# Band-gap analysis of one-dimensional photonic crystals and conditions for gap closing

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In this paper an analytical theory for arbitrary one-dimensional periodic media is presented. The analysis relies on the mathematical properties of Hill's equation. It is shown that the position of the band gaps can be obtained by quite simple expressions. As a special case, a one-dimensional multilayered medium (conventional photonic crystal) is studied. An exact formula for the location of the gap edges is derived for an infinite number of gaps, for both polarizations, at arbitrary angle of incidence. The gap closing conditions and the difference between the even- and the odd-numbered gaps are obtained. An extension for periodic structures with an arbitrary number of different layers is also presented. This method can be useful for the design of photonic crystal devices.

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## I. INTRODUCTION

Photonic-band-gap materials have been intensively investigated during the last ten years both experimentally and theoretically.[1–6] For the most part, the theoretical works were numerical[3,6] or included approximate analytical calculations.[1,2] However, exact analytical expressions for such parameters like the gap location, the gap width, and the position of the gap closing points (the points where gap width vanishes) for all gaps are still not available. Having these analytical expressions is a significant advantage which allows us to understand the behavior of the system, to simplify the calculations and alleviate the design of photonic crystal. In this paper, we focus on an exact analytical investigation of one-dimensional photonic crystals, with no simplifying assumptions, and show that the position of band gaps and the gap closing conditions for an infinite number of gaps can be obtained by quite simple analytical formulas.

The one-dimensional periodic problem is usually solved by using the transfer matrix method[7,8] or the plane wave expansion method.[3,6] In this paper, however, we present a different mathematical approach, which relies on the mathematical properties of Hill's equation,[9–12] and provide a different insight into the problem. Using this formalism we get some interesting conclusions that have not been reported previously to our knowledge.

A linear second-order differential equation of the form $u''+a(x)u=0$, where $a(x)$ is a periodic function of $x$, is known as an equation of the Hill type.[9–12] This equation was first introduced and investigated by Hill in his study of the motion of the moon in 1877. Since then Hill's equation has appeared in many applications and has been the subject of numerous analytic studies.[9–12] Here we apply the theory of Hill's equation to study the properties of photonic crystals.

First we demonstrate the analysis for an arbitrary periodic medium, with $n(x)$ being an arbitrary periodic refractive index. We find the conditions for the gap edges and explain the difference between even and odd gaps.

Next, we examine a special case, namely, an ordinary one-dimensional photonic crystal, which is made of a periodic multilayer medium. We show the equivalence between the present analysis and the transfer matrix method by getting the same dispersion relation. The dispersion relation that has been derived for infinite layered medium using the transfer matrix method[7,8,4] is

$$K(\beta,\omega) = \frac{1}{L}\cos^{-1}\left(\frac{A+D}{2}\right), \tag{1}$$

where $A$ and $D$ are the diagonal elements of a $2\times 2$ translation matrix, $L$ is the length of a period, and $K$ is a Bloch wave number. The expressions for $A$ and $D$, for the $I$-layered periodic structure, are given in Appendix A. The frequencies at band-gap edges are usually found by setting $\cos(KL) \equiv \pm 1$ in Eq. (1) and solving the transcendental equation numerically. However, some analytical calculations are possible. The derivation of the expression for the edges of the first band gap was published previously.[1,2]

In our paper we present the extended formula for the frequencies of gap edges and gap width for an infinite number of gaps, for both TE polarization (where the electric field is perpendicular to the plane of incidence) and TM polarization (the electric field is parallel to the plane of incidence) at arbitrary angle of incidence. We show that our formula includes the expressions that have been derived earlier.

It is well known that the gap width of one-dimensional photonic crystals strongly depends on the incident angle of light. Moreover, it is sensitive to polarization, leading to a polarization-dependent gap. For some angles, the gap width vanishes and the gap closes. Finding these closing points (the angle and the frequency) for both TE and TM polarizations is an important issue, which will allow us to design photonic crystals for suitable applications. For example, knowing these closing points helps to create an omnidirectional reflector, operating in several distinct frequency ranges by use of only a single photonic crystal.[15,16] Usually, these closing points are found graphically, using the band structure diagram.[4,5] In this paper, however, we provide the exact mathematical criterion for gap closing points as a consequence of the presented analysis. We also prove mathematically that the first band gap never closes for the TE wave and has only one closing point for the TM wave, at the Brewster angle. This important property of one-dimensional photonic crystals has been observed earlier[5] and used to construct the omnidirectional reflector.[4] Here we provide the analytical verification of this behavior.

## II. THEORETICAL BACKGROUND

We consider an infinite periodic one-dimensional material in the $x$-$z$ plane, with periodicity in the $x$ direction and homogeneity in $z$ and $y$. Assuming a plane wave, the wave vector is $\boldsymbol{k}=k_x\hat{x}+k_z\hat{z}$ (per definition we take $k_y=0$). In order to study the properties of electromagnetic waves in this structure we should solve Maxwell's equations, which reduce to the two-dimensional wave equation

$$\frac{\partial^2 \boldsymbol{E}(x,z,t)}{\partial x^2}+\frac{\partial^2 \boldsymbol{E}(x,z,t)}{\partial z^2}=\frac{n^2(x)}{c^2}\frac{\partial^2 \boldsymbol{E}(x,z,t)}{\partial t^2} \tag{2}$$

assuming a dependence of

$$\boldsymbol{E}(x,z,t)=E(x)\exp(ik_z z)\exp(-i\omega t), \tag{3}$$

we obtain the Helmoltz equation, which is a type of Hill's equation:[9–12]

$$\frac{d^2E(x)}{dx^2}+\left(n^2(x)\frac{\omega^2}{c^2}-k_z^2\right)E(x)=0 \tag{4}$$

where the refractive index $n(x)$ is a periodic real-valued function with period $L$, namely, $n(x+L)=n(x)$.

Let $E_1(x)$ and $E_2(x)$ be two different solutions of (4) satisfying the initial conditions

$$E_1(x=0)=1,$$
$$E_1'(x=0)=0, \tag{5a}$$
$$E_2(x=0)=0,$$
$$E_2'(x=0)=1. \tag{5b}$$

These solutions are called normalized solutions of (4). The general solution of (4) for any given boundary conditions $E(x=0)=C_1$ and $E'(x=0)=C_2$ can be expressed in the form[9–11]

$$E(x)=C_1E_1(x)+C_2E_2(x) \tag{6}$$

where $C_1$ and $C_2$ are arbitrary chosen constants.

Employing the Floquet-Bloch theorem, for the solutions in a periodic structure, we obtain[3,6,8]

$$E(x+L)=E(x)\exp(iKL) \tag{7}$$

where $K$ is the Bloch wave number.

Therefore, we look for the solutions of Eq. (4) that have the form

$$E(x+L)=pE(x),$$
$$E'(x+L)=pE'(x), \tag{8}$$

where for convenience we denote

$$p=\exp(iKL). \tag{9}$$

By substituting Eq. (6) in condition (8) we get a set of homogeneous equations for $C_1$ and $C_2$, which can have a solution only if its determinant vanishes for every value of $x$. In particular, for $x=0$, we obtain

$$\begin{vmatrix} E_1(L)-p & E_2(L) \\ E_1'(L) & E_2'(L)-p \end{vmatrix}=0. \tag{10}$$

Since the expression $E_1(x)E_2'(x)-E_1'(x)E_2(x)$ is the Wronskian of the differential equation, we find that it is constant and, from the initial conditions, we find that its value is equal to unity. Thus, using $E_1(L)E_2'(L)-E_1'(L)E_2(L)=1$, the determinantal equation for $p$ becomes

$$p^2-F(\omega,k_z)p+1=0 \tag{11}$$

where

$$F(\omega,k_z)=E_1(\omega,k_z,L)+E_2'(\omega,k_z,L). \tag{12}$$

Note that $k_z$ depends on $\omega$ and the function $F(\omega,k_z)$ depends only on the values and derivatives of normalized solutions $[E_1(x)$ and $E_2(x)]$ in $x=L$. Because the coefficients of Eq. (4) are real, the function $F(\omega,k_z)$, called the Hill's determinant, always remains real.[12]

Equation (11) is a characteristic equation for the differential equation (4). If $p_1$ and $p_2$ are two roots of this equation, then $p_1p_2=1$ and $p_1+p_2=F(\omega,k_z)$.The roots of Eq. (11) are given by

$$p_{1,2}=\frac{F(\omega,k_z)\pm\sqrt{F(\omega,k_z)^2-4}}{2}. \tag{13}$$

If Eq. (11) has two different roots, there are two different solutions of (4) with the same boundary conditions, namely, $E(x)$ and $\tilde{E}(x)$, which satisfy

$$E(x+L)=p_1E(x),$$
$$\tilde{E}(x+L)=p_2\tilde{E}(x). \tag{14}$$

Now we examine three regions, for various choices of $\omega$ and $k_z$, for which $|F(\omega,k_z)|<2$, $|F(\omega,k_z)|>2$, and $|F(\omega,k_z)|=2$.

(I) If $|F(\omega,k_z)|<2$, for some fixed $\omega$ and $k_z$, then both $p_1$ and $p_2$ are complex conjugates of unit magnitude [see Eq. (13)]. Therefore we have $p_{1,2}=e^{\pm iKL}$, where $K$ is real.[9–11] Thus, for any values of $\omega$ and $k_z$ that satisfy $F|(\omega,k_z)|<2$ we get an allowed propagating solution that takes the form of the Bloch wave.

(II) If $|F(\omega,k_z)|>2$, then both $p_1$ and $p_2$ are real and since $p_1p_2=1$, one of them (say $p_1$) is greater than unity and the other (say $p_2$) is smaller than unity. Employing Eq. (14) we get $E(x+nL)=p_1^nE(x)$, and therefore $E(x)$ is unbounded, not an allowed solution. On the other hand, $\tilde{E}(x+nL)=p_2^n\tilde{E}(x)$; therefore $\tilde{E}(x)$ is a decaying function. Thus, the values of $\omega$ that satisfy $|F(\omega,k_z)|>2$ correspond to the decaying solutions of Eq. (4) and constitute the region that we call the band gap. Here $p_{1,2}=\exp(\pm iKL)$, where $K$ is a complex number.

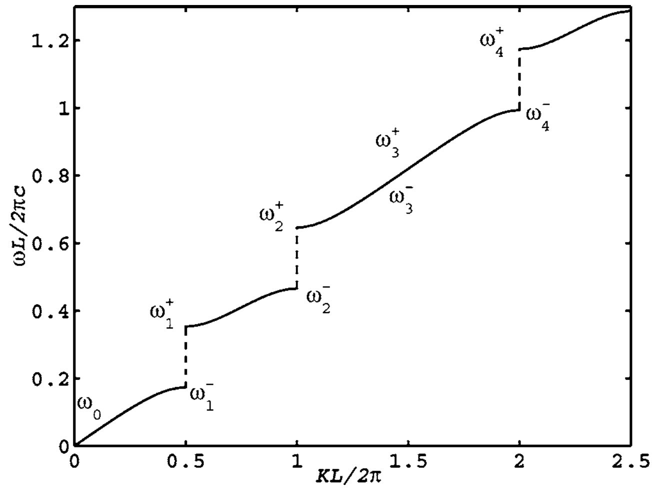


FIG. 1. Schematic description of the normalized gap edges $\omega_n^\pm$ as function of the normalized Bloch wave number $K$.

(III) The most interesting region consists of values of $\omega$ for which $|F(\omega,k_z)|=2$. This is a boundary between the regions I and II; therefore this is a condition for the gap edges. In this case we have two different solutions of Eq. (11), which are both double roots. For $F(\omega,k_z)=2$ we have $p_1=p_2=1$; therefore $K=2\pi m/L$, where $m$ is an integer. For $F(\omega,k_z)=-2$ we have $p_1=p_2=-1$, where $K=(2m+1)\pi/L$. Employing Eq. (14) we find that when $F(\omega,k_z)=2$, the electric field has a period $L$, i.e., $E(x+L)=E(x)$, whereas for $F(\omega,k_z)=-2$, the electric field satisfies $E(x+L)=-E(x)$.

In order to obtain more information about the gap edges we find the values of $\omega$ for which $F(\omega,k_z)=\pm 2$ and therefore $p_{1,2}=\pm 1$.

We consider Eq. (4) with initial conditions (5) and two different boundary conditions, obtained from Eq. (8):

$$\begin{aligned} E(0) &= E(L), \\ E'(0) &= E'(L) \end{aligned} \quad \text{for } p_1=p_2=1 \tag{15}$$

and

$$\begin{aligned} E(0) &= -E(L), \\ E'(0) &= -E'(L) \end{aligned} \quad \text{for } p_1=p_2=-1. \tag{16}$$

The values of $\omega$ which satisfy (15) we call the edges of the even gap, whereas the values of $\omega$ which satisfy (16) are the edges of the odd gap. There are an infinite number[9–11] of real values of $\omega$, which satisfy both Eqs. (4), (5) and Eq. (15) or (16). We let $\omega_m$ be all these values for $m=0,1,2,3,\ldots$ and as explained above they correspond to the band-gap edges. It is clear that for $\omega_0=0$ Eq. (4) has a simple solution $E(x)=1$. The values of $\omega$ that correspond to the even gaps $[F(\omega,k_z)=2]$ for a given propagation angle are

$$0=\omega_0<\omega_2^-\leqslant\omega_2^+<\omega_4^-\leqslant\omega_4^+\cdots<\omega_{2m}^-\leqslant\omega_{2m}^+<\cdots \tag{17}$$

and the values that correspond to the odd gaps $[F(\omega,k_z)=-2]$ are

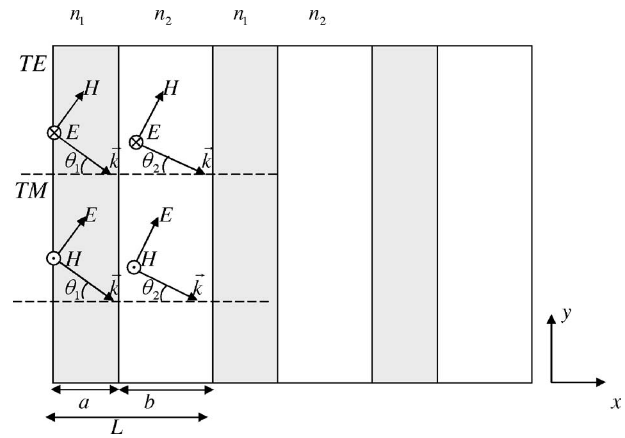


FIG. 2. Electromagnetic wave propagation in a one-dimensional photonic crystal for TE and TM polarizations.

$$\omega_1^-\leqslant\omega_1^+<\omega_3^-\leqslant\omega_3^+<\cdots<\omega_{2m+1}^-\leqslant\omega_{2m+1}^+<\cdots. \tag{18}$$

These values occur in the order

$$0=\omega_0<\omega_1^-\leqslant\omega_1^+<\omega_2^-\leqslant\omega_2^+<\omega_3^-\leqslant\omega_3^+<\omega_4^-\leqslant\omega_4^+<\cdots. \tag{19}$$

The values $\omega_m^2/c^2$ are called characteristic values. That the characteristic values of Hill's equations are arranged in such a sequence is well known in mathematics and called the oscillation theorem.[9–11]

If $\omega$ lies in any of the intervals $(\omega_m^-,\omega_m^+)$ $(m=0,1,2,3,\ldots)$ we obtain that Eq. (4) has only forbidden (not propagating) solutions $[|F(\omega,k_z)|>2]$. These intervals are the band gaps. If $\omega$ lies in any complementary intervals $(\omega_{m-1}^+,\omega_m^-)$, we have propagating allowed solutions $[|F(\omega,k_z)|>2]$; these intervals are called passbands.

Thus, the values of $\omega_m^\pm$, which are solutions of the equation $F(\omega,k_z)=\pm 2$, correspond to band-gap edges, so that $\omega_m^-$ is the initial point of the $m$ gap and $\omega_m^+$ is the end point of the $m$ gap. The order of the values of $\omega_m^\pm$ for some given propagation angle is shown schematically in Fig. 1.

The equality signs in (17)–(19) show that some of the gaps may be absent, whereas the passbands can never disappear. The gap number $m$ will be absent if $\omega_m^-=\omega_m^+$ (see for example $\omega_3^\pm$ in Fig. 1); this special case will be considered later below.

The above analysis is valid for every real-valued arbitrary periodic refractive index $n(x)$. In photonic crystals we are usually interested in functions $n(x)$ which are piecewise constant. In these particular cases a simple expression for values of $\omega_m^\pm$ can be found.

As a special case we consider the alternating dielectric regions of indices $n_1$ and $n_2$ which have width $a$ and $b$ with $L=a+b$ the lattice period. However, the presented formalism can be extended for periodic layered media with more than two different layers (see Appendix A) and thus can be used as an approximation for graded-index periodic structures.

We consider

$$n(x) = \begin{cases} n_1, & 0 \le x \le a, \\ n_2, & a < x \le L, \end{cases} \tag{20}$$

as is shown in Fig. 2.

First, we consider the TE modes of this structure. The electric field $E(x)$ is in the $y$ direction and satisfies (4). The solutions of Eq. (4) in any layer are combinations of $\sin(x)$ and $\cos(x)$. Therefore, the functions $E_1(x)$ and $E_2(x)$ of electric field which solve Eq. (4) and satisfy the conditions (5) are also linear combinations of $\sin(x)$ and $\cos(x)$. The boundary conditions for the TE mode require continuity of the electric field [both $E_1(x)$ and $E_2(x)$] and its derivative at the interface. Therefore

$$E_1(x,\omega) = \begin{cases} \cos(k_1 x), & 0 \le x \le a, \\ \cos(k_1 a)\cos[k_2(x-a)] - \dfrac{k_1}{k_2}\sin(k_1 a)\sin[k_2(x-a)], & a < x \le L, \end{cases}$$

$$E_2(x,\omega) = \begin{cases} \dfrac{\sin(k_1 x)}{k_1}, & 0 \le x \le a, \\ \dfrac{\sin(k_1 a)}{k_1}\cos[k_2(x-a)] + \cos(k_1 a)\dfrac{\sin[k_2(x-a)]}{k_2}, & a < x \le L, \end{cases} \tag{21}$$

where $k_{1,2} = \sqrt{(n_{1,2}\omega/c)^2 - k_z^2} = n_{1,2}\omega \cos\theta_{1,2}/c$ and $\theta_{1,2}$ are propagation ray angles in each layer $n_{1,2}$ (see Fig. 2). The constants in (21) were chosen to satisfy conditions (5) and the continuity conditions of the TE mode. The solutions with other initial conditions can be expressed as

$$E(x,\omega) = C_1 E_1(x,\omega) + C_2 E_2(x,\omega). \tag{22}$$

We are interested now in finding the function $F(\omega,k_z)$. By using (21), we obtain

$$F(\omega,k_z) = B\cos\left(\frac{\omega}{c}\delta\right) + (2-B)\cos\left(\frac{\omega}{c}\gamma\right) \tag{23}$$

where

$$B = 1 + \frac{1}{2}\left(\frac{n_1\cos\theta_1}{n_2\cos\theta_2} + \frac{n_2\cos\theta_2}{n_1\cos\theta_1}\right) \tag{24}$$

and

$$\delta = n_1 a\cos\theta_1 + n_2 b\cos\theta_2,$$

$$\gamma = n_1 a\cos\theta_1 - n_2 b\cos\theta_2. \tag{25}$$

The propagation angles $\theta_1$ and $\theta_2$ in Eqs. (24) and (25) are related to each other by Snell's law. Note that by using the property of the roots of Eq. (11), $p_1 + p_2 = F(\omega,k_z)$, and substituting the definitions of $F(\omega,k_z)$ from Eq. (23) and $p_{1,2} = e^{\pm iKL}$, we get the same dispersion relation that is obtained using the transfer matrix approach [see Eq. (1)]. Here, we get this expression as a special case from the more general analysis.

Following the previous discussion, the values $\omega_m^{\pm}$, which are the band-gap edges, satisfy $F(\omega_m^{\pm},k_z) = \pm 2$, that is,

$$B\cos\left(\frac{\omega_m^{\pm}}{c}\delta\right) + (2-B)\cos\left(\frac{\omega_m^{\pm}}{c}\gamma\right) = \pm 2. \tag{26}$$

Equation (26) can be solved by applying the Rouche theorem.[13,14] The solution has the form

$$\omega_m^{\pm} = \frac{c}{\delta}(m\pi \pm 2r_m^{\pm}), \quad m = 1,2,3\ldots, \tag{27}$$

where $0 \le r_m^{\pm} < \pi/2$ is different for even and odd gaps and found from

$$\sin r_{2s}^{\pm} = \left|\sin\frac{\gamma}{\delta}(s\pi \pm r_{2s}^{\pm})\right|\sqrt{\frac{B-2}{B}} \quad \text{for } s = 1,2,\ldots \tag{28}$$

and

$$\sin r_{2s+1}^{\pm} = \left|\cos\frac{\gamma}{\delta}\left(s\pi + \frac{\pi}{2} \pm r_{2s+1}^{\pm}\right)\right|\sqrt{\frac{B-2}{B}} \quad \text{for } s = 0,1,2,\ldots \tag{29}$$

These are results for TE polarization. To find the solution for TM polarization, we use the fact that the function $n(x)$ is piecewise constant. Therefore, we should solve the Helmoltz equation (4) with conditions (5) for the magnetic field $H$, in a manner similar to (21) and choose the constants that satisfy the continuity conditions for the magnetic field and its derivative. Thus, we get the same expression for the gap edges, but with $B$ defined in a different way, namely,

$$B_{TM} = 1 + \frac{1}{2}\left(\frac{n_2\cos\theta_1}{n_1\cos\theta_2} + \frac{n_1\cos\theta_2}{n_2\cos\theta_1}\right). \tag{30}$$

Note that for $m=1$, Eq. (27) provides the expression that was obtained in Ref. 1 for the first band gap. Our formula, how-

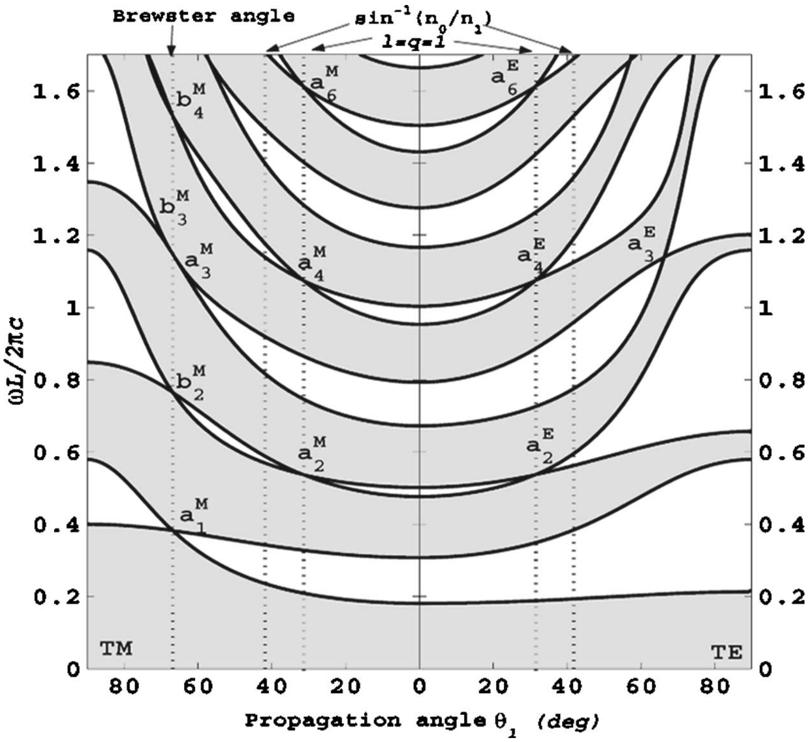


FIG. 3. The normalized band frequencies as function of the propagation angle $\theta_1$, for the first six bands for a one-dimensional photonic crystal, with $n_1=1.5$ and $n_2=3.5$ and layer widths $a$ and $b$ such that $a/b=8/3$. The right panel is for TE polarization, whereas the left panel is for TM polarization. Vertical dotted lines are for the maximum internal angle, assuming $n_0=1$ and for some gap closing points.

ever, includes an infinite number of band gaps. Although the above expression gives $r_m^{\pm}$ in implicit form it can be easily found using, for example, the bisection method. Because $r_m^{\pm}$ is bounded between 0 and $\pi/2$ it can easily be applied. In addition, some analytical expressions can be found to approximate (28) and (29), using simplifying assumptions.[1,2] However, for some particular cases the values of $\omega_m^{\pm}$ for the gap edges can be found explicitly as pointed out in Sec. IV. The extension of Eqs. (27)–(29) for an arbitrary number of layers per period is presented in Appendix A.

## III. APPLICATIONS AND DISCUSSION

Even in their implicit form, expressions (27)–(30) are quite useful. First, these formulas significantly simplify the calculations of band-gap structures. For example, it helps to plot the projected band structure diagram in a much easier way. The projected band structure is used to investigate photonic crystals for arbitrary directions of propagation.[4,5] Examples of such structures are shown in Figs. 3 and 4. The figures show normalized frequency as a function of propa-

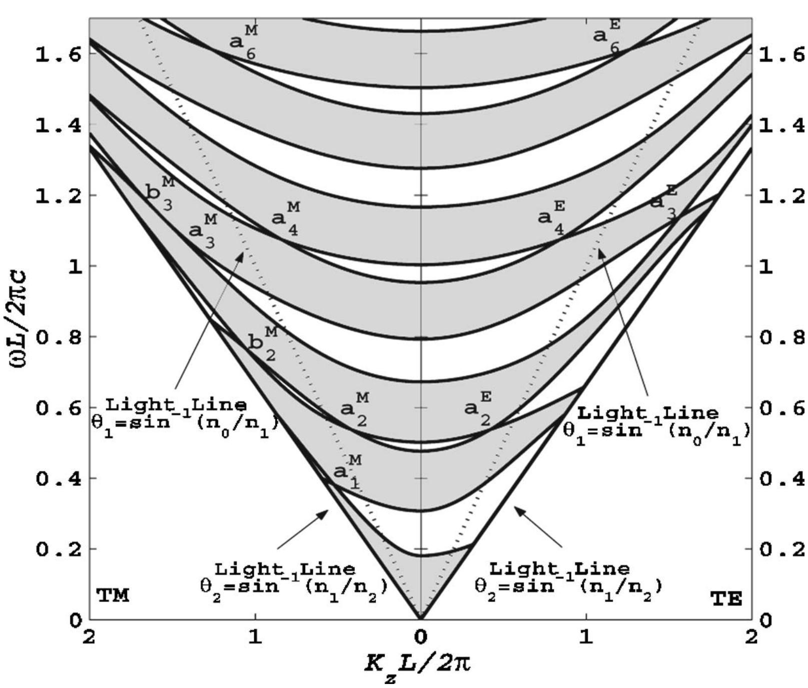


FIG. 4. Projected band structure of the first six bands. The photonic crystal parameters are the same as in Fig. 3.

gating angle $\theta_1$ (Fig. 3) or as a function of tangential component of the wave vector (Fig. 4). To plot these diagrams we need just to find the boundaries between the allowed (dark) regions and the gaps (bright regions), using expressions (27)–(29), and by scanning the angle from 0 to 90°. Thus, the gaps are between lines $\omega_m^-(\theta_1)$ and $\omega_m^+(\theta_1)$, and the propagating electromagnetic waves are between lines $\omega_{m-1}^+(\theta_1)$ and $\omega_m^-(\theta_1)$ (see Fig. 3). Figure 4 is obtained from Fig. 3, using $k_z=\omega n_1 \sin\theta_1/c=\omega n_2 \sin\theta_2/c$.

Another important application of the expressions (27)–(29) is the ability to calculate the extent of the gap. From Eq. (27) we find the expression for the gap width:

$$\Delta\omega_m=\omega_m^+-\omega_m^-=\frac{2c}{\delta}(r_m^+ + r_m^-), \quad m=1,2,3\ldots . \tag{31}$$

It is obvious that when $r_m^+=r_m^-=0$, $\Delta\omega_m$ vanishes and the gap has zero width; it is defined as the "empty gap" or gap closing. The gap closing point can be found from band structure diagrams, like Figs. 3 and 4. These points are marked by $a_1^M$ for the first TM gap, $a_2^M, b_2^M$ for the second TM gap, $a_3^M, b_3^M$ for the third TM gap and so on, whereas $a_2^E$ is for the second TE, $a_3^E$ for the third TE, and so on.

In contrast, the conditions for gap closing are easily derived from (28) and (29), without using these plots (for derivation see Appendixes B and C). The resulting conditions are presented below.

(i) The condition for gap closing for both TE and TM waves is as follows. If for some angles $\theta_1$ in layer $n_1$ and $\theta_2$ in layer $n_2$, we have

$$n_1 a(\cos\theta_1)l=n_2 b(\cos\theta_2)q \tag{32}$$

where $l$ and $q$ are integers, then all gaps numbered $i(q+l)$, $i=1,2,3\ldots$, have zero width for these angles. We say that at these points the gap closes. For example, if $n_1 a\cos\theta_1=2n_2 b\cos\theta_2$, every gap number $3i$ closes ($i=1,2,3\ldots$) at these angles and if $n_1 a\cos\theta_1=n_2 b\cos\theta_2$ every gap number $2i$, namely, every even gap, closes at these angles.

Note that the relation between $\theta_1$ and $\theta_2$ in Eq. (32) is defined by Snell's law. In addition, the condition (32) is the same for both TE and TM polarizations, because (32) does not depend on $B$, which is the only parameter that distinguishes between two polarizations. Therefore, these gap closing points are identical for both polarizations.

(ii) For the TM wave, however, there is an additional condition for gap closing:

$$\tan\theta_1=\frac{n_2}{n_1}. \tag{33}$$

It corresponds to the Brewster angle.[5,7] At this point there is no reflection of TM waves and therefore there is no band gap. The Brewster angle condition (33) can be directly derived from Eqs. (27)–(30) (see Appendix C for details).

Next, we find the expression for closed gap frequency of gap number $m$ by setting $r_m^{\pm}=0$ in Eq. (27):

$$\omega_m^{\pm}=\frac{c\pi m}{\delta}. \tag{34}$$

Another interesting conclusion from the gap closing conditions (i) and (ii) is that the first TE gap never closes, whereas the first TM gap has only one closing point, at the Brewster angle. [It can be proved by setting $m=0$ and $r_1^{\pm}=0$ in Eq. (26) and noting that there is no solution to this equation for TE polarization and only one solution for TM polarization. The TM closing point corresponds to $B_{TM}=0$, which is exactly the Brewster angle condition as explained in Appendix C]. This important property of the first band gap, which allows omnidirectional reflection, has been demonstrated earlier,[4,5] but has not been explained mathematically. Here this property is obtained as a consequence of conditions (i) and (ii).

Note also that the higher gaps commonly do not have this property. However, by the proper design we can prevent band gap closing also for the higher-order gaps.

The presented analysis and the derived expressions are valid for infinite photonic crystals. However, it can be also used to approximate the finite structure. The reflectivity spectrum of finite multilayers tends to the reflectivity spectrum of the infinite multilayer exponentially with the number of periods $N$. Thus, if $N$ is sufficiently large, the equations developed for an infinite system can be used as a good approximation for a finite structure as well.

In this case Eqs. (24), (25), (30), and (32) can be expressed in terms of $\theta_0$, the incident angle, and $n_0$, the refractive index of ambient medium, using Snell's law:

$$n_0\sin\theta_0=n_1\sin\theta_1=n_2\sin\theta_2. \tag{35}$$

From Snell's law we can see that the propagating angle $\theta_2$ is restricted to the range $0\leqslant\theta_2\leqslant\sin^{-1}(n_1/n_2)$, assuming $n_1<n_2$, and if we are considering the finite structure, the propagating angle $\theta_1$ is restricted to the range $0\leqslant\theta_1\leqslant\sin^{-1}(n_0/n_1)$. The upper boundaries of these ranges, the light lines, are depicted in Figs. 3 and 4.

As a numerical example we consider a one-dimensional photonic crystal with refractive indices $n_1=1.5$ and $n_2=3.5$ and layers width $a$ and $b$, respectively, such that $a/b=8/3$. The refractive indices are chosen close to ones of $SiO_2$ and Si. Both Figs. 3 and 4 show projected band diagrams of this photonic crystal. The dotted lines are for the maximum internal angle (the light line), assuming $n_0=1$ and for the gap closing points. To verify our conclusions (i) and (ii), we examine every gap closing point in either Fig. 3 or Fig. 4 and find which condition every point corresponds to.

As we expected, the first TE gap never closes and the first TM gap has one closing point $a_1^M$, corresponding to $\theta_1=66.8°$ (see Fig. 3). This is exactly the Brewster angle defined by $\theta_B=\tan^{-1}(n_2/n_1)$. The second gap has zero width at $a_2^E$ for TE polarization and at $a_2^M$ for TM polarization, both at $\theta_1=31.5°$. In this case $n_1 a\cos\theta_1=n_2 b\cos\theta_2$, which is exactly the first condition for zero width gap with $l=q=1$, and as was indicated earlier it is identical for both polarizations. Moreover, from the first condition it follows that if $\Delta\omega_2=0$, then every even gap closes exactly at the same angle. See, for example, $a_4^E$, $a_4^M$ and $a_6^E$, $a_6^M$, all corresponding to the same $\theta_1=31.5°$. Next, we examine $b_2^M$. This is also a Brewster angle point just like $a_1^M$. The other points that match the Brewster angle condition are $b_3^M$ and $b_4^M$ (see Fig. 3). At all these points the TM polarization can not be reflected; therefore the gap closes. In the third band gap there are two additional points $a_3^E$ and $a_3^M$, at $\theta_1=66.3°$, that give $2n_1a\cos\theta_1=n_2b\cos\theta_2$. That is, these points satisfy the first condition for gap closing with $l=2$ and $q=1$. In this particular case the condition states that every gap number $3i$ will have a zero width at this angle, for $i=1,2,3\ldots$.

We observe that for higher-order gaps there are more closing points. If for a given angle there is a closing point, there is an infinite number of closing points at this angle due to the higher gaps.

## IV. SOME SPECIAL CASES

As was mentioned before, for some special cases the $\omega_m^{\pm}$ can be found explicitly. In this section we point out some of these cases.

The simplest solution is obtained if $\gamma=0$ or from (25) if

$$n_1 a\cos\theta_1 = n_2 b\cos\theta_2. \tag{36}$$

Employing Eqs. (27)–(29) we obtain the expression for even-gap edges:

$$\omega_{2s}^{\pm}=\frac{2\pi c s}{\delta},\quad s=1,2,3\ldots, \tag{37}$$

whereas for odd-gap edges

$$\omega_{2s+1}^{\pm}=c\frac{(2s+1)\pi\pm 2\sin^{-1}\sqrt{\frac{B-2}{B}}}{\delta},\quad s=0,1,2,3\ldots. \tag{38}$$

Hence, the width of all even gaps is zero and the width of all odd gaps is constant (independent of $s$) and given by

$$\Delta\omega_{2s+1}=\frac{4c}{\delta}\sin^{-1}\sqrt{\frac{B-2}{B}}. \tag{39}$$

Note that for the normal propagation in a quarter-wave stack, ($k_1a=k_2b=\pi/2$), the condition (36) holds; therefore every even gap in a quarter-wave stack will be closed for $\theta=0$ and the width of odd gaps is given by Eq. (39). The expression for the width of the first gap for a quarter-wave stack is presented also in Refs. 1 and 8 for $\theta=0$, and in Refs. 4 and 5 for arbitrary angles. All these expressions are included in Eq. (39).

A simple expression for the gap edges can also be derived if $\gamma/\delta$ is a rational number. For example if $\gamma=\delta/2$, which corresponds to $n_1a\cos\theta_1=3n_2b\cos\theta_2$, then the even-gap edges are located at

$$\omega_{4s}^{\pm}=\frac{4\pi s}{\delta}c,$$

$$\omega_{4s+2}^{\pm}=c\frac{(4s+2)\pi\pm 2\cos^{-1}[(2+B)/2B]}{\delta}, \tag{40}$$

whereas the odd-gap edges are located at

$$\omega_{4s+1}^{\pm}=c\frac{(4s+1)\pi\pm 2\sin^{-1}d_{\pm}}{\delta},$$

$$\omega_{4s+3}^{\pm}=c\frac{(4s+3)\pi\pm 2\sin^{-1}d_{\pm}}{\delta}, \tag{41}$$

where $d_{\pm}=\pm[B-2\pm\sqrt{(B-2)^2+8B(B-2)}]/4B$, $0<d_{\pm}<\pi/2$. As indicated in the previous section, the width of gaps of order $m=4s$ vanishes for $s=1,2,3\ldots$.

## V. CONCLUSIONS

In this paper we presented a study of one-dimensional band-gap materials using a mathematical formalism based on the analysis of Hill's equation. We derived the exact formula of the gap edge's location for an infinite number of gaps, for both TE and TM polarizations at arbitrary angle of incidence. In addition, the formula for the gap width was derived and the gap closing conditions were given for an infinite number of gaps. We also proved mathematically that the first band gap never closes for TE polarization and has only one closing point for TM polarization, at the Brewster angle.

This simple analysis and the derived expressions may be useful for the design of photonic crystal devices, as well as for the understanding of their properties.

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## APPENDIX A: EXTENSION FOR THE PERIODIC STRUCTURE WITH ARBITRARY NUMBER OF DIFFERENT LAYERS

We consider a periodic structure of $I$ layers per period:

$$n(x)=\begin{cases} n_1, & 0=a_0<x<a_1,\\ n_2, & a_1<x<a_2,\\ \vdots & \\ n_I, & a_{I-1}<x<a_I=L\end{cases} \tag{A1}$$

where $L$ is a the period, namely, $n(x+L)=n(x)$, $n_i$ is the refractive index of the layer number $i$, and $i=1,\ldots,I$. Using the technique explained in Sec. II, we find the same dispersion relation that is obtained for the two-layered structure [see Eq. (1)].

However, for $I$ layers $A$ and $D$ are defined by

$$A=(A_I^{(1)}+k_IB_I^{(2)})\cos(k_Id_I),$$

$$D=(B_I^{(1)}-k_IA_I^{(2)})\sin(k_Id_I), \tag{A2}$$

where $k_i=\sqrt{(n_i\omega/c)^2-k_z^2}=n_i\omega\cos\theta_i/c$, $\theta_i$ is the propagation angle in the layer number $i$, and $d_i$ is the width of the layer number $i$, defined by $d_i=a_i-a_{i-1}$. Note that $a_0=0$ and $a_I=L$. The coefficients $A_I^{(1,2)}$ and $B_I^{(1,2)}$ are found recursively:

$$A_i^{(1,2)} = A_{i-1}^{(1,2)} \cos(k_{i-1}d_{i-1}) + B_{i-1}^{(1,2)} \sin(k_{i-1}d_{i-1}) \quad (\text{TE,TM}),$$

$$B_i^{(1,2)} = -\frac{k_{i-1}}{k_i}[A_{i-1}^{(1,2)} \sin(k_{i-1}d_{i-1}) - B_{i-1}^{(1,2)} \cos(k_{i-1}d_{i-1})] \quad (\text{TE}),$$

$$B_i^{(1,2)} = -\frac{n_i^2 k_{i-1}}{n_{i-1}^2 k_i}[A_{i-1}^{(1,2)} \sin(k_{i-1}d_{i-1}) - B_{i-1}^{(1,2)} \cos(k_{i-1}d_{i-1})] \quad (\text{TM}),$$

$$A_1^{(1)} = 1, \quad B_1^{(2)} = 1/k_1, \quad B_1^{(1)} = A_1^{(2)} = 0 \quad (\text{TE,TM}). \tag{A3}$$

In the same way we obtain the expression for band-gap edges of the gap number $m$

$$\omega_m^{\pm} = \frac{c(m\pi \pm 2r_m^{\pm})}{\sum_{i=1}^{I} \eta_i d_i}, \quad m = 1,2,3 \ldots , \tag{A4}$$

where $\eta_i = n_i \cos \theta_i$. As before, the function $r_m^{\pm}$ is different for even and odd gaps. For even gaps it is found from

$$0 = C_1 \sin^2 r_{2s}^{\pm} + \sum_{j=1}^{I} C_2^j \sin^2\left( \frac{-\eta_j d_j + \sum_{i\neq j}^{I} \eta_i d_i}{\sum_{i=1}^{I} \eta_i d_i}(\pi s \pm r_{2s}^{\pm}) \right) + \sum_{\substack{j,h \\ j\neq h}}^{I} C_3^{jh} \sin^2\left( \frac{-\eta_j d_j - \eta_h d_h + \sum_{i\neq j\neq h}^{I} \eta_i d_i}{\sum_{i=1}^{I} \eta_i d_i}(\pi s \pm r_{2s}^{\pm}) \right) + \cdots + C_{I+1} \sin^2 r_{2s}^{\pm}, \tag{A5}$$

whereas for odd gaps the $r_m^{\pm}$ is found from

$$0 = C_1 \sin^2 r_{2s+1}^{\pm} + \sum_{j=1}^{I} C_2^j \cos^2\left( \frac{-\eta_j d_j + \sum_{i\neq j}^{I} \eta_i d_i}{\sum_{i=1}^{I} \eta_i d_i}(\pi s + \pi/2 \pm r_{2s+1}^{\pm}) \right) + \sum_{\substack{j,h \\ j\neq h}}^{I} C_3^{jh} \cos^2\left( \frac{-\eta_j d_j - \eta_h d_h + \sum_{i\neq j\neq h}^{I} \eta_i d_i}{\sum_{i=1}^{I} \eta_i d_i}(\pi s + \pi/2 \pm r_{2s+1}^{\pm}) \right) + \cdots + C_{I+1} \sin^2 r_{2s+1}^{\pm}, \tag{A6}$$

where

$$C_1 = C_{I+1} = (0.5)^{I-2} + \sum_{\substack{i,p \\ i<p}}^{I} B_{ip} + \sum_{\substack{i,p,l,q \\ i<p<l<q}}^{I} B_{iplq} + \sum_{i<p<l<q<j<n}^{I} B_{ijnlpq} + \cdots ,$$

$$C_2^j = C_I^j = (0.5)^{I-2} + \sum_{\substack{i,p \\ i<p}}^{I} (-1)^{\delta_{ij}}(-1)^{\delta_{pj}} B_{ip} + \sum_{\substack{i,p,l,q \\ i<p<l<q}}^{I} (-1)^{\delta_{ij}}(-1)^{\delta_{pj}}(-1)^{\delta_{lj}}(-1)^{\delta_{qj}} B_{iplq} + \cdots ,$$

$$C_3^{jh} = C_{I-1}^{jh} = (0.5)^{I-2} + \sum_{\substack{i,p \\ i<p}}^{I} (-1)^{\delta_{ij}}(-1)^{\delta_{pj}}(-1)^{\delta_{ih}}(-1)^{\delta_{ph}} B_{ip} + \cdots ,$$

$$\vdots \tag{A7}$$

and

$$\delta_{ij} = \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases} \tag{A8}$$

The constants in (A7) are defined as follows:

$$B_{ij} = \begin{cases} (1/2)^{I-1}(\eta_i/\eta_j + \eta_j/\eta_i) & \text{(TE)}, \\ (1/2)^{I-1}(n_i^2\eta_i/n_j^2\eta_j + n_j^2\eta_j/n_i^2\eta_i) & \text{(TM)}, \end{cases} \tag{A9}$$

$$B_{ij,\ldots,lm} = \begin{cases} (1/2)^{I-1}(\eta_i,\ldots,\eta_l/\eta_j,\ldots,\eta_m + \eta_j,\ldots,\eta_m/\eta_i,\ldots,\eta_l) & \text{(TE)}, \\ (1/2)^{I-1}\left(\dfrac{n_i^2\eta_i}{n_j^2\eta_j}\cdots\dfrac{n_l^2\eta_l}{n_m^2\eta_m} + \dfrac{n_j^2\eta_j}{n_i^2\eta_i}\cdots\dfrac{n_m^2\eta_m}{n_l^2\eta_l}\right) & \text{(TM)}. \end{cases} \tag{A10}$$

## APPENDIX B: DERIVATION OF GAP CLOSING CONDITIONS

We want to find the solution of Eqs. (28) and (29) with the requirement $r_m^{\pm}=0$.

In order that even gaps will vanish

$$0 = \sin(s\pi\gamma/\delta), \quad s = 1,2,\ldots\,. \tag{B1}$$

This equation gives two solutions, namely, $\gamma=0$ and $\gamma/\delta=(q-l)/(q+l)$, where $q$ and $l$ are integers. Using the definitions for $\gamma$ and $\delta$ [Eq. (25)], we obtain the first solution corresponding to condition (32), given in the text with $l=q=1$. The second solution corresponds to condition (32) with $l,q\geqslant 1$.

Next, to find the condition for odd-gap closing, one should solve the equation

$$0 = \cos\frac{\gamma}{\delta}(s\pi + \pi/2), \quad s = 0,1,2,\ldots\,. \tag{B2}$$

The solution is $\gamma/\delta=(q-l)/(q+l)$, where $q+l$ and $q-l$ are both odd. This condition is also equivalent to the first condition (i) of the gap closing.

## APPENDIX C: DERIVATION OF THE BREWSTER ANGLE CONDITION

From Eqs. (28) and (29) we see that an additional condition for $r_m^{\pm}=0$ is $B-2=0$. For the TE mode, the solution of this equation does not exist. For the TM mode, however, this condition gives

$$\frac{k_1}{k_2} = \frac{n_1^2}{n_2^2}. \tag{C1}$$

After setting the expressions for $k_1=n_1\omega\cos\theta_1/c$ and $k_2=n_2\omega\cos\theta_2/c$, we get

$$\frac{\cos\theta_1}{\cos\theta_2} = \frac{n_1}{n_2}. \tag{C2}$$

Applying Snell's law gives $\theta_1+\theta_2=90°$ and therefore $\tan\theta_1=n_2/n_1=\tan\theta_B$.

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