Surface acoustic waves on one-dimensional phononic crystals of general anisotropy: Existence considerations

A. N. Darinskii[1,2] and A. L. Shuvalov[3]

[1]*Institute of Crystallography FSRC "Crystallography and Photonics", Russian Academy of Sciences, Leninskii pr. 59, Moscow 119333, Russia*

[2]*National University of Science and Technology "MISIS", Leninsky pr. 4, Moscow 119049, Russia*

[3]*Université de Bordeaux, CNRS, UMR 5295, 33405 Talence, France*

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Existence of surface acoustic waves on the boundary of half-infinite one-dimensional phononic crystals is investigated. The structure is formed of perfectly bonded solid nonpiezoelectric layers of general anisotropy. The layers are parallel to the substrate surface. It is shown that at most three surface waves can exist in a stopband. The number of surface waves on the structure with a given order of layers is correlated with the number of surface waves on the structure where the order of layers is reversed, namely, in total at most three surface waves occur within a stopband. However, if the layers are arranged so that the period is symmetric with respect to its midplane, "symmetric" period, then at most one surface wave exists per stopband on the phononic crystal-vacuum boundary. A criterion of the occurrence of such a wave in the lowest stopband is found. No surface acoustic wave exists in the lowest stopband on the mechanically clamped surface but one surface wave can occur in the other stopbands. The case of "symmetric" period has no relation to crystallographic symmetry. In particular, it occurs in half-infinite two-layered phononic crystals where the thickness of the exterior layer of the substrate is half the thickness of the interior layers of the same material.

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I. INTRODUCTION

During the last decades much attention has been paid to acoustic waves in phononic crystals [1–3]. The simplest option is a one-dimensional (1D) phononic crystal, a periodically layered medium. Even in this case the band structure of frequency spectra results in intriguing peculiarities in the behavior of the reflection and transmission coefficients [4,5]. Notice that the results obtained in studying the elastic wave propagation in 1D phononic crystals are useful for understanding the properties of low-frequency acoustic phonons in semiconductor superlattices [6–8].

The boundary of phononic crystals is able to support surface acoustic waves (SAWs) just as the boundary of homogeneous solids [9]. SAWs on 1D phononic crystals with layers parallel to the surface truncating the structure were studied extensively (see [4] for a review). In particular, shear horizontally polarized (SH) SAWs in nonpiezoelectric and piezoelectric phononic crystals [10–17], sagittally polarized two-partial SAWs [18–21], fully coupled three-partial SAWs [22–25], and leaky SAWs [17,21,25] were investigated. The scalar setup of elastic SH waves is a special case, for it allows analytical insight into the link between the inhomogeneity profile and the existence of SH SAW in layered or continuously periodic structures [16]. Note that the SAW propagation on periodic solid-fluid structures [5,26] and on solid-fluid Fibonacci superlattices [27] was also intensively studied analytically and numerically.

Despite a large amount of results, the question of actual existence and number of SAWs on 1D phononic crystals still remains open. This work fills in this gap as applied to solid structures with perfectly bonded layers. We prove a number of statements concerning the existence of SAWs on half-infinite nonpiezoelectric 1D phononic structures of general anisotropy. In other words, our considerations do not take advantage of any properties related to a particular crystallographic symmetry. It appears that ideas put forward in order to study the SAW propagation in homogeneous substrates are applicable to the SAW existence problem in periodic structures. We mean the theorems concerning the existence of SAWs on half-infinite homogeneous purely elastic anisotropic substrates [28,29] (see also [30–32]).

Our paper is arranged as follows. In Sec. II we briefly remind some general relations, which hold true for plane waves in nonpiezoelectric substrates. Section III discusses the properties of the transfer matrix. Section IV is devoted to the SAW existence problem in 1D phononic crystals. Section V presents numerical examples illustrating our general conclusions. The results of our study are summarized in Sec. VI. In the Appendix an important property of matrices involved in our considerations is proved.

II. ELASTIC WAVES IN NONPIEZOELECTRIC SUBSTRATES

Let an elastically anisotropic medium occupy the half-space $\mathbf{nr} > 0$, where $\mathbf{n}$ is the unit normal to the boundary and $\mathbf{r} = (x_1, x_2, x_3)$ is the radius vector. The unit vector $\mathbf{m}$ is perpendicular to $\mathbf{n}$ and specifies the direction of propagation of a plane harmonic wave $\mathbf{u}(\mathbf{r}, t)$ along the surface $\mathbf{nr} = 0$. The displacement $\mathbf{u}(\mathbf{r}, t)$ is usually sought for in the form

$$\mathbf{u}(\mathbf{r}, t) = \mathbf{A}(y)e^{i[k(\mathbf{mr})-\omega t]}, \quad (1)$$

where the vector function $\mathbf{A}(y)$ describes the dependence of the displacement on the distance $y = \mathbf{nr}$ from the boundary, k is the wave number, and ω is the frequency. The wave field satisfies the equation [9]

$$\frac{\partial \sigma_{ij}}{\partial x_j} = -\rho\omega^2 u_i, \tag{2}$$

where $\sigma_{ij} = c_{ijkl}\partial u_k/\partial x_l$ are the components of the mechanical stress tensor $\hat{\sigma}$ in a solid with elastic moduli $c_{ijkl}, i, j, k, l = 1, 2, 3$, u_i, $i = 1, 2, 3$, are the components of $\mathbf{u}(\mathbf{r}, t)$ and ρ is the density. In addition, the boundary conditions at $y = 0$ and in the depth $y \to \infty$ must be fulfilled.

The boundary conditions at $y = 0$ commonly involve traction $\mathbf{F} = \mathbf{F}(0)$, where $\mathbf{F}(y) = \hat{\sigma}\mathbf{n}$, or/and displacement $\mathbf{A} = \mathbf{A}(0)$. The displacement-traction field described by the vector column $\xi(y) = (\mathbf{A}(y),\ \mathbf{L}(y))^t$, where $\mathbf{L}(y) = ik^{-1}\mathbf{F}(y)$, obeys a set of six first-order differential equations [33]

$$\frac{1}{ik}\frac{d\xi}{dy} = \hat{\mathbf{N}}\xi \tag{3}$$

with the 6×6 real matrix

$$\hat{\mathbf{N}} = -\begin{Bmatrix} (nn)^{-1}(nm) & (nn)^{-1} \\ (mn)(nn)^{-1}(nm) - (mm) + \rho v^2\hat{\mathbf{I}} & (mn)(nn)^{-1} \end{Bmatrix} \tag{4}$$

constructed from 3×3 matrices of the type (ab) with components $(ab)_{IJ} = a_k c_{kIJl} b_l$, $\mathbf{a}$ and $\mathbf{b}$ are vectors, $v = \omega/k$ is the velocity of the wave field along the surface, and $\hat{\mathbf{I}}$ is the 3×3 unit matrix.

When the medium is homogeneous, i.e., $\hat{\mathbf{N}}$ is a constant, solutions of Eq. (3) are linear superpositions of the partial waves $\xi_\alpha(y) = \xi_\alpha \exp[ikp_\alpha y]$, where $\xi_\alpha = (\mathbf{A}_\alpha,\ \mathbf{L}_\alpha)^t$ and p_α satisfy the eigenvalue problem

$$\hat{\mathbf{N}}\xi_\alpha = p_\alpha\xi_\alpha, \quad \alpha = 1, \ldots, 6. \tag{5}$$

The properties of $\hat{\mathbf{N}}$ and its eigenvectors are comprehensively discussed in Refs. [31–35]. We shall take advantage of the symmetry relation

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

where

$$\hat{\mathbf{T}} = \begin{Bmatrix} \hat{\mathbf{O}} & \hat{\mathbf{I}} \\ \hat{\mathbf{I}} & \hat{\mathbf{O}} \end{Bmatrix} \tag{7}$$

and $\hat{\mathbf{O}}$ is the 3×3 zero matrix. Therefore, the eigenvectors ξ_α can be orthonormalized,

$$(\hat{\mathbf{T}}\xi_\alpha)^t\xi_\beta = \delta_{\alpha\beta}, \tag{8}$$

where $\delta_{\alpha\beta}$ is the Kronecker symbol.

If the medium is vertically inhomogeneous but homogeneous along any horizontal directions, i.e., for any orientations of $\mathbf{m}$, then the wave field is still sought for in the form (1). An important role is played by the transfer matrix $\hat{\mathbf{M}}$ which expresses the mechanical displacement and traction at plane $y = y_a$ in terms of these characteristics referred to plane $y = y_b$: $\xi_a = \hat{\mathbf{M}}\xi_b$, where $\xi_{a,b}$ are the ξ vectors at $y_{a,b}$, respectively.

Let the layer between $y = y_a$ and $y = y_b$ be homogeneous. By virtue of Eqs. (5) and (8),

$$\hat{\mathbf{M}} = \sum_{\alpha=1}^{6} e^{ikhp_\alpha}\xi_\alpha \otimes \hat{\mathbf{T}}\xi_\alpha = e^{ikh\hat{\mathbf{N}}}, \tag{9}$$

where the symbol $\otimes$ stands for the dyadic product and $h = y_a - y_b$. The transfer matrix of n perfectly bonded layers of thicknesses $h_1, h_2, \ldots, h_n$ is the product of the transfer matrices $\hat{\mathbf{M}}_i = \exp[ikh_i\hat{\mathbf{N}}_i]$, where $\hat{\mathbf{N}}_i$ is the $\hat{\mathbf{N}}$ matrix (4) of i^{th} layer:

$$\hat{\mathbf{M}} = \hat{\mathbf{M}}_n\hat{\mathbf{M}}_{n-1}\ldots\hat{\mathbf{M}}_1 = e^{ikh_n\hat{\mathbf{N}}_n}e^{ikh_{n-1}\hat{\mathbf{N}}_{n-1}}\ldots e^{ikh_1\hat{\mathbf{N}}_1}. \tag{10}$$

The propagation of plane modes in 1D phononic crystals, where the neighboring layers are perfectly bonded with each other, can be analyzed in terms of six-component vector columns $\zeta_\alpha = (\mathbf{A}_\alpha,\ \mathbf{L}_\alpha)^t$ formed of the displacement vector and the traction similar to the eigenvectors ξ_α of the matrix $\hat{\mathbf{N}}$. Given the value of k in Eq. (1), the frequency spectrum is found from the condition that the vectors $\zeta_{\alpha,a}$ and $\zeta_{\alpha,b}$ at the two boundaries $y = y_a$ and $y = y_b$ of a structure period, respectively, are collinear, $\zeta_{\alpha,a} = \gamma_\alpha\zeta_{\alpha,b}$, the parameter γ_α being independent of the period number. In other words, ζ_α and γ_α solve the eigenvalue problem for the transfer matrix $\hat{\mathbf{M}}$ (10) of a single period,

$$\hat{\mathbf{M}}\zeta_\alpha = \gamma_\alpha\zeta_\alpha, \quad \alpha = 1, \ldots, 6. \tag{11}$$

We shall call eigensolutions of Eq. (11) partial modes with understanding that the displacement-traction field of the mode α inside layer 1 is $\zeta_\alpha(y) = \exp(iky\hat{\mathbf{N}}_1)\zeta_\alpha$, inside the next layer $\zeta_\alpha(y) = \exp(iky\hat{\mathbf{N}}_2)\exp(ikh_1\hat{\mathbf{N}}_1)\zeta_\alpha$, etc.

If $|\gamma_\alpha| = 1$, then this mode freely moves through the infinite phononic crystal like a bulk mode in a homogeneous solid. Within certain frequency intervals (stopbands) $|\gamma_\alpha| \neq 1$. In this instance, the wave field at the boundaries of periods decreases or increases with distance from a fixed boundary. If the eigenvector ζ_α is referred to boundary $y = 0$, then the ζ vector at boundary $y = nH$ of the nth period is $\zeta_\alpha^{(n)} = \gamma_\alpha^n\zeta_\alpha$. The modes with $|\gamma_\alpha| \neq 1$ are analogs of inhomogeneous modes with $\mathrm{Im}(p_\alpha) \neq 0$ in homogeneous substrates. They can be used to construct wave fields in confined structures, e.g., SAWs.

III. PROPERTIES OF THE TRANSFER MATRIX

Our analysis of the SAW existence on the surface of 1D phononic crystals will be based on general properties of the transfer matrix $\hat{\mathbf{M}}$ (10). Let us assume that the period is "symmetric": The period involves an odd number of layers $n = 2m + 1$, layers i and $n + 1 - i$, $i = 1, \ldots, m$, are identical but there is no restriction on their crystallographic symmetry. In this instance the transfer matrix reads as

$$\begin{aligned}\hat{\mathbf{M}}_S &= \hat{\mathbf{M}}_1\hat{\mathbf{M}}_2\ldots\hat{\mathbf{M}}_{m+1}\ldots\hat{\mathbf{M}}_2\hat{\mathbf{M}}_1 \\ &= e^{ikh_1\hat{\mathbf{N}}_1}e^{ikh_2\hat{\mathbf{N}}_2}\ldots e^{ikh_{m+1}\hat{\mathbf{N}}_{m+1}}\ldots e^{ikh_2\hat{\mathbf{N}}_2}e^{ikh_1\hat{\mathbf{N}}_1}.\end{aligned} \tag{12}$$

It is noteworthy that a two-layered structure can always be viewed as a structure with symmetric period. Indeed, one can choose the center planes of layers 1 as the period boundaries to obtain

$$\hat{\mathbf{M}}_S = e^{ikh_1\hat{\mathbf{N}}_1}e^{ikh_2\hat{\mathbf{N}}_2}e^{ikh_1\hat{\mathbf{N}}_1} \tag{13}$$

(the thickness of layer 1 equals $2h_1$).

Due to Eq. (6) [36],

$$(\hat{\mathbf{T}}\hat{\mathbf{M}}_S)^t = \hat{\mathbf{T}}\hat{\mathbf{M}}_S, \tag{14}$$

wherefrom it follows that the eigenvectors of $\hat{\mathbf{M}}_S$ can be introduced orthonormalized

$$(\hat{\mathbf{T}}\zeta_\alpha)^t \zeta_\beta = \delta_{\alpha\beta}. \tag{15}$$

In addition,

$$\hat{\mathbf{M}}_S^{-1} = \hat{\mathbf{M}}_S^*, \tag{16}$$

so

$$\hat{\mathbf{M}}_S^* \zeta_\alpha^* = \gamma_\alpha^* \zeta_\alpha^* \quad \text{and} \quad \hat{\mathbf{M}}_S^* \zeta_\alpha = \gamma_\alpha^{-1} \zeta_\alpha. \tag{17}$$

Hence, if γ_α is an eigenvalue of $\hat{\mathbf{M}}_S$, then $1/\gamma_\alpha^*$ is also an eigenvalue. Thus, the eigenvalues of $\hat{\mathbf{M}}_S$ appear pairwise either as

$$\gamma_\alpha = |\gamma_\alpha| e^{i\varphi_\alpha}, \quad \gamma_{\alpha+3} = \frac{1}{|\gamma_\alpha|} e^{i\varphi_\alpha}, \quad |\gamma_\alpha| \neq 1, \tag{18}$$

or

$$\gamma_\alpha = e^{i\varphi_\alpha}, \quad \gamma_{\alpha+3} = e^{i\varphi_{\alpha+3}}, \tag{19}$$

where φ_α and $\varphi_{\alpha+3}$ are real. In the former case $\gamma_\alpha = 1/\gamma_{\alpha+3}^*$. Hence, ζ_α and $\zeta_{\alpha+3}$ can be introduced in such a way that

$$\zeta_\alpha^* = \zeta_{\alpha+3}. \tag{20}$$

In the latter case, $\gamma_\alpha = 1/\gamma_\alpha^*$. Accordingly, the vectors ζ_α and ζ_α^* prove to be collinear. Hence, the eigenvectors ζ'_α and $\zeta'_{\alpha+3}$ not obeying the normalization condition (15) can be purely real. When normalized, one of the eigenvectors is purely real and the other is purely imaginary depending on which of the products $(\hat{\mathbf{T}}\zeta'_\alpha)^t\zeta'_\alpha$ and $(\hat{\mathbf{T}}\zeta'_{\alpha+3})^t\zeta'_{\alpha+3}$ is positive. These products are of opposite sign since they are proportional to the energy flow carried by modes α and $\alpha + 3$ perpendicular to the layers, respectively. As it has been already mentioned, this pair of eigensolutions corresponds to two modes freely propagating in the infinite periodic structure.

In the general case, "asymmetric" period, by virtue of Eq. (6) the transfer matrix (10) of the single period possesses the property [24]

$$\hat{\mathbf{T}}(\hat{\mathbf{T}}\hat{\mathbf{M}})^t = \hat{\mathbf{T}}\hat{\mathbf{M}}^t\hat{\mathbf{T}} = \hat{\mathbf{M}}^{*-1}. \tag{21}$$

According to Ref. [37], if a matrix fulfills relation (21), then its eigenvalues also appear in pairs either (18) or (19).

We multiply Eq. (11) by $(\hat{\mathbf{T}}\zeta_\beta^*)^t$ from the left,

$$(\hat{\mathbf{T}}\zeta_\beta^*)^t \hat{\mathbf{M}}\zeta_\alpha = \gamma_\alpha (\hat{\mathbf{T}}\zeta_\beta^*)^t \zeta_\alpha, \tag{22}$$

and transform the left-hand side of Eq. (22),

$$\begin{aligned}(\hat{\mathbf{T}}\zeta_\beta^*)^t \hat{\mathbf{M}}\zeta_\alpha &= (\hat{\mathbf{T}}\zeta_\beta^*)^t \hat{\mathbf{M}}\hat{\mathbf{T}}\hat{\mathbf{T}}\zeta_\alpha = (\hat{\mathbf{T}}\zeta_\beta^*)^t (\hat{\mathbf{T}}\hat{\mathbf{M}}^t)^t \hat{\mathbf{T}}\zeta_\alpha \\ &= (\hat{\mathbf{T}}\hat{\mathbf{M}}^t\hat{\mathbf{T}}\zeta_\beta^*)^t \hat{\mathbf{T}}\zeta_\alpha = (\hat{\mathbf{T}}\zeta_\beta^*)^t \zeta_\alpha/\gamma_\beta^*. \end{aligned} \tag{23}$$

Hence, $(\hat{\mathbf{T}}\zeta_\beta^*)^t\zeta_\alpha = 0$ when $\gamma_\alpha \neq 1/\gamma_\beta^*$.

Thus, if $\gamma_\alpha = |\gamma_\alpha| e^{i\varphi_\alpha}$ with $|\gamma_\alpha| \neq 1$, then one can put

$$(\hat{\mathbf{T}}\zeta_\beta^*)^t \zeta_\alpha = \delta_{\alpha+3,\beta}. \tag{24}$$

A specific case is met when $\gamma_\alpha = e^{i\varphi_\alpha}$ and $\gamma_{\alpha+3} = e^{i\varphi_{\alpha+3}}$. In this instance, the eigenvectors describe a pair of bulk modes. Therefore, one of the products $(\hat{\mathbf{T}}\zeta_\alpha^{\prime *})^t\zeta'_\alpha$ and $(\hat{\mathbf{T}}\zeta_{\alpha+3}^{\prime *})^t\zeta'_{\alpha+3}$ of the non-normalized eigenvectors $\zeta'_{\alpha,\alpha+3}$ is positive and the other is negative since these products are proportional to the energy flow perpendicular to layers (the mode is incident in the former case and reflected in the latter case). Hence, the following normalization conditions can be adopted:

$$\begin{aligned}(\hat{\mathbf{T}}\zeta_\beta^*)^t \zeta_\alpha &= \delta_{\alpha\beta} \quad \text{if the mode } \alpha \text{ is incident,} \\ (\hat{\mathbf{T}}\zeta_\beta^*)^t \zeta_\alpha &= -\delta_{\alpha\beta} \quad \text{if the mode } \alpha \text{ is reflected.}\end{aligned} \tag{25}$$

Note that $(\hat{\mathbf{T}}\zeta_\alpha^*)^t\zeta_\alpha = 0$ when $|\gamma_\alpha| \neq 1$ shows that the decaying and growing modes do not carry the energy perpendicular to layers.

The above-listed properties are valid provided that the eigenvalues of the transfer matrix are distinct which generally holds true. However, given the vectors $\mathbf{n}$ and $\mathbf{m}$ as well as the value of k, at secluded values of the frequency ω, or the velocity $v = \omega/k$, coinciding eigenvalues can appear. Two options are met. In spite of coincidence there are still six linearly linearly independent eigenvectors (semisimple degeneracy). There also can be that the matrix possesses less than six eigenvectors (nonsemisimple degeneracy). The similar types of degeneracy occur with the eigenvalues of the matrix $\hat{\mathbf{N}}$. For instance, $\hat{\mathbf{N}}$ is nonsemisimply degenerate at the velocities at which the so-called limiting bulk waves appear, that is, the bulk waves with group velocity perpendicular to $\mathbf{n}$ [28,31]. Analogous nonsemisimple degeneracy of the transfer matrix takes place at the frequencies separating passbands and stopbands. The properties of the degenerate transfer matrix and its eigenvectors can be investigated by analogy with the analysis of the properties of the matrix $\hat{\mathbf{N}}$ [31–35].

IV. EXISTENCE OF SURFACE WAVES

We assume that boundary $y = 0$ of the half-infinite phononic crystal is simultaneously the boundary of the period. If the exterior half-space is vacuum, then the traction is to vanish at $y = 0$. It is also of interest to investigate the mechanically clamped surface which implies the vanishing of the mechanical displacement at $y = 0$. In particular, the fact of existence or nonexistence of SAWs on the mechanically clamped surface can allow one to make predictions regarding interfacial waves on the contact between two half-infinite media. Some hints can be extracted from the examination of Refs. [38,39] where waves on a contact between two homogeneous solids are studied.

The boundary conditions generally put three relations on the characteristics of the wave field, so the wave field should involve at least three partial modes in order to satisfy these relations. Besides, the SAW field is to decrease to zero as y tends to infinity. Therefore, a SAW generally occurs only within "full" stopbands, that is, within frequency intervals where, given the k value, the magnitudes of all six eigenvalues of the transfer matrix are not equal to unity, so three eigensolutions with $|\gamma_\alpha| < 1$ can be selected. We put $|\gamma_\alpha| < 1$ at $\alpha = 1, 2, 3$.

Within a "full" stopband $\omega_{\min} < \omega < \omega_{\max}$ the displacement-traction vector $\zeta_{\text{SAW}} = (\mathbf{A}_{\text{SAW}}, \mathbf{L}_{\text{SAW}})^t$ of SAW field is representable at $y = 0$ as a linear combination of three eigenvectors of the transfer matrix,

$$\zeta_{\mathrm{SAW}} = \sum_{\alpha=1}^{3} b_\alpha \zeta_\alpha. \quad (26)$$

The coefficients b_α are to be such that either $\mathbf{L}_{\mathrm{SAW}} = 0$ or $\mathbf{A}_{\mathrm{SAW}} = 0$. The former equality requires the linear dependence of the vectors $\mathbf{L}_{1,2,3}$. The SAW frequency ω_{SAW} is a root of the equation $\det(\hat{\mathbf{L}}_{123}) = 0$, where $\hat{\mathbf{L}}_{123}$ is the 3×3 matrix which columns are the vectors $\mathbf{L}_{1,2,3}$. The condition $\mathbf{A}_{\mathrm{SAW}} = 0$ will be fulfilled at a frequency which satisfies the equation $\det(\hat{\mathbf{A}}_{123}) = 0$, where $\hat{\mathbf{A}}_{123}$ is the 3×3 matrix which columns are the vectors $\mathbf{A}_{1,2,3}$. We shall investigate separately the cases where the period of the substrate is symmetric and asymmetric.

A. Symmetric period

Let us form the real 6×6 matrix

$$\hat{\Upsilon} = i\sum_{\alpha=1}^{3}[\zeta_\alpha \otimes \hat{\mathbf{T}}\zeta_\alpha - \zeta_{\alpha+3} \otimes \hat{\mathbf{T}}\zeta_{\alpha+3}]$$
$$= i\sum_{\alpha=1}^{3}[\zeta_\alpha \otimes \hat{\mathbf{T}}\zeta_\alpha - \zeta_\alpha^* \otimes \hat{\mathbf{T}}\zeta_\alpha^*] = \begin{pmatrix} \hat{\mathbf{S}} & \hat{\mathbf{Q}} \\ \hat{\mathbf{B}} & \hat{\mathbf{S}}^t \end{pmatrix}, \quad (27)$$

where $\hat{\mathbf{S}}$, $\hat{\mathbf{Q}}$, and $\hat{\mathbf{B}}$ are the 3×3 blocks of $\hat{\Upsilon}$, the matrices $\hat{\mathbf{Q}}$ and $\hat{\mathbf{B}}$ being symmetric.

The matrix $\hat{\Upsilon}$ is an analog of the so-called integral Stroh matrix introduced in [28,29]. The integral Stroh matrix is defined in [28,29] as the integral of a matrix $\hat{\mathbf{N}}(\theta)$ over the angle θ from 0 to 2π, where $\hat{\mathbf{N}}(\theta)$ is obtained from Eq. (4) by substituting the vectors $\mathbf{m}' = \mathbf{m}\cos\theta - \mathbf{n}\sin\theta$ and $\mathbf{n}' = \mathbf{m}\sin\theta + \mathbf{n}\cos\theta$ for $\mathbf{m}$ and $\mathbf{n}$, respectively, and $c_{ijkl} - \rho v^2\delta_{jk}m_i m_l$ for c_{ijkl}. The integration way, which comes from the theory of dislocations in anisotropic solids [40], is not applicable to the cases under consideration and one has to demonstrate that matrix (27) does not diverge inside full stopbands at frequencies where the transfer matrix falls into nonsemisimple degeneracy (see Appendix).

The degeneracy issue arises because the eigenvector ζ_d, which corresponds to the degenerate eigenvalue of the nonsemisimply degenerate $\hat{\mathbf{M}}_S$, is self-orthogonal in the sense $(\hat{\mathbf{T}}\zeta_d)^t\zeta_d = 0$ [cf. Eq. (15)]. Hence, if, e.g., the non-normalized eigenvectors $\zeta'_{\alpha,\beta}$ coalesce to ζ_d, then the dyads $\zeta_\gamma \otimes \hat{\mathbf{T}}\zeta_\gamma$, $\gamma = \alpha, \beta$, formed of the vectors $\zeta_{\alpha,\beta}$, which are normalized according to Eq. (15), diverge. The analysis shows that if the degeneracy happens in the stopband, then $\hat{\Upsilon}$ involves the sum of the divergent dyads. The sum does not diverge and $\hat{\Upsilon}$ remains finite. The degeneracy of $\hat{\mathbf{M}}_S$ at the band edge is such that the difference of the divergent dyads enters $\hat{\Upsilon}$. The difference diverges, so does $\hat{\Upsilon}$. Note that $(\hat{\mathbf{T}}\zeta_d)^t\zeta_d = 0$ at a band edge reflects the fact that the bulk mode associated with ζ_d has zero-energy flow perpendicular to the layers.

Due to Eq. (15)

$$\hat{\Upsilon}^2 = \begin{pmatrix} \hat{\mathbf{S}}^2 + \hat{\mathbf{Q}}\hat{\mathbf{B}} & \hat{\mathbf{S}}\hat{\mathbf{Q}} + \hat{\mathbf{Q}}\hat{\mathbf{S}}^t \\ \hat{\mathbf{B}}\hat{\mathbf{S}} + \hat{\mathbf{S}}^t\hat{\mathbf{B}} & \hat{\mathbf{S}}^{t2} + \hat{\mathbf{B}}\hat{\mathbf{Q}} \end{pmatrix} = -\begin{pmatrix} \hat{\mathbf{I}} & \hat{\mathbf{O}} \\ \hat{\mathbf{O}} & \hat{\mathbf{I}} \end{pmatrix} \quad (28)$$

and

$$\hat{\Upsilon}\zeta_\alpha = i\zeta_\alpha, \quad \hat{\Upsilon}\zeta_{\alpha+3} = -i\zeta_{\alpha+3}, \quad \alpha = 1, 2, 3. \quad (29)$$

In view of Eq. (29), the surface impedance $\hat{\mathbf{Z}}$ and admittance $\hat{\mathbf{Y}}$ relating displacement with traction,

$$\mathbf{L}_\alpha = -i\hat{\mathbf{Z}}\mathbf{A}_\alpha, \quad \mathbf{A}_\alpha = i\hat{\mathbf{Y}}\mathbf{L}_\alpha, \ \alpha = 1, 2, 3 \quad (30)$$

can be expressed in terms of the matrices $\hat{\mathbf{S}}$, $\hat{\mathbf{Q}}$, and $\hat{\mathbf{B}}$:

$$\hat{\mathbf{Z}} = -\hat{\mathbf{Q}}^{-1} - i\hat{\mathbf{Q}}^{-1}\hat{\mathbf{S}}, \quad \hat{\mathbf{Y}} = \hat{\mathbf{B}}^{-1} + i\hat{\mathbf{B}}^{-1}\hat{\mathbf{S}}^t. \quad (31)$$

The real parts $\hat{\mathbf{Z}}$ and $\hat{\mathbf{Y}}$ are symmetric matrices. From Eq. (28) it follows that their imaginary parts $-\hat{\mathbf{Q}}^{-1}\hat{\mathbf{S}}$ and $\hat{\mathbf{B}}^{-1}\hat{\mathbf{S}}^t$ are antisymmetric matrices. Hence, $\hat{\mathbf{Z}}$ and $\hat{\mathbf{Y}}$ are Hermitian matrices within a full stopband.

Due to the completeness of the set of eigenvectors,

$$\sum_{\alpha=1}^{3}[\zeta_\alpha \otimes \hat{\mathbf{T}}\zeta_\alpha + \zeta_{\alpha+3} \otimes \hat{\mathbf{T}}\zeta_{\alpha+3}] = \begin{pmatrix} \hat{\mathbf{I}} & \hat{\mathbf{O}} \\ \hat{\mathbf{O}} & \hat{\mathbf{I}} \end{pmatrix}, \quad (32)$$

and Eq. (20), which is valid in a full stopband for $\alpha = 1, 2, 3$, one has

$$\hat{\mathbf{B}} = 2i\sum_{\alpha=1}^{3}\mathbf{L}_\alpha \otimes \mathbf{L}_\alpha, \quad \hat{\mathbf{Q}} = 2i\sum_{\alpha=1}^{3}\mathbf{A}_\alpha \otimes \mathbf{A}_\alpha. \quad (33)$$

Therefore,

$$\det(\hat{\mathbf{B}}) = -8i\det(\hat{\mathbf{L}}_{123})^2, \quad \det(\hat{\mathbf{Q}}) = -8i\det(\hat{\mathbf{A}}_{123})^2. \quad (34)$$

As a result, the equation on the SAW frequency can be written in the form $\det(\hat{\mathbf{Z}}) = 0$ or $\det(\hat{\mathbf{B}}) = 0$ and $\det(\hat{\mathbf{Y}}) = 0$ or $\det(\hat{\mathbf{Q}}) = 0$.

The properties of $\hat{\mathbf{Z}}$, $\hat{\mathbf{Y}}$, $\hat{\mathbf{B}}$, and $\hat{\mathbf{Q}}$ can be established with the help of a relation between the impedance and the surface Lagrangian £ of the time-averaged Lagrange function of harmonic wave fields which decay with distance towards the interior of the substrate. Like in the case of homogeneous substrate [28,29] (see also [41]),

$$£ = \frac{1}{8}(\mathbf{F}^*\mathbf{A} + \mathbf{F}\mathbf{A}^*) = -\frac{k}{4}\mathbf{A}^*\hat{\mathbf{Z}}\mathbf{A}, \quad (35)$$

where $\mathbf{A}$ and $\mathbf{F} = \hat{\sigma}\mathbf{n} = -ik\mathbf{L}$ are the displacement and the traction at the surface, respectively. In deriving this expression, the fact is used that the equation of motion for an elastic field moving in a homogeneous solid along $\mathbf{m}$ with velocity v can be written in the form $\partial\sigma'_{ij}/\partial x_i = 0$, where $\sigma'_{ij} = [c_{ijkl} - \rho v^2 m_i m_l \delta_{jk}]\partial u_k/\partial x_l$ [28,41]. Accordingly, the Lagrange function for the fields obeying the equation of motion can be brought into the form

$$L = -\frac{1}{2}\int \sigma'_{ij}\frac{\partial u_j}{\partial x_i}dV = \frac{1}{2}\int \sigma'_{ij}n_i u_j dS, \quad (36)$$

where $\mathbf{n}$ is the internal normal to the surface S. Equation (36) can be applied to wave (1) in each layer. The contraction $\sigma'_{ij}n_i$ reduces to the traction $\sigma_{ij}n_i = F_j$ since $\mathbf{n}$ is perpendicular to $\mathbf{m}$. The traction and displacement are continuous and the internal normals are counterdirected in neighboring layers. As a result, we arrive at Eq. (35).

By analogy with considerations of SAWs on homogeneous substrates, we find that

$$\hat{\mathbf{Z}} \text{ and } \hat{\mathbf{Y}} \text{ are positive-definite matrices at } \omega = 0, \quad (37)$$

$$\frac{\partial\hat{\mathbf{Z}}}{\partial\omega} \text{ is a negative-definite matrix in full stopbands,} \quad (38)$$

$$\frac{\partial\hat{\mathbf{Y}}}{\partial\omega} \text{ is a positive-definite matrix in full stopbands.} \quad (39)$$

Equation (37) is due to the fact that at $\omega = 0$ the Lagrangian is the energy of the static field with sign "minus." The latter two properties follow from the fact that the partial derivative $\partial L/\partial v$ is positive since it equals twice the kinetic energy divided by v and that, given the displacement $\mathbf{A}$ on the surface, $\partial \pounds/\partial v = -k^2\mathbf{A}^*(\partial\hat{\mathbf{Z}}/\partial\omega)\mathbf{A}/4$.

In accordance with Eq. (37), for an arbitrary real vector $\mathbf{a}$ the contractions $\mathbf{a}\hat{\mathbf{Z}}\mathbf{a} \equiv -\mathbf{a}\hat{\mathbf{Q}}^{-1}\mathbf{a}$ and $\mathbf{a}\hat{\mathbf{Y}}\mathbf{a} \equiv \mathbf{a}\hat{\mathbf{B}}^{-1}\mathbf{a}$ are positive at $\omega = 0$. Hence,

$$\hat{\mathbf{B}} \text{ is a positive-definite matrix at } \omega = 0, \tag{40}$$

$$\hat{\mathbf{Q}} \text{ is a negative-definite matrix at } \omega = 0. \tag{41}$$

Analogously, $\mathbf{a}(\partial\hat{\mathbf{Z}}/\partial\omega)\mathbf{a} \equiv -\mathbf{a}(\partial\hat{\mathbf{Q}}^{-1}/\partial\omega)\mathbf{a}$ and $\mathbf{a}(\partial\hat{\mathbf{Y}}/\partial\omega)\mathbf{a} \equiv \mathbf{a}(\partial\hat{\mathbf{B}}^{-1}/\partial\omega)\mathbf{a}$. In view of Eqs. (38) and (39), the matrices $\partial\hat{\mathbf{Q}}^{-1}/\partial\omega$ and $\partial\hat{\mathbf{B}}^{-1}/\partial\omega$ are positive definite in full stopbands. By differentiating the spectral decomposition of the matrices $\hat{\mathbf{Q}}^{-1}$ and $\hat{\mathbf{B}}^{-1}$ and using the orthogonality of each normalized eigenvector to its derivative, we find that the frequency derivatives of their eigenvalues are positive in full stopbands. Hence,

$$\text{the eigenvalues of } \hat{\mathbf{Q}} \text{ and } \hat{\mathbf{B}} \text{ decrease with increasing frequency in full stopbands.} \tag{42}$$

We remind that $\hat{\mathbf{Q}}$ and $\hat{\mathbf{B}}$ are real symmetric matrices, so their eigenvalues are real.

Further, by virtue of Eq. (29), $\mathbf{L}_{\mathrm{SAW}} = 0$ entails $\hat{\mathbf{B}}\mathbf{A}_{\mathrm{SAW}} = 0$ and $\hat{\mathbf{B}}\mathbf{A}^*_{\mathrm{SAW}} = 0$. The vectors $\mathbf{A}_{\mathrm{SAW}}$ and $\mathbf{A}^*_{\mathrm{SAW}}$ are not collinear. Otherwise, the eigenvectors of the transfer matrix would be linearly dependent, once $\mathbf{L}_{\mathrm{SAW}} = \mathbf{L}^*_{\mathrm{SAW}} = 0$. Therefore, we conclude that two eigenvalues of $\hat{\mathbf{B}}$ vanish, i.e.,

$$\text{the eigenvalues of } \hat{\mathbf{B}} \text{ vanish pairwise inside full stopbands.} \tag{43}$$

The noncollinearity of $\mathbf{A}_{\mathrm{SAW}}$ and $\mathbf{A}^*_{\mathrm{SAW}}$ can also be proved by noting that, in the case of collinearity, $\mathbf{A}_{\mathrm{SAW}}$ is collinear to a real vector $\mathbf{A}_0$ which is to satisfy the relation $\hat{\mathbf{S}}\mathbf{A}_0 = i\mathbf{A}_0$ but it cannot be valid since $\hat{\mathbf{S}}$ is a real matrix.

For analogous reasons, from the relations $\hat{\mathbf{Q}}\mathbf{L}_{\mathrm{SAW}} = 0$, which holds true when $\mathbf{A}_{\mathrm{SAW}} = 0$, it follows that

$$\text{the eigenvalues of } \hat{\mathbf{Q}} \text{ vanish pairwise inside full stopbands.} \tag{44}$$

None of the three eigenvalues of $\hat{\mathbf{B}}$ and $\hat{\mathbf{Q}}$ can tend to infinity within full stopbands because all elements of the matrices are finite within these bands. Accordingly,

$$\text{the determinants of } \hat{\mathbf{B}} \text{ and } \hat{\mathbf{Q}} \text{ can vanish only once within full stopbands.} \tag{45}$$

References [28,29] investigate the existence of SAWs on homogeneous substrates within the subsonic velocity interval $0 < v < v_{\mathrm{lim}}$, where v_{lim} is the velocity along the substrate surface of the slowest limiting bulk wave, that is, all partial modes are inhomogeneous when $v < v_{\mathrm{lim}}$. Homogeneous bulk modes appear at $v \geqslant v_{\mathrm{lim}}$. In periodic structures, an analog of the subsonic interval is the frequency interval $0 < \omega < \omega_{\mathrm{lim}}$, where ω_{lim} is a threshold frequency above which the passband for a pair of modes appears, given the value of the wave number k in Eq. (1). We shall call the interval $0 < \omega < \omega_{\mathrm{lim}}$ the lowest stopband. At $\omega > \omega_{\mathrm{lim}}$ the transfer matrix can have at least two distinct eigenvalues $\exp(i\varphi_\alpha)$ and $\exp(i\varphi_{\alpha+3})$, and at $\omega = \omega_{\mathrm{lim}}$ these two eigenvalues coalesce. Accordingly, the analog of the limiting bulk wave at $v = v_{\mathrm{lim}}$ in the homogeneous substrate is the mode associated at $\omega = \omega_{\mathrm{lim}}$ with the coalescing eigenvalues of the transfer matrix. This mode at $\omega = \omega_{\mathrm{lim}}$ will also be called limiting. The transfer matrix is nonsemisimple degenerate at ω_{lim} and its degenerate eigenvector ζ_d, which is mentioned in the beginning of this section, corresponds to the limiting mode. Like the limiting wave on the homogeneous substrate, the limiting wave at $\omega = \omega_{\mathrm{lim}}$ may leave the surface of the layered substrate traction free. By analogy, such a limiting wave will be called exceptional.

The comparison shows that the properties of the matrices $\hat{\mathbf{Z}}$, $\hat{\mathbf{Y}}$ as well as of $\hat{\mathbf{Q}}$, $\hat{\mathbf{B}}$, and $\hat{\mathbf{S}}$ within the interval $0 < \omega < \omega_{\mathrm{lim}}$ are identical to those of their counterparts involved in the theory of SAWs in the subsonic interval on the homogeneous substrate [28,29]. Therefore, the existence theorems [28,29] are applicable to SAWs in the lowest stopband on 1D phononic crystals with symmetric period. As to the other full stopbands, the conclusions appear to be somewhat different because nothing is known about the signs of the eigenvalues of the matrices $\hat{\mathbf{Z}}$, etc., at the edges ω_{min}, ω_{max} of these bands.

Summing up, in the case of symmetric period, the following statements hold true for full stopbands corresponding to a fixed value of the tangential wave number k:

at most 1 SAW exists on the mechanically free surface in any full stopband, (46)

the SAW on the free surface necessarily exists in the stopband $0 < \omega < \omega_{\mathrm{lim}}$
unless the limiting mode at $\omega = \omega_{\mathrm{lim}}$ is exceptional,
if the limiting mode is exceptional, then the SAW does not need to exist within the range $0 < \omega < \omega_{\mathrm{lim}}$, (47)

at most 1 SAW exists on the clamped surface in any full stopband, except $0 < \omega < \omega_{\mathrm{lim}}$, (48)

the SAW cannot exist on the mechanically clamped surface in the stopband $0 < \omega < \omega_{\mathrm{lim}}$. (49)

Statements (46) and (48) are direct consequences of property (45). The determinant of $\hat{\mathbf{Q}}$ cannot vanish within the stopband $0 < \omega < \omega_{\mathrm{lim}}$, because due to Eqs. (41) and (42) the matrix $\hat{\mathbf{Q}}$ is negative definite within this stopband, so (49) holds true.

At the lowest stopband edge ω_{lim} the matrix $\hat{\mathbf{B}}$ diverges and one of its eigenvalues tends to minus infinity if the limiting mode is not exceptional. If the limiting mode is exceptional, then $\hat{\mathbf{B}}$ does not diverge. In view of Eqs. (40) and (45), we arrive at (47). The matrices $\hat{\mathbf{B}}$ and $\hat{\mathbf{Q}}$ also diverge at the edges ω_{min}, ω_{max} of the other full stopbands unless the limiting modes satisfy the condition of the free or clamped surface, respectively. But, this divergency does not lead necessarily to the vanishing of eigenvalues inside the stopband and, hence, to the existence of SAWs, because the sign of the eigenvalues of the matrices at ω_{min} and ω_{max} is not detectable.

Apparently, the exceptional limiting mode is a specific situation. Hence, the SAW on the free surface of phononic crystals with symmetric period practically always exists in the lowest stopband.

When the sagittal plane spanned by the vectors **n** and **m** is the plane of symmetry, or the structure is composed of isotropic layers, there are four sagittally polarized modes and two SH modes, the two sets of modes being totally independent of one another. It may be that the stopband $0 < \omega < \omega_{\lim}^{(SH)}$ of SH waves is formally the lowest full stopband, but the sagittally polarized SAW does not exist in the interval $0 < \omega < \omega_{\lim}^{(SH)}$ since it falls into the interval $\omega_{\lim}^{(SH)} < \omega < \omega_{\lim}$, where $\omega_{\lim}$ is the edge of the passband for the sagittally polarized waves. The explanation is that the limiting SH mode at $\omega_{\lim}^{(SH)}$ on the substrate with symmetric period is always exceptional [16], so the uncertainty regarding the SAW in the interval $0 < \omega < \omega_{\lim}^{(SH)}$ matches (47). Note that the SH SAW cannot exist in $0 < \omega < \omega_{\lim}^{(SH)}$ [16].

B. Asymmetric period

The sum (26) now involves three eigenvectors $\alpha = 1, 2, 3$ of the transfer matrix **M** (10) corresponding to the case of asymmetric period. We introduce the matrix

$$\hat{\Xi} = i\sum_{\alpha=1}^{3}[\zeta_\alpha \otimes \hat{\mathbf{T}}\zeta_{\alpha+3}^* - \zeta_{\alpha+3} \otimes \hat{\mathbf{T}}\zeta_\alpha^*] = \begin{Bmatrix} \hat{\Xi}_{11} & \hat{\Xi}_{12} \\ \hat{\Xi}_{21} & \hat{\Xi}_{22} \end{Bmatrix}. \tag{50}$$

The matrix $\hat{\Xi}$ does not diverge in the stopbands (see Appendix). The "suspicious" points are those where the transfer matrix $\hat{\mathbf{M}}$ is nonsemisimple degenerate. The matrix $\hat{\Xi}$, like the matrix $\hat{\mathbf{\Upsilon}}$ in the analogous case, will involve divergent dyads. Inside the stopband such dyads are summed up and the divergent terms cancel out. None of the elements of $\hat{\Xi}$ diverge. In contrast, at a band edge the divergent dyads are subtracted from one another in the expression of $\hat{\Xi}$. The difference preserves divergent terms, so some elements of $\hat{\Xi}$ diverge.

Due to Eq. (24)

$$\hat{\Xi}\zeta_\alpha = i\zeta_\alpha, \quad \hat{\Xi}\zeta_{\alpha+3} = -i\zeta_{\alpha+3}, \quad \alpha = 1, 2, 3, \tag{51}$$

$$\hat{\Xi}^2 = \begin{pmatrix} \hat{\Xi}_{11}^2 + \hat{\Xi}_{12}\hat{\Xi}_{21} & \hat{\Xi}_{11}\hat{\Xi}_{12} + \hat{\Xi}_{12}\hat{\Xi}_{22} \\ \hat{\Xi}_{21}\hat{\Xi}_{11} + \hat{\Xi}_{22}\hat{\Xi}_{21} & \hat{\Xi}_{22}^2 + \hat{\Xi}_{21}\hat{\Xi}_{12} \end{pmatrix} = -\begin{pmatrix} \hat{\mathbf{I}} & \hat{\mathbf{O}} \\ \hat{\mathbf{O}} & \hat{\mathbf{I}} \end{pmatrix}. \tag{52}$$

The 3×3 blocks $\hat{\Xi}_{ij}$ of $\hat{\Xi}$ are not real matrices:

$$(\hat{\mathbf{T}}\hat{\Xi})^t = \hat{\mathbf{T}}\hat{\Xi}^* \tag{53}$$

and, hence,

$$\hat{\Xi}_{22} = \hat{\Xi}_{11}^{t*}, \quad \hat{\Xi}_{12} = \hat{\Xi}_{12}^{t*}, \quad \hat{\Xi}_{21} = \hat{\Xi}_{21}^{t*}. \tag{54}$$

Below, we are making use of the properties of the impedances and admittances relating $\mathbf{A}_\alpha$ and $\mathbf{L}_\alpha$ as well as $\mathbf{A}_{\alpha+3}$ and $\mathbf{L}_{\alpha+3}$:

$$\mathbf{L}_\alpha = -i\hat{\mathbf{Z}}\mathbf{A}_\alpha, \quad \mathbf{A}_\alpha = i\hat{\mathbf{Y}}\mathbf{L}_\alpha, \tag{55}$$

$$\mathbf{L}_{\alpha+3} = i\hat{\mathbf{Z}}'\mathbf{A}_{\alpha+3}, \quad \mathbf{A}_{\alpha+3} = -i\hat{\mathbf{Y}}'\mathbf{L}_{\alpha+3}, \tag{56}$$

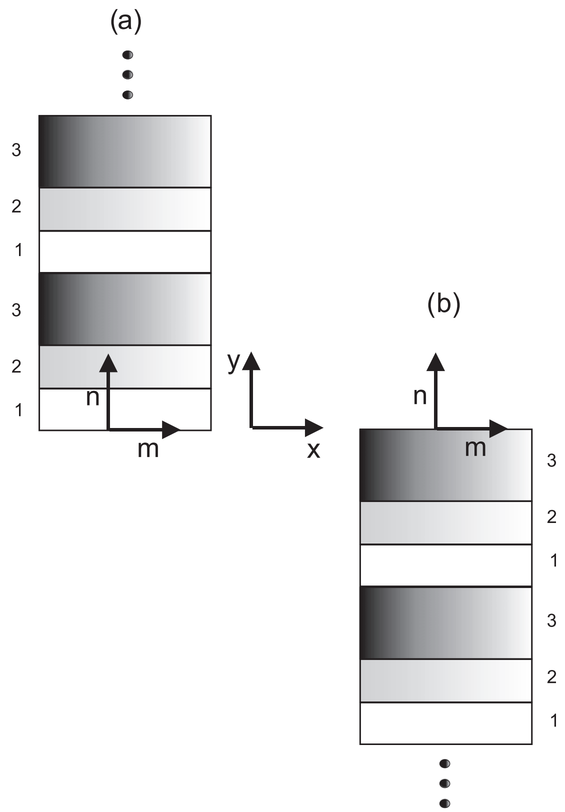

FIG. 1. "Direct" periodic structure with order of layers 1-2-3 (a) and "reversed" structure where the order of layers is 3-2-1 (b).

where $\alpha = 1, 2, 3$. In view of (51),

$$\hat{\mathbf{Z}} = -\hat{\Xi}_{12}^{-1} - i\hat{\Xi}_{12}^{-1}\hat{\Xi}_{11}, \quad \hat{\mathbf{Y}} = \hat{\Xi}_{21}^{-1} + i\hat{\Xi}_{21}^{-1}\hat{\Xi}_{22}, \tag{57}$$

$$\hat{\mathbf{Z}}' = -\hat{\Xi}_{12}^{-1} + i\hat{\Xi}_{12}^{-1}\hat{\Xi}_{11}, \quad \hat{\mathbf{Y}}' = \hat{\Xi}_{21}^{-1} - i\hat{\Xi}_{21}^{-1}\hat{\Xi}_{22}. \tag{58}$$

The four matrices are Hermitian since, due to Eqs. (52) and (54), the matrices $\hat{\Xi}_{12}$ and $\hat{\Xi}_{21}$ are Hermitian while the matrices $\hat{\Xi}_{12}^{-1}\hat{\Xi}_{11}$ and $\hat{\Xi}_{21}^{-1}\hat{\Xi}_{22}$ are anti-Hermitian.

We use expression (10) of the transfer matrix $\hat{\mathbf{M}}$ under reservation that the substrate occupies the half-space $(\mathbf{nr}) > 0$, where **n** is the internal normal [see Fig. 1(a)]. The assumption that the three eigenvectors ζ_α, $\alpha = 1, 2, 3$, are associated with decaying fields applies to $\hat{\mathbf{M}}$ (10). Let the substrate occupy the half-space $(\mathbf{nr}) < 0$, where **n** is the external normal, and the order of layers is reversed [see Fig. 1(b)]. The vectors **m** and **n** and the elastic constants are specified in the old coordinate system. In this instance, the transfer matrix of the "reversed" structure

$$\hat{\mathbf{M}}' = e^{-ikh_1\hat{\mathbf{N}}_1} \dots e^{-ikh_{n-1}\hat{\mathbf{N}}_{n-1}} e^{-ikh_n\hat{\mathbf{N}}_n} \tag{59}$$

is the inverse of the transfer matrix $\hat{\mathbf{M}}$ (10) of the "direct" structure. Therefore, the six eigenvalues and eigenvectors of $\hat{\mathbf{M}}'$ are $(1/\gamma_\alpha, \zeta_\alpha)$ and $(1/\gamma_{\alpha+3}, \zeta_{\alpha+3})$, where $\alpha = 1, 2, 3$. Since $1/|\gamma_{\alpha+3}| = |\gamma_\alpha| < 1$, $\alpha = 1, 2, 3$, now the vectors $\mathbf{A}_{\alpha+3}$ and $\mathbf{L}_{\alpha+3}$ are associated with decaying fields. Therefore, within a full stopband the displacement-traction field

$\zeta'_{\rm SAW} = (\mathbf{A}'_{\rm SAW}, \mathbf{L}'_{\rm SAW})^t$, which correspond to a SAW on the reversed structure, is representable at $y = 0$ as a linear combination $\zeta'_{\rm SAW} = \sum_{\alpha=1}^{3} b'_\alpha \zeta_{\alpha+3}$. The SAW frequency $\omega_{\rm SAW}$ on the mechanically free surface is a root of the equation $\det(\hat{\mathbf{L}}_{456}) = 0$, and on the clamped surface $\omega_{\rm SAW}$ is a root of the equation $\det(\hat{\mathbf{A}}_{456}) = 0$, where the symbols $\hat{\mathbf{L}}_{456}$ and $\hat{\mathbf{A}}_{456}$ stand for the matrices which columns are the vectors $\mathbf{L}_{4,5,6}$ and $\mathbf{A}_{4,5,6}$, respectively.

As it has already been indicated, the properties of the impedance and admittance relating the displacement and traction of a field, which decays with distance into the depth of the substrate, are found using the fact that the surface Lagrangian £ for such a field can be expressed in terms of these matrices. Equation (35), which involves the impedance $\hat{\mathbf{Z}}$, is obtained under assumption that the vector $\mathbf{n}$ is the internal normal. If $\mathbf{n}$ is the external normal, then $£' = -(\mathbf{F}'^*\mathbf{A}' + \mathbf{F}'\mathbf{A}'^*)/8$ [cf. Eq. (35)]. The insertion of $\mathbf{F}' = -ik\mathbf{L}' = k\hat{\mathbf{Z}}'\mathbf{A}'$ yields $£' = -k\mathbf{A}'^*\hat{\mathbf{Z}}'\mathbf{A}'/4$, i.e., £′ and £ [Eq. (35)] are expressed identically in terms of the impedances. Hence, $\hat{\mathbf{Z}}$ and $\hat{\mathbf{Z}}'$, as well as $\hat{\mathbf{Y}}$ and $\hat{\mathbf{Y}}'$, exhibit alike properties.

Thus,

$$\hat{\mathbf{Z}},\ \hat{\mathbf{Z}}',\ \hat{\mathbf{Y}},\ \text{and}\ \hat{\mathbf{Y}}'\ \text{are positive-definite matrices at}\ \ \omega = 0, \tag{60}$$

$$\frac{\partial\hat{\mathbf{Z}}}{\partial\omega}\ \text{and}\ \frac{\partial\hat{\mathbf{Z}}'}{\partial\omega}\ \text{are negative-definite matrices in full stopbands,} \tag{61}$$

$$\frac{\partial\hat{\mathbf{Y}}}{\partial\omega}\ \text{and}\ \frac{\partial\hat{\mathbf{Y}}'}{\partial\omega}\ \text{are positive-definite matrices in full stopbands.} \tag{62}$$

The properties of the matrices $\hat{\Xi}_{12}$ and $\hat{\Xi}_{21}$ are also required. Combining Eqs. (50) and the completeness relation

$$\sum_{\alpha=1}^{3}[\zeta_\alpha \otimes \hat{\mathbf{T}}\zeta^*_{\alpha+3} + \zeta_{\alpha+3} \otimes \hat{\mathbf{T}}\zeta^*_\alpha] = \begin{Bmatrix} \hat{\mathbf{I}} & \hat{\mathbf{O}} \\ \hat{\mathbf{O}} & \hat{\mathbf{I}} \end{Bmatrix} \tag{63}$$

results in

$$\hat{\Xi}_{12} = 2i\sum_{\alpha=1}^{3}\mathbf{A}_\alpha \otimes \mathbf{A}^*_{\alpha+3},\quad \hat{\Xi}_{21} = 2i\sum_{\alpha=1}^{3}\mathbf{L}_\alpha \otimes \mathbf{L}^*_{\alpha+3}. \tag{64}$$

Hence,

$$\det(\hat{\Xi}_{12}) = -8i\det(\hat{\mathbf{A}}_{123})\det(\hat{\mathbf{A}}^*_{456}), \tag{65}$$

$$\det(\hat{\Xi}_{21}) = -8i\det(\hat{\mathbf{L}}_{123})\det(\hat{\mathbf{L}}^*_{456}), \tag{66}$$

so the frequencies of SAWs in the "direct" structure [Fig. 1(a)] and the "reversed" structure [Fig. 1(b)] fulfill the equations $\det(\hat{\Xi}_{12}) = 0$ or $\det(\hat{\Xi}_{21}) = 0$ depending on the boundary conditions.

Since

$$\hat{\Xi}_{12}^{-1} = -(\hat{\mathbf{Z}} + \hat{\mathbf{Z}}')/2,\quad \hat{\Xi}_{21}^{-1} = (\hat{\mathbf{Y}} + \hat{\mathbf{Y}}')/2, \tag{67}$$

from Eqs. (60)–(62) it follows that

$$\hat{\Xi}_{21}\ \text{is a positive-definite matrix at}\ \ \omega = 0, \tag{68}$$

$$\hat{\Xi}_{12}\ \text{is a negative-definite matrix at}\ \ \omega = 0, \tag{69}$$

the eigenvalues of $\hat{\Xi}_{12}$ and $\hat{\Xi}_{21}$ decrease
with increasing frequency in full stopbands (70)

[cf. properties (40)–(42) of the matrices $\hat{\mathbf{Q}}$ and $\hat{\mathbf{B}}$]. The eigenvalues of $\hat{\Xi}_{12}$ and $\hat{\Xi}_{21}$ are real because these matrices are Hermitian. Unlike the eigenvalues of $\hat{\mathbf{Q}}$ and $\hat{\mathbf{B}}$, the eigenvalues of $\hat{\Xi}_{12}$ and $\hat{\Xi}_{21}$ do not need to vanish in pairs. None of the eigenvalues of $\hat{\Xi}_{12}$ and $\hat{\Xi}_{21}$ can tend to infinity inside a full stopband because all elements of $\hat{\Xi}_{12}$ and $\hat{\Xi}_{21}$ are finite (see Appendix). In view of this fact and Eq. (70),

the determinants of $\hat{\Xi}_{12}$ and $\hat{\Xi}_{21}$ can vanish
at most three times within a full stopband. (71)

A reservation to (71) concerns $\hat{\Xi}_{12}$. By virtue of Eqs. (69) and (70),

$\hat{\Xi}_{12}$ is a negative-definite matrix in the lowest stopband (72)

and, hence,

the determinant of $\hat{\Xi}_{12}$ cannot vanish
in the lowest stopband. (73)

The determinant of $\hat{\Xi}_{21}$ can vanish in any full stopband. By Eq. (66), the condition $\det(\hat{\Xi}_{21}) = 0$ entails either $\det(\hat{\mathbf{L}}_{123}) = 0$, or $\det(\hat{\mathbf{L}}^*_{456}) = 0$, or $\det(\hat{\mathbf{L}}_{123}) = \det(\hat{\mathbf{L}}^*_{456}) = 0$. If the latter option happens, then the coefficients b_α and b'_α, $\alpha = 1,2,3$, can be chosen in such a way that $\mathbf{L}_{\rm SAW} = \sum_{\alpha=1}^{3} b_\alpha\mathbf{L}_\alpha = 0$ and $\mathbf{L}'_{\rm SAW} = \sum_{\alpha=1}^{3} b'_\alpha\mathbf{L}_{\alpha+3} = 0$. When $\mathbf{L}_{\rm SAW} = \mathbf{L}'_{\rm SAW} = 0$, it follows from Eq. (51) that $\hat{\Xi}_{21}\mathbf{A}_{\rm SAW} = \hat{\Xi}_{21}\mathbf{A}'_{\rm SAW} = 0$, where $\mathbf{A}_{\rm SAW} = \sum_{\alpha=1}^{3} b_\alpha\mathbf{A}_\alpha$ and $\mathbf{A}'_{\rm SAW} = \sum_{\alpha=1}^{3} b'_\alpha\mathbf{A}_{\alpha+3}$. The vectors $\mathbf{A}_{\rm SAW}$ and $\mathbf{A}'_{\rm SAW}$ cannot be collinear if $\mathbf{L}_{\rm SAW} = \mathbf{L}'_{\rm SAW} = 0$ since otherwise the eigenvectors of the transfer matrix fall into linear dependence. Therefore, $\hat{\Xi}_{21}\mathbf{A}_{\rm SAW} = \hat{\Xi}_{21}\mathbf{A}'_{\rm SAW} = 0$ implies that two eigenvalues of $\hat{\Xi}_{21}$ vanish under condition $\det(\hat{\mathbf{L}}_{123}) = \det(\hat{\mathbf{L}}^*_{456}) = 0$.

As a result, we conclude that

at most three SAWs exist on the mechanically free surface
in a full stopband, (74)

in sum, the number of SAWs on the free surfaces of
the direct and reversed structures
does not exceed 3 in a full stopband. (75)

Analogous statements are valid regarding SAWs on the mechanically clamped surface:

at most three SAWs exist on the mechanically clamped
surface in a full stopband, (76)

in sum, the number of SAWs on the clamped surfaces of
the direct and reversed structures
does not exceed 3 in a full stopband. (77)

Due to Eqs. (65) and (73),

SAW does not exist in the lowest stopband
if the surface is mechanically clamped. (78)

At the edges of the stopbands, excluding $\omega = 0$, the matrices $\hat{\Xi}_{21}$ and $\hat{\Xi}_{12}$ diverge and one of three eigenvalues of each matrix tends to infinity unless the limiting bulk mode satisfies the condition of the free or clamped surface, respectively. Let us consider the lowest stopband. By virtue of Eq. (68), all the eigenvalues of $\hat{\Xi}_{21}$ are positive and in view of (70) we arrive at the following conclusion:

in the lowest stopband, at least one SAW exists
on the mechanically free surface
provided that the limiting mode does not satisfy
the condition of the free surface. (79)

The situation where the limiting mode satisfies the condition of free surface, i.e., the occurrence of the exceptional limiting mode, is fairly specific. Therefore, one can argue that at least one SAW practically always occurs in the lowest stopband either in the case of the direct structure or in the case of the reversed one. Like in the case of symmetric period, the divergency of the matrices at the edges of the other stopbands does not allow any conclusions to be made regarding SAWs.

If the sagittal plane is the plane of crystallographic symmetry, then the relevant 2×2 diagonal blocks of the 3×3 matrices $\hat{\mathbf{Z}}$, $\hat{\mathbf{Z}}'$, etc., pertain to sagittally polarized SAWs. The remaining diagonal element of each matrix characterizes SH SAWs. Accordingly, in a full stopband for sagittally modes, at most two sagittally polarized SAWs can exist and in total not more than two SAWs can exist on the direct and reversed structures. Unlike the case of symmetric period, the limiting SH mode at the upper edge of the lowest stopband has nonzero traction [16]. Therefore, at least one SAW, sagittally polarized SAW or SH SAW, exists in this band on the free surface of either direct or reversed structure. One SH SAW exists in the lowest stopband for SH modes on the free surface of either direct or reversed structure. At most one SH SAW on the free and the clamped surface is allowed to exist in a SH stopband of one of these two structures.

All these conclusions are applicable to structures made of elastically isotropic layers where the modes are naturally split into SH-polarized and sagittally polarized ones. The results of numerical computations and analytic evaluations carried out in Refs. [10–24] exemplify permissible options of their occurrence (see also Sec. V).

We assumed that $k \neq 0$ in Eq. (1). If $k = 0$, then, after having changed the definition of the vector $\mathbf{L}$, e.g., $\mathbf{L} = ik_0^{-1}\mathbf{F}$, where k_0 has the meaning of a wave number, one arrives at the eigenvalue problem of type (5) for a matrix slightly different from the matrix $\hat{\mathbf{N}}$ (4) but possessing equivalent properties. The factor k_0 appears in Eq. (35) instead of k. The expression $L_s = 0.5\sigma_{ij}n_iu_j$ for the surface Lagrangian L_s of a homogeneous solid should be derived in a different manner in order to validate its applicability at $k = 0$. Namely, one can write the bulk Lagrangian L_b in the form $L_b = 0.5(\rho\omega^2\sum_{i=1}^{3}u_i^2 - \sigma_{ij}\partial u_j/\partial x_i)$ and use Eq. (2) to obtain $L = \int L_b dV = 0.5\int \sigma_{ij}n_iu_j dS$ [cf. Eq. (36) and the discussion around it]. The properties of the matrices $\hat{\mathbf{Z}}$, $\hat{\mathbf{Y}}$, etc., also remain valid, excluding those which hold true only in the stopband $0 < \omega < \omega_{\rm lim}$, since at $k = 0$ all the stopbands begin from nonzero frequencies. Accordingly, statements (46), (48), and (74)–(77) cover the case $k = 0$ as well. Note that the results obtained for structures composed of isotropic layers are in agreement with these statements (see Refs. [12,13,18,42]).

V. SURFACE WAVES ON InAs-GaSb SUPERLATTICES

As an example, we discuss the SAW spectrum on the InAs-GaSb superlattice. Notice that from the viewpoint of the electron-hole band properties this superlattice is of interest by the fact that the minimum of the conduction band of InAs is lower than the maximum of the valence band of GaSb [7].

The substrate with symmetric period will be referred to as the InAs/GaSb/InAs or GaSb/InAs/GaSb substrate depending on which of the layers, InAs or GaSb, is exterior, respectively. Analogously, the substrate with asymmetric period will be referred to as the InAs/GaSb or GaSb/InAs substrate. In accordance of our terminology, GaSb/InAs is the reversed InAs/GaSb substrate. Besides, we consider InAs/GaSb and GaSb/InAs structures with exterior layer of intermediate thickness in order to track the transformation of SAWs with changing period from asymmetric to symmetric.

We assume that the thicknesses $h_{\rm InAs}$ and $h_{\rm GaSb}$ of the InAs and GaSb layers are identical, except possibly the exterior layer which is characterized by the thickness h, and use the dimensionless parameter $\omega H/v_0$, where ω is the frequency, $H = (h_{\rm InAs} + h_{\rm GaSb})/2\pi$ and $v_0 = 3\times10^3$ m/s. The layer boundaries are (001) planes and the direction of propagation is [100], so the modes are split into SH polarized modes and modes polarized in the sagittal plane (010) or, for short, sagittally polarized modes. The material constants are taken from site [43]: $c_{11} = 8.34\times10^{10}$ N/m^2, $c_{12} = 4.54\times10^{10}$ N/m^2, $c_{44} = 3.95\times10^{10}$ N/m^2, $\rho = 5680$ kg/m^3 for InAs and $c_{11} = 8.83\times10^{10}$ N/m^2, $c_{12} = 4.02\times10^{10}$ N/m^2, $c_{44} = 4.32\times10^{10}$ N/m^2, $\rho = 5614$ kg/m^3 for GaSb. The weak piezoelectric effect is ignored. We put $k = 2.5k_B$ in Eq. (1), where $k_B = 1/H$ is the Brillouin wave number.

Figure 2 depicts the dependence of the magnitudes of the three eigenvalues of the transfer matrix on $\omega H/v_0$ within the interval from 1.8 to 2.4. Note that the transfer matrices $\hat{\mathbf{M}}$ and $\hat{\mathbf{M}}_S$ have identical eigenvalues in our case.

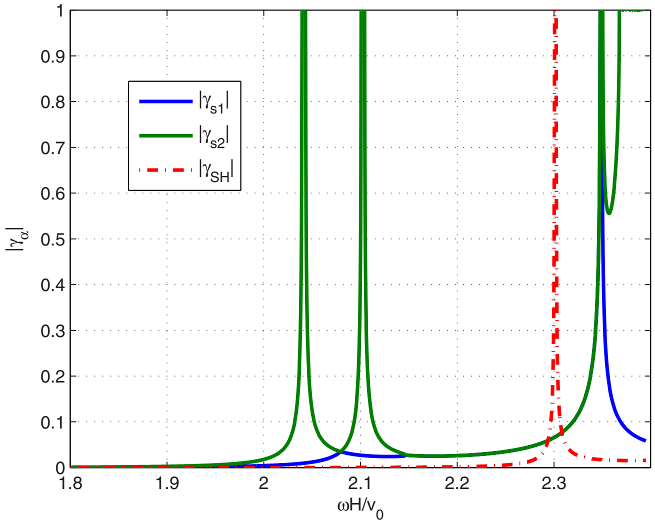

FIG. 2. Magnitudes of eigenvalues of the transfer matrix vs the parameter $\omega H/v_0$ at $k = 2.5k_B$. The eigenvalues $\gamma_{s1,s2}$ and $\gamma_{\rm SH}$ characterize the sagittally polarized and SH modes, respectively.

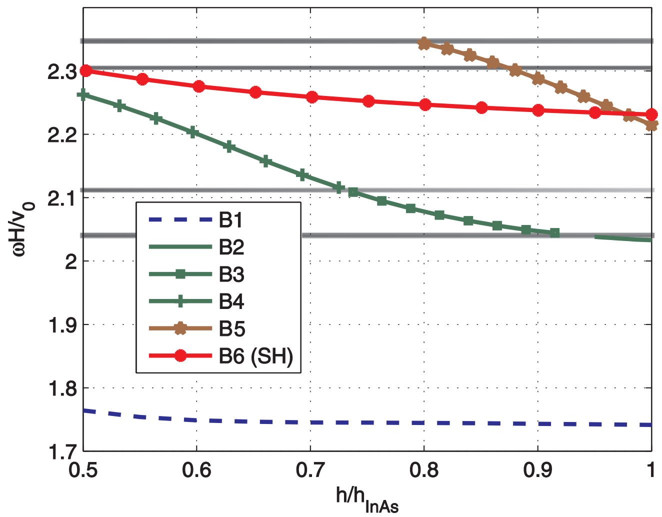

FIG. 3. SAW branches vs thickness h of the exterior layer InAs at $k = 2.5k_B$. Mechanically free surface. Sagittally polarized SAWs: branches B1-B5. SH SAW: branch B8. Gray lines: passbands. The SH-mode passband is near $\omega H/v_0 = 2.3$.

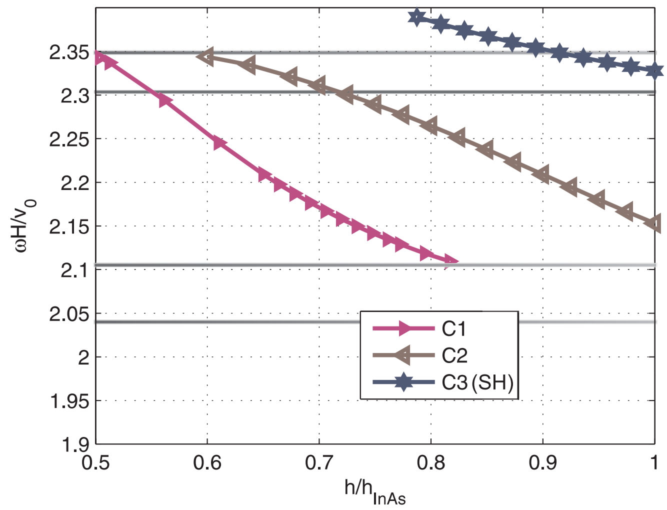

FIG. 4. SAW branches vs thickness h of the exterior layer InAs at $k = 2.5k_B$. Mechanically clamped surface. Sagittally polarized SAWs: branches C1, C2. SH SAWs: branch C3. Gray lines: passbands. The SH-mode passband is near $\omega H/v_0 = 2.3$.

Below $\omega H/v_0 = 1.8$ all three eigenvalues are hardly different from zero. The passbands appear within very narrow intervals of $\omega H/v_0$ values at which the absolute value of at least one of the eigenvalues is equal to unity. Nevertheless, even such a band structure significantly modifies the SAW propagation as compared with that on homogeneous InAs or GaSb substrates.

The SAW frequencies at $k = 2.5k_B$ as functions of the thickness of the exterior InAs layer are shown in Fig. 3. The surface is mechanically free. The values $h/h_{\text{InAs}} = 0.5$ and $h/h_{\text{InAs}} = 1$ correspond to the InAs/GaSb/InAs and InAs/GaSb substrates, respectively. The lowest branch B1 practically represents the SAW on the half-infinite InAs substrate, because at $k = 2.5k_B$ the penetration depth of this wave is so small that it propagates as if the exterior layer were infinitely thick. The $\omega H/v_0$ value corresponding to the SAW velocity on InAs equals 1.74.

In accordance with the general statement (46), one SAW exists on the mechanically free surface of InAs/GaSb/InAs in the lowest stopband $\omega H/v_0 < 2.04$. InAs/GaSb supports two waves in the lowest stopband. The second SAW on the free surface (branch B2) is also sagittally polarized, like the first one. It occurs near the edge of the stopband where the magnitudes of the eigenvalues $\gamma_{s1,s2}$ associated with sagittally polarized modes are not very small (Fig. 2). Such a closeness to the band edge correlates with the fact that the half-infinite homogeneous substrate supports only one SAW [28,29]. This restriction implies that the second SAW cannot appear in the frequency range where $|\gamma_{s1,s2}|$ are extremely small since then the influence of the structure inhomogeneity on SAWs is minor.

With decreasing h/h_{InAs} the SAW frequency approaches the band edge. Branch B2 disappears on reaching the band edge at $h/h_{\text{InAs}} \approx 0.95$ but reappears as branches B3 and B4 in higher stopbands. The end of branch B4 at $h/h_{\text{InAs}} = 0.5$ is the sagitally polarized SAW in the third full stopband for sagittally polarized modes.

A sagittally polarized SAW on the free surface of InAs/GaSb exists in the third stopband. It gives rise to branch B5 which ends at the upper edge of the stopband when $h/h_{\text{InAs}} \approx 0.8$. Branch B6 of SH SAWs on the free surface goes from a frequency below the edge of the lowest stopband of SH waves (InAs/GaSb substrate) towards this edge. At $h/h_{\text{InAs}} = 0.5$, i.e., on InAs/GaSb/InAs substrate, one has the exceptional limiting SH mode. SH SAWs do not exist inside the lowest stopband on structures with symmetric period but the limiting bulk wave corresponding to the edge of this stopband satisfies the condition of the free surface [16]. Branch B8 lies near the band edge since SH SAWs do not exist on the free surface of half-infinite homogeneous nonpiezoelectric substrates, so this SAW can appear on layered substrates within a frequency interval where the relevant eigenvalue of the transfer matrix is not very small (γ_{SH} in Fig. 2).

SAWs also exist on the clamped surface (Fig. 4). Branch C1 of sagittally polarized SAWs begins at the upper edge of the stopband and ends at the lower edge of the band when $h/h_{\text{InAs}} \approx 0.81$. There is one more branch of sagittally polarized SAWs (branch C2). This branch begins at a frequency lying inside the third stopband ($h/h_{\text{InAs}} = 1$, i.e., InAs/GaSb substrate), goes upward, and ends at the upper edge of the third stopband when $h/h_{\text{InAs}} \approx 0.6$. On the clamped surface of InAs/GaSb, the SH SAW occurs in the second SH stopband (branch C3).

Note that all branches shown in Figs. 3–5 exist in stopbands common for sagittally and SH polarized waves. Therefore, these SAWs also exist in the vicinity of [100] direction.

The SAW spectrum on the InAs-GaSb superlattice under the same conditions, but with exterior GaSb layer, is shown in Fig. 5. SH SAWs do not exist either on the free or clamped surface. To be more exact, the limiting SH bulk wave at the upper edge of the lowest SH stopband satisfies the condition of the free surface of the GaSb/InAs/GaSb substrate. This wave disappears once $h/h_{\text{GaSb}} > 0.5$. An explanation of this fact is that the SH stopband edge is below the SH bulk wave velocity in GaSb ($\omega H/v_0 = 2.78$), so adding a "fast" GaSb layer destroys the wave on GaSb/InAs/GaSb substrate similarly to

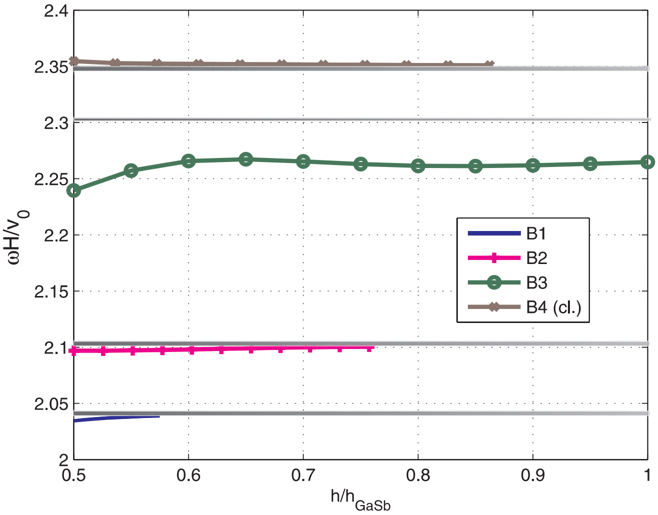

FIG. 5. SAW branches as functions of the thickness h of the exterior layer GaSb at $k = 2.5k_B$. Sagittally polarized SAWs on the free surface (branches B1–B3) and on the clamped surface (branch B4). GaSb/InAs/GaSb substrate: $h/h_{\mathrm{GaSb}} = 0.5$. GaSb/InAs substrate: $h/h_{\mathrm{GaSb}} = 1$. Gray lines: passbands. The SH-mode passband is near $\omega H/v_0 = 2.3$.

what happens when a fast layer is placed on a homogeneous substrate. On the contrary, the SH stopband edge is above the SH bulk velocity in InAs ($\omega H/v_0 = 2.2$) and, hence, adding an InAs layer slows down the limiting SH bulk wave on the free surface of the InAs/GaSb/InAs substrate, giving rise to a branch of SH SAWs (B6 in Fig. 3).

The only SAW on GaSb/InAs substrate exists at $\omega H/v_0 < 2.3$ when the surface is mechanically free and the frequency belongs to the third stopband for sagittally polarized modes. This SAW resembles very closely the SAW on the half-infinite GaSb substrate coming about at the velocity $v = 2724$ m/s which corresponds to $\omega H/v_0 = 2.27$. With decreasing h/h_{GaSb} the SAW on GaSb/InAs continuously transforms to the SAW on GaSb/InAs/GaSb, the $\omega H/v_0$ value still approximately equaling 2.27.

Apart from the SAW inside the third stopband, GaSb/InAs/GaSb supports the SAW on the clamped surface near the lower edge of the fourth stopband, the SAW on the free surface near the upper edge of the second stopband of sagittally polarized modes, and the SAW on the free surface within the lowest stopband. Since the $\omega H/v_0$ value corresponding the SAW on the half-infinite GaSb substrate is above the edge of the lowest stopband, it is natural that the SAW exists in the lowest stopband near its edge where $|\gamma_{s1,s2}|$ is large enough for the presence of other layers to affect the solution of the boundary-value problem (see Fig. 2).

The absence of the SH SAW on the free surface of GaSb/InAs in the lowest stopband for SH waves agrees with general conclusions (the end of the previous section). The SH SAW exists on InAs/GaSb in this stopband and, therefore, it cannot exist on GaSb/InAs. The existence of the SAW on the free surface of GaSb/InAs in the third stopband agrees with general conclusions as well. There are one SAW on InAs/GaSb (branch B5 in Fig. 3) and one SAW on GaSb/InAs in this stopband. The number of SAWs on InAs/GaSb/InAs and GaSb/InAs/GaSb substrates in higher stopbands are also in agreement with general statements (46) and (48).

The InAs/GaSb superlattice is an example of two-layered phononic crystals with asymmetric period which at certain values of the wave number k support two sagittally polarized SAWs in the lowest stopband when the exterior layer is of one sort of material but support no SAW in this stopband if the exterior layer is of the other material. The W/Al half-infinite superlattice studied in Ref. [18] is a structure of different type. Having asymmetric period, it supports one sagittally polarized SAW in the lowest stopband within an interval of k values independently of which layer is exterior but outside this k interval one sagittally polarized SAW exists in the lowest stopband if the exterior layer is W and no SAW exists in the lowest stopband if the exterior layer is Al.

Note that in Ref. [25], SAW branches on the mechanically free surface of GaAs/AlAs superlattices with different external layers were computed. By our classification, this is the case of asymmetric period in mutually reversed structures GaAs/AlAs and AlAs/GaAs. The plane of propagation is (001) and the direction changes from [100] until [110]. In the lowest stopband, two SAW branches on GaAs/AlAs and one branch on AlAs/GaAs are found. In the second full stopband, there one SAW on GaAs/AlAs and one SAW on AlAs/GaAs. These results also agree with our general statements.

VI. CONCLUDING REMARKS

In this work, a number of rigorous statements are proved regarding the existence of SAWs on half-infinite 1D nonpiezoelectric phononic crystals of general anisotropy. In particular, not more than one SAW exists on the mechanically free surface of structures in which the layers are placed "symmetrically" within the period. The existence criterion for this SAW in the lowest stopband is established. The simplest example of the substrate with "symmetric" period is an appropriately truncated two-layered periodic structure. If the period is "asymmetric," then at most three SAWs can occur in a "full" stopband. A correlation between the number of SAWs on the phononic crystal with given order of layers and on the phonic crystal with the reversed order of layers is found: at most three SAWs can exist in total.

Our work reveals a close methodological similarity between the analysis of the SAW propagation on homogeneous substrates and the analysis of the SAW propagation on phononic crystals, especially in the case of structures with symmetric period. This fact allows us to think that a large amount of acoustic wave problems solved for homogeneous anisotropic substrates by using and developing the method [28–30] are also solvable for phononic crystals. Among such problems are the existence of interfacial waves at various types of contact between two elastically anisotropic solids [38,39], specific features of the propagation of fast, or "supersonic", SAWs as well as of leaky SAWs [44–47]. The counterpart of a "supersonic" SAW on homogeneous substrate is a nonattenuating SAW existing within a passband of a phononic crystal (see, e.g., [25]). The list of problems potentially solvable in the case of phononic crystals can be extended by referring to the fact that the mathematical formalism [33] allows the analysis of general properties of the bulk acoustic wave reflection/transmission in homogeneous solids of general anisotropy [46–50], the derivation of explicit secular equations for SAWs and interfacial waves in generally anisotropic or low symmetric structures [51–58].

Our results can be extended to half-infinite functionally graded periodic structures where the matrix $\hat{\mathbf{N}}$ [Eq. (4)] is a continuous periodic function of the depth coordinate. The only difference is that the transfer matrix is the multiplicative integral of $\hat{\mathbf{N}}$ expanding into the Peano series [37].

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APPENDIX

Let the matrix $\hat{\mathbf{M}}_S$ be nonsemisimply degenerate at a frequency ω_d falling into a full stopband. For instance, $\gamma_2 = \gamma_3 = \gamma_d$ and $\zeta_2 = \zeta_3 = \zeta_d$ at ω_d. In parallel, in view of Eqs. (18) and (20) $\gamma_5 = \gamma_6 = 1/\gamma_d^*$ and $\zeta_5 = \zeta_6 = \zeta_d^*$. The nonsemisimple degeneracy implies

$$\hat{\mathbf{M}}_S\zeta_\alpha = \gamma_\alpha\zeta_\alpha, \quad \alpha = 1,4$$
$$\hat{\mathbf{M}}_S\zeta_d = \gamma_d\zeta_d, \quad \hat{\mathbf{M}}_S\zeta_g = \gamma_d\zeta_g + \zeta_d,$$
$$\hat{\mathbf{M}}_S\zeta_d^* = \zeta_d^*/\gamma_d^*, \quad \hat{\mathbf{M}}_S\zeta_g' = \zeta_g'/\gamma_d^* + \zeta_d^*, \tag{A1}$$

where ζ_g and ζ_g' are the generalized eigenvectors of $\hat{\mathbf{M}}_S$. The eigenvectors and generalized eigenvectors form a complete set of linearly independent vectors [37]. Since ζ_g is a complex vector, the six vectors ζ_1, $\zeta_4 \equiv \zeta_1^*$, ζ_d, ζ_d^*, ζ_g, and ζ_g^* are also linearly independent. Hence, the vectors ζ_g^* and ζ_g' must be collinear. The equality $\hat{\mathbf{M}}_S^* = \hat{\mathbf{M}}_S^{-1}$ yields

$$\hat{\mathbf{M}}_S\zeta_g^* = \frac{1}{\gamma_d^*}\zeta_g^* - \frac{1}{\gamma_d^{*2}}\zeta_d^*. \tag{A2}$$

Therefore, $\zeta_g' = -\gamma_d^{*2}\zeta_g^*$.

Due to $(\hat{\mathbf{T}}\hat{\mathbf{M}}_S)^t = \hat{\mathbf{T}}\hat{\mathbf{M}}_S$ and $\hat{\mathbf{M}}_S^* = \hat{\mathbf{M}}_S^{-1}$ all the products of the type $(\hat{\mathbf{T}}\zeta_\alpha)^t\zeta_\beta$ of the vectors in Eq. (A1) vanish, except $(\hat{\mathbf{T}}\zeta_1)^t\zeta_1$ and $(\hat{\mathbf{T}}\zeta_g)^t\zeta_d$. We put $(\hat{\mathbf{T}}\zeta_1)^t\zeta_1 = 1$ and $(\hat{\mathbf{T}}\zeta_g)^t\zeta_d = 1$, so the completeness relation for $\zeta_{1,d,g}$ and $\zeta_{1,d,g}^*$ reads as

$$\hat{\Upsilon}_1 + \hat{\Upsilon}_1^* = \begin{pmatrix} \hat{\mathbf{I}} & \hat{\mathbf{O}} \\ \hat{\mathbf{O}} & \hat{\mathbf{I}} \end{pmatrix}, \tag{A3}$$

where

$$\hat{\Upsilon}_1 = \zeta_1 \otimes \hat{\mathbf{T}}\zeta_1 + \zeta_d \otimes \hat{\mathbf{T}}\zeta_g + \zeta_g \otimes \hat{\mathbf{T}}\zeta_d. \tag{A4}$$

Using the orthogonality relations and the properties of $\hat{M}_S$, one can find that in the vicinity of ω_d the eigenvalues $\gamma_{2,3}$ and eigenvectors $\zeta_{2,3}$ which fulfill the normalization condition $(\zeta_\alpha\hat{\mathbf{T}})^t\zeta_\beta = \delta_{\alpha\beta}$ (15) are of the form

$$\gamma_{2,3} = \gamma_d \pm \Delta\gamma + O(\Delta\gamma^2),$$
$$\zeta_{2,3} = \frac{\zeta_d \pm \Delta\gamma\zeta_g}{\sqrt{\pm 2\Delta\gamma}} + O(\Delta\gamma^{3/2}), \tag{A5}$$

where $\Delta\gamma = \sqrt{(\hat{\mathbf{T}}\zeta_d)^t\Delta\hat{\mathbf{M}}_S\zeta_d}$ and $\Delta\hat{\mathbf{M}}_S = (\partial\hat{\mathbf{M}}_S/\partial\omega)\Delta\omega$. Besides, $\gamma_{5,6} = 1/\gamma_{2,3}^*$ and $\zeta_{5,6} = \zeta_{2,3}^*$.

The substitution into Eq. (27) of the expressions (A6) for $\zeta_{2,3}$ and $\zeta_{2,3}^*$ yields $\hat{\Upsilon} = \hat{\Upsilon}_1 - \hat{\Upsilon}_1^* + O(\Delta\gamma)$, i.e., all elements of $\hat{\Upsilon}$ are finite at the point of degeneracy in the full stopband.

The degeneracy of $\hat{\mathbf{M}}_S$ at the band edge is due to a different coalescence. One of the three eigenvalues γ_α, $\alpha = 1,2,3$, merges with one of the three eigenvalues $\gamma_{\alpha+3} = 1/\gamma_\alpha^*$. The expressions of the eigenvalues, which coalesce at the band edge, are similar to Eq. (A5) of $\zeta_{2,3}$. But, in the present case $\hat{\Upsilon}$ contains the difference of the divergent dyads. The terms of the type $1/\sqrt{\Delta\gamma}$ do not cancel out, so certain elements of $\hat{\Upsilon}$ can tend to infinity as the frequency approaches the band edge.

Let us assume that the general transfer matrix $\hat{\mathbf{M}}$ [Eq. (10)] is nonsemisimple degenerate at a frequency ω_d inside the full stopband as a result of the coalescence $\gamma_2 = \gamma_3 = \gamma_d$ and, accordingly, $\gamma_5 = \gamma_6 = 1/\gamma_d^*$. The eigenvalue problem for $\hat{\mathbf{M}}$ reads then as

$$\hat{\mathbf{M}}\zeta_\alpha = \gamma_\alpha\zeta_\alpha, \quad \alpha = 1,4$$
$$\hat{\mathbf{M}}\zeta_{d3} = \gamma_d\zeta_{d3}, \quad \hat{\mathbf{M}}\zeta_{g3} = \gamma_d\zeta_{g3} + \zeta_{d3},$$
$$\hat{\mathbf{M}}\zeta_{d6} = \zeta_{d6}/\gamma_d^*, \quad \hat{\mathbf{M}}\zeta_{g6} = \zeta_{g6}/\gamma_d^* + \zeta_{d6}, \tag{A8}$$

where ζ_{g3} and ζ_{g6} are the generalized eigenvectors. Since $(\hat{\mathbf{T}}\hat{\mathbf{M}})^t = \hat{\mathbf{T}}\hat{\mathbf{M}}^{*-1}$, all the products $(\hat{\mathbf{T}}\zeta_\alpha^*)^t\zeta_\beta$ vanish, except $(\hat{\mathbf{T}}\zeta_1^*)^t\zeta_4$ and $(\hat{\mathbf{T}}\zeta_{g6}^*)^t\zeta_{d3} = -\gamma_d^2(\hat{\mathbf{T}}\zeta_{d6}^*)^t\zeta_{g3}$. We put $(\hat{\mathbf{T}}\zeta_1^*)^t\zeta_4 = 1$ and $(\hat{\mathbf{T}}\zeta_{d6}^*)^t\zeta_{g3} = 1$. Under this condition, the completeness relation acquires the form

$$\hat{\Xi}_1 + \hat{\Xi}_2 = \begin{pmatrix} \hat{\mathbf{I}} & \hat{\mathbf{O}} \\ \hat{\mathbf{O}} & \hat{\mathbf{I}} \end{pmatrix}, \tag{A9}$$

where

$$\hat{\Xi}_1 = \zeta_1 \otimes \hat{\mathbf{T}}\zeta_4^* + \zeta_{g3} \otimes \hat{\mathbf{T}}\zeta_{d6}^* - \frac{1}{\gamma_d^2}\zeta_{d3} \otimes \hat{\mathbf{T}}\zeta_{g6}^*, \tag{A11}$$

$$\hat{\Xi}_2 = \zeta_4 \otimes \hat{\mathbf{T}}\zeta_1^* + \zeta_{d6} \otimes \hat{\mathbf{T}}\zeta_{g3}^* - \frac{1}{\gamma_d^{*2}}\zeta_{g6} \otimes \hat{\mathbf{T}}\zeta_{d3}^*. \tag{A12}$$

At $\omega \neq \omega_d$ the vectors $\zeta_{2,3}$ and $\zeta_{5,6}$ can fulfill the normalization condition $(\hat{\mathbf{T}}\zeta_{\alpha+3}^*)^t\zeta_\alpha = 1$. Expanding $\zeta_{2,3}$ and $\zeta_{5,6}$, which are normalized in this way, and the eigenvalues $\gamma_{2,3,5,6}$ in the neighborhood of ω_d, we obtain that in the lowest approximation

$$\gamma_{2,3} = \gamma_d \pm \Delta\gamma + O(\Delta\gamma^2), \quad \gamma_{5,6} = \frac{1}{\gamma_{2,3}^*}, \tag{A13}$$

$$\zeta_{2,3} = \frac{\zeta_{d3} \pm \Delta\gamma\zeta_{g3}}{\sqrt{\pm 2\Delta\gamma}} + O(\Delta\gamma^{3/2}), \tag{A14}$$

$$\zeta_{5,6} = \frac{\zeta_{d6} \mp \Delta\gamma^*\zeta_{g6}/\gamma_d^{*2}}{\sqrt{\pm 2\Delta\gamma^*}} + O(\Delta\gamma^{3/2}), \tag{A15}$$

where $\Delta\gamma = \sqrt{(\hat{\mathbf{T}}\zeta_{d6}^*)^t\Delta\hat{\mathbf{M}}\zeta_{d3}}$, $\Delta\hat{\mathbf{M}} = (\partial\hat{\mathbf{M}}/\partial\omega)\Delta\omega$, the upper sign in (A13)–(A15) corresponds to the subscripts $\alpha = 2,5$. Thus, we eventually find that the matrix $\hat{\Xi}$ [Eq. (50)] tends to $\hat{\Xi} = \hat{\Xi}_1 - \hat{\Xi}_2$ as $\omega \to \omega_d$, where $\hat{\Xi}_{1,2}$ are given by Eqs. (A11) and (A12).

The degeneracy of $\hat{\mathbf{M}}$ at the band edge occurs as a result of the coalescence of one of the three eigenvalues γ_α, $\alpha = 1,2,3$, with one of the three eigenvalues $\gamma_{\alpha+3} = 1/\gamma_\alpha^*$. The elements of the matrix $\hat{\Xi}$ diverge since the divergent terms do not cancel out in this case.

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