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This paper studies the existence of electromagnetic surface waves localized on a boundary of half-infinite periodic superlattices formed by an arbitrary periodic sequence of layers of homogeneous or functionally graded materials with generally anisotropic dielectric permittivity and magnetic permeability tensors. The geometry in question implies either two superlattices attached together to form a photonic bicrystal or else a superlattice in contact with vacuum or any other homogeneous dielectric or metal. Using the formalism of transfer and impedance matrices, a series of statements is proved on the maximum number of surface waves which may exist within a forbidden band at a fixed tangential wave number. This number embraces possible occurrences of surface waves in a given bicrystal and in its counterpart obtained by swapping the upper and lower superlattices. A maximum total number of surface waves in both these structures with an arbitrary arrangement of their unit cells is 2 in the lowest forbidden band (extending from zero frequency) and 4 in any upper forbidden band. The same statements apply to the case where one of the half spaces is occupied by a homogeneous material. A factor 2 smaller number of surface waves occur in a bicrystal composed of superlattices with a symmetric arrangement of unit cells. The existence considerations are further specialized for the surface waves with TE and TM polarizations.

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I. INTRODUCTION

Theoretical and experimental investigation of bulk and localized (surface) waves in periodic optical structures called photonic crystals has been a focus of attention for a few decades [1–4]. Active studies in this field are stimulated by potentially vast areas of application, such as antenna engineering [3,5], optical communication systems [6–8], and optical sensors [9–12]. Various topics of interest concern, among other issues, the band structure of electromagnetic wave spectra, the reflection and refraction of bulk waves, and the occurrence of surface electromagnetic waves (SEWs). Theoretical analysis of the propagation of electromagnetic waves in two- and three-dimensional photonic crystals is essentially based on numerical methods [3,4,13,14]. The case of one-dimensional photonic crystals, or superlattices, admits closed-form analytical results for some basic wave parameters, particularly when the crystal is fabricated of optically isotropic materials and has a simple structure. For instance, a bilayered superlattice composed of isotropic materials allows a simple explicit expression of the transfer matrix and hence of the reflection and refraction coefficients as well as of the dispersion equation for surface waves (see [15,16]). Within the above framework, explicit calculations have proved fruitful for studying different aspects of the SEW propagation in half-infinite superlattices under different boundary conditions [15–22], in finite superlattices on a substrate [23,24], and in quasiperiodic [25,26] and functionally graded [27–29] superlattices. At the same time, it is well known that the SEW dispersion equation even for the simplest setups is a transcendental one, i.e., it does not admit a closed-form solution, and, moreover, its formulation for more general cases of anisotropic superlattices with a complex arrangement of unit cells (period) is virtually implicit. Thus a direct approach to finding SEWs usually comes down to a numerical procedure which has to be implemented anew for each new set of material data and the frequency and wave-number values. Evidently, such strategy is by construction unable to yield an insight into the SEW existence conditions in general. The latter task requires some special analytical approaches.

A similar challenge is faced in acoustics. A general method for successful solving of the existence problem for the surface acoustic waves in anisotropic homogeneous elastic and piezoelectric solids was developed and applied in [30–33]. The method rested on the so-called Stroh formulation of the wave equation together with the constitutive relations [34], which was complemented by introduction of the surface impedance matrices linked to the energy quantities [35]. This approach combined with the transfer-matrix technique was recently extended to surface waves in one-dimensional phononic crystals [36–40].

In contrast to acoustic waves, no SEWs exist on an interface between half-infinite homogeneous isotropic solids unless the dielectric permittivity of one of them is negative [41]. However, if at least one of the adjoined solids is optically anisotropic, then its dielectric permittivity does not need to be negative for admitting a surface wave. Such waves were investigated via explicit calculations in a series of publications

[42–57]. Existence of SEWs in dielectric materials with generally anisotropic permittivity was studied in [58,59]. Adapting the concepts of the Stroh integral matrix and the surface impedances from the acoustic-wave theory [30–33] to the case of the Maxwell equations and invoking the Lagrangian density of electromagnetic field, it was shown that at most one dispersionless SEW can exist at the interface between two anisotropic homogeneous half spaces [59].

The present paper is concerned with the existence of SEWs in superlattices formed by arbitrary periodic repetition of layers of homogeneous or functionally graded materials possessing generally anisotropic dielectric permittivity and magnetic permeability but being nongyrotropic and nonabsorbing. As usual, the assumption of no losses implies in practical terms referring the consideration to frequency ranges of negligible absorption. Our approach to formulating and analyzing the SEW dispersion equation stems from the methodology developed in [30–33] for homogeneous elastic media and modified for phononic crystals in [36–40]. We will use the general properties of the transfer matrix through a period and of the appropriately defined impedance matrices. It is worth noting that, in contrast to the formalism of [58,59], the treatment developed in our paper operates without the need for the "optical" integral Stroh matrix and Lagrangian density of electromagnetic fields and, additionally, it involves magnetic anisotropy as well as takes into account the frequency dependence of dielectric permittivity and magnetic permeability. Such a framework allows us to establish the maximum possible number of SEWs for a forbidden band (wave number being fixed) which may exist on an interface of a photonic bicrystal composed of two half-infinite superlattices. The results obtained for the general setting of the problem will be specialized for particular cases such as a superlattice bounded by a homogeneous medium (e.g., vacuum), a superlattice with a symmetrically arranged unit cell, and a superlattice of a certain crystallographic symmetry for which the sought SEWs consist of uncoupled TE or TM modes.

Note that the issue of symmetry appears in the paper in different senses. First of all, it is assumed throughout that any given regular stratification is observed strictly, i.e., there is no dispersion of thickness of layers and no structural defects affecting wave spectra (otherwise see, e.g., [60–62]; this aspect is also touched upon in Sec. IV). At the same time, we will see that the properties of waves propagating in a perfectly periodic material depend essentially on whether the unit cell is formed of layers arranged in the symmetric or in any asymmetric stacking order. Another matter is anisotropy, or crystallographic symmetry of the constituent materials. Its impact is especially manifested when it allows for electromagnetic waves of transverse polarizations. Considerations of the paper concern materials of unrestricted anisotropy, i.e., of any crystallographic symmetry; however, an additional focus is set on the case of TE and TM waves in view of their wide relevance to practical applications.

The paper is organized as follows. Definition and basic properties of the transfer matrices and the impedance matrices related to photonic superlattices are given in Sec. II. The results on the existence of SEWs in adjoined superlattices and in superlattices on a homogeneous substrate or in contact with vacuum are presented in Sec. III. Numerical examples are discussed in Sec. IV. The conclusions are recapitulated in Sec. V. The proofs of some key properties of the impedance and related matrices are provided in Appendices A and B.

II. TRANSFER MATRIX AND IMPEDANCE MATRICES

A. Transfer matrix

Consider an optically anisotropic nongyrotropic and nonabsorbing medium. Taking the stratification direction as the axis Z, assume an electromagnetic wave of the form

$$\begin{pmatrix}\mathbf{E}(\mathbf{r},t)\\ \mathbf{H}(\mathbf{r},t)\end{pmatrix}=\begin{pmatrix}\mathbb{E}(z)\\ \mathbb{H}(z)\end{pmatrix}e^{i(kx-\omega t)}, \tag{1}$$

where $\mathbf{E}$ and $\mathbf{H}$ are the vectors of electric and magnetic fields, $\mathbf{r}$ is the radius vector, and ω and k are frequency and wave number. As applied to the wave (1), the Maxwell equations can be cast into a system of four ordinary differential equations:

$$\frac{d\boldsymbol{\xi}}{dz}=i\hat{\mathbf{N}}\boldsymbol{\xi}, \tag{2}$$

where the vector $\boldsymbol{\xi}(z)$ is composed of xth and yth components of amplitudes $\mathbb{E}(z)$ and $\mathbb{H}(z)$ [15,16,58,59,63]. We choose to take

$$\boldsymbol{\xi}(z)=\begin{pmatrix}\mathbf{u}\\ \mathbf{v}\end{pmatrix},\quad \mathbf{u}(z)=\begin{pmatrix}-\mathbb{E}_y\\ \mathbb{H}_y\end{pmatrix},\quad \mathbf{v}(z)=\begin{pmatrix}\mathbb{H}_x\\ \mathbb{E}_x\end{pmatrix}. \tag{3}$$

The corresponding matrix $\hat{\mathbf{N}}$ in a layer takes the form

$$\hat{\mathbf{N}}=\begin{pmatrix}-k\frac{\mu_{xz}}{\mu_{zz}} & \omega m_{xy} & \omega m_{xx} & 0\\ -\omega\epsilon_{xy} & -k\frac{\varepsilon_{xz}}{\varepsilon_{zz}} & 0 & \omega\epsilon_{xx}\\ \omega\epsilon_{yy}-\frac{k^2}{\omega\mu_{zz}} & k\left(\frac{\varepsilon_{yz}}{\varepsilon_{zz}}-\frac{\mu_{yz}}{\mu_{zz}}\right) & -k\frac{\mu_{xz}}{\mu_{zz}} & -\omega\epsilon_{xy}\\ k\left(\frac{\varepsilon_{yz}}{\varepsilon_{zz}}-\frac{\mu_{yz}}{\mu_{zz}}\right) & \omega m_{yy}-\frac{k^2}{\omega\varepsilon_{zz}} & \omega m_{xy} & -k\frac{\varepsilon_{xz}}{\varepsilon_{zz}}\end{pmatrix}, \tag{4}$$

where the SI system of units is adopted,

$$\epsilon_{ij}=\varepsilon_{ij}-\varepsilon_{iz}\varepsilon_{jz}\varepsilon_{zz}^{-1};\ m_{ij}=\mu_{ij}-\mu_{iz}\mu_{jz}\mu_{zz}^{-1},\ i,j=x,y, \tag{5}$$

ε_{ij} and μ_{ij} are the components of tensors of dielectric permittivity $\hat{\boldsymbol{\varepsilon}}$ and magnetic permeability $\hat{\boldsymbol{\mu}}$, respectively. By construction, the matrix $\hat{\mathbf{N}}$ satisfies the symmetry

$$(\hat{\mathbf{T}}\hat{\mathbf{N}})^t=\hat{\mathbf{T}}\hat{\mathbf{N}}, \tag{6}$$

where the subscript t means transpose and

$$\hat{\mathbf{T}}=\begin{pmatrix}\hat{\mathbf{0}} & \hat{\mathbf{I}}\\ \hat{\mathbf{I}} & \hat{\mathbf{0}}\end{pmatrix} \tag{7}$$

with $\hat{\mathbf{0}}$ and $\hat{\mathbf{I}}$ being zero and identity 2×2 matrices.

Suppose that the stratified medium is periodically layered and its unit cell consists of n layers of thicknesses h_i ($i=1,\dots,n$), each characterized by the matrix $\hat{\mathbf{N}}_i$ (4). Denote by $\hat{\mathbf{M}}(H,0)\equiv\hat{\mathbf{M}}$ the transfer matrix relating the vector of amplitudes (3) at the opposite edges $z=0$ and $z=\sum_{i=1}^{n}h_i\equiv H$ of a unit cell, so that $\boldsymbol{\xi}(H)=\hat{\mathbf{M}}\boldsymbol{\xi}(0)$ and

$$\hat{\mathbf{M}}=\hat{\mathbf{M}}_n\dots\hat{\mathbf{M}}_2\hat{\mathbf{M}}_1, \tag{8}$$

where $\hat{\mathbf{M}}_i$ is a transfer matrix through the ith layer. If this layer is homogeneous, then $\hat{\mathbf{M}}_i = \exp(ih_i\hat{\mathbf{N}}_i)$; if it is functionally graded, then $\hat{\mathbf{M}}_i = \widehat{\int}[\hat{\mathbf{I}} + i\hat{\mathbf{N}}_i(z)dz]$, where $\widehat{\int}$ is the multiplicative integral over the given ith layer [64]. In either case, due to (6) and the fact that any matrix $\hat{\mathbf{N}}_i$ in the assumed absence of absorption is real, the matrix $\hat{\mathbf{M}}$ satisfies the equality

$$\hat{\mathbf{M}}^{-1} = \hat{\mathbf{T}}\hat{\mathbf{M}}^{\dagger}\hat{\mathbf{T}}, \tag{9}$$

where † means Hermitian conjugation. Note that the subsequent analysis does not in any way engage an explicit form of the transfer matrix $\hat{\mathbf{M}}$ and rests solely on its general properties.

In view of (9), the eigenvalues γ_α of $\hat{\mathbf{M}}$,

$$\hat{\mathbf{M}}\boldsymbol{\zeta}_\alpha = \gamma_\alpha\boldsymbol{\zeta}_\alpha, \quad \alpha = 1, \dots, 4, \tag{10}$$

are pairwise related, namely,

$$\text{either } |\gamma_\alpha| = |\gamma_{\alpha+2}| = 1 \tag{11a}$$

$$\text{or } \gamma_\alpha = 1/\gamma^*_{\alpha+2}, \ |\gamma_\alpha| \neq 1, \quad \alpha = 1, 2, \tag{11b}$$

where $*$ indicates complex conjugation. Denote the components of an eigenvector of $\hat{\mathbf{M}}$ by

$$\boldsymbol{\zeta}_\alpha = \begin{pmatrix} \mathbf{U}_\alpha \\ \mathbf{V}_\alpha \end{pmatrix}, \quad \alpha = 1, \dots, 4. \tag{12}$$

By construction, the components of eigenvector $\boldsymbol{\zeta}_\alpha$ have the same physical dimension as the corresponding components of the vector $\boldsymbol{\xi}$ (3). Let an eigenvector $\boldsymbol{\zeta}_\alpha$ be the initial value for Eq. (2) at a period edge. Then the amplitude of the corresponding wave solution, or eigenmode, $\boldsymbol{\xi}_\alpha(z)$, taken at the consecutive period edges in the positive direction of the Z axis, either is constant ($|\gamma_\alpha| = 1$) or increases ($|\gamma_\alpha| > 1$) or decreases ($|\gamma_\alpha| < 1$). Aiming to study the localized wave solutions, we are concerned only with the forbidden bands defined as the areas of the plane (ω, k) where the absolute values of both pairs of the eigenvalues γ_α are not equal to unity [see (11b)]. The numbering of γ_α's in the forbidden bands will hereafter follow the rule

$$|\gamma_\alpha| < 1 < |\gamma_{\alpha+2}|, \ \alpha = 1, 2. \tag{13}$$

Owing to (9), the eigenvectors $\boldsymbol{\zeta}_\alpha$ within a forbidden band obey a particular orthogonality which, being complemented by the normalization condition, reads as

$$\boldsymbol{\zeta}^{\dagger}_\alpha\hat{\mathbf{T}}\boldsymbol{\zeta}_\beta = \mathbf{U}^{\dagger}_\alpha\mathbf{V}_\beta + \mathbf{V}^{\dagger}_\alpha\mathbf{U}_\beta = \delta_{|\alpha-\beta|,2}, \tag{14}$$

where $\alpha, \beta = 1, \dots, 4$, and $\delta_{\alpha,\beta}$ is the Kronecker symbol.

The above-listed properties pertain to a transfer matrix through a unit cell with an arbitrary arrangement of constituent layers. These properties take a more specific form in the particular case of a unit cell which remains the same after inverting the sequence of constituent layers (in other words, after the unit cell has been mentally cut along the midplane orthogonal to Z and its upper and lower halves swapped with each other). We will call such a unit cell symmetric and any otherwise arranged unit cell asymmetric. Thus a unit cell of $2n + 1$ layers is symmetric when its ith and $(2n + 2 - i)$th layers are identical. Accordingly, Eq. (8) applied to the transfer matrix through a symmetric unit cell takes the form

$$\hat{\mathbf{M}}^{(S)} = \hat{\mathbf{M}}_1 \dots \hat{\mathbf{M}}_n\hat{\mathbf{M}}_{n+1}\hat{\mathbf{M}}_n \dots \hat{\mathbf{M}}_1, \tag{15}$$

where the superscript S means "symmetric." In consequence, a general identity (9) splits into two independent equalities

$$(\hat{\mathbf{T}}\hat{\mathbf{M}}^{(S)})^t = \hat{\mathbf{T}}\hat{\mathbf{M}}^{(S)}, \tag{16a}$$

$$\hat{\mathbf{M}}^{(S)-1} = \hat{\mathbf{M}}^{(S)*}, \tag{16b}$$

which imply that the eigenvalues of $\hat{\mathbf{M}}^{(S)}$ satisfy the same relations (11) as those of $\hat{\mathbf{M}}$ while Eq. (14) is modified to the form

$$\boldsymbol{\zeta}^t_\alpha\hat{\mathbf{T}}\boldsymbol{\zeta}_\beta = \delta_{\alpha\beta}, \quad \alpha, \beta = 1, \dots, 4. \tag{17}$$

In addition, the eigenvectors of $\hat{\mathbf{M}}^{(S)}$ in a forbidden band can be introduced so that

$$\boldsymbol{\zeta}_\alpha = \boldsymbol{\zeta}^*_{\alpha+2}, \ \alpha = 1, 2. \tag{18}$$

B. Impedance matrices

Let us introduce the matrices

$$\hat{\mathbf{Z}} = -i\hat{\mathbf{V}}\hat{\mathbf{U}}^{-1}, \tag{19a}$$

$$\hat{\mathbf{Z}}' = i\hat{\mathbf{V}}'\hat{\mathbf{U}}'^{-1}, \tag{19b}$$

where

$$\hat{\mathbf{U}} = (\mathbf{U}_1, \mathbf{U}_2), \quad \hat{\mathbf{V}} = (\mathbf{V}_1, \mathbf{V}_2), \\ \hat{\mathbf{U}}' = (\mathbf{U}_3, \mathbf{U}_4), \quad \hat{\mathbf{V}}' = (\mathbf{V}_3, \mathbf{V}_4) \tag{20}$$

are 2×2 matrices the columns of which are formed by the upper and lower parts $\mathbf{U}_\alpha$ and $\mathbf{V}_\alpha$ of the eigenvectors $\boldsymbol{\zeta}_\alpha$ (12). Multiplying Eqs. 19(a) and 19(b), respectively, by $\hat{\mathbf{U}}$ and $\hat{\mathbf{U}}'$ from the right and expanding the result in columns of matrices (20) yields the equalities

$$\mathbf{V}_\alpha = i\hat{\mathbf{Z}}\mathbf{U}_\alpha, \ \mathbf{V}_{\alpha+2} = -i\hat{\mathbf{Z}}'\mathbf{U}_{\alpha+2}, \ \alpha = 1, 2. \tag{21}$$

The matrices $\hat{\mathbf{Z}}$ and $\hat{\mathbf{Z}}'$ considered in a forbidden band are Hermitian, as may be observed from the identities

$$\hat{\mathbf{U}}^{\dagger}\hat{\mathbf{V}} + \hat{\mathbf{V}}^{\dagger}\hat{\mathbf{U}} = \hat{\mathbf{0}}, \ \ \hat{\mathbf{U}}'^{\dagger}\hat{\mathbf{V}}' + \hat{\mathbf{V}}'^{\dagger}\hat{\mathbf{U}}' = \hat{\mathbf{0}}, \tag{22}$$

which follow from Eq. (14).

The matrices $\hat{\mathbf{Z}}$ and $\hat{\mathbf{Z}}'$ appear in the SEW dispersion equation and thereby play a pivotal role in our considerations, which is similar to the role of the impedance matrix in the theory of surface acoustic waves [30–33]. For this reason, we shall also call them the impedance matrices, although their definition (19) does not match the classical meaning of an electromagnetic wave impedance as the measure of proportionality between the electric field and the magnetic field. It will be seen that using the impedances defined by (19) is helpful for pinpointing some essential properties of the SEW existence problem, particularly those in the lowest forbidden band.

In the case of a symmetric unit cell, the matrices $\hat{\mathbf{U}}'$ and $\hat{\mathbf{V}}'$ in the forbidden bands are equal to $\hat{\mathbf{U}}^*$ and $\hat{\mathbf{V}}^*$ [see (18)]. Hence the impedances $\hat{\mathbf{Z}}^{(S)}$ and $\hat{\mathbf{Z}}^{(S)\prime}$ are interrelated as

$$\hat{\mathbf{Z}}^{(S)\prime} = \hat{\mathbf{Z}}^{(S)*} = \hat{\mathbf{Z}}^{(S)t}. \tag{23}$$

Some more properties of the impedance matrices $\hat{\mathbf{Z}}$, $\hat{\mathbf{Z}}'$, and $\hat{\mathbf{Z}}^{(S)}$ are established in Appendix A. One of them, namely, the sign definiteness of frequency derivatives, is unreservedly valid for generally anisotropic superlattices with frequency

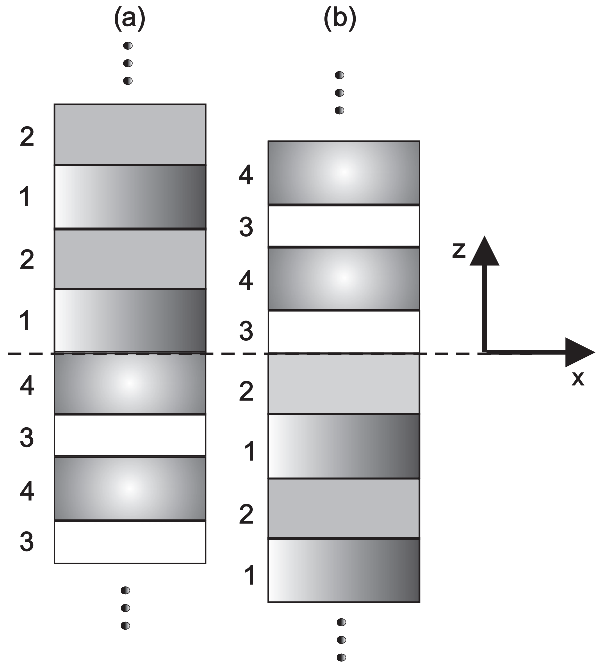

FIG. 1. Example of direct (a) and complementary (b) bicrystals composed of two-layer half-infinite superlattices $J = 1$ (layers 1 and 2) and $J = 2$ (layers 3 and 4).

independent dielectric permittivity and magnetic permeability, and it is also true when they are frequency dependent and either the wave field (1) is taken with $k = 0$ or k is arbitrary but the superlattice obeys the monoclinic symmetry (see the precise formulation in Appendix A). Note that the latter setting is predominant in practice. Our subsequent considerations of the SEW existence are referred to one or the other of the above cases.

III. EXISTENCE OF SURFACE ELECTROMAGNETIC WAVES

A. Bicrystal with asymmetric unit cells

Consider a photonic bicrystal formed of two half-infinite superlattices periodic along a common axis Z and having asymmetric unit cells. Choose the origin $z = 0$ of the axis Z at the interface of the bicrystal. Let the labels $J = 1$ and 2 correspond to the superlattices located at $z \geqslant 0$ and at $z \leqslant 0$, respectively. Referring to the given bicrystal as a "direct" one, we introduce in parallel a "complementary" bicrystal which consists of the superlattice $J = 2$ at $z \geqslant 0$ and of the superlattice $J = 1$ at $z \leqslant 0$. For a better grasp of these two structures, one may view the upper part of the direct bicrystal and the lower part of the complementary one as two halves of a bisected infinite superlattice $J = 1$ and, in turn, the lower and the upper parts of, respectively, direct and complementary bicrystal as the halves of a bisected infinite superlattice $J = 2$ (Fig. 1). We will see that general considerations for existence of SEWs involve both direct and complementary bicrystals at once.

Equation (8) defines the transfer matrices $\hat{\mathbf{M}}^{(J)}$ $(J = 1, 2)$ along the positive z direction in the given superlattices, so that the spatial evolution of the wave field along the positive and negative z directions away from the interface $z = 0$ is determined, respectively, by the matrices $\hat{\mathbf{M}}^{(1)} \equiv \hat{\mathbf{M}}^{(1)}(T_1, 0)$ and $\hat{\mathbf{M}}^{(2)-1} \equiv \hat{\mathbf{M}}^{(2)}(0, T_2)$ in the direct bicrystal and by the matrices $\hat{\mathbf{M}}^{(2)}$ and $\hat{\mathbf{M}}^{(1)-1}$ in the complementary one. Recall that a matrix and its inverse have the same set of eigenvectors and mutually inverse sets of eigenvalues. Hence the definition (11) implies the same band structure for the direct and complementary bicrystals. The SEW localized at the interface $z = 0$, i.e., turning to zero at the infinite depth, may generally exist only within the overlaps of the forbidden bands of the lower and upper half-infinite superlattices, which we will refer to as simply the forbidden bands (of a bicrystal).

Consider a direct bicrystal. Assuming that ω and k belong to a forbidden band and sticking to the eigenvalue numbering (13) inside the band, the SEW solution of Eq. (2) should have the form of linear superpositions $\boldsymbol{\xi}^{(+)}(z) = \sum_{\alpha=1}^{2} c_\alpha \boldsymbol{\xi}_\alpha^{(1)}(z)$ at $z \geqslant 0$ and $\boldsymbol{\xi}^{(-)}(z) = \sum_{\alpha=3}^{4} d_\alpha \boldsymbol{\xi}_\alpha^{(2)}(z)$ at $z \leqslant 0$, each solution being generated by its initial value $\boldsymbol{\xi}^{(+)}(0) = \sum_{\alpha=1}^{2} c_\alpha \boldsymbol{\zeta}_\alpha^{(1)}$ and $\boldsymbol{\xi}^{(-)}(0) = \sum_{\alpha=3}^{4} d_\alpha \boldsymbol{\zeta}_\alpha^{(2)}$ at $z = 0$. The continuity of the tangential components of the electric and magnetic fields implies that

$$\sum_{\alpha=1}^{2} c_\alpha \boldsymbol{\zeta}_\alpha^{(1)} = \sum_{\alpha=3}^{4} d_\alpha \boldsymbol{\zeta}_\alpha^{(2)}, \tag{24}$$

or, equivalently,

$$\mathbf{U} = \mathbf{U}', \quad \hat{\mathbf{Z}}^{(1)}\mathbf{U} = -\hat{\mathbf{Z}}'^{(2)}\mathbf{U}', \tag{25}$$

where $\mathbf{U} = \sum_{\alpha=1}^{2} c_\alpha \mathbf{U}_\alpha^{(1)}$, $\mathbf{U}' = \sum_{\alpha=3}^{4} d_\alpha \mathbf{U}_\alpha^{(2)}$, and $\hat{\mathbf{Z}}^{(1)}$, $\hat{\mathbf{Z}}'^{(2)}$ are the impedance matrices defined by (19) for the superlattices 1 and 2, respectively. Hence, the sought dispersion equation for SEWs in the direct bicrystal is

$$\det \hat{\mathbf{Z}}_B = 0 \ \text{ with } \ \hat{\mathbf{Z}}_B = \hat{\mathbf{Z}}^{(1)} + \hat{\mathbf{Z}}'^{(2)}, \tag{26}$$

where the subscript B implies "bicrystal." By precisely the same arguments the dispersion equation for SEWs in the complementary bicrystal is

$$\det \hat{\mathbf{Z}}_B' = 0 \ \text{ with } \ \hat{\mathbf{Z}}_B' = \hat{\mathbf{Z}}^{(2)} + \hat{\mathbf{Z}}'^{(1)}. \tag{27}$$

For analyzing the number of solutions of Eqs. (26) and (27), it proves helpful to introduce an auxiliary matrix

$$\hat{\mathbf{G}}_B = \hat{\mathbf{Z}}_B + \hat{\mathbf{Z}}_B' = \hat{\mathbf{G}}^{(1)} + \hat{\mathbf{G}}^{(2)}, \tag{28}$$

where

$$\hat{\mathbf{G}}^{(J)} = \hat{\mathbf{Z}}^{(J)} + \hat{\mathbf{Z}}'^{(J)}, \quad J = 1, 2. \tag{29}$$

The matrix $\hat{\mathbf{G}}_B$ can be expanded in two equivalent forms:

$$\hat{\mathbf{G}}_B = \sum_{\alpha=1}^{2} (\chi_\alpha \mathbf{e}_\alpha \otimes \mathbf{e}_\alpha^* + \chi_\alpha' \mathbf{e}_\alpha' \otimes \mathbf{e}_\alpha'^*) \tag{30a}$$

$$= \sum_{J=1}^{2} \sum_{\alpha=1}^{2} \sigma_\alpha^{(J)} \mathbf{t}_\alpha^{(J)} \otimes \mathbf{t}_\alpha^{(J)*}, \tag{30b}$$

where χ_α, χ_α', $\sigma_\alpha^{(J)}$ and $\mathbf{e}_\alpha$, $\mathbf{e}_\alpha'$, $\mathbf{t}_\alpha^{(J)}$ $(\alpha = 1, 2;\ J = 1, 2)$ are the eigenvalues and the orthonormal eigenvectors of the Hermitian matrices $\hat{\mathbf{Z}}_B$, $\hat{\mathbf{Z}}_B'$, and $\hat{\mathbf{G}}^{(J)}$, respectively, and $\otimes$ is a dyadic product. By (26) and (27), zeros of $\chi_\alpha(\omega, k)$ and of $\chi_\alpha'(\omega, k)$ define the sought SEW dispersion branches for the direct and complementary bicrystals, respectively. In the following, we analyze the number of SEW solutions per a forbidden band at fixed k, the upper and lower frequency edges of which will be denoted by ω_l and ω_u, respectively ($\omega_l = 0$ for the lowest band).

Consider the lowest forbidden band $0 < \omega < \omega_u$. As shown in Appendix A, the eigenvalues χ_α of $\hat{\mathbf{Z}}_B$ are positive near $\omega = 0$, decrease with growing ω, and have no poles within this band. Hence,

> given a fixed k, at most two SEWs can exist in the lowest forbidden band of a bicrystal.

It is understood that this formulation applies independently to the direct and complementary bicrystals. However, a stronger statement can be deduced via Eq. (30). Note first that, by (A14), the eigenvalues $\sigma_\alpha^{(J)}$ stay positive in the lowest forbidden band. Regarding χ_α and χ'_α, it can be shown that at least two of these four must remain positive throughout the lowest band. Indeed, assume that this is not so and, say, only $\chi_1 > 0$ while $\chi_2 < 0$ and $\chi'_{1,2} < 0$ at some frequency within $0 < \omega < \omega_u$. Then a Hermitian contraction of (30a) and (30b) with the eigenvector $\mathbf{e}_2$ yields incompatible inequalities:

$$\mathbf{e}_2^\dagger \hat{\mathbf{G}}_B \mathbf{e}_2 = \sum_{J=1}^{2}\sum_{\alpha=1}^{2} \sigma_\alpha^{(J)} \left|\mathbf{t}_\alpha^{(J)\dagger}\mathbf{e}_2\right|^2 > 0,$$
$$\mathbf{e}_2^\dagger \hat{\mathbf{G}}_B \mathbf{e}_2 = \chi_2 + \sum_{\alpha=1}^{2} \chi'_\alpha |\mathbf{e}_\alpha'^\dagger \mathbf{e}_2|^2 < 0. \tag{31}$$

Hence the above assumption cannot hold true and not more than two of χ_α and χ'_α, being positive near $\omega = 0$, may become negative within the lowest band. Since they decrease continuously, this means that χ_α and χ'_α may have not more than two zeros for two at $0 < \omega < \omega_u$. Therefore we can conclude that

> given a fixed k, at most two SEWs can exist in total in the lowest forbidden band of the direct and complementary bicrystals.

The latter formulation means that if two SEWs in the lowest forbidden band occur for the direct bicrystal then none of them may occur for the complementary one and vice versa, whereas if there is a single SEW for one of the bicrystal structures then there may be no more then one SEW for the other (this being said, it is clear that there may be a single SEW existing in only one of the bicrystals or there may be no SEWs in the lowest band at all).

Consider an upper forbidden band $\omega_l < \omega < \omega_u$. In contrast to the previous case of the lowest band, the eigenvalues of the matrices $\hat{\mathbf{Z}}_B$, $\hat{\mathbf{Z}}'_B$, and $\hat{\mathbf{G}}^{(J)}$, being decreasing functions of ω, do not need to be positive at the lower band edge $\omega_l (\neq 0)$ and they may have one pole each at $\omega_l < \omega < \omega_u$. Suppose first that none of them has a pole. The number of zeros of the eigenvalues χ_α and χ'_α of $\hat{\mathbf{Z}}_B$ and $\hat{\mathbf{Z}}'_B$ within the band in this case is bounded by 4. Note that the occurrence of maximum number implies that all four $\chi_\alpha, \chi'_\alpha$ are positive near ω_l and negative near ω_u, which is indeed a possible option but it requires two of the four eigenvalues $\sigma_\alpha^{(J)}$ of $\hat{\mathbf{G}}^{(J)}$ to be positive and two negative at the band edges. Next assume that one of χ_α, χ'_α has a pole at some frequency ω_p inside the band and hence so does one of $\sigma_\alpha^{(J)}$ ($\alpha = 1, 2;\ J = 1, 2$). It could seem at first glance that the eigenvalues χ_α and χ'_α in this case may altogether have as many as five zeros at $\omega_l < \omega < \omega_u$ (including two zeros of the same eigenvalue branch vanishing below and above its pole). However, such a state of affairs is barred. Indeed, as mentioned above, its prerequisite is that all four $\chi_\alpha, \chi'_\alpha$ are positive near ω_l and negative near ω_u, and the former condition can come about only if two of $\sigma_\alpha^{(J)}$ are positive and two are negative at ω_l. By (A14), none of the eigenvalues $\sigma_\alpha^{(J)}$ may vanish in a forbidden band, hence the pole occurs for the branch $\sigma_\alpha^{(J)}(\omega)$ that is negative near ω_l. It then follows that one of $\sigma_\alpha^{(J)}$ is negative and three are positive at $\omega_p < \omega < \omega_u$, say $\sigma_1^{(1)} < 0$ and $\sigma_2^{(1)}$, $\sigma_\alpha^{(2)} > 0$. Provided this is so, a Hermitian contraction of $\hat{\mathbf{G}}_B$ (30) with the eigenvector $\mathbf{t}_2^{(1)}$ at ω near ω_u yields incompatible inequalities

$$\mathbf{t}_2^{(1)\dagger} \hat{\mathbf{G}}_B \mathbf{t}_2^{(1)} = \sum_{\alpha=1}^{2} \left(\chi_\alpha \left|\mathbf{t}_2^{(1)\dagger}\mathbf{e}_\alpha\right|^2 + \chi'_\alpha \left|\mathbf{t}_2^{(1)\dagger}\mathbf{e}'_\alpha\right|^2\right) < 0,$$
$$\mathbf{t}_2^{(1)\dagger} \hat{\mathbf{G}}_B \mathbf{t}_2^{(1)} = \sigma_2^{(1)} + \sum_{\alpha=1}^{2} \sigma_\alpha^{(2)} \left|\mathbf{t}_2^{(1)\dagger}\mathbf{t}_\alpha^{(2)}\right|^2 > 0, \tag{32}$$

which rules out the possibility of existence of more than four SEWs in the case of one eigenvalue pole. Applying similar argumentation to one-by-one analysis of other possible cases, where two, three, or all four eigenvalue branches have poles, renders the same conclusion. Thus,

> given a fixed k, at most four SEWs can exist in total in an upper forbidden band of the direct and complementary bicrystals.

B. Bicrystal with symmetric unit cells

Consider a bicrystal composed of two half-infinite periodic superlattices with a symmetric unit cell each. By virtue of Eq. (23), the SEW dispersion equation for the direct bicrystal [see (26)] can be specialized to the form

$$\det \hat{\mathbf{Z}}_B^{(S)} = 0 \ \text{ with } \ \hat{\mathbf{Z}}_B^{(S)} = \hat{\mathbf{Z}}^{(S,1)} + \hat{\mathbf{Z}}^{(S,2)t}, \tag{33}$$

while Eq. (27) is obviously equivalent to (33). This means that there is no need for invoking a complementary bicrystal and the auxiliary matrix (28). Instead, the full insight follows from simultaneous analysis of the impedances $\hat{\mathbf{Z}}^{(S,J)}$ ($J = 1, 2$) and their real parts.

Let us write the matrices $\hat{\mathbf{Z}}_B^{(S)}$ and $\mathrm{Re}\hat{\mathbf{Z}}_B^{(S)}$ as

$$\hat{\mathbf{Z}}_B^{(S)} = \sum_{\alpha=1}^{2} \chi_\alpha^{(S)} \mathbf{e}_\alpha^{(S)} \otimes \mathbf{e}_\alpha^{(S)*}, \tag{34}$$

$$\mathrm{Re}\hat{\mathbf{Z}}_B^{(S)} = \sum_{J=1}^{2}\sum_{\alpha=1}^{2} \nu_\alpha^{(J)} \mathbf{p}_\alpha^{(J)} \otimes \mathbf{p}_\alpha^{(J)}, \tag{35}$$

where $\chi_\alpha^{(S)}$ and $\mathbf{e}_\alpha^{(S)}$ are the eigenvalues and orthonormal eigenvectors of the matrix $\hat{\mathbf{Z}}_B^{(S)}$ while $\nu_\alpha^{(J)}$ and $\mathbf{p}_\alpha^{(J)}$ are the eigenvalues and orthonormal eigenvectors of the matrices $\mathrm{Re}\hat{\mathbf{Z}}^{(S,J)}$ ($\alpha = 1, 2;\ J = 1, 2$). Note that a contraction of a Hermitian matrix $\hat{\mathbf{Z}}_B^{(S)}$ with an arbitrary real vector $\mathbf{q}$ coincides with that of its real part, i.e.,

$$\sum_{\alpha=1}^{2} \chi_\alpha^{(S)} \left|\mathbf{q}^t \mathbf{e}_\alpha^{(S)}\right|^2 = \sum_{J=1}^{2}\sum_{\alpha=1}^{2} \nu_\alpha^{(J)} \left(\mathbf{q}^t \mathbf{p}_\alpha^{(J)}\right)^2. \tag{36}$$

Consider the lowest forbidden band $0 < \omega < \omega_u$. According to Appendix A, all four eigenvalues $\nu_\alpha^{(J)}$ are positive within this band and both $\chi_\alpha^{(S)}$ are positive near $\omega = 0$ and decrease continuously. Hence the quantity (36) is positive throughout the band, so at least one of the eigenvalues $\chi_\alpha^{(S)}$ must remain positive whereas the other one may vanish only once. Recalling that zero of $\chi_\alpha^{(S)}$ is the solution of the SEW dispersion Eq. (33), we conclude that

> given a fixed k, at most one SEW can exist in the lowest forbidden band of a bicrystal with symmetric unit cells.

In an upper forbidden band $\omega_l < \omega < \omega_u$, the eigenvalues $\chi_\alpha^{(S)}$ and $\nu_\alpha^{(J)}$ are not sign definite near the lower edge ω_l and may have poles within the band. Suppose first that both $\chi_\alpha^{(S)}$ are continuous. Since they are decreasing functions of ω, the maximum number of their zeros in this case is 2. Next assume the presence of poles. By (A18), each of the two pairs of eigenvalues $\nu_\alpha^{(1)}$ and $\nu_\alpha^{(2)}$of Re$\hat{\mathbf{Z}}^{(1)}$ and Re$\hat{\mathbf{Z}}^{(2)}$ may have one pole and hence the eigenvalues $\chi_\alpha^{(S)}$ of $\hat{\mathbf{Z}}_B$ may have one or two poles per an upper forbidden band. In both cases, the analysis of Eq. (30) with account for the property of $\nu_\alpha^{(J)}$ to have no zeros inside forbidden bands (see Appendix A) leads to the same conclusion that the eigenvalues of $\hat{\mathbf{Z}}_B$ can turn to zero at most twice. Thus,

> given a fixed k, at most two SEWs can exist in an upper forbidden band of a bicrystal with symmetric unit cells.

Note that if only one of the two half-infinite superlattices forming a given bicrystal has a symmetric unit cell while the other superlattice has an asymmetric one, then the maximum admissible number of SEWs is described by statements formulated in Sec. III A.

C. SEWs in a superlattice - homogeneous medium structure

Let us address the case where a half-infinite superlattice is bounded by a homogeneous dielectric. The four eigenvalues of a constant matrix $\hat{\mathbf{N}}$ (4), which are equal to i times wave numbers along the axis Z, are complex valued at frequencies smaller than a certain critical value $\omega_L(k)$. The impedances $\hat{\mathbf{Z}}^{(H)}$ and $\hat{\mathbf{Z}}'^{(H)}$ of a homogeneous medium are defined similarly to (19) but with the eigenvectors of $\hat{\mathbf{N}}$ in place of those of the transfer matrix $\hat{\mathbf{M}}$. When taken in the range $\omega < \omega_L$, the matrices $\hat{\mathbf{Z}}^{(H)}$ and $\hat{\mathbf{Z}}'^{(H)}$ are Hermitian and satisfy $\hat{\mathbf{Z}}'^{(H)} = \hat{\mathbf{Z}}^{(H)t}$. Their eigenvalues are positive at $\omega \to 0$ and decrease continuously with growing ω. [Note also that the impedance of a superlattice with a symmetric unit cell has the same properties within the lowest forbidden band as those of the impedance of a homogeneous material].

Assume a half-infinite superlattice with asymmetric unit cell and consider in parallel two configurations: the one where the given superlattice and homogeneous medium occupy, respectively, the half spaces $z \geqslant 0$ and $z \leqslant 0$ (a direct structure) and the other one where they swap their places (a complementary structure). Note that the latter complementary structure is equivalent to the configuration where the homogeneous half space is at $z \leqslant 0$ (like for the direct structure), whereas the superlattice located at $z \geqslant 0$ differs from the given superlattice in that the unit cell of the former is obtained from the unit cell of the latter by inverting the sequence of layers. The dispersion equations defining the SEWs in these structures are given by (26) and (27) with $J = 1$ related to the given superlattice and with $\hat{\mathbf{Z}}^{(2)}$ and $\hat{\mathbf{Z}}'^{(2)}$ replaced, respectively, with the impedances $\hat{\mathbf{Z}}^{(H)}$ and $\hat{\mathbf{Z}}'^{(H)}$ of the homogeneous medium. According to the above-mentioned properties of $\hat{\mathbf{Z}}^{(H)}$ and $\hat{\mathbf{Z}}'^{(H)}$, the existence considerations for SEWs in this case are similar to those developed in Secs. III A and III B. Specifically, it follows that

> if a half-infinite superlattice has an asymmetric unit cell, then, for a fixed k and $\omega < \omega_L$, at most two SEWs in the lowest forbidden band and at most four SEWs per upper forbidden bands can exist in total in the direct and complementary superlattice - homogeneous dielectric structures;

and

> if a half-infinite superlattice has a symmetric unit cell, then, for a fixed k and $\omega < \omega_L$, at most one SEW in the lowest forbidden band and at most two SEWs per upper forbidden bands can exist in the superlattice bounded by a homogeneous dielectric.

A different situation may occur for a superlattice coated by a metal film with isotropic dielectric permittivity $\varepsilon/\varepsilon_0 = 1 - \omega_p^2/\omega^2$, where ε_0 is the absolute permittivity and ω_p is the plasma frequency (the Drude model without dissipation). Let the film be thick enough to behave as a half-infinite medium with respect to optical wavelengths. Then its impedance is a diagonal matrix $\hat{\mathbf{Z}}^{(M)} = \mathrm{diag}(Z_{11}^{(M)}, Z_{22}^{(M)})$ with the elements

$$Z_{11}^{(M)} = \frac{c\varepsilon_0}{\omega}\sqrt{k^2c^2 + \omega_p^2 - \omega^2},$$
$$Z_{22}^{(M)} = -\frac{\omega}{\varepsilon_0 c(\omega_p^2 - \omega^2)}\sqrt{k^2c^2 + \omega_p^2 - \omega^2}, \tag{37}$$

where c is the speed of light. We consider the frequency range $\omega < \omega_p$. According to (37), $Z_{11}^{(M)}$ in this range is positive and tends to infinity as $\omega \to 0$, while $Z_{22}^{(M)}$ is negative, vanishes at $\omega = 0$ and tends to minus infinity as $\omega \to \omega_p$. Both $Z_{11}^{(M)}$ and $Z_{22}^{(M)}$ monotonically decrease with increasing frequency.

A negative value of $Z_{22}^{(M)}$ is in contrast to the positive definiteness of the impedance of periodic or homogeneous dielectric materials at low frequency. Hence a particular dissimilarity of the SEW properties can be expected in the lowest forbidden band $0 < \omega < \omega_u$ (let $\omega_u < \omega_p$). It is evident that the dispersion Eqs. (26) and (27) with $\hat{\mathbf{Z}}_B = \hat{\mathbf{Z}} + \hat{\mathbf{Z}}^{(M)}$ and $\hat{\mathbf{Z}}'_B = \hat{\mathbf{Z}}' + \hat{\mathbf{Z}}^{(M)}$ at fixed k and $0 < \omega < \omega_u$ may have up to two roots each, since the eigenvalues of the matrices $\hat{\mathbf{Z}}_B$ and $\hat{\mathbf{Z}}'_B$ are positive at $\omega \to 0$ and decrease continuously with increasing frequency in this range. Thus the maximum possible number of SEWs in the lowest forbidden band of a superlattice in contact with metal is 2, which is the same as in the case of a contact with a homogeneous or periodic dielectric (see the corresponding statements above and in Sec. III A). At the same time, the maximum total number of SEWs, embracing their occurrences in both direct and complementary structures, is no longer 2, as it was in the case of a contact with a dielectric, but may equal 3. To show this, consider the matrices $\hat{\mathbf{G}}_B = \hat{\mathbf{G}}^{(1)} + \hat{\mathbf{G}}^{(2)}$ with $\hat{\mathbf{G}}^{(1)} = \hat{\mathbf{Z}} + \hat{\mathbf{Z}}'$ and $\hat{\mathbf{G}}^{(2)} = 2\hat{\mathbf{Z}}^{(M)}$ defined by analogy with Eqs. (28) and (29). Both eigenvalues of $\hat{\mathbf{G}}^{(1)}$ in the lowest forbidden band are positive, as is the eigenvalue $Z_{11}^{(M)}$, while $Z_{22}^{(M)}$ is negative. Therefore, taking a contraction of $\hat{\mathbf{G}}^{(J)}$ with the eigenvector $\mathbf{e} = (1\ 0)^t$ of $\hat{\mathbf{Z}}^{(M)}$ corresponding to $Z_{11}^{(M)}$ yields

$$\mathbf{e}^t \hat{\mathbf{G}} \mathbf{e} = \mathbf{e}^t \hat{\mathbf{Z}}_B \mathbf{e} + \mathbf{e}^t \hat{\mathbf{Z}}'_B \mathbf{e} > 0, \tag{38}$$

hence at least one of the four eigenvalues of the matrices $\hat{\mathbf{Z}}_B$ and $\hat{\mathbf{Z}}'_B$ must stay positive throughout the lowest forbidden band. Thus it follows that

> if a half-infinite superlattice with an asymmetric unit cell is coated by metal, then the maximum total number of SEWs which can exist at fixed k in the direct and complementary structures inside their lowest forbidden band is 3.

Regarding a superlattice with symmetric unit cell, the restriction on the maximum number of SEWs in the lowest forbidden band, which must not exceed 1 in the case of a contact with a dielectric, can also be relaxed when the superlattice is in contact with metal. Reasoning similarly as above, it can be demonstrated that the latter case admits existence of two SEWs at maximum in the lowest band.

D. TE and TM SEWs

Let the layers constituting a superlattice possess a common plane of symmetry parallel to the sagittal plane XZ and/or a twofold symmetry axis orthogonal to XZ (this implies crystallographic symmetry of a monoclinic or higher type). Then the xy and yz components of the dielectric permittivity and magnetic permeability tensors are zero. As a result, Eq. (2) with the matrix of coefficients (4) splits into the following two systems describing, respectively, the TE- and TM-polarized modes:

$$\frac{d}{dz}\begin{pmatrix} -e_y \\ h_x \end{pmatrix} = i\begin{pmatrix} 0 & \omega m_{xx} \\ \omega\varepsilon_{yy} - \frac{k^2}{\omega\mu_{zz}} & 0 \end{pmatrix}\begin{pmatrix} -e_y \\ h_x \end{pmatrix}, \tag{39}$$

$$\frac{d}{dz}\begin{pmatrix} h_y \\ e_x \end{pmatrix} = i\begin{pmatrix} 0 & \omega\epsilon_{xx} \\ \omega\mu_{yy} - \frac{k^2}{\omega\varepsilon_{zz}} & 0 \end{pmatrix}\begin{pmatrix} h_y \\ e_x \end{pmatrix}, \tag{40}$$

where $(-e_y\ h_x)^t = (-\mathbb{E}_y\ \mathbb{H}_x)^t e^{ik\varphi_\varepsilon}$ and $(h_y\ e_x)^t = (\mathbb{H}_y\ \mathbb{E}_x)^t e^{ik\varphi_\mu}$ with $\varphi_\varepsilon = \sum_{i=1}^n h_i(\varepsilon_{xz}/\varepsilon_{zz})_i$ and $\varphi_\mu = \sum_{i=1}^n h_i(\mu_{xz}/\mu_{zz})_i$, the sum being taken over n layers of a unit cell (replaced by an integral if the unit cell is functionally graded). Since both TE and TM modes are described by similar equations, we will refer our analysis to the TE modes and then extend the conclusions to the TM modes. Note that similar considerations for the acoustic analogy, which is related to the so-called shear horizontal waves, may be found, e.g., in [65,66].

Denote the transfer matrix associated with Eq. (39) by $\hat{\mathbf{M}}_{\mathrm{TE}}$. Zero trace of the matrix of coefficients in (39) implies that $\det \hat{\mathbf{M}}_{\mathrm{TE}} = 1$ and therefore, by virtue of Eq. (9), $\hat{\mathbf{M}}_{\mathrm{TE}}$ has real diagonal elements and purely imaginary off-diagonal elements. Mutually inverse eigenvalues $\gamma_1 = 1/\gamma_2$ of $\hat{\mathbf{M}}_{\mathrm{TE}}$ are given by

$$\gamma_\alpha = \tfrac{1}{2}[\mathrm{tr}\hat{\mathbf{M}}_{\mathrm{TE}} \pm \sqrt{(\mathrm{tr}\hat{\mathbf{M}}_{\mathrm{TE}})^2 - 4}], \quad \alpha = 1, 2, \tag{41}$$

where $\mathrm{tr}\hat{\mathbf{M}}_{\mathrm{TE}} = M_{11} + M_{22}$. Considering the interior of TE forbidden bands, which are determined by the inequality $\mathrm{tr}\hat{\mathbf{M}}_{\mathrm{TE}} > 2$, let us denote the eigenvalue with an absolute value smaller than 1 by γ (i.e., $|\gamma| < 1$). The TE impedances

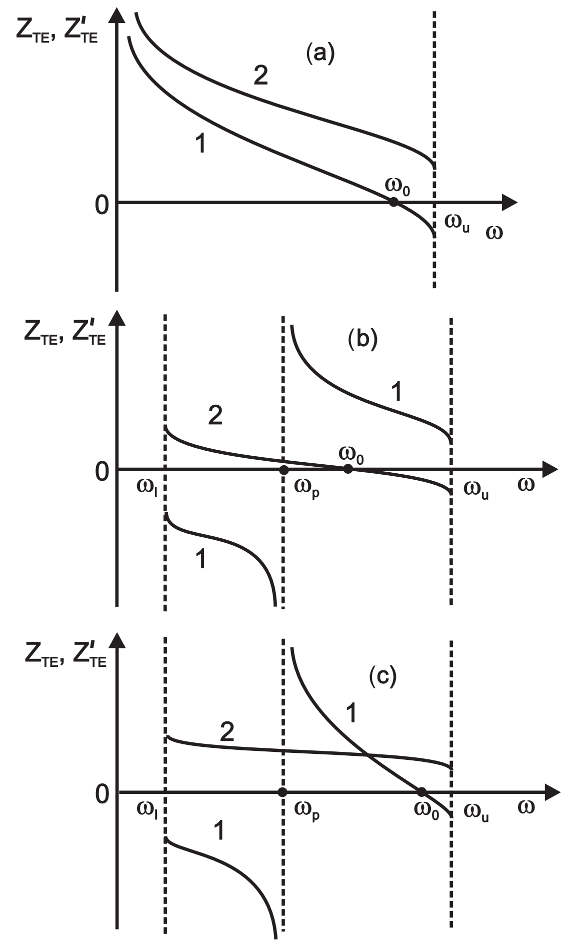

FIG. 2. Frequency dependence of impedances Z_{TE} and Z'_{TE} in the lowest (a) and upper (b, c) forbidden bands of a superlattice with asymmetric unit cell. One of the curves 1 and 2 depicts $Z_{\mathrm{TE}}(\omega)$ and the other is $Z'_{\mathrm{TE}}(\omega)$.

Z_{TE} and Z'_{TE} defined by analogy with Eq. (19) via the eigenvectors of the matrix $\hat{\mathbf{M}}_{\mathrm{TE}}$ are real scalars:

$$Z_{\mathrm{TE}} = \frac{\gamma - M_{11}}{\overline{\overline{M}}_{12}}, \quad Z'_{\mathrm{TE}} = \frac{M_{11} - 1/\gamma}{\overline{\overline{M}}_{12}}, \tag{42}$$

where $\overline{\overline{M}}_{ij} \equiv \mathrm{Im} M_{ij} = -iM_{ij}$ $(i, j = 1, 2,\ i \neq j)$.

In consequence of the general features of the impedance matrices proved in Appendix A, Z_{TE} and Z'_{TE} in forbidden bands are decreasing functions of ω at any fixed k. Note also from (42) that the equality $Z_{\mathrm{TE}} = -Z'_{\mathrm{TE}}$ holds at the edges of a forbidden band (where $\gamma = 1/\gamma$) but cannot occur inside this band (where $\gamma \neq 1/\gamma$). Using these facts allows one to ascertain the key properties of $Z_{\mathrm{TE}}(\omega)$ and $Z'_{\mathrm{TE}}(\omega)$. They read that Z_{TE} and Z'_{TE} considered in any upper forbidden band must have in total one pole and one zero, so that either one of Z_{TE} and Z'_{TE} has a pole and the other has zero or else both zero and pole occur for one of the impedances Z_{TE} and Z'_{TE} while the other has none. In turn, one of Z_{TE} and Z'_{TE} considered in the lowest forbidden band has zero but none of them has a pole. Some possible options of the shape of functions $Z_{\mathrm{TE}}(\omega)$ and $Z'_{\mathrm{TE}}(\omega)$ are shown in Fig. 2.

Let us argue the above-stated propositions. Guaranteed existence of a pole within an upper forbidden band is readily seen from the fact that a decreasing function $Z_{\rm TE}$ and an increasing function $-Z'_{\rm TE}$ cannot start from a common value at one band edge and end up at a common value at the other edge (as they must) without having a first-order pole in between. Further properties are easy to visualize by drawing a two-valued function formed by $Z_{\rm TE}$ and $-Z'_{\rm TE}$. It is evident that a single pole of the functions $Z_{\rm TE}$ or $Z'_{\rm TE}$ implies that one of them must also have a single zero inside the band, while the occurrence of more than one pole is ruled out since otherwise it would lead to the equality of $Z_{\rm TE}$ and $-Z'_{\rm TE}$ inside the band, which is not possible. A different state of affairs takes place in the lowest forbidden band $0 < \omega < \omega_u$, where $Z_{\rm TE}$ and $Z'_{\rm TE}$ tend to positive infinity at $\omega \to 0$ (see Appendix A). In this case, sketching $Z_{\rm TE}$ and $-Z'_{\rm TE}$ confirms that no pole can exist due to inequality of $Z_{\rm TE}$ and $-Z'_{\rm TE}$ throughout the band, while their equality at ω_u necessitates one zero for either $Z_{\rm TE}$ or $Z'_{\rm TE}$.

In the case of an asymmetric unit cell, a single zero and a single pole appropriately "shared" between $Z_{\rm TE}$ and $Z'_{\rm TE}$ generally occur strictly inside the forbidden band. As an exceptional occasion, either of them may come about at the band edge, which is the case if M_{12} happens to vanish at this edge. On the other hand, this is always so when the unit cell is symmetric. Then, by (16a), $M_{11} = M_{22}$ and $\gamma = M_{11} - \mathrm{sign}(M_{11})\sqrt{M_{11}^2 - 1}$ where $M_{11}^2 - 1 = M_{12}M_{21} > 0$, so both TE impedances merge into one impedance $Z_{\rm TE}^{(S)}$ given by

$$Z_{\rm TE}^{(S)} = \mathrm{sign}(M_{11}\overline{\overline{M}}_{12})\sqrt{-\frac{M_{21}}{M_{12}}}. \tag{43}$$

At the edges of the upper forbidden bands, the corresponding equality $\gamma = 1/\gamma$ implies that either M_{12} or M_{21} must turn to zero and hence the decreasing function $Z_{\rm TE}^{(S)}$ either tends to plus infinity at the lower band edge and turns to zero at the upper edge or it turns to zero at the lower edge and tends to minus infinity at the upper edge. Since $Z_{\rm TE}^{(S)}$ must tend to positive infinity at $\omega \to 0$, the former of the two above options is always the case in the lowest forbidden band. Note for completeness that the pole or zero of $Z_{\rm TE}^{(S)}$ moves away from the band edge into the band interior in the extraordinary case when M_{12} and M_{21} at this edge vanish simultaneously.

Now we are in the position to examine the existence of the SEWs of TE and TM polarization. Assume a bicrystal for which both constituent half spaces admit TE and TM modes propagating in the sagittal plane XZ. The dispersion equations (26) and (27) each split into two scalar equations, so that

$$Z_{\rm TE}^{(1)} + Z_{\rm TE}^{\prime(2)} = 0,\ Z_{\rm TE}^{\prime(1)} + Z_{\rm TE}^{(2)} = 0 \tag{44}$$

define the TE SEWs in the given (direct) and complementary bicrystals, respectively, and the same equations hold for the TM SEWs. Based on the outlined properties of the TE and TM impedances and a simple graphical analysis, we can formulate the following statements. If either or both parts of a monoclinic bicrystal have a unit cell of a generic (asymmetric) arrangement, then

> given a fixed k, at most one TE-SEW (one TM-SEW) in the lowest TE (TM) forbidden band and at most two TE-SEWs (two TM-SEWs) in any upper TE (TM) band, respectively, can exist in total for the direct and complementary bicrystals.

If both upper and lower parts have symmetric unit cells, then

> no TE-SEW (no TM-SEW) exists in the lowest forbidden band and at most one TE-SEW (one TM-SEW) at a fixed k can exist in an upper TE (TM) forbidden band.

These statements can be given a stronger formulation provided that the forbidden bands of the two superlattices constituting a bicrystal coincide with each other. Then the above-formulated upper bound becomes the only and necessary option, namely, one TE SEW (one TM SEW) must exist for either a direct or a complementary bicrystal within the lowest forbidden band and two TE SEWs (one TM SEWs) in total must exist in any upper forbidden band. Note that two half-infinite superlattices of the same period have identical band structure when they can be viewed as being cut from the same infinite superlattice along different cross-section planes and then adjusted to each other (see Sec. IV).

Let us briefly discuss SEWs occurring at the interface of a superlattice with a homogeneous dielectric when both media are of appropriate crystallographic symmetry and admit TE and TM modes. The impedances $Z_{\rm TE}^{(H)}$ and $Z_{\rm TM}^{(H)}$ of TE and TM modes in a homogeneous medium, being defined by analogy with (19) but in terms of eigenvectors of the coefficient matrices of Eqs. (39) and (40), are

$$Z_{\rm TE}^{(H)} = \frac{1}{\omega\sqrt{m_{xx}\mu_{zz}}}\sqrt{k^2 - \varepsilon_{yy}\mu_{zz}\omega^2}, \tag{45a}$$

$$Z_{\rm TM}^{(H)} = \frac{1}{\omega\sqrt{\epsilon_{xx}\varepsilon_{zz}}}\sqrt{k^2 - \varepsilon_{zz}\mu_{yy}\omega^2}. \tag{45b}$$

Both $Z_{\rm TE}^{(H)}$ and $Z_{\rm TM}^{(H)}$ are real and positive at frequencies lower than the critical values $\omega_L^{(TE)}(k)$ and $\omega_L^{(TM)}(k)$, which are the roots of the equations $k/\sqrt{\varepsilon_{yy}\mu_{zz}} = \omega$ and $k/\sqrt{\varepsilon_{zz}\mu_{yy}} = \omega$, respectively, and both are decreasing functions of ω within this frequency range. The aforementioned conclusions on the number of TE and TM SEWs in a bicrystal embrace the case of a superlattice bounded by a homogeneous medium; what is interesting is that those statements can be given a stronger form. For example, let a superlattice with an asymmetric unit cell occupy the half space $z \geqslant 0$. If its TE impedance $Z_{\rm TE}$ at some fixed k has both a pole at $\omega_p^{\rm (TM)}$ and a zero at $\omega_0^{\rm (TE)}$ within an upper forbidden band, then the inequality $\omega_p^{\rm (TE)} < \omega_0^{\rm (TE)}$ is sufficient for the existence of one and only one TE SEW in this band while the inverse inequality $\omega_0^{\rm (TE)} < \omega_p^{\rm (TE)}$ is necessary for possible occurrence of two TE SEWs. In the case of a superlattice with a symmetric unit cell, existence of a single SEW in an upper forbidden band is ensured or ruled out when zero of $Z_{\rm TE}$ occurs at the upper or lower band edge, respectively.

Let the adjoined homogeneous medium be metal, so that Eq. (45) is specialized into the form (37) with the TM impedance being negative. The latter particularity reveals itself in permitting the existence of one TM SEW in the lowest forbidden band of a superlattice with symmetric unit cell bounded by metal while this was banned in the case of a contact with a dielectric.

IV. NUMERICAL EXAMPLES

The purpose of this section is to illustrate the above theoretical results and, most importantly, to demonstrate that the

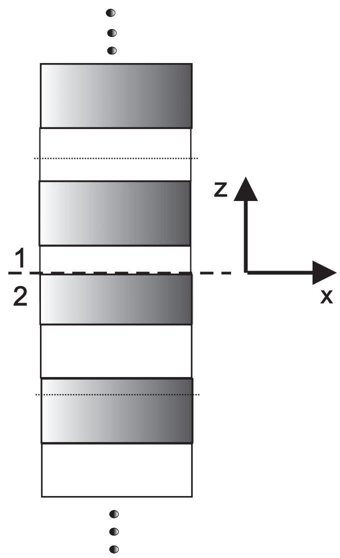

FIG. 3. A bicrystal composed of layers A (white) and B (gray) materials. All layers are of the same thickness except for the two "defect" A and B layers 1 and 2. The bold dashed line is the interface between the half-infinite A/B/A and B/A/B superlattices; dotted lines indicate edges of the unit cells.

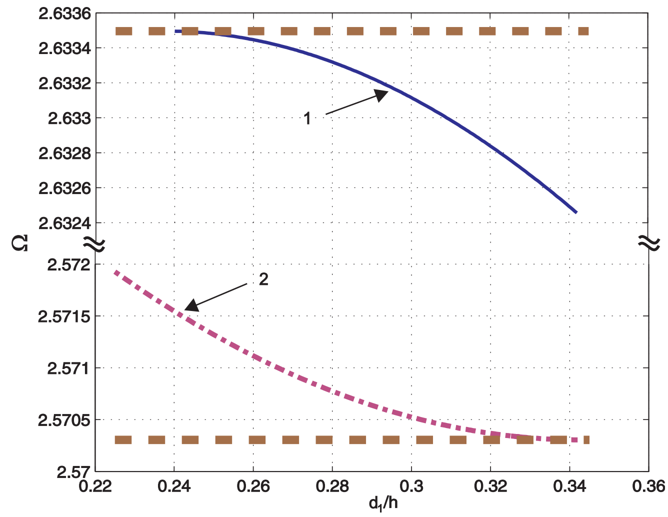

FIG. 4. Dimensionless frequency $\Omega \equiv \omega H/c$ of two TE SEWs (curves 1 and 2) at fixed $kH = 5.6$ vs the relative thickness d_1/h of the terminal AlAs layer adjacent from above to the internal interface of the AlAs/GaAs/AlAs–GaAs/AlAs/GaAs bicrystal with a period $H = 2h$. The relative thickness of the terminal layer GaAs adjacent to the interface from below is d_2/h=0.35. Horizontal dashed lines show the forbidden band edges.

established maximum for a possible number of SEWs per a forbidden band is attainable, i.e., that this number of SEWs can exist in a band and, hence, this is really a maximum rather than an upper bound. Since the occurrence of the maximum number of SEWs is a special rather than a generic occasion, we will use not only real but also fictitious materials with physically admissible parameters in order to facilitate the search task.

As a structural model, we will consider a most transparent representation of a bicrystal, namely, an infinite structure of alternating layers of two types A and B which are all of the same thickness h except a single defect cell. In the first set of examples, we will assume this cell to also be an A/B bilayer with thicknesses d_1 and d_2, where $d_1, d_2 < h$ (Fig. 3). Such structure may equally be seen as a bicrystal consisting of two half-infinite periodic superlattices, the interface $z = 0$ of which is that between the A and B defect layers. They consist of three-layer unit cells of the same thickness $H = 2h$ separated by virtual interfaces drawn inside a "physical" layer, so that one superlattice (the upper one in Fig. 3) has a A/B/A unit cell with successive layer thicknesses $\{d_1, h, h - d_1\}$ and the other (lower in Fig. 3) has a B/A/B unit cell with layer thicknesses $\{d_2, h, h - d_2\}$ (here the thicknesses are listed in the order away from the interface $z = 0$). Both unit cells are asymmetric provided that $d_{1,2} \neq h/2$. It may also be helpful to think of this bicrystal as obtained via bisecting two identical infinite superlattices of A and B layers of identical thickness along two different planes inside the layers of different types (i.e., one plane inside layer A, the other inside layer B) and then putting together the half space lying above one plane and the half space lying below the other plane. Similar conjunction of the other two half spaces yields a complementary bicrystal. The upper and lower superlattices of such a pair of bicrystals have the same band structure because the transfer matrices over the period $[z_0, z_0 + H]$ counted from different reference points z_0 of an infinite periodic sequence are similar matrices and hence possess the same set of eigenvalues.

We proceed with an example of two TE SEWs in a forbidden band (k being fixed) of a bicrystal with asymmetric unit cells. According to the foregoing analysis, if the constituent half-infinite superlattices have the same band structure (which is the case in hand, see above), then two TE SEWs are guaranteed to come about in total in the direct and/or complementary bicrystals. We are interested to find an example where both these TE SEWs occur in one given bicrystal, that is, when one of the dispersion equations (44) has two solutions (then the other has none). Figure 2(b) indicates that for this to happen, i.e., for the two functions $Z_{\mathrm{TE}}^{(I)}$ and $-Z_{\mathrm{TE}}^{\prime(J)}$ $(I, J = 1, 2;\ I \neq J)$ to intersect twice, one of them must be continuous while the other must have a pole and the band-edge values of the continuous function must be greater than those of the discontinuous one. Let us simulate such a situation for the aforementioned structural model with cubic AlAs and GaAs as the materials A and B. The principal crystallographic axes of the corresponding layers are mutually aligned and assumed parallel to the axes X, Y, and Z. The relative dielectric permittivities used in the calculation are

$$\frac{\varepsilon_{yy}}{\varepsilon_0} = \begin{cases} 2.0792 + \frac{6.0840\lambda^2}{\lambda^2 - 0.2822^2} + \frac{1.9\lambda^2}{\lambda^2 - 27.62^2} & \text{(AlAs)}, \\ 5.743 + \frac{5.1\lambda^2}{\lambda^2 - 0.2257} & \text{(GaAs)}, \end{cases} \tag{46}$$

where the wavelength $\lambda = 2\pi c/\omega$ is counted in microns and is confined to the interval $\lambda > 0.92$ μm, in which the attenuation of electromagnetic waves in AlAs and GaAs is negligibly small. These material data are approximated from the results of [67] and taken from [68]. The layer thickness is set to be $h = 0.2$ μm.

Figure 4 demonstrates the occurrence of two TE SEWs in an upper forbidden band of the AlAs/GaAs/AlAs–GaAs/AlAs/GaAs bicrystal assembled according to Fig. 3. It is seen that two waves exist within a certain range of values of thickness d_1 of the terminal AlAs layer of the upper superlattice (the period $H = 2h$ being kept constant). Beyond this range, one of the TE SEWs disappears in the given bicrystal and hence appears in the complementary GaAs/AlAs/GaAs–AlAs/GaAs/AlAs bicrystal.

Let us now seek an example of two TE SEWs in a superlattice–homogeneous dielectric structure. Two TE SEWs come about provided that the frequency dependence of the impedance $Z_{\rm TE}$ of the superlattice corresponds to curve 1 shown in Fig. 2(c) and that $Z_{\rm TE}(\omega_l) > -Z^{(H)}_{\rm TE}(\omega_l)$ and $Z_{\rm TE}(\omega_u) < -Z^{(H)}_{\rm TE}(\omega_u)$. However, since the impedance $Z^{(H)}_{\rm TE}$ (45a) involves only one adjustment parameter ε_{yy} (contrary to several material and geometrical parameters available for the impedance of a superlattice), a simultaneous occasion of the above-mentioned inequalities between the band-edge values of $Z_{\rm TE}$ and $Z^{(H)}_{\rm TE}$, which is required for the existence of two TE SEWs, turns out to be a rather tight constraint. We have failed to model occurrence of two TE SEWs in realistic cases and will exemplify them for a fictitious superlattice, the unit cell of which consists of three nonmagnetic orthotropic layers with the relative dielectric permittivities $\varepsilon_{yy}/\varepsilon_0$ equal to 10, 4, and 20 (data for the terminal layer are mentioned first), and a homogeneous half space with $\varepsilon_{yy}/\varepsilon_0$ of 8.75. For this set of data, two solutions ω_1 and ω_2 of the TE SEW dispersion equation $Z_{\rm TE} + Z^{(H)}_{\rm TE} = 0$ emerge in a forbidden band very close to its edges ω_l and ω_u, respectively. For instance, if the layer relative thicknesses are 0.075, 0.2, and 0.125 μm, respectively, then $\omega_1/\omega_l - 1 \approx 3 \times 10^{-3}$ and $1 - \omega_2/\omega_u \approx 4 \times 10^{-4}$.

Our next objective is to confirm that a direct bicrystal with an asymmetric unit cell and the corresponding complementary bicrystal can support in total two SEWs in the lowest forbidden band and four SEWs in an upper one. With this task in mind, we will consider once again an infinite structure of alternating equidistant layers A and B containing a single structural defect, which is now a single layer, say of A type, of a "perturbed" thickness d, where $d \neq h$ and $d < 2h$. Similarly to the above model with a defect bilayer, the present structure may be seen as a bicrystal formed by half-infinite periodic superlattices, each having A/B/A unit cells with successive layer thicknesses $\{d_1, h, h - d_1\}$ for one half space and $\{d_2, h, h - d_2\}$ for the other (two thickness sets are ordered in the opposite senses with respect to the axis Z), where $d_1 + d_2 = d$ with arbitrary $d_1 < d$. The latter implies that the interface $z = 0$ between the bicrystal halves may be taken at an arbitrary point of the Z axis inside the defect layer. Independence of the defect modes (the sought SEWs) from the position of this putative interface is physically obvious and may certainly be confirmed in formal terms.

Having specified the above structure as a direct bicrystal, the complementary bicrystal (as is defined in the opening paragraph of Sec. III A) is a similar structure of A and B layers of the same thickness h except for a defect A layer of thickness $2h - d$. In the subsequent calculations, d is taken to be $d = 0.9h$ ($\neq 0.5h$ so that the A/B/A unit cells are asymmetric). The A and B layers are assumed to be uniaxial with optical axes perpendicular to the XZ plane, nonmagnetic, and having relative dielectric permittivities $\varepsilon^{(A)}_{xx}/\varepsilon_0 = \varepsilon^{(A)}_{zz}/\varepsilon_0 = 7.8$, $\varepsilon^{(A)}_{yy}/\varepsilon_0 = 10$ and $\varepsilon^{(B)}_{xx}/\varepsilon_0 = \varepsilon^{(B)}_{zz}/\varepsilon_0 = 1.15$, $\varepsilon^{(B)}_{yy}/\varepsilon_0 = 2$, respectively. These values ensure that, given the value $kH = 2\pi$ (which is kept fixed hereafter), the lowest forbidden bands of TE and TM waves propagating in the XZ plane practically coincide with each other and so do the first upper forbidden bands. The common frequency ranges of these lowest and upper bands are $0 < \Omega < 2.604$ and $2.67 < \Omega < 3.684$, where $\Omega \equiv \omega H/c$.

Under these conditions, we find by computations that the direct and complementary bicrystals each support one TE SEW and one TM SEW in the upper forbidden band at frequencies $\Omega^{\rm TE}_d = 2.703$ and $\Omega^{\rm TM}_d = 2.735$, respectively. The complementary bicrystal supports one TE SEW and one TM SEW in the same band at $\Omega^{\rm TE}_c = 3.572$ and $\Omega^{\rm TM}_c = 3.608$. Within the lowest forbidden band, no SEW occurs in the direct bicrystal, whereas one TE SEW and one TM SEW come about for the complementary bicrystal at $\Omega^{\rm TE}_c = 2.592$ and $\Omega^{\rm TM}_c = 2.539$. These data are actually enough to confirm the possibility of the desired occasion of as many as two SEWs in the lowest band and four SEWs in an upper band for direct and complementary bicrystals in total. These wave solutions occur as SEWs of general polarization when the propagation direction X slightly deviates from the symmetry plane (010). For instance, let them make an angle 10°; then the lowest forbidden band is $0 < \Omega < 2.605$ and it contains two solutions for SEWs propagating in the complementary bicrystal with frequencies $\Omega^{(1)}_c = 2.541$ and $\Omega^{(2)}_c = 2.582$, while the first upper band is $2.662 < \Omega < 3.673$ and it contains two pairs of SEW solutions for the direct and complementary bicrystals at frequencies $\Omega^{(1)}_d = 2.694$, $\Omega^{(2)}_d = 2.738$ and $\Omega^{(3)}_c = 3.56$, $\Omega^{(4)}_c = 3.612$, respectively.

Finally, let us give an example of the maximum possible number of SEWs in a bicrystal with symmetric unit cells. For this purpose, we turn back to the A/B structure with a defect bilayer shown in Fig. 3 and take the thicknesses of A and B layers of the defect cell to be $d_1 = d_2 = h/2$, which renders the A/B/A and B/A/B unit cells of the upper and lower half spaces to be symmetric. The properties of layers A and B are kept the same as in the above example, hence so is the band structure (which is not affected by the values of d_1, d_2). The wave number is fixed as $kH = 2\pi$. The lowest forbidden band $0 < \Omega < 2.604$ is void of both TE and TM SEWs which is in agreement with the corresponding conclusion of Sec. III D. The first upper forbidden band $2.67 < \Omega < 3.684$ contains the frequencies $\Omega^{\rm TE} = 3.091$ and $\Omega^{\rm TM} = 3.408$ of one TE SEW and one TM SEW. Now let us modify the bicrystal by rotating its upper half as a whole about the Z axis by an angle $\theta = 10^\circ$ clockwise and its lower half by the same angle θ anticlockwise. The band structure of the "twisted" bicrystal changes only slightly, but the former TE and TM modes propagating in the XZ plane couple and acquire a general polarization. We find two such SEWs at frequencies $\Omega^{(1)} = 3.079$ and $\Omega^{(2)} = 3.414$. Additionally, one SEW emerges in the lowest forbidden band, though at frequency ω quite close to the band edge ω_u, namely, $1 - \omega/\omega_u = 4.58 \times 10^{-5}$. Thus we observe the existence of two SEWs in an upper forbidden band and of one SEW in the lowest band, which, according to

Sec. III B, is the maximum number of such waves admitted in a bicrystal with symmetric unit cells.

V. CONCLUDING REMARKS

We have established the maximum number of SEWs which may exist at a fixed tangential wave number in a forbidden band of a photonic bicrystal. The latter is formed of two half-infinite superlattices consisting of periodically assembled optically anisotropic uniaxial or biaxial nongyrotropic and nonabsorbing layers. The results apply to the materials with frequency independent dielectric permittivity $\hat{\boldsymbol{\varepsilon}}$ and magnetic permeability $\hat{\boldsymbol{\mu}}$ of general anisotropy, or to the materials of monoclinic and higher crystallographic symmetry with frequency dependent $\hat{\boldsymbol{\varepsilon}}$ and $\hat{\boldsymbol{\mu}}$, or to any anisotropic materials with dispersive $\hat{\boldsymbol{\varepsilon}}$ and $\hat{\boldsymbol{\mu}}$ in the special case $k=0$ [the latter implying that the wave field (1) varies along the stratification direction only]. In the case of generic (asymmetric) arrangement of the unit cell, the established number is the sum of the number of SEWs in a given ("direct") bicrystal with the number of SEWs in its complementary counterpart, which is obtained by swapping upper and lower superlattices of the direct one (without turning any of them upside down). The so-defined maximum number of SEWs is 2 for the lowest forbidden band originating at $\omega=0$ and 4 for any upper forbidden band regardless of the anisotropy and arrangement of the unit cells. A more stringent prediction follows in the case when both adjoined superlattices have symmetrically arranged unit cells invariant relative to the midplane. Such a bicrystal admits at most one SEW in the lowest forbidden band and at most two SEWs in any upper band. The same statements as above apply in the case when a superlattice is bounded by an arbitrary homogeneous dielectric. At the same time, certain additional options concerning SEWs in the lowest forbidden band arise when a superlattice is in contact with metal. The results obtained for SEWs of arbitrary polarization have also been specialized for the TE- and TM-polarized SEWs. For instance, the maximum possible number of either TE SEWs or TM SEWs occurring in total in the direct and complementary bicrystals is 1 in a lowest forbidden band and 2 in any upper forbidden band (the bands for TE and TM modes being independent of each other). All above conclusions equally apply to the SEWs in functionally graded photonic bicrystals.

As already mentioned, the results of the paper are obtained under a widely used no-loss assumption which underlies the standard concept of the allowed and forbidden bands and also renders the impedance matrices Hermitian. A rigorous account for an absorption in the formalism of wave propagation in periodic media is a rather intricate issue, since the Bloch wave number becomes complex valued throughout and so the notion of band structure is no longer as straightforward as it is in the no-loss case. This general problem is beyond the scope of the present paper. However, it is evident that a weak enough absorption should not change the number of SEWs, unless the SEW dispersion branch comes too close to the edge of the forbidden band where its periodicity-induced attenuation is relatively low and therefore even a weak absorption may drastically affect the wave type.

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APPENDIX A

We start from considering the limit $\omega\to 0$. Taking note that the matrix $\hat{\mathbf{N}}$ (4) diverges in this limit, it is helpful to replace the vector $\boldsymbol{\xi}(z)$ and the matrix $\hat{\mathbf{N}}$ in Eq. (2) with the vector

$$\boldsymbol{\xi}^{\omega}(z)=\begin{pmatrix}\mathbf{u}^{\omega}\\ \mathbf{v}\end{pmatrix}=\hat{\mathbf{S}}\boldsymbol{\xi}(z)\ \text{ with }\hat{\mathbf{S}}=\begin{pmatrix}\frac{1}{\omega}\mathbf{I} & \mathbf{0}\\ \mathbf{0} & \mathbf{I}\end{pmatrix}\tag{A1}$$

and with the corresponding matrix $\hat{\mathbf{N}}^{\omega}=\hat{\mathbf{S}}\hat{\mathbf{N}}\hat{\mathbf{S}}^{-1}$, so that

$$\hat{\mathbf{N}}^{\omega}=\begin{pmatrix}-k\frac{\mu_{xz}}{\mu_{zz}} & \omega m_{xy} & m_{xx} & 0\\ -\omega\epsilon_{xy} & -k\frac{\varepsilon_{xz}}{\varepsilon_{zz}} & 0 & \epsilon_{xx}\\ \omega^2\epsilon_{yy}-\frac{k^2}{\mu_{zz}} & \omega k\left(\frac{\varepsilon_{yz}}{\varepsilon_{zz}}-\frac{\mu_{yz}}{\mu_{zz}}\right) & -k\frac{\mu_{xz}}{\mu_{zz}} & -\omega\epsilon_{xy}\\ \omega k\left(\frac{\varepsilon_{yz}}{\varepsilon_{zz}}-\frac{\mu_{yz}}{\mu_{zz}}\right) & \omega^2 m_{yy}-\frac{k^2}{\varepsilon_{zz}} & \omega m_{xy} & -k\frac{\varepsilon_{xz}}{\varepsilon_{zz}}\end{pmatrix}.\tag{A2}$$

All elements of $\hat{\mathbf{N}}^{\omega}$ remain finite at $\omega\to 0$ and hence so are all components of $\boldsymbol{\xi}^{\omega}(z)$. The transfer matrix $\hat{\mathbf{M}}^{\omega}=\hat{\mathbf{S}}\hat{\mathbf{M}}\hat{\mathbf{S}}^{-1}$ of Eq. (2) redefined to include $\boldsymbol{\xi}^{\omega}(z)$ and $\hat{\mathbf{N}}^{\omega}$ has the same eigenvalues as $\hat{\mathbf{M}}$ while its eigenvectors are $\boldsymbol{\xi}^{\omega}_{\alpha}=(\mathbf{U}^{\omega}_{\alpha}\ \mathbf{V}_{\alpha})^t$ with $\mathbf{U}^{\omega}_{\alpha}=\omega^{-1}\mathbf{U}_{\alpha}$. Insertion into Eq. (21) yields $\mathbf{V}_{\alpha}=i\hat{\mathbf{Z}}^{\omega}\mathbf{U}^{\omega}_{\alpha}$ and $\mathbf{V}_{\alpha+2}=-i\hat{\mathbf{Z}}'^{\omega}\mathbf{U}^{\omega}_{\alpha+2}$ $(\alpha=1,2)$, where the impedances $\hat{\mathbf{Z}}^{\omega}=\omega\hat{\mathbf{Z}}$ and $\hat{\mathbf{Z}}'^{\omega}=\omega\hat{\mathbf{Z}}'$ stay finite at $\omega\to 0$.

Next, using the Maxwell equations, let us represent the quasistatic limit $\omega\to 0$ of the time-averaged energy density $W=\frac{1}{4}(\mathbf{E}^{\dagger}\mathbf{D}+\mathbf{H}^{\dagger}\mathbf{B})$ of the wave $\boldsymbol{\xi}^{\omega}=(\mathbf{u}^{\omega}\ \mathbf{v})^t$ as

$$\begin{aligned}4W(z)\big|_{\omega\to 0}&=\frac{d}{dz}\mathrm{Im}(\mathbf{v}^{\dagger}\mathbf{u}^{\omega})\big|_{\omega\to 0}\\ &=\mathbf{v}^{\dagger}\hat{\mathbf{N}}^{\omega}_{12}\mathbf{v}-\mathbf{u}^{\omega\dagger}\hat{\mathbf{N}}^{\omega}_{21}\mathbf{u}^{\omega}>0,\end{aligned}\tag{A3}$$

where $\hat{\mathbf{N}}^{\omega}_{12}$ and $\hat{\mathbf{N}}^{\omega}_{21}$ are the upper and lower 2×2 off-diagonal blocks of $\hat{\mathbf{N}}^{\omega}$. The inequality in (A3) follows from positiveness of energy and may be confirmed indeed via substituting $\hat{\mathbf{N}}^{\omega}_{12}$ and $\hat{\mathbf{N}}^{\omega}_{21}$ from (A2).

Let the eigenvector $\boldsymbol{\xi}_\alpha^\omega$ of $\hat{\mathbf{M}}^\omega$ be the initial condition at the edge $z=0$ of a unit cell. Then the solution $\boldsymbol{\xi}_\alpha^\omega(z)=(\mathbf{u}^\omega\ \mathbf{v})^t$ taken at the other edge $z=H$ is $\boldsymbol{\xi}_\alpha^\omega(H)=\gamma_\alpha\boldsymbol{\zeta}_\alpha^\omega$. Integrating the zth derivative of $\mathrm{Im}(\mathbf{v}_\alpha^\dagger\mathbf{u}_\alpha^\omega)|_{\omega\to 0}$ over a period H and applying inequality (A3) yields

$$\int_0^H \frac{d}{dz}\mathrm{Im}\big(\mathbf{v}_\alpha^\dagger\mathbf{u}_\alpha^\omega\big)\big|_{\omega\to 0}dz=(|\gamma_\alpha|^2-1)\mathrm{Im}\big(\mathbf{V}_\alpha^\dagger\mathbf{U}_\alpha^\omega\big)\big|_{\omega\to 0}>0. \tag{A4}$$

It follows that $|\gamma_\alpha|^2_{\omega\to 0}\neq 1$ and so, in view of (11b), the semiaxis $\omega=0$, $k\neq 0$ on the (ω,k) plane is always an origin of a forbidden band. Keeping ω within this band, consider the wave solution $\boldsymbol{\xi}^\omega(z)$ the initial value of which at $z=0$ is an arbitrary linear combination $\boldsymbol{\xi}^\omega(0)\equiv(\mathbf{U}^\omega\ \mathbf{V})^t=\sum_{\alpha=1}^2 c_\alpha\boldsymbol{\zeta}_\alpha^\omega$ of two eigenvectors corresponding to the eigenvalues $|\gamma_\alpha|<1$ $(\alpha=1,2)$. Hence such $\boldsymbol{\xi}^\omega(z)$ decays to zero at $z\to\infty$ and so certainly does a scalar product $\mathbf{v}^\dagger\mathbf{u}^\omega$ of the components of this solution. Therefore taking into account piecewise continuous differentiability of $\boldsymbol{\xi}^\omega(z)$ and integrating the derivative of $\mathrm{Im}(\mathbf{v}^\dagger\mathbf{u}^\omega)$ from zero to ∞ yields

$$\int_0^\infty \frac{d}{dz}\mathrm{Im}(\mathbf{v}^\dagger\mathbf{u}^\omega)\big|_{\omega\to 0}dz = -\mathrm{Im}(\mathbf{v}^\dagger\mathbf{u}^\omega)\big|_{\omega\to 0,\ z=0}=\mathbf{U}^{\omega\dagger}\hat{\mathbf{Z}}^\omega\mathbf{U}^\omega\big|_{\omega\to 0}>0, \tag{A5}$$

where $\mathbf{U}^\omega=\sum_{\alpha=1}^2 c_\alpha\mathbf{U}_\alpha^\omega$ is an arbitrary vector and Hermiticity of $\hat{\mathbf{Z}}^\omega$ was used. Similar reasoning with respect to the wave $\boldsymbol{\xi}^\omega(z)$ generated in the half space $z\leqslant 0$ by the initial condition $\boldsymbol{\xi}^\omega(0)=\sum_{\alpha=3}^4 d_\alpha\boldsymbol{\zeta}_\alpha^\omega$ and vanishing at $z\to-\infty$ due to $|\gamma_\alpha|>1$ $(\alpha=3,4)$ results in the inequality $\mathbf{U}'^{\omega\dagger}\hat{\mathbf{Z}}'^\omega\mathbf{U}'^\omega|_{\omega\to 0}>0$, where $\mathbf{U}'^\omega=\sum_{\alpha=3}^4 d_\alpha\mathbf{U}_\alpha^\omega$ is an arbitrary vector. Thus we conclude that

$$\hat{\mathbf{Z}}=\frac{1}{\omega}\hat{\mathbf{Z}}^\omega \text{ and } \hat{\mathbf{Z}}'=\frac{1}{\omega}\hat{\mathbf{Z}}'^\omega \text{ are positive definite matrices at } \omega\to 0. \tag{A6}$$

Further we pass to the initial formulation of Eq. (2) and consider the whole frequency range. At this stage let us assume that at a fixed k

$$k\frac{\partial}{\partial\omega}\left(\frac{\varepsilon_{iz}}{\varepsilon_{zz}}\right)=0,\ \ k\frac{\partial}{\partial\omega}\left(\frac{\mu_{iz}}{\mu_{zz}}\right)=0,\ \ i=x,y, \tag{A7}$$

i.e., the derivatives vanish or/and $k=0$. Then using Eqs. (2), (4), and (6) we find that

$$-i\frac{d}{dz}\left(\boldsymbol{\xi}^\dagger\hat{\mathbf{T}}\frac{\partial\boldsymbol{\xi}}{\partial\omega}\right)=\boldsymbol{\xi}^\dagger\hat{\mathbf{T}}\frac{\partial\hat{\mathbf{N}}}{\partial\omega}\boldsymbol{\xi}=\mathbf{E}_\tau^\dagger\hat{\mathbf{A}}_E\mathbf{E}_\tau+\mathbf{H}_\tau^\dagger\hat{\mathbf{A}}_H\mathbf{H}_\tau>0, \tag{A8}$$

where $\mathbf{E}_\tau=(\mathbb{E}_x\ \mathbb{E}_y)^t$, $\mathbf{H}_\tau=(\mathbb{H}_x\ \mathbb{H}_y)^t$,

$$\hat{\mathbf{A}}_E=\frac{\partial}{\partial\omega}\left(\omega\hat{\boldsymbol{\epsilon}}-\frac{k^2}{\omega\mu_{zz}}\hat{\mathbf{I}}'\right),\ \ \hat{\mathbf{A}}_H=\frac{\partial}{\partial\omega}\left(\omega\hat{\boldsymbol{m}}-\frac{k^2}{\omega\varepsilon_{zz}}\hat{\mathbf{I}}'\right),$$

$\hat{\mathbf{I}}'$ is a 2×2 matrix with elements $I'_{ij}=\delta_{i2}\delta_{j2}$, and the elements of matrices $\hat{\boldsymbol{\epsilon}}$ and $\hat{\boldsymbol{m}}$ are defined in (5) (note that $\hat{\boldsymbol{\epsilon}}$ and $\hat{\boldsymbol{m}}$ are the inverses of the upper 2×2 diagonal blocks of matrices $\hat{\boldsymbol{\varepsilon}}^{-1}$ and $\hat{\boldsymbol{\mu}}^{-1}$ in the adopted basis X,Y,Z). The matrices $\hat{\mathbf{A}}_E$ and $\hat{\mathbf{A}}_H$ are positive definite, because so are the matrices $\partial(\omega\hat{\boldsymbol{\varepsilon}})/\partial\omega$ and $\partial(\omega\hat{\boldsymbol{\mu}})/\partial\omega$ [69,70] and hence also $\partial(\omega\varepsilon_{zz})/\partial\omega$, $\partial(\omega\mu_{zz})/\partial\omega$ and $\partial(\omega\hat{\boldsymbol{\epsilon}})/\partial\omega$, $\partial(\omega\hat{\boldsymbol{m}})/\partial\omega$.

As the next step, consider an arbitrary forbidden band and let the two-partial wave solution $\boldsymbol{\xi}(z)=(\mathbf{u}\ \mathbf{v})^t$ be defined by the initial value $\boldsymbol{\xi}(0)\equiv(\mathbf{U}\ \mathbf{V})^t=\sum_{\alpha=1}^2 c_\alpha\boldsymbol{\zeta}_\alpha$ at $z=0$, where $\boldsymbol{\zeta}_\alpha=(\mathbf{U}_\alpha\ \mathbf{V}_\alpha)^t$ are the eigenvectors of $\hat{\mathbf{M}}$ corresponding to its eigenvalues $|\gamma_\alpha|<1$ $(\alpha=1,2)$. Assume the coefficients $c_\alpha=c_\alpha(\omega)$ to be chosen so that $\mathbf{U}=\sum_{\alpha=1}^2 c_\alpha\mathbf{U}_\alpha$ is an arbitrary but constant vector (independent of frequency). Taking this into account and integrating the left-hand side of (A8) in z from zero to ∞ yields

$$-i\int_0^\infty\frac{d}{dz}\left[\boldsymbol{\xi}^\dagger\hat{\mathbf{T}}\frac{\partial\boldsymbol{\xi}}{\partial\omega}\right]dz=i\left(\mathbf{U}^\dagger\frac{\partial\mathbf{V}}{\partial\omega}+\mathbf{V}^\dagger\frac{\partial\mathbf{U}}{\partial\omega}\right)=-\mathbf{U}^\dagger\frac{\partial\hat{\mathbf{Z}}}{\partial\omega}\mathbf{U}. \tag{A9}$$

A similar integration from zero to $-\infty$ for the wave decaying into the depth of a half space $z\leqslant 0$ shows that a Hermitian form $U'^\dagger\frac{\partial\hat{\mathbf{Z}}'}{\partial\omega}U'$, where $\mathbf{U}'=\sum_{\alpha=3}^4 d_\alpha\mathbf{U}'_\alpha$ is an arbitrary constant vector, also has the inverse sign of (A8). Thus we conclude that

$$\frac{\partial\hat{\mathbf{Z}}}{\partial\omega} \text{ and } \frac{\partial\hat{\mathbf{Z}}'}{\partial\omega} \text{ are negative definite matrices in forbidden bands.} \tag{A10}$$

provided that (A7) is fulfilled. Our consideration of the SEW in superlattices is largely based on the result (A10). For this reason, let us accentuate the cases when (A7) and hence (A10) are ensured.

(1) The layers are generally anisotropic and arbitrarily oriented but $\hat{\boldsymbol{\varepsilon}}$ and $\hat{\boldsymbol{\mu}}$ are independent of frequency.

(2) $\hat{\boldsymbol{\varepsilon}}$ and $\hat{\boldsymbol{\mu}}$ are frequency dependent but the layers are monoclinic and oriented so that the stratification axis Z, i.e., the normal to the layer interfaces, is either parallel to a symmetry axis or perpendicular to the plane of symmetry (hence the off-diagonal elements ε_{iz} and μ_{iz} with $i=x,y$ are identically zero).

(3) The layers are generally anisotropic and $\hat{\boldsymbol{\varepsilon}}$ and $\hat{\boldsymbol{\mu}}$ are frequency dependent but $k=0$.

It is clear that property (A10) remains valid even if none of the above conditions is observed but the frequency derivatives of $\varepsilon_{iz}/\varepsilon_{zz}$ and μ_{iz}/μ_{zz} $(i=x,y)$ are just too small to counteract the sign definite terms in (A8). Note also that, in view of Eqs. (39) and (40), the scalar impedances of TE and TM modes always satisfy (A10).

Of a particular significance for the analysis of SEWs is the matrix

$$\begin{aligned}\hat{\mathbf{G}}&=\hat{\mathbf{Z}}+\hat{\mathbf{Z}}'=-i(\hat{\mathbf{V}}\hat{\mathbf{U}}^{-1}-\hat{\mathbf{V}}'\hat{\mathbf{U}}'^{-1})\\&=-i(\hat{\mathbf{V}}\hat{\mathbf{U}}^{-1}+\hat{\mathbf{U}}'^{\dagger-1}\hat{\mathbf{V}}'^\dagger)\\&=-i\hat{\mathbf{U}}'^{\dagger-1}(\hat{\mathbf{U}}'^\dagger\hat{\mathbf{V}}+\hat{\mathbf{V}}'^\dagger\hat{\mathbf{U}})\hat{\mathbf{U}}^{-1}=-i(\hat{\mathbf{U}}\hat{\mathbf{U}}'^\dagger)^{-1}.\end{aligned} \tag{A11}$$

As a sum of $\hat{\mathbf{Z}}$ and $\hat{\mathbf{Z}}'$, the matrix $\hat{\mathbf{G}}$ is also a Hermitian matrix, is positive definite at $\omega\to 0$, and has a negative definite derivative with respect to ω in forbidden bands. Moreover, it can be confirmed that none of the elements of matrix $\hat{\mathbf{G}}^{-1}$ can diverge inside forbidden bands (see Appendix B). Let us formulate these properties of $\hat{\mathbf{G}}$ in terms of its eigenvalues denoted by σ_α $(\alpha=1,2)$. Note that σ_α should be understood as eigenvalues of a physically dimensionless matrix representing the numerical values of elements G_{ij} of $\hat{\mathbf{G}}$ in whichever system of physical units. It is clear that one or the other choice of units changes the magnitude of the eigenvalues but does not touch their real-valuedness, signs, zeros, and poles, which are the actual issues of our interest. Neither can a choice of physical units affect the sign of frequency derivatives of σ_α's. They are always negative due to negative definiteness of matrix $\partial\hat{\mathbf{G}}/\partial\omega$ (although its eigenvalues are not equal to $\partial\sigma_\alpha/\partial\omega$).

It follows from the above that σ_α are real and satisfy the inequalities

$$\sigma_\alpha > 0,\ \alpha = 1, 2,\ \text{in the vicinity of } \omega = 0, \tag{A12}$$

$$\frac{\partial\sigma_\alpha}{\partial\omega} < 0,\ \alpha = 1, 2,\ \text{in forbidden bands}, \tag{A13}$$

$$\sigma_\alpha \neq 0,\ \alpha = 1, 2,\ \text{in forbidden bands}. \tag{A14}$$

Combining properties (A12) with (A14) shows that

$$\begin{aligned}&\sigma_\alpha,\ \alpha = 1, 2,\ \text{have no poles}\\ &\text{in the lowest forbidden band},\end{aligned} \tag{A15}$$

while combining(A13) with (A14) and taking into account that σ_α's do not need to be positive at the lower edge of upper forbidden bands reveals that each of

$$\begin{aligned}&\text{each of } \sigma_\alpha,\ \alpha = 1, 2,\ \text{may have one pole}\\ &\text{in an upper forbidden band}.\end{aligned} \tag{A16}$$

Note that if $\hat{\mathbf{G}}$ has a diverging eigenvalue then so does either $\hat{\mathbf{Z}}$ or $\hat{\mathbf{Z}}'$. Therefore the eigenvalues λ_α and λ'_α ($\alpha = 1, 2$) of $\hat{\mathbf{Z}}$ and $\hat{\mathbf{Z}}'$, being positive at $\omega \to 0$ and decreasing with growing ω in forbidden bands, have no poles in the lowest forbidden band and may have at most two poles in total in an upper forbidden band.

In the case of a symmetric unit cell, combining Eqs. (23) and (A10) yields

$$\hat{\mathbf{G}}^{(S)} = 2\mathrm{Re}\hat{\mathbf{Z}}^{(S)} = -i(\hat{\mathbf{U}}\hat{\mathbf{U}}^t)^{-1}. \tag{A17}$$

The eigenvalues ν_α ($\alpha = 1, 2$) of $\mathrm{Re}\hat{\mathbf{Z}}^{(S)} = \frac{1}{2}\hat{\mathbf{G}}^{(S)}$ certainly retain the properties (A12)–(A15). A new feature, which is due to Eq. (A17), is that the poles of ν_α may come about only simultaneously, since $\det(\hat{\mathbf{G}}^{(S)-1}) = -(\det\hat{\mathbf{U}})^2$ and hence $\det(\hat{\mathbf{G}}^{(S)-1})$ vanishes at $\det\hat{\mathbf{U}} = 0$ together with its frequency derivative. Thus property (A16) is modified as follows:

$$\begin{aligned}&\nu_\alpha,\ \alpha = 1, 2,\ \text{in an upper forbidden band}\\ &\text{are either continuous or have one common pole}.\end{aligned} \tag{A18}$$

APPENDIX B

The fact that the matrix

$$\hat{\mathbf{G}}^{-1} = i\hat{\mathbf{U}}\hat{\mathbf{U}}'^{\dagger} = i\sum_{\alpha=1}^{2}\mathbf{U}_\alpha \otimes \mathbf{U}^*_{\alpha+2} \tag{B1}$$

does not diverge in forbidden bands is not evident at the secluded values $(\omega, k)_d$ where the degeneracy $\gamma_1 = \gamma_2$ and hence $\gamma_3 = \gamma_4$ of the eigenvalues γ_α of the transfer matrix $\hat{\mathbf{M}}$ occurs such that it renders $\hat{\mathbf{M}}$ non-semi-simple (not diagonalizable). When ω, k tend to $(\omega, k)_d$, the eigenvectors $\boldsymbol{\zeta}_\alpha = (\mathbf{U}_\alpha\ \mathbf{V}_\alpha)^t$ of $\hat{\mathbf{M}}$ tend to infinity and hence so may do the elements of $\hat{\mathbf{G}}^{-1}$. On the other hand, divergence of individual dyads in (B1) does not necessarily mean divergence of their sum. We shall prove that in fact all elements of $\hat{\mathbf{G}}^{-1}$ stay finite at $(\omega, k)_d$ and hence everywhere within any forbidden band.

Let us first note that $\hat{\mathbf{G}}^{-1}$ is i times the upper off-diagonal block of the matrix $\sum_{\alpha=1}^{2}\boldsymbol{\zeta}_\alpha \otimes \hat{\mathbf{T}}\boldsymbol{\zeta}^*_{\alpha+2}$ so that its components may be written as

$$(\hat{\mathbf{G}}^{-1})_{ij} = i\sum_{\alpha=1}^{2}(\boldsymbol{\zeta}_\alpha \otimes \hat{\mathbf{T}}\boldsymbol{\zeta}^*_{\alpha+2})_{i,j+2} \equiv i\sum_{\alpha=1}^{2}a_\alpha^{(i,j+2)},$$
$$i, j = 1, 2;\ \alpha = 1, 2. \tag{B2}$$

With this in mind, let us consider each (ij)th element of the matrix identities

$$\hat{\mathbf{M}}^m = \sum_{\alpha=1}^{2}\left(\gamma_\alpha^m\boldsymbol{\zeta}_\alpha \otimes \hat{\mathbf{T}}\boldsymbol{\zeta}^*_{\alpha+2} + \gamma_{\alpha+2}^m\boldsymbol{\zeta}_{\alpha+2} \otimes \hat{\mathbf{T}}\boldsymbol{\zeta}^*_\alpha\right),$$
$$m = 0, \ldots, 3, \tag{B3}$$

in the proximity of $(\omega, k)_d$ as a system of four equations

$$\sum_{\alpha=1}^{2}\left(\gamma_\alpha^m a_\alpha^{(ij)} + \gamma_{\alpha+2}^m a_{\alpha+2}^{(ij)}\right) = b_m^{(ij)},\ i, j = 1, \ldots, 4, \tag{B4}$$

where $a_\alpha^{(ij)}$ is defined in (B2), $a_{\alpha+2}^{(ij)} = (\boldsymbol{\zeta}_{\alpha+2} \otimes \hat{\mathbf{T}}\boldsymbol{\zeta}^*_\alpha)_{ij}$, and $b_m^{(ij)} = (\hat{\mathbf{M}}^m)_{ij}$. The solution of each system is

$$a_\beta^{(ij)} = \frac{\Delta_\beta^{(ij)}}{D}, \beta = 1, \ldots, 4,\ \text{ with } D = \prod\nolimits_{1\leqslant n<\beta\leqslant 4}(\gamma_\beta - \gamma_n), \tag{B5}$$

where D is the so-called Vandermonde determinant and $\Delta_\beta^{(ij)}$ is obtained from the matrix of coefficients of system (B4) by replacing its βth column with the column $b_m^{(ij)}$. It follows from (B5) that

$$\sum_{\alpha=1}^{2}a_\alpha^{(ij)} = \frac{\Lambda^{(ij)}}{D} - 1,\ \ i, j = 1, \ldots, 4, \tag{B6}$$

where $\Lambda^{(ij)} = \Delta_1^{(ij)} + \Delta_2^{(ij)} + D$ is the determinant of the 4×4 matrix $\hat{\boldsymbol{\Lambda}}^{(ij)}$ with components $[\Lambda^{(ij)}]_{n\beta} = b_{n-1}^{(ij)} + \gamma_\beta^{n-1}$ at $\beta = 1, 2$ and $[\Lambda^{(ij)}]_{n\beta} = \gamma_\beta^{n-1}$ at $\beta = 3, 4$ ($n = 1, \ldots, 4$). It can be verified that

$$\Lambda^{(ij)} = (\gamma_2 - \gamma_1)(\gamma_4 - \gamma_3)\tilde{\Lambda}^{(ij)}, \tag{B7}$$

where the determinant $\tilde{\Lambda}^{(ij)}$ is always finite. As a result, the product $(\gamma_2 - \gamma_1)(\gamma_4 - \gamma_3)$ cancels in $\Lambda^{(ij)}/D$ and hence the left-hand side of Eq. (B6) remains finite even if (ω, k) coincides with $(\omega, k)_d$ where $\gamma_1 = \gamma_2$ and $\gamma_3 = \gamma_4$. Thus, comparing (B2) and (B6), we can conclude that the matrix $\hat{\mathbf{G}}^{-1}$ is assuredly finite inside forbidden bands. If the transfer matrix $\hat{\mathbf{M}}$ is defined on a symmetric unit cell, then $\hat{\mathbf{G}}^{-1}$ reduces to $\frac{1}{2}(\mathrm{Re}\hat{\mathbf{Z}}^{(S)})^{-1} = i\hat{\mathbf{U}}\hat{\mathbf{U}}^t$ and so it is $(\mathrm{Re}\hat{\mathbf{Z}}^{(S)})^{-1}$ which takes over the property of having no poles within forbidden bands.

Note in conclusion that, contrary to the interior of forbidden bands, the matrix $\hat{\mathbf{G}}^{-1}$ may diverge at their edges, since they are conditioned by the degeneracy $\gamma_\alpha = \gamma_{\alpha+2}$ ($\alpha = 1$ or 2) and the latter generally blows up the ratios $\Lambda^{(ij)}/D$.

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