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Linear periodic and quasiperiodic anisotropic layered media with arbitrary orientation of optic axis—A numerical study

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Abstract. We study numerically the linear properties of periodic and quasiperiodic anisotropic layered media. Each anisotropic slab can have arbitrary orientation of optic axis. We apply the general numerical code to recover the known results for solc filters. We propose novel periodic structures where the location and width of the gaps can be controlled easily. We also study the transmission properties of a Fibonacci sequence of anisotropic layers and show the interesting features like self-similarity and scaling.

Keywords. Layered media; birefringence

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1. Introduction

In the past few decades there has been considerable interest in layered anisotropic structures [1–7]. This is because of the various applications these structures have. These include narrow band solc filters, polarizers, etc. The study of anisotropic layered media is of utmost importance from an altogether different angle. Most of the second order nonlinear materials are anisotropic in character. In order to have a theoretical understanding of second order nonlinear optical processes in layered configuration, it is imperative to know the properties of its linear analogue. The knowledge of the forward and backward fundamental wave amplitudes in each layer is necessary to calculate the source polarization in each layer [5]. Thus the knowledge of linear properties is a first step to explore the nonlinear properties.

The general theory of anisotropic layered media is well understood [2–7]. It is well-known that the theory for anisotropic layers with arbitrarily oriented optic axis involves 4×4 matrices and in general a computer program is needed to calculate the transmission and reflection coefficients. Our interest in linear anisotropic layered medium is motivated by its importance in the context of nonlinear studies. We developed a very general computer code which can cope with any number and sequence of linear uniaxial or biaxial layers with arbitrary orientation of optic axes for arbitrary angle of incidence. We have applied the code to recover the known results, for example, for solc filters [3]. We have proposed some novel periodic structures where the location and the widths of the gaps can be easily controlled. We have also carried out numerical investigations of Fibonacci sequences [8–12] of anisotropic layers and revealed the self-similarity and scaling features. To the best of our knowledge, such studies for uniaxial crystals have not been carried out in the past. All through our paper we have used the same anisotropic material and just varied the orientation of the optic axis from layer to layer. Thus, all the gaps and other features reported in this paper appear as a consequence of anisotropy.

In § 2 we recall the essential mathematical background for the matrix formalism. In § 3 we present the numerical results for both periodic and quasiperiodic structures and in § 4 we conclude the paper.

2. Mathematical background

In this section we present the essential mathematical background for calculating the reflection and transmission coefficients of layered anisotropic media. The theory is applicable to any (uniaxial or biaxial) anisotropic layers with arbitrary orientation of optic axis and for arbitrary angle of incidence. It was mentioned earlier that a general theory is well understood. We will follow Yeh [3] in recalling the essential steps though there are equivalent methods by other authors [2, 5].

Consider the system shown in figure 1, consisting of N anisotropic layers with plane of stratification along the xy plane. For any specific jth layer the dielectric tensor $\overleftrightarrow{\varepsilon}$ in the xyz basis can be expressed as follows:

$$\overleftrightarrow{\varepsilon} = A \begin{pmatrix} \varepsilon_1 & 0 & 0 \\ 0 & \varepsilon_2 & 0 \\ 0 & 0 & \varepsilon_3 \end{pmatrix} A^{-1}, \tag{1}$$

where $\varepsilon_k (k = 1, 2, 3)$ are the components of the tensor for the jth layer along the principal axes, and A is the general rotation matrix which can be expressed in terms of the Euler angles θ, φ and ψ. In choosing the form of A we stick to the x-convention [13]. It may be noted here that simple rotations in the coordinate planes can be affected as follows:

yz rotation: by varying θ with $\varphi = \psi = 0$,

xy rotation: by varying φ with $\theta = \psi = 0$,

zx rotation: by varying θ with $\varphi = -\psi = \pi/2$.

It may be noted here that the method of Yeh [3] can be generalized to include the description of Faraday rotation and gyrotropic media. However, it lacks the generality

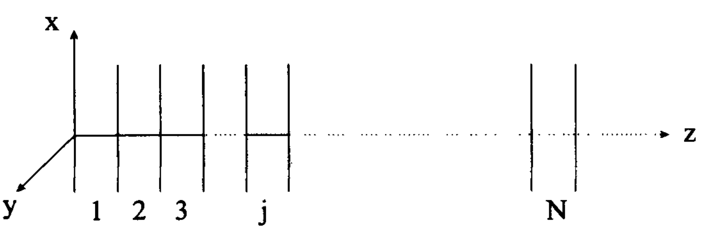

Figure 1. Schematic view of the layered medium.

of the approach developed by Berreman [2] which in principle can handle a broader class of media.

For fields having the dependence $\exp i[k_0(\alpha x + \beta y + \gamma z) - \omega t]$ with $k_0 = \omega/c$, the wave equation takes the following form

$$\mathbf{k} \times \mathbf{k} \times \mathbf{E} + k_0^2 \overleftrightarrow{\varepsilon} \cdot \mathbf{E} = 0, \quad \mathbf{k} = k_0(\alpha, \beta, \gamma). \tag{2}$$

The homogeneity of the layered medium in the xy plane implies that α and β remain the same throughout the layered medium. Equation (2) represents a set of three homogeneous equations with respect to the three cartesian components of **E**. The nontriviality of **E** imposes the following condition on the allowed values of γ:

$$\sum_{s=0}^{4} a_s \gamma^s = 0 \tag{3}$$

with

$$a_0 = \alpha^2(\alpha^2 \varepsilon_{xx} - \varepsilon_{xx}\varepsilon_{yy} - \varepsilon_{zz}\varepsilon_{xx} + \varepsilon_{zx}^2 + \varepsilon_{xy}^2) + \varepsilon_{xx}\varepsilon_{yy}\varepsilon_{zz}$$
$$+ 2\varepsilon_{xy}\varepsilon_{yz}\varepsilon_{zx} - \varepsilon_{zx}^2\varepsilon_{yy} - \varepsilon_{xy}^2\varepsilon_{zz} - \varepsilon_{yz}^2\varepsilon_{xx}, \tag{4}$$

$$a_1 = 2\alpha(\varepsilon_{xy}\varepsilon_{yz} - \varepsilon_{zx}\varepsilon_{yy} + \alpha^2 \varepsilon_{zx}), \tag{5}$$

$$a_2 = \alpha^2(\varepsilon_{xx} + \varepsilon_{zz}) - \varepsilon_{zz}(\varepsilon_{xx} + \varepsilon_{yy}) + \varepsilon_{zx}^2 + \varepsilon_{yz}^2, \tag{6}$$

$$a_3 = 2\varepsilon_{zx}\alpha, \tag{7}$$

$$a_4 = \varepsilon_{zz}. \tag{8}$$

In writing eqs (3)–(8) we have assumed (without any loss of generality) that the wave vector **k** lies on the xz plane (i.e. $\beta = 0$). The four (in general distinct) eigenvalues given by the solution of (3) leads to the eigenvectors which can be easily determined from (2). It may be noted here that (5) of Yeh [3], for the eigenvectors is not always applicable, which can be easily verified, for example, for A representing identity transformation, or coordinate rotation by $\pi/2$ about, say x axis. In determining the eigenvectors corresponding to a specific root of (3) we have adopted the following procedure. We substitute a particular solution for γ in the matrix corresponding to (2) and construct the adjoint matrix. Next we identify any nonzero element in the adjoint matrix. The corresponding minor is a basis minor which leads to the eigenvectors. If all the elements of the adjoint matrix are zeros (i.e. the rank of the coefficient matrix equals one) we refer to the nonzero element of the coefficient matrix. The corresponding components of the eigenvector are zero. The other two components are chosen in order to maintain the orthogonality of the ordinary and extraordinary components. Let the electric field eigenvectors be denoted by $\mathbf{p}_\sigma (\sigma = 1, 2, 3, 4)$. The corresponding magnetic field vectors can be expressed in terms of $\mathbf{p}_\sigma$ as follows.

$$\mathbf{q}_\sigma = (-\gamma p_{\sigma y}, \gamma p_{\sigma x} - \alpha p_{\sigma z}, \alpha p_{\sigma y}). \tag{9}$$

In terms of the eigenvectors the transfer matrix for a particular layer of width d can be expressed as follows:

$$M = DPD^{-1} \tag{10}$$

where D is the (4 × 4) dynamical matrix given by

$$D=\begin{pmatrix} p_{1x} & p_{2x} & p_{3x} & p_{4x} \\ q_{1y} & q_{2y} & q_{3y} & q_{4y} \\ p_{1y} & p_{2y} & p_{3y} & p_{4y} \\ q_{1x} & q_{2x} & q_{3x} & q_{4x} \end{pmatrix}, \tag{11}$$

and P is the propagation matrix (4 × 4) having the form

$$P=\mathrm{diag}(e^{-i\gamma_1 d}, e^{-i\gamma_2 d}, e^{-i\gamma_3 d}, e^{-i\gamma_4 d}). \tag{12}$$

The dynamical matrix given by (11) is defined such that it becomes block diagonal in the absence of mode coupling. Thus the amplitudes of the electric field vector corresponding to γ_1 and γ_2 (γ_3 and γ_4) represent the wave of the same polarization.

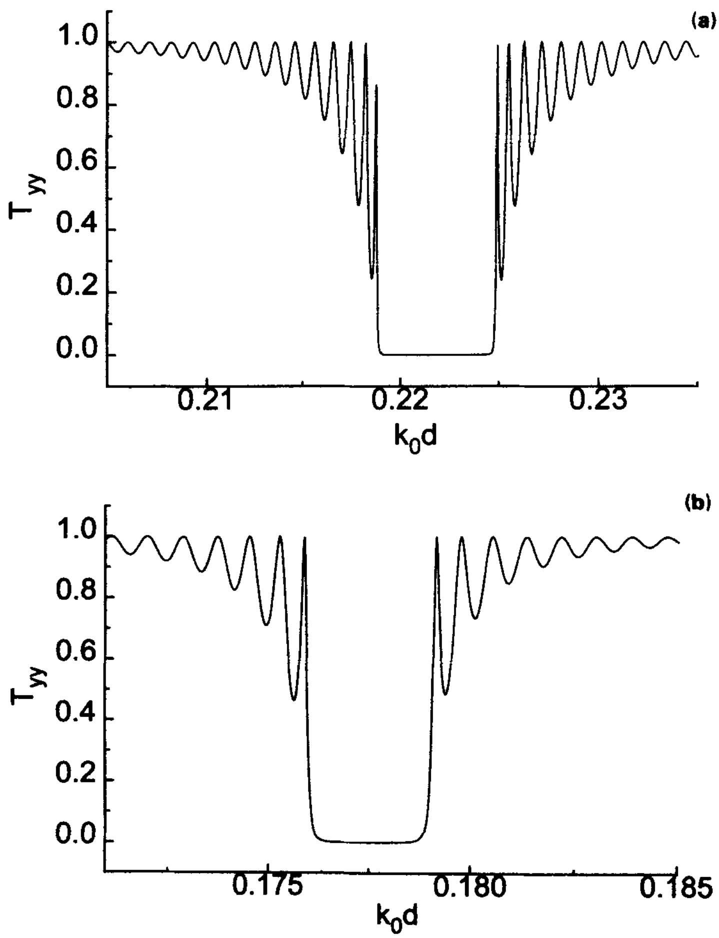

Figure 2. Transmission coefficient T_{yy} as a function of $k_0 d$ (in units of π) for (**a**) $N_m = 4$ and (**b**) $N_m = 5$ for $N_p = 100$, $n_0 = 2{\cdot}3$, $n_e = 2{\cdot}208$, $n_i = n_f = 2{\cdot}3$.

In fact in the absence of damping and evanescent waves, root of (3) are real and occur in pairs with opposite signs, representing the forward and backward propagating plane waves. We choose $\gamma_1, \gamma_3 (\gamma_2, \gamma_4)$ to represent the forward (backward) waves. The characteristic matrix $M^{(T)}$ for the layered medium with N layers can be written as

$$M^{(T)} = \prod_{j=1}^{N} M^{(j)}. \tag{13}$$

In (13) superscript j refers to the jth layer with dielectric tensor $\overleftrightarrow{\varepsilon}^{(j)}$ and width $d^{(j)}$. In order to relate the amplitudes of the waves in the medium of incidence and in the final medium one needs to know the corresponding dynamical matrices. The relation between the amplitudes can be expressed as follows:

$$\begin{pmatrix} A_{i+} \\ A_{i-} \\ B_{i+} \\ B_{i-} \end{pmatrix} = (D^{(i)})^{-1} M^{(T)} D^{(t)} \begin{pmatrix} A_{t+} \\ 0 \\ B_{t+} \\ 0 \end{pmatrix}, \tag{14}$$

where A_{i+}, A_{i-} and A_{t+} (B_{i+}, B_{i-}, B_{t+}) represent the amplitudes corresponding to the incident, reflected and transmitted x polarized (y-polarized) wave. We also assumed that the wave is incident from the left of the structure. Superscript $i(t)$ in the dynamical matrices refers to the medium of incidence (transmission). With the help of (14) four types of transmission coefficients can be defined:

$$T_{xx} = \left| \frac{A_{t+}}{A_{i+}} \right|^2_{B_{i+}=0}, \tag{15}$$

$$T_{xy} = \left| \frac{B_{t+}}{A_{i+}} \right|^2_{B_{i+}=0}, \tag{16}$$

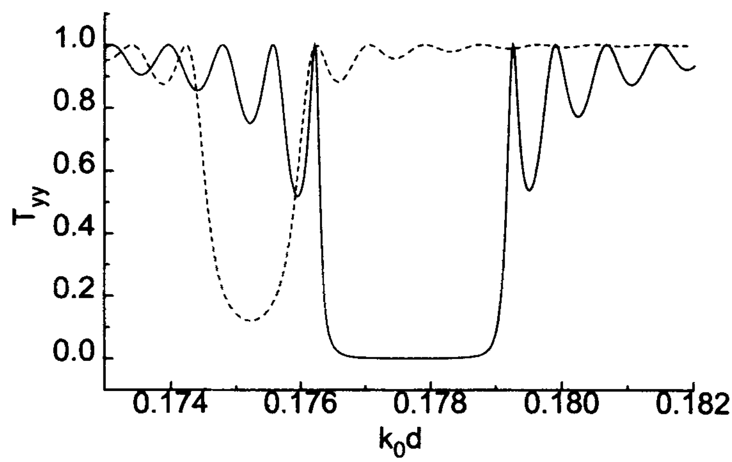

Figure 3. Transmission coefficient T_{yy} for periodic variation of θ as per eq. (20) in the text for $N_m = 5$, $N_p = 100$. The solid (dashed) curve is for $\theta_m = 0{\cdot}4\pi$ ($\theta_m = 0{\cdot}2\pi$). Other parameters are as in figure 2.

$$T_{yx} = \left|\frac{A_{t+}}{B_{i+}}\right|^2_{A_{i+}=0}, \tag{17}$$

$$T_{yy} = \left|\frac{B_{t+}}{B_{i+}}\right|^2_{A_{i+}=0}. \tag{18}$$

The various reflection coefficients can be defined in an analogous manner.

3. Numerical results and discussion

In this section, we present the results of our numerical investigations of periodic and quasiperiodic layered structures. A general Fortran code was developed along the lines discussed in the previous section which can deal with any number and sequence of anisotropic layers with arbitrary orientation of the optic axis and for arbitrary angle of incidence. In all our calculations we have chosen the same anisotropic medium and only varied the orientation of the optic axis from layer to layer. It is well-known that a periodic variation in the orientation of optic axis along the plane of stratification can lead to well defined band gaps. This has already been exploited to create very narrow

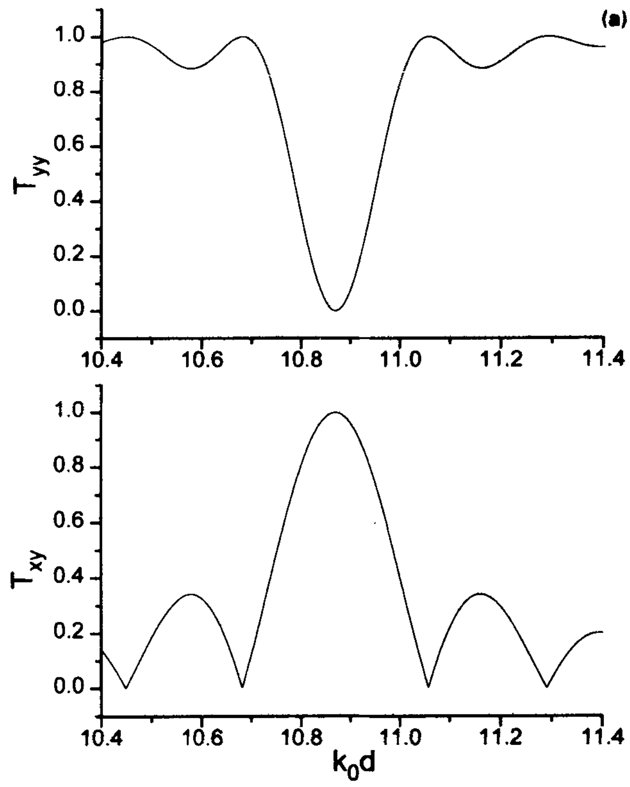

Figure 4a.

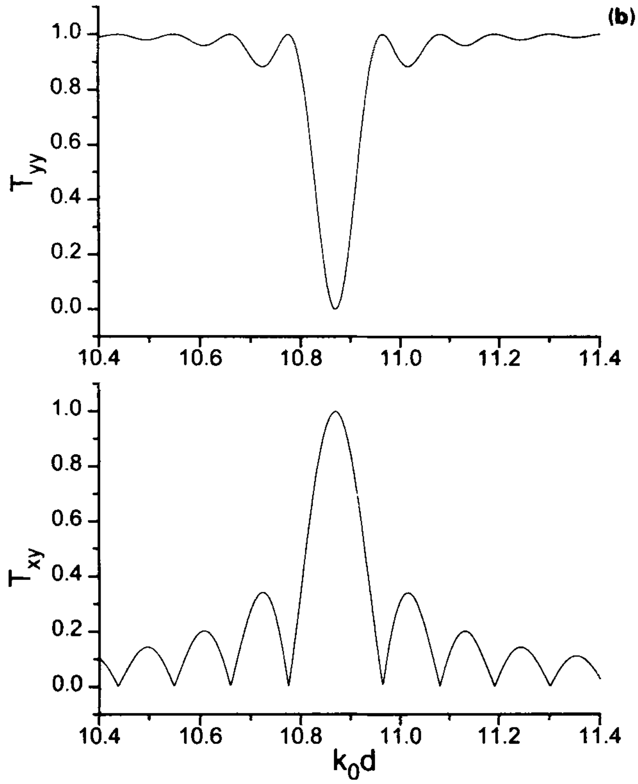

Figure 4b.

Figure 4. Transmission coefficient T_{yy} and T_{xy} as a function of $k_0 d$ (in units of π) for a solc filter for (**a**) $N_p = 50$ and (**b**) $N_p = 100$. Other parameters are as follows: $n_0 = 2{\cdot}3$, $n_e = 2{\cdot}208$, $n_i = n_f = 2{\cdot}3$, $\varepsilon_1 = \varepsilon_3 = n_0^2$ and $\varepsilon_2 = n_e^2$.

band solc filters. However, to the best of our knowledge, the case where the orientation of the optic axis is changed on the plane of incidence in a periodic fashion has not been dealt with in sufficient detail. Thus, in dealing with periodic structures we consider two cases, namely, (a) optic axis on the *yz* plane and (b) optic axis on *xy* plane. In the context of quasiperiodic structures also, we deal with the above two cases though our code can handle any other orientation. In all our calculations we have chosen the anisotropic material to be uniaxial and we have considered normal incidence (i.e. $\alpha = 0$). In what follows we present the results separately for periodic and quasiperiodic structures.

3.1 *Periodic anisotropic layered media*

(a) *Optic axis on the yz plane*: In this case we take $\varepsilon_1 = \varepsilon_2 = n_0^2$ and $\varepsilon_3 = n_e^2$. It is clear that, with optic axis on the *yz* plane the ordinary waves will have *x*-polarization and there is no polarization mixing (i.e. $T_{xy} = T_{yx} = 0$). So far as the ordinary waves are concerned, the layered medium will act as uniform slab having the total width of the structure and the ordinary refractive index n_0. Since there is no coupling between the x and y polarized waves and the matrix $M^{(T)}$ has block diagonal structure, one could have a 2×2 matrix formalism for this particular case. One may be tempted to think that in the context of the extraordinary waves one can replace the anisotropic layers by isotropic ones with θ dependent refractive indices. This approach is not correct since the eigenvectors as well as their projection on the plane of layers depend on θ. We consider a layered medium consisting of N_p stacks. Each stack is assumed to have N_m layers each with width d. In a jth layer the Euler angles are given by

$$\theta_j = \frac{(j-1)}{N_m} 2\pi, \varphi_j = \psi_j = 0, \quad j = 1, \ldots, N_m, \tag{19}$$

$$\theta_j = \theta_m \sin\left[\frac{(j-1)}{N_m} 2\pi\right], \varphi_j = \psi_j = 0, \quad j = 1, \ldots, N_m. \tag{20}$$

Equation (19) corresponds to the situation when the optic axis is rotated through 2π in each stack. Obviously, the period of the structure will depend on the value of N_m.

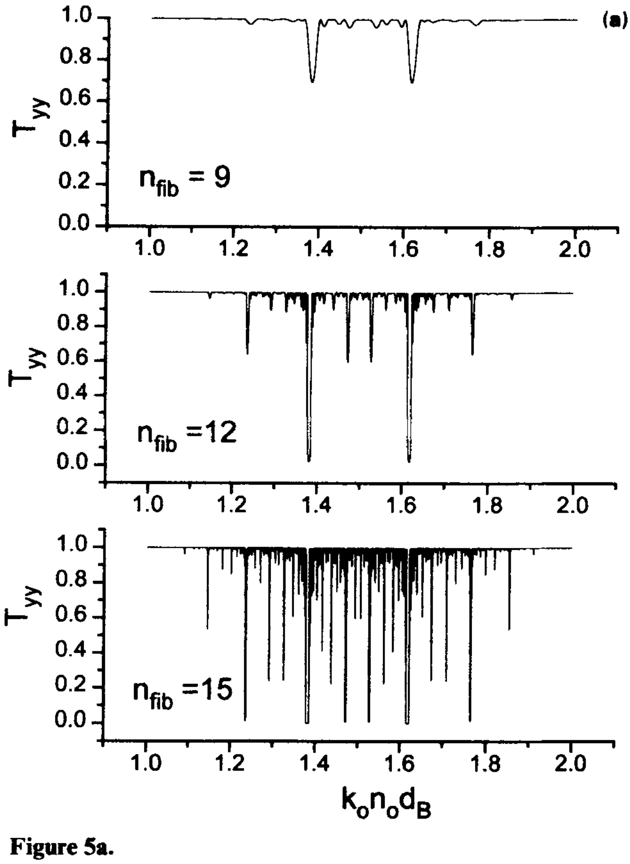

Figure 5a.

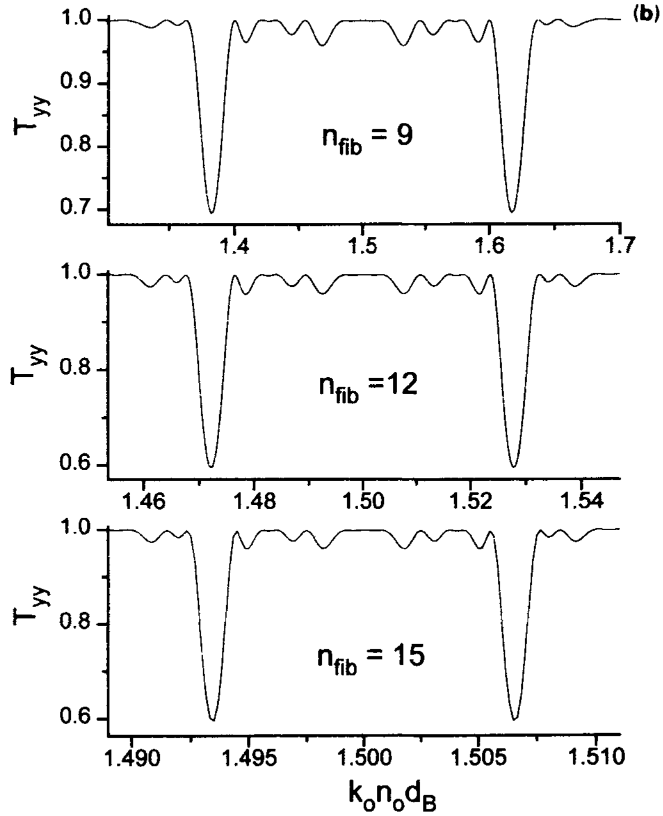

Figure 5b.

Figure 5. (**a**) Transmission coefficient T_{yy} as a function of $k_0 n_0 d_B$ (in units of π) for the Fibonacci sequence for $n_{\rm fib} = 9$, 12 and 15 (top to bottom) and (**b**) expanded version of (a). Other parameters are as follows: $n_0 = 2{\cdot}3$, $n_e = 2{\cdot}208$, $n_i = n_f = 2{\cdot}3$, $\theta_A = \pi/2$, $\theta_B = 0$, $\psi_A = \psi_B = \varphi_A = \varphi_B = 0$, $\varepsilon_1 = \varepsilon_2 = n_0^2$ and $\varepsilon_3 = n_e^2$.

Equation (20) corresponds to the situation where θ is varied in a periodic fashion with amplitude of modulation given by θ_m. The purpose of this special case is to show that the bandwidth of the gap can be controlled by varying the depth of modulation θ_m. The results of (19) are shown in figure 2a (for $N_m = 4$ and $N_p = 100$) and in figure 2b (for $N_m = 5$ and $N_p = 100$), where we have plotted T_{yy} as a function of $k_0 d$. Other parameters were chosen as follows: $n_0 = 2{\cdot}3$, $n_e = 2{\cdot}208$ (corresponding to $LiNbO_3$ at $\lambda = 0{\cdot}633\ \mu$m), $n_i = n_f = 2{\cdot}3$. It is clear that for $N_m = 4$ a period consists of effectively two slabs and the gaps occur at [3],

$$k_0 d(n_0 + n_e) = m\pi, \quad m \text{ integer}. \tag{21}$$

With the increasing number of periods the gap becomes more well defined. The location of the gap can be controlled by changing N_m. The results for $N_m = 5$ and $N_p = 100$ are shown in figure 2b. However, for a specified N_m one does not have much control over the width of the gap. This can be achieved by introducing an extra parameter as in (20). We have shown this in figure 3 where results are plotted for two different values of θ_m, namely $\theta_m = 0{\cdot}2\pi$ and $0{\cdot}4\pi$. It is clear from figure 3 that we can double the gap width by doubling the depth of modulation.

(b) *Optic axis on xy plane*: The main purpose of this subsection is to show the applicability of our code to recover known results. We take $\varepsilon_1 = \varepsilon_3 = n_0^2$ and $\varepsilon_2 = n_e^2$. Note that we have taken the optic axis along the y axis (in the last section the optics axis was along z axis). This is just to enable us to affect the rotations on the relevant planes in a direct fashion. xy rotation is affected by varying φ from layer to layer and keeping $\theta = \psi = 0$. The structure is assumed to consist of N_p periods. Each period (labeled by A and B) having two slabs (with equal width d and with $\varphi_a = +\delta$ and $\varphi_b = -\delta$), where $\delta = \pi/(8N_p)$ such that the Bragg-solc condition is satisfied. The solc resonances occur [3] at

$$k_0 d(n_0 - n_e) = m\pi, \quad m\text{-integer} \tag{22}$$

and one of these resonances are shown in figure 4a ($N_p = 50$) and 4b ($N_p = 100$). The following parameters were chosen for calculations: $n_0 = 2{\cdot}3, n_e = 2{\cdot}208, n_i = n_f = 2{\cdot}3$. We have plotted T_{yy} and T_{xy} as functions of $k_0 d$. The curves for T_{xx} and T_{yx} are analogous. As expected for solc filters, at solc resonances the conversion of x polarization to y and

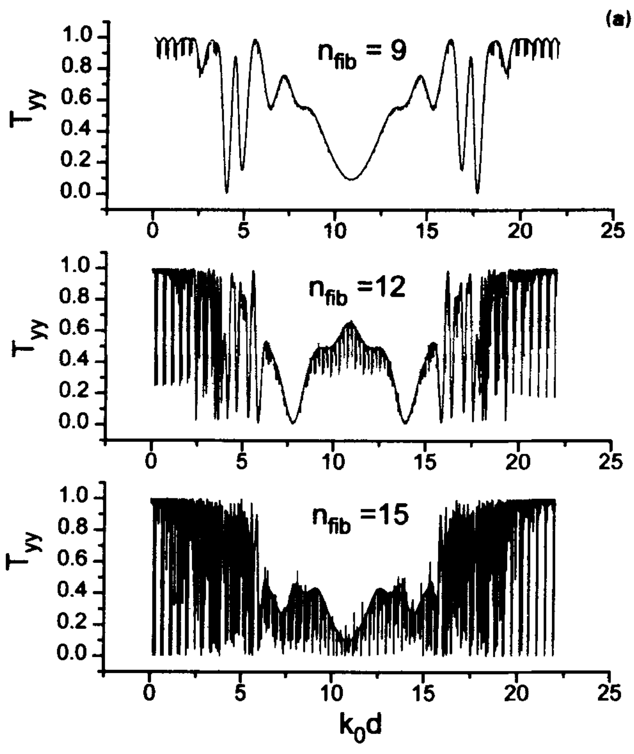

Figure 6a.

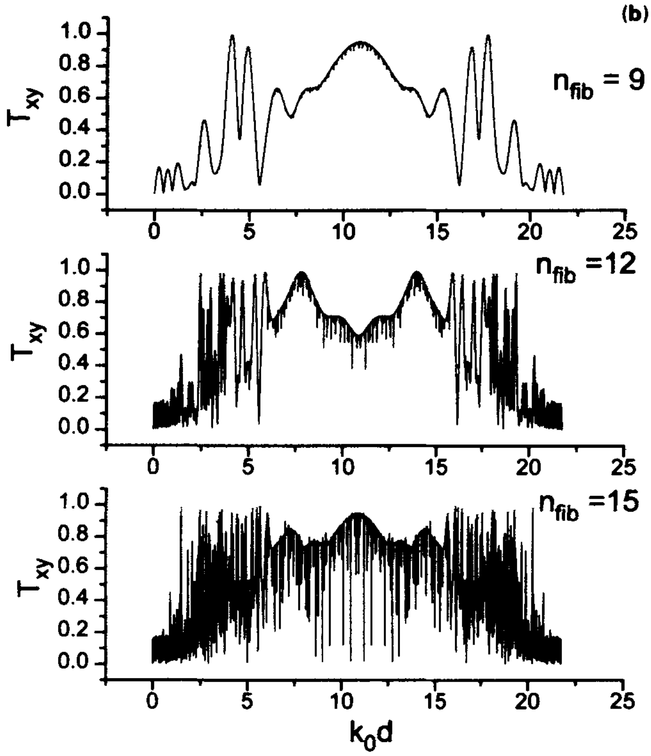

Figure 6b.

Figure 6. Transmission coefficient (**a**) T_{yy} and (**b**) T_{xy} for $n_{\mathrm{fib}} = 9$, 12 and 15 (curves from top to bottom) for the Fibonacci sequence. Other parameters are as follows: $n_0 = 2{\cdot}3$, $n_e = 2{\cdot}208$, $n_i = n_f = 2{\cdot}3$, $\varphi_A = -\delta$, $\varphi_B = \delta$, $\theta_A = \theta_B = \psi_A = \psi_B = 0$, $\varepsilon_1 = \varepsilon_3 = n_0^2$ and $\varepsilon_2 = n_e^2$.

vice versa is maximized. Moreover, one can drastically narrow down the band width with an increase in the number of periods (compare figures 4a and 4b).

3.2 *Quasiperiodic anisotropic layered medium*

We consider two types of anisotropic layers, namely A and B, with widths d_A and d_B respectively, and Euler angles $\theta_A, \varphi_A, \psi_A$ and $\theta_B, \varphi_B, \psi_B$, respectively. The Fibonacci sequence and the Fibonacci numbers are generated using the following recursion scheme

$$S_{j+1} = S_{j-1} S_j, F_{j+1} = F_{j-1} + F_j \tag{23}$$

with $S_0 = A$, $S_1 = B$ and $F_0 = F_1 = 1$. As mentioned earlier such layered media can exhibit interesting features like self similarity and scaling and they have been probed to explore weak localization in optics [8, 9]. Like in the periodic case we consider the two specific situations and present the results separately.

(a) *Optic axis on the yz plane*: For this case we take $\varepsilon_1 = \varepsilon_2 = n_0^2$ and $\varepsilon_3 = n_e^2$. $\theta_A = \pi/2$, $\varphi_A = \psi_A = 0$ and $\theta_B = 0$, $\varphi_B = \psi_B = 0$, $n_e d_A = n_0 d_B$. The numerical values were chosen to be $n_0 = 2{\cdot}3$, $n_e = 2{\cdot}208$, $n_i = n_f = 2{\cdot}3$. The results for Fibonacci generations $n_{\rm fib} = 9$, 12 and 15 are shown in figure 5a. A comparison of the plots on figure 5a reveals their self similarity. In order to have a more direct proof of the same, we have selected specific portions and expanded the horizontal axis and shown the same curves in figure 5b. Note the different scales of the horizontal axis. The self similarity features are obvious from figure 5b.

(b) *Optic axis on the xy plane*: We take $\varepsilon_1 = \varepsilon_3 = n_0^2$ and $\varepsilon_2 = n_e^2$, $\theta_A = \psi_A = 0$, $\varphi_A = -\delta$, $\theta_B = \psi_B = 0$, $\varphi_B = \delta$. The results for $T_{yy}(T_{xy})$ for $n_{\rm fib} = 9$, 12 and 15 are shown in figure 6a (figure 6b). The parameters chosen for calculations were as follows: $n_0 = 2{\cdot}3$, $n_e = 2{\cdot}208$, $n_i = n_f = 2{\cdot}3$, $\delta = 0{\cdot}1$. It can be easily seen from figures 6a and 6b that the curves corresponding to $n_{\rm fib} = 9$ and 15 are self similar. Like in Kohmoto and Sutherland 1987, for the chosen geometry and set of parameters the corresponding dynamical map has a six-cycle and thus features repeat after six generations. It may also be noted that the scale factor is very close to one. This is because we have chosen the constituent slabs to be of the same material and a change in the orientation of the optic axis in the xy plane by an angle 0·1 leads to a weakly quasiperiodic medium. In order to prove this, one needs to calculate the invariants associated with the dynamical matrix map, which can be treated as a measure of quasiperiodicity. Investigation are on to study these features in more detail and they will be reported elsewhere.

4. Conclusions

In conclusion, we have developed a very general code to deal with anisotropic layered media and applied the code to various periodic and quasiperiodic layered structures. In particular, we have dealt with the case where the optic axis is rotated on the plane of incidence and showed that the location and width of the gaps can be controlled simply by changing the depth of modulation of the angle of rotation. We have also investigated quasiperiodic layered media with optic axis on the plane of incidence or on the plane of stratification. In both the cases we have demonstrated the self similarity and scaling in the transmission coefficients. In this paper we restricted ourselves only to normal incidence though our code can also handle cases of oblique incidence. It is well-known that in case of oblique incidence one can excite the guided and surface modes which are of great practical importance. Such studies are underway and will be reported elsewhere.

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