2b) and (3.1), namely, solving \(I^{(o)} T A_1 x_1 = 0, I^{(o)} T z_2 = 0\). The steps proceed similarly to Case II-1. \(S = \{0\}\) is equivalent to \(\begin{bmatrix} I^{(o)} U_{\tilde{n}_{123}} & I^{(o)} U_1 \end{bmatrix}\) is of full column rank, where \(U_1 = [u_{1,1}], u_{1,1} := V_{n_3}(1) \otimes V_{n_1}(1) \otimes V_{n_1}(1)\).

Case III-3. \(A_\ell, \ell = 1, 2\) are singular, but \(A_3\) is nonsingular. The only proper \(z_3 = 0\). By the form of \(A_1, A_2\) in (2.5), we have:

(1) \(m_1 = 0\): it is similar to the combination of Case I-1 and Case III-2(1).

\(A_1\) is singular \(\iff \frac{i_1 + k \cdot \hat{a}_1}{n_1} \in \mathbb{Z}\) for some \(i_1 \iff k \cdot \hat{a}_1 = 0\),

\(A_2\) is singular \(\iff \frac{i_2 + k \cdot \hat{a}_2}{n_2} \in \mathbb{Z}\) for some \(i_2 \iff k \cdot \hat{a}_2 = 0\).

In detail,

\[
(I^{n_3}_{3})^H x_1 = -\delta_3[[I^{n_3}_{3}]^H A_3 I^{n_3}_{3}]^{-1} (I^{n_3}_{3})^H z_1,
\]

and

\[
(I^{n_3}_{3})^H x_1 = -\delta_3[[I^{n_3}_{3}]^H A_3 I^{n_3}_{3}]^{-1} (I^{n_3}_{3})^H z_2.
\]

This forces \((I^{n_3}_{3})^H z_1 = (I^{n_3}_{3})^H z_2\).

Then, consider (3.2b) and (3.1), namely, solving \(I^{(o)} T A_1 x_1 = 0, I^{(o)} T z_1 = 0, I^{(o)} T z_2 = 0\). For ease, we mainly discuss the case in which the related index sets are nonempty. Inserting the solution of (3.2a) into (3.2b), we have

\[
0 = \begin{bmatrix} I^{(o)} T A_1 x_1 \\ I^{(o)} T z_1 \\ I^{(o)} T z_2 \\ (I^{n_3}_{3})^H (z_1 - z_2) \end{bmatrix} = \begin{bmatrix} I^{(o)} T I^{n_3}_{3} A_1 x_1 \\ I^{(o)} T I^{n_3}_{3} z_1 \\ I^{(o)} T I^{n_3}_{3} z_2 \\ (I^{n_3}_{3})^H (z_1 - z_2) \end{bmatrix} = \begin{bmatrix} I^{(o)} T A_1 x_1 \\ I^{(o)} T z_1 \\ I^{(o)} T z_2 \\ (I^{n_3}_{3})^H (z_1 - z_2) \end{bmatrix},
\]

where \(\tilde{T} = \begin{bmatrix} I^{(o)} T I^{n_3}_{3} \\ I^{(o)} T I^{n_3}_{3} z_2 \\ I^{(o)} T I^{n_3}_{3} z_2 \\ I^{(o)} T I^{n_3}_{3} x_1 \\ I^{(o)} T I^{n_3}_{3} x_2 \\ I^{(o)} T I^{n_3}_{3} x_2 \end{bmatrix}\). This equation has

\[
I^{(o)} T I^{n_3}_{3} z_2 = I^{(o)} T I^{n_3}_{3} x_2
\]

only trivial solutions, as long as

\[
\begin{bmatrix} I^{(o)} T I^{n_3}_{3} \\ I^{(o)} T I^{n_3}_{3} z_1 \\ I^{(o)} T I^{n_3}_{3} x_1 \end{bmatrix}
\]

is of full column rank. Thus

\[
S = \{0\}, \text{ as long as } \begin{bmatrix} I^{(o)} U_{\tilde{n}_{123}} \\ I^{(o)} U_{\tilde{n}_{23}} \\ I^{(o)} U_{\tilde{n}_{123}} \end{bmatrix}
\]

is of full column rank.

(2) \(m_1 \neq 0\): it is similar to Case III-3(1), considering the combination of Case I-1 and Case II-2(2). Thus \(S = \{0\}\), as long as

\[
\begin{bmatrix} I^{(o)} U_{\tilde{n}_{123}} \\ I^{(o)} U_{\tilde{n}_{23}} \\ I^{(o)} U_{\tilde{n}_{123}} \end{bmatrix}
\]

is of full column rank.
Case III-2. $A_{\ell}, \ell = 1, 3$ are singular, but $A_2$ is nonsingular. It is similar to Case III-1, considering the combination of Case II-1 and Case II-3.

Case III-1. $A_{\ell}, \ell = 2, 3$ are singular, but $A_1$ is nonsingular. It is similar to Case III-1, considering the combination of Case II-2 and Case II-3.

Case IV. $A_{\ell}, \ell = 1, 2, 3$ are all singular.

(1) $m_1 = 0, \tilde{m}_1 = 0, m_2 = 0$: it is similar to Case III-1(1), considering the combination of Case II-1, Case II-2, and Case II-3. Since $A_{g} = A_1^{g} + A_2^{g} + A_3^{g} \succ 0$, we know $\mathcal{I}_1 \cap \mathcal{I}_2 \cap \mathcal{I}_3 = \emptyset$. Note that $(I_{g}^{2, \tau} \mathcal{Z}_2)^{H}_z = (I_{g}^{2, \tau} \mathcal{Z}_2)^{H}_{z_2}$, $(I_{g}^{2, \tau} \mathcal{Z}_2)^{H}_z = (I_{g}^{2, \tau} \mathcal{Z}_2)^{H}_{z_3}$, and $(I_{g}^{2, \tau} \mathcal{Z}_2)^{H}_z = (I_{g}^{2, \tau} \mathcal{Z}_2)^{H}_{z_2}$. Thus, $S = \{0\}$, as long as

$$
\begin{bmatrix}
I^{(o)}u_{\tilde{r}_{123}} & I^{(o)}u_{\tilde{r}_{12}} & I^{(o)}u_{\tilde{r}_{23}} & I^{(o)}u_{\tilde{r}_{13}} & I^{(o)}u_{n_1}\nI^{(o)}u_{\tilde{r}_{12}} & I^{(o)}u_{\tilde{r}_{13}} & I^{(o)}u_{n_1} & I^{(o)}u_{n_2} & I^{(o)}u_{n_3} & I^{(o)}u_{1}\nI^{(o)}u_{\tilde{r}_{23}} & I^{(o)}u_{\tilde{r}_{13}} & I^{(o)}u_{n_1} & I^{(o)}u_{n_2} & I^{(o)}u_{n_3} & I^{(o)}u_{1}\nI^{(o)}u_{\tilde{r}_{12}} & I^{(o)}u_{\tilde{r}_{13}} & I^{(o)}u_{n_1} & I^{(o)}u_{n_2} & I^{(o)}u_{n_3} & I^{(o)}u_{1}\nI^{(o)}u_{\tilde{r}_{12}} & I^{(o)}u_{\tilde{r}_{13}} & I^{(o)}u_{n_1} & I^{(o)}u_{n_2} & I^{(o)}u_{n_3} & I^{(o)}u_{1}\nI^{(o)}u_{\tilde{r}_{12}} & I^{(o)}u_{\tilde{r}_{13}} & I^{(o)}u_{n_1} & I^{(o)}u_{n_2} & I^{(o)}u_{n_3} & I^{(o)}u_{1}
\end{bmatrix}
$$

is of full column rank.

(2) other cases: everything is similar.

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

$$
I^{(o)}u_{\tilde{r}_{123}}, I^{(o)}u_{\tilde{r}_{12}}, I^{(o)}u_{\tilde{r}_{23}}, I^{(o)}u_{\tilde{r}_{13}}, I^{(o)}u_{n_1}, I^{(o)}u_{n_2}, I^{(o)}u_{n_3}, I^{(o)}u_{1}
$$

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 $\mathcal{G}_1 = \{i_1, i_2, i_3\} \subset \mathcal{D}_o$:
then $(P_{g})^{T}I^{(o)}u_{\tilde{n}_{123}} = (P_{g})^{T}I^{(o)}u_{\tilde{n}_{12}} = (P_{g})^{T}I^{(o)}u_{\tilde{n}_{23}} = (P_{g})^{T}I^{(o)}u_{\tilde{n}_{13}} = (P_{g})^{T}I^{(o)}u_{\tilde{n}_{1}}$(hemispherical projection). Since $|\eta_{\tilde{n}_{123}}| = 1$ and the upper square block of $V_{n_1 \times \tilde{n}_{123}}(\eta_{\tilde{n}_{123}}) \in V_{n_1 \times \tilde{n}_{123}}(\eta_{\tilde{n}_{123}})$, the DFT matrix of size $\tilde{n}_{123}$ that is nonsingular, we know $(P_{g})^{T}I^{(o)}u_{\tilde{n}_{123}}$ is of full column rank, and so is $I^{(o)}u_{\tilde{n}_{123}}$. Similarly, $I^{(o)}u_{\tilde{n}_{12}}, I^{(o)}u_{\tilde{n}_{13}}, I^{(o)}u_{n_1}$ are of full column rank.

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

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

As a result, we have the lemma.

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