PHYSICAL REVIEW E **69**, 016612 (2004)

Semiclassical coupled-wave theory and its application to TE waves in one-dimensional photonic crystals

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(Received 2 September 2003; published 29 January 2004)

A semiclassical coupled-wave theory is developed for TE waves in one-dimensional periodic structures. The theory is used to calculate the bandwidths and reflection/transmission characteristics of such structures, as functions of the incident wave frequency. The results are in good agreement with exact numerical simulations for an arbitrary angle of incidence and for any achievable refractive index contrast on a period of the structure.

DOI: 10.1103/PhysRevE.69.016612 PACS number(s): 03.50.De, 03.65.Sq, 42.70.Qs

I. INTRODUCTION

Photonic crystals, which are repetitive dielectric structures, have attracted considerable attention during the last 15 years, as they hold promise of applications in photonic devices. The ideal three-dimensional (3D) photonic crystal would exhibit absolute photonic band gaps (forbidden bands) in which the propagation of light is prohibited in any direction. That is, it would behave as an omnidirectional mirror in a specified frequency range. However, to achieve a complete 3D photonic band gap one has to build a perfect 3D dielectric lattice from materials with a refractive index contrast of 2 or more, which is still a challenging technological problem [1].

Fortunately, it has recently been shown [2,3] that a 1D periodic structure with high refractive index contrast can serve as such a photonic crystal. This has sparked another surge of interest in wave propagation through one-dimensional layered periodic structures [4–7]. The common theoretical methods include the Floquet-Bloch approach, coupled-wave theory, and the transfer matrix method. Among these three, the coupled-wave approach offers superior physical insight and moreover gives simple analytical results in limiting cases.

The assumptions of conventional coupled-wave theory [8–10] (which is equally applicable to both 2D slanted gratings, and 1D periodic structures) include neglect of second derivatives of the field amplitudes and retention of just one diffracted wave (in addition to the transmitted wave). As a result, the final system of coupled-wave equations contains only two first-order differential equations which can be solved analytically. Unfortunately, these approximations often lead to obviously incorrect results. This occurs in the case of high refractive index contrast, which is required for a 1D photonic crystal.

Rigorous coupled-wave theory [11,12] allows for the presence of all possible diffracted waves in the cases of 2D or 3D periodic structures, and takes into account the second derivatives of the field amplitudes as well. The resulting system of coupled-wave equations is exact but involves an infinite number of second-order differential equations. In practice, the infinite set must be truncated by discarding the higher-order diffracted waves. The order of the approximate set of equations depends on the required precision of the final result. Therefore, rigorous coupled-wave theory is particularly suitable for numerical calculations. In that sense it is analogous to the Floquet-Bloch approach, while it has the advantage of a clear physical interpretation. One can say that rigorous coupled-wave theory or the Floquet-Bloch approach is better suited for specific calculations than for deriving general properties of wave propagation in periodic structures. Moreover, the rigorous coupled-wave theory is not directly applicable to 1D periodic structures (pure reflection gratings), as the transition of the slant angle from near zero to exactly zero involves a singularity [11].

The transfer matrix method for one-dimensional periodic structures [13,14] is exact and particularly suitable for structures with homogeneous constituent layers. However, the analytical expressions for the widths of forbidden and allowed bands in terms of characteristic physical parameters, such as refractive indices and thicknesses of the constituent layers, are difficult to analyze even for a bilayer period.

In light of the above, a theory that should be analytically as simple as the conventional coupled-wave theory but provide more accurate results in the case of high refractive index contrast (deep gratings) is desirable for the description of wave propagation in 1D photonic crystals. A suitable candidate is a semiclassical version of the Kogelnik coupled-wave theory. This semiclassical coupled-wave theory was initially introduced in [15] for normal incidence in 1D structures and was thoroughly reviewed in [16] for the same case. Other recent efforts to improve the conventional coupled-wave theory in the case of high refractive index contrast include [17–20]. However, in our opinion, the semiclassical version of the coupled-wave theory is a better choice for 1D structures as it provides accurate and relatively simple analytical results for the bandwidths and reflection/transmission characteristics.

The purpose of this paper is twofold. First, we extend the semiclassical coupled wave theory to the case of oblique propagation of TE electromagnetic waves in 1D periodic structures and show the relation between the solutions obtained within the approximations of this theory and Bloch waves. Second, we work out the second approximation of the semiclassical coupled-wave theory, which turns out to be essentially exact for any achievable ratio of the refractive indices of the layers comprising the 1D photonic crystal.

In the following section, this coupled-wave method is developed in terms of two counterpropagating waves, including not only variable amplitudes as in conventional theory, but also variable (geometric-optics) phases. Then we find the relation between the solutions in terms of coupled waves and in terms of Floquet-Bloch functions. This allows us to construct a simple analytical expression for the Bloch phase, which is a key parameter for determination of band structure. These results are illustrated in Sec. III to obtain the widths of forbidden bands and reflection/transmission characteristics of a periodic bilayered dielectric structure for arbitrary angle of incidence and arbitrary ratio of the refractive indices. Another example in that section shows how to apply our theory to a periodic structure with a continuous profile of the refractive index. The conclusions are summarized in Sec. IV.

II. SEMICLASSICAL COUPLED WAVE THEORY

A. Derivation of basic equations

We consider a transparent (no absorption) slab whose normal is the z axis, occupying the region $0<z<L$. The index of refraction $n(z)=n(z+d)$ varies periodically in the z direction, but does not depend on x or y. The dielectric permittivity $\epsilon(z)$ is the square of the refractive index: $\epsilon(z)=n^2(z)$. Monochromatic plane waves with angular frequency ω and vacuum wave number $k=\omega/c$ propagate inside the medium parallel to the xz plane. For TE polarized waves, i.e., for waves with $\mathbf{E}$ perpendicular to the plane of wave propagation,

$$\mathbf{E}=E(z)\hat{\mathbf{e}}_y\exp[i(k\beta x-\omega t)],$$

$$\mathbf{H}=[H_x(z)\hat{\mathbf{e}}_x+H_z(z)\hat{\mathbf{e}}_z]\exp[i(k\beta x-\omega t)]. \tag{1}$$

Maxwell's equations inside the periodic medium reduce to the wave equation

$$\frac{d^2E(z)}{dz^2}+k^2[n^2(z)-\beta^2]E(z)=0, \tag{2}$$

where $k\beta$ is the (constant) x component of the wave vector of modulus $k(z)=\omega n(z)/c$ inside the medium. If a TE polarized wave impinges on the periodic medium from the region $z<0$, then

$$\beta=n_0\sin\theta_0, \tag{3}$$

where n_0 is the refractive index of the region $z<0$ and θ_0 is the angle of incidence measured from the normal.

Equation (2) with an arbitrary periodic function $n(z)$ is the Hill equation. According to Floquet-Lyapunov theory, its general solution can be written as a superposition of two Bloch waves,

$$E(z)=Fp_1(z)\exp(i\alpha z)+Gp_2(z)\exp(-i\alpha z),$$

$$p_{1,2}(z)=p_{1,2}(z+d). \tag{4}$$

The quantity α is a so-called characteristic index that is generally complex ($\alpha=\alpha'+i\alpha''$) and related to the Bloch phase by $\phi=\alpha d$. One can see that the peculiarities of wave propagation through a periodic structure depend mainly on the dispersion relation $\alpha=\alpha(k)$, which is conveniently written in the form of the dispersion equation $\cos\phi(k)$ as a function of k. There are two physically different regions of parameters for our structure. In the first, where $|\cos\phi|<1$, so ϕ is real, the forward Bloch wave $p_1(z)$ propagates without attenuation; these we call allowed bands. In the second, ϕ is complex ($|\cos\phi|>1$), and the forward Bloch wave is exponentially damped, even in the absence of real absorption. Such regions are called forbidden bands. Physically, in the forbidden bands, especially around their centers, the accumulated Fresnel reflection from variations of the refractive index $n(z)$ over the period results in an increase of the amplitude of the backward Bloch wave at the expense of the forward wave, leading to an increase of the reflection probability.

The essence of the semiclassical coupled-wave theory is as follows. It is based on use of the approximation of geometrical optics, which is related to the WKB approach in quantum mechanics. It provides a good approximation when the properties of the medium change slowly over one wavelength. A general solution in the approximation of geometrical optics is a superposition of two waves $A^{\pm}\exp[\pm i\psi(z)]/[n^2(z)-\beta^2]^{1/4}$ [21]. In the semiclassical coupled-wave theory we assume that the amplitudes $A^{\pm}$ depend on z as well. This additional z dependence allows for some small transformation of forward waves into backward waves and vice versa as the waves advance over one period, going beyond the geometrical-optics approximation. Therefore, instead of Bloch waves, we seek a solution of the Hill equation (2) in terms of two counterpropagating waves with slowly varying amplitudes $A^{(\pm)}(z)$ and geometric-optics phases $\pm\psi(z)$, i.e.,

$$E(z)=\frac{A^{(+)}(z)}{[n^2(z)-\beta^2]^{1/4}}\exp[i\psi(z)]+\frac{A^{(-)}(z)}{[n^2(z)-\beta^2]^{1/4}}\times\exp[-i\psi(z)], \tag{5}$$

where

$$\psi(z)=k\int_0^z\sqrt{n^2(z')-\beta^2}dz', \tag{6}$$

and one can see that $\psi(z+d)=\psi(z)+\psi(d)$. For the magnetic field we seek a solution in the form

$$H_x(z)=-[n^2(z)-\beta^2]^{1/4}A^{(+)}(z)\exp[i\psi(z)]+[n^2(z)-\beta^2]^{1/4}A^{(-)}(z)\exp[-i\psi(z)],$$

$$H_z(z)=\frac{\beta A^{(+)}(z)}{[n^2(z)-\beta^2]^{1/4}}\exp[i\psi(z)]+\frac{\beta A^{(-)}(z)}{[n^2(z)-\beta^2]^{1/4}}\times\exp[-i\psi(z)]. \quad (7)$$

After the substitution of expressions (5) and (7), Maxwell's equations, or, equivalently, the wave equation (12), become an identity if the amplitudes $A^{(\pm)}(z)$ satisfy the system

$$\frac{dA^{(+)}(z)}{dz}=S^{(-)}(z)A^{(-)}(z),$$

$$\frac{dA^{(-)}(z)}{dz}=S^{(+)}(z)A^{(+)}(z), \quad (8)$$

where

$$S^{(\pm)}(z)=\frac{n(z)}{2[n^2(z)-\beta^2]}\frac{dn(z)}{dz}\exp[\pm 2i\psi(z)]. \quad (9)$$

The system (8) is exact. Introducing the phase averaged refractive index $n_{av,\beta}=\psi(d)/kd$, i.e.,

$$n_{av,\beta}=\frac{1}{d}\int_0^d\sqrt{n^2(z')-\beta^2}dz', \quad (10)$$

we find that the quantities $S^{(\pm)}(z)\exp(\mp 2ikn_{av,\beta}z)$ are periodic functions that can be Fourier expanded as

$$S^{(\pm)}(z)e^{\mp 2ikn_{av,\beta}z}=\sum_{m=-\infty}^{m=+\infty}s_m^{(\pm)}e^{i2\pi mz/d}. \quad (11)$$

The coefficients $s_m^{(\pm)}$ can be expressed in a form which is particularly suitable for layered periodic structures with piecewise continuous $n(z)$:

$$s_m^{(\pm)}=\frac{1}{2d}\mathrm{P}\int_0^d\frac{n(z)}{n^2(z)-\beta^2}\frac{dn(z)}{dz}\times\exp\left[2i\left(\pm\psi(z)\mp kn_{av,\beta}z-\frac{\pi}{d}mz\right)\right]dz+\frac{1}{4d}\sum_j\ln\left[\frac{n^2(z_j+0)-\beta^2}{n^2(z_j-0)-\beta^2}\right]\times\exp\left[2i\left(\pm\psi(z_j)\mp kn_{av,\beta}z_j-\frac{\pi}{d}mz_j\right)\right]. \quad (12)$$

The P implies a principal value integral, and the sum over $j=1,2,\ldots$ takes into account the contribution to $s_m^{(\pm)}$ of jumps in the refractive index $n(z)$ at the points of discontinuity z_j within the period. If a discontinuity in $n(z)$ occurs at the beginning or at the end of a period, we should take this discontinuity into account only once, say at the beginning of the period. The quantities $n(z_j\pm 0)$ are the limiting values of the refractive index $n(z)$ to the right/left of a point of discontinuity z_j. Physically, the coefficients $s_m^{(\pm)}$ represent the magnitude of coupling between the two counterpropagating waves (5) due to the mth Fourier components of the functions $S^{\pm}(z)$.

We can now average over rapid oscillations to obtain from the exact system (8) an approximate and simpler set of equations. In practice, the main contribution to the exact solutions of Eq. (8) is provided by the slowly varying components of the coefficients $S^{\pm}(z)$. It is reasonable to start the analysis from the so-called Bragg resonances $k_q=\pi q/(n_{av,\beta}d)$, $q=1,2,3,\ldots$, of our periodic structure, which coincide with the centers of the forbidden bands in the zeroth approximation. Now, introducing the detuning δ_q from the qth Bragg resonance

$$kn_{av,\beta}=\frac{\pi}{d}q+\delta_q, \quad -\frac{\pi}{2d}<\delta_{q\neq 1}<\frac{\pi}{2d}, \quad -\frac{\pi}{d}<\delta_1<\frac{\pi}{2d}, \quad (13)$$

we can rewrite Eq. (11) in the form

$$S^{(+)}(z)=\left[s_{-q}^{(+)}+\sum_{m\neq -q}s_m^{(+)}e^{i2\pi(m+q)z/d}\right]e^{2i\delta_q z},$$

$$S^{(-)}(z)=\left[s_q^{(-)}+\sum_{m\neq q}s_m^{(-)}e^{i2\pi(m-q)z/d}\right]e^{-2i\delta_q z}. \quad (14)$$

We see from Eq. (12) that $s_{-m}^{(+)}$ is just the complex conjugate of $s_m^{(-)}$. Therefore, introducing the notation $s_m^{(-)}\equiv s_m$ and a new set of functions $B^{(\pm)}(z)=A^{(\pm)}(z)\exp(\pm i\delta_q z)$, we obtain from the system (8) a new one in the form

$$\frac{dB^{(+)}(z)}{dz}=i\delta_q B^{(+)}(z)+\left[s_q+\sum_{m\neq q}s_m e^{i2\pi(m-q)z/d}\right]B^{(-)}(z),$$

$$\frac{dB^{(-)}(z)}{dz}=-i\delta_q B^{(-)}(z)+\left[s_q^*+\sum_{m\neq q}s_m^* e^{-i2\pi(m-q)z/d}\right]B^{(+)}(z). \quad (15)$$

This system is still exact. If all $s_m d<1$ and $\delta_q d<1$, we can use the method of averaging [22] to obtain an approximate solution. Further, we will find that this method gives reasonable results even in cases where some of the $s_m d>1$ and/or $\delta_q d>1$.

Following Ref. [22], we represent $B^{(\pm)}(z)$ as a superposition of slowly varying terms $\overline{B}^{(\pm)}(z)$ plus a sum of small oscillatory terms:

$$B^{(+)}(z)=\overline{B}^{(+)}(z)+v_1(z)\overline{B}^{(-)}(z)+v_2(z)\overline{B}^{(+)}(z)+\cdots,$$

$$B^{(-)}(z)=\overline{B}^{(-)}+v_1^*(z)\overline{B}^{(+)}(z)+v_2^*(z)\overline{B}^{(-)}(z)+\cdots, \quad (16)$$

where the unknown function $v_1(z)$ is a linear function of small quantities $(s_m d,\ \delta_q d)$ in the system (15), $v_2(z)$ is bilinear, and so on. For the slowly varying terms $\overline{B}^{(\pm)}(z)$ we have a system

$$\frac{d\overline{B}^{(+)}(z)}{dz}=i\delta_q\overline{B}^{(+)}(z)+c_1\overline{B}^{(-)}(z)+c_2\overline{B}^{(+)}(z)+\cdots,$$

$$\frac{d\overline{B}^{(-)}(z)}{dz}=-i\delta_q\overline{B}^{(-)}(z)+c_1^*\overline{B}^{(+)}(z)+c_2^*\overline{B}^{(-)}(z)+\cdots, \tag{17}$$

where the unknown coefficient c_1 is a linear function of small quantities $s_m d$ and $\delta_q d$, the unknown coefficient c_2 is a bilinear function, and so on. Substituting the solution (16) into Eq. (15) and taking into account Eq. (17), we obtain (for the details see the Appendix)

$$c_1=s_q, \quad c_2=\frac{id}{2\pi}\sum_{m\neq q}\frac{|s_m|^2}{m-q-\delta_q d/\pi}, \tag{18}$$

and

$$v_1(z)=-\frac{id}{2\pi}\sum_{m\neq q}\frac{s_m e^{i2\pi(m-q)z/d}}{m-q-\delta_q d/\pi}. \tag{19}$$

In the first approximation of small $s_m d$ and $\delta_q d$, the functions $B^{(\pm)}(z)$ are replaced by slowly varying terms $\overline{B}^{(\pm)}(z)$, which can be found from the system obtained by averaging Eqs. (15) over one period:

$$\frac{d\overline{B}^{(+)}(z)}{dz}=i\delta_q\overline{B}^{(+)}(z)+s_q\overline{B}^{(-)}(z),$$

$$\frac{d\overline{B}^{(-)}(z)}{dz}=-i\delta_q\overline{B}^{(-)}(z)+s_q^*\overline{B}^{(+)}(z). \tag{20}$$

Therefore, the functions $B^{(\pm)}(z)$ in the first approximation have the form

$$B_1^{(+)}(z)=(\gamma_1-i\delta_q)Fe^{-\gamma_1 z}+s_qGe^{\gamma_1 z},$$

$$B_1^{(-)}(z)=(-s_q^*)Fe^{-\gamma_1 z}+G(\gamma_1-i\delta_q)Ge^{\gamma_1 z}, \tag{21}$$

where F and G are constants that depend on the boundary conditions, and

$$\gamma_1(k)=\sqrt{|s_q(k)|^2-\delta_q^2}. \tag{22}$$

The second approximation to the functions $B^{(\pm)}(z)$ takes into account not only the slowly varying terms $\overline{B}^{(\pm)}(z)$ but also the first oscillatory terms $v_1(z)\overline{B}^{(\pm)}(z)$ [see Eq. (16)]; and the slowly varying terms $\overline{B}^{(\pm)}(z)$ themselves should be calculated in the second approximation, i.e., from the system

$$\frac{d\overline{B}^{(+)}(z)}{dz}=i\delta_q\overline{B}^{(+)}(z)+s_q\overline{B}^{(-)}(z)+c_2\overline{B}^{(+)}(z),$$

$$\frac{d\overline{B}^{(-)}(z)}{dz}=-i\delta_q\overline{B}^{(-)}(z)+s_q^*\overline{B}^{(+)(z)}(z)+c_2^*\overline{B}^{(-)}(z), \tag{23}$$

rather than from the system (20). Therefore, the final expressions for the functions $B^{(\pm)}(z)$ in the second approximation take the form

$$B_2^{(+)}(z)=[(\gamma_2-i\eta_q)-s_q^*v_1(z)]Fe^{-\gamma_2 z}+[s_q+(\gamma_2-i\eta_q)v_1(z)]Ge^{\gamma_2 z},$$

$$B_2^{(-)}(z)=[-s_q^*+(\gamma_2-i\eta_q)v_1^*(z)]Fe^{-\gamma_2 z}+[(\gamma_2-i\eta_q)+s_qv_1^*(z)]Ge^{\gamma_2 z} \tag{24}$$

with

$$\gamma_2(k)=\sqrt{|s_q(k)|^2-\eta_q^2}, \tag{25}$$

where $\eta_q=\delta_q-ic_2$ is a real number.

We can now write the final expressions for the electric field in terms of two counterpropagating waves (5) inside the periodic structure in the first and second approximations as

$$E^{(1)}(z)=\frac{F(\gamma_1-i\delta_q)e^{-\gamma_1 z}+Gs_qe^{\gamma_1 z}}{(n^2(z)-\beta^2)^{1/4}}e^{i[\psi(z)-\delta_q z]}+\frac{F(-s_q^*)e^{-\gamma_1 z}+G(\gamma_1-i\delta_q)e^{\gamma_1 z}}{(n^2(z)-\beta^2)^{1/4}}e^{-i[\psi(z)-\delta_q z]} \tag{26}$$

and

$$E^{(2)}(z)=\frac{F[(\gamma_2-i\eta_q)-s_q^*v_1(z)]e^{-\gamma_2 z}+G[s_q+(\gamma_2-i\eta_q)v_1(z)]e^{\gamma_2 z}}{(n^2(z)-\beta^2)^{1/4}}e^{i[\psi(z)-\delta_q z]}+\frac{F[-s_q^*+(\gamma_2-i\eta_q)v_1^*(z)]e^{-\gamma_2 z}+G[\gamma_2-i\eta_q+s_qv_1^*(z)]e^{\gamma_2 z}}{(n^2(z)-\beta^2)^{1/4}}e^{-i[\psi(z)-\delta_q z]}, \tag{27}$$

or in terms of two Bloch waves (4) as

$$E^{(1)}(z)=F\frac{(\gamma_1-i\delta_q)e^{i[\psi(z)-\delta_q z]}-s_q^*e^{-i[\psi(z)-\delta_q z]}}{[n^2(z)-\beta^2]^{1/4}}e^{-\gamma_1 z}+G\frac{s_qe^{i[\psi(z)-\delta_q z]}+(\gamma_1-i\delta_q)e^{-i[\psi(z)-\delta_q z]}}{[n^2(z)-\beta^2]^{1/4}}e^{\gamma_1 z} \tag{28}$$

and

$$E^{(2)}(z)=F\frac{[\gamma_2-i\eta_q-s_q^*v_1(z)]e^{i[\psi(z)-\delta_q z]}-[s_q^*-(\gamma_2-i\eta_q)v_1^*(z)]e^{-i[\psi(z)-\delta_q z]}}{(n^2(z)-\beta^2)^{1/4}}e^{-\gamma_2 z}$$
$$+G\frac{[s_q+(\gamma_2-i\eta_q)v_1(z)]e^{i[\psi(z)-\delta_q z]}+[\gamma_2-i\eta_q+s_q v_1^*(z)]e^{-i[\psi(z)-\delta_q z]}}{[n^2(z)-\beta^2]^{1/4}}e^{\gamma_2 z}. \qquad (29)$$

From the expressions (28) and (29), we easily obtain that in each zone along the k axis $\pi(-\frac{1}{2}+q)/(n_{av,\beta}d)<k<\pi(\frac{1}{2}+q)/(n_{av,\beta}d)$ [see Eq. (13)] the characteristic index α and the Bloch phase ϕ in the first and second approximations take the forms

$$\alpha_{1,2}=\frac{\pi}{d}q+i\gamma_{1,2}, \quad \phi_{1,2}=\pi q+i\gamma_{1,2}d. \qquad (30)$$

In forbidden bands, where $|s_q|>|\delta_q|$ (first approximation) or $|s_q|>|\eta_q|$ (second approximation), $\gamma_{1,2}$ is a real positive number. In allowed bands, where $|s_q|<|\delta_q|$ (first approximation) or $|s_q|<|\eta_q|$ (second approximation) $\gamma_{1,2}$ is a purely imaginary number: $\gamma_1=i|\gamma_1|$ if $\delta_q<0$ and $\gamma_1=-i|\gamma_1|$ if $\delta_q>0$; $\gamma_2=i|\gamma_2|$ if $\eta_q<0$ and $\gamma_2=-i|\gamma_2|$ if $\eta_q>0$.

In the first approximation, according to Eqs. (22) and (13), the right k_R and left k_L boundaries of the forbidden band with the center $k_q=\pi q/(n_{av,\beta}d)$ can be found from the equations

$$k_R n_{av,\beta}-\pi q/d=|s_q(k_R)|,$$
$$\pi q/d-k_L n_{av,\beta}=|s_q(k_L)|. \qquad (31)$$

Adding these two equations, we obtain the width of the forbidden band to be

$$w_q=\frac{|s_q(k_R)|+|s_q(k_L)|}{n_{av,\beta}}\approx 2\frac{|s_q(k_q)|}{n_{av,\beta}}, \qquad (32)$$

where $s_q(k_q)$ is the coupling coefficient at the Bragg resonance. We will see from the figures that this is a very accurate approximation.

B. Reflection and transmission

First, we calculate the reflection and transmission coefficients for a wave incident on a matched periodic structure. By matched, we mean that the refractive index is continuous across the exterior boundaries at $z=0$ and $z=L$, i.e., there is no Fresnel reflection from them. As a result, reflection by the entire system $0<z<L$ is determined only by Bragg reflection from the periodic structure itself.

Equation (5) represents a solution of the Hill equation (1) in terms of right- and left-moving components. Therefore, the amplitude Bragg reflection and transmission coefficients for a wave incident on the structure from the left, i.e., from the region $z<0$, can be found from the expressions

$$r_B=\frac{A^{(-)}(0)}{[n^2(0)-\beta^2]^{1/4}}\exp[-i\psi(0)],$$

$$t_B=\frac{A^{(+)}(L)}{[n^2(L)-\beta^2]^{1/4}}\exp[i\psi(L)], \qquad (33)$$

under the conditions

$$\frac{A^{(+)}(0)}{[n^2(0)-\beta^2]^{1/4}}\exp[i\psi(0)]=1,$$

$$\frac{A^{(-)}(L)}{[n^2(L)-\beta^2]^{1/4}}\exp[-i\psi(L)]=0. \qquad (34)$$

The first relation in Eq. (34) is just a normalization condition, while the second expresses the radiation principle: no propagation of a left-moving wave in the region $z>L$. From these conditions we can find the constants F and G to be substituted into expressions (33) for the reflection and transmission amplitudes. The final results in the first and second approximations are

$$r_B^{(1)}=\frac{-s_q^*\sinh(\gamma_1 L)}{\gamma_1\cosh(\gamma_1 L)-i\delta_q\sinh(\gamma_1 L)},$$

$$t_B^{(1)}=\frac{\gamma_1 e^{i\pi Nq}}{\gamma_1\cosh(\gamma_1 L)-i\delta_q\sinh(\gamma_1 L)}, \qquad (35)$$

$$r_B^{(2)}=\frac{(-s_q^*-2i\,\eta_q u^*+s_q u^{*2})\sinh(\gamma_2 L)}{(1-|u|^2)\gamma_2\cosh(\gamma_2 L)-i[(1+|u|^2)\eta_q-2\,\mathrm{Im}(s_q u^*)]\sinh(\gamma_2 L)},$$

$$t_B^{(2)}=\frac{(1-|u|^2)\gamma_2 e^{i\pi Nq}}{(1-|u|^2)\gamma_2\cosh(\gamma_2 L)-i[(1+|u|^2)\eta_q-2\,\mathrm{Im}(s_q u^*)]\sinh(\gamma_2 L)},\qquad(36)$$

where $u=v_1(0)$.

As we have already mentioned, $\gamma_{1,2}$ is real and positive in forbidden bands and becomes a purely imaginary number in allowed bands. Therefore, for reflection and transmission in allowed bands it is more natural to use the expressions in terms of the characteristic index $\alpha_{1,2}$, which is a real number in these bands. These expressions follow immediately from Eqs. (35) and (36), if we take into account Eq. (30):

$$r_B^{(1)}=\frac{-s_q^*\sin(\alpha_1 L)}{(\alpha_1-\pi q/d)\cos(\alpha_1 L)-i\,\delta_q\sin(\alpha_1 L)},$$

$$t_B^{(1)}=\frac{(\alpha_1-\pi q/d)e^{i\pi Nq}}{(\alpha_1-\pi q/d)\cos(\alpha_1 L)-i\,\delta_q\sin(\alpha_1 L)},\qquad(37)$$

$$r_B^{(2)}=\frac{(-s_q^*-2i\,\eta_q u^*+s_q u^{*2})\sin(\alpha_2 L)}{(1-|u|^2)(\alpha_2-\pi q/d)\cos(\alpha_2 L)-i[(1+|u|^2)\eta_q-2\,\mathrm{Im}(s_q u^*)]\sin(\alpha_2 L)},$$

$$t_B^{(2)}=\frac{(1-|u|^2)(\alpha_2-\pi q/d)e^{i\pi Nq}}{(1-|u|^2)(\alpha_2-\pi q/d)\cos(\alpha_2 L)-i[(1+|u|^2)\eta_q-2\,\mathrm{Im}(s_q u^*)]\sin(\alpha_2 L)}.\qquad(38)$$

For an arbitrary (nonmatched) periodic structure, the field $E(z)$ of a TE polarized wave (1) in the region outside the periodic structure takes the form

$$E(z)=e^{ik\sqrt{n_0^2-\beta^2}z}+r_\Sigma e^{-ik\sqrt{n_0^2-\beta^2}z},\quad z<0,$$

$$E(z)=t_\Sigma e^{ik\sqrt{n_s^2-\beta^2}(z-L)},\quad z>L,\qquad(39)$$

where n_s is the refractive index of the region $z>L$. Then, the amplitude reflection r_Σ and transmission t_Σ coefficients of an arbitrary (nonmatched) periodic structure can be found from the matrix equation

$$\begin{pmatrix}1\\ r_\Sigma\end{pmatrix}=\begin{pmatrix}1/t_0 & r_0/t_0\\ r_0/t_0 & 1/t_0\end{pmatrix}\begin{pmatrix}1/t_B & r_B^*/t_B^*\\ r_B/t_B & 1/t_B^*\end{pmatrix}\begin{pmatrix}1/t_s & r_s/t_s\\ r_s/t_s & 1/t_s\end{pmatrix}\times\begin{pmatrix}t_\Sigma\\ 0\end{pmatrix},\qquad(40)$$

where the Fresnel coefficients

$$r_0=\frac{\sqrt{n_0^2-\beta^2}-\sqrt{[n(0)]^2-\beta^2}}{\sqrt{n_0^2-\beta^2}+\sqrt{[n(0)]^2-\beta^2}},$$

$$t_0=\frac{2\sqrt{n_0^2-\beta^2}}{\sqrt{n_0^2-\beta^2}+\sqrt{[n(0)]^2-\beta^2}},$$

$$r_s=\frac{\sqrt{[n(L)]^2-\beta^2}-\sqrt{n_s^2-\beta^2}}{\sqrt{[n(L)]^2-\beta^2}+\sqrt{n_s^2-\beta^2}},$$

$$t_s=\frac{2\sqrt{[n(L)]^2-\beta^2}}{\sqrt{[n(L)]^2-\beta^2}+\sqrt{n_s^2-\beta^2}}\qquad(41)$$

are responsible for the reflection and transmission on the boundaries of the structure. In these formulas $n(0)$ and $n(L)$ are the refractive indices of our periodic structure at the points $z=0$ and $z=L$.

The expressions (35) and (37) for the reflection and transmission coefficients in the first approximation of the semiclassical coupled-wave theory have the same form as those in the conventional coupled-wave theory [9,10,16], if we take into account the fact that the coupling coefficient $s_m^{(-)}\equiv s_m$ of the semiclassical theory plays the same role as the coupling coefficient is_m^{con} of the conventional theory and $s_{-m}^{(+)}\equiv s_m^*$ plays the same role as $-is_{-m}^{con}$. However, the semiclassical theory even in the first approximation differs from the conventional one in several respects. First, the positions of the Bragg resonances are different: $k_q n_{av,\beta}d=\pi q$ (semiclassical) and $k_q\sqrt{\varepsilon_{av}-\beta^2}d=\pi q$ (conventional). This leads to a more accurate determination of the centers of the forbidden bands k_q and, as a result, to a more accurate estimation of the detuning δ_q.

Second, the magnitudes of the coupling coefficients $s_{\mp m}^{(\pm)}$ in the semiclassical theory are determined by expression (12) rather than by $s_{\pm m}^{con}=k\varepsilon_{\pm m}/(2\sqrt{\varepsilon_{av}-\beta^2})$ as in the conven-

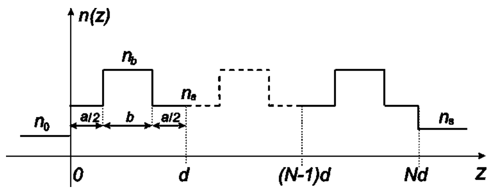

FIG. 1. Two-layered periodic dielectric structure (bilayer photonic crystal).

tional theory. [Here ε_{av} is the average value of the dielectric permittivity $\varepsilon(z)$ over the period of the structure and ε_m($m=1,2,\ldots$) is the mth Fourier harmonic of this function.] As a result, the coupling coefficients $s^{(\pm)}_{\mp m}$ of the semiclassical theory take into account multiwave diffraction by periodic inhomogeneities of $\varepsilon(z)$ because this periodically modulated function makes its appearance under the integral sign in the expression (12), $\varepsilon(z)=n^2(z)$. This is the key point of departure of our semiclassical theory from the conventional (Kogelnik) one, where only one diffracted wave $\exp(-ik\sqrt{\varepsilon_{av}-\beta^2}z)$ [in addition to the transmitted wave $\exp(ik\sqrt{\varepsilon_{av}-\beta^2}z)$] was assumed to exist within the periodic structure.

Finally, the initial approximations of the conventional coupled-wave theory include neglecting boundary diffraction, i.e., it is assumed that $\varepsilon_0\approx\varepsilon_{av}\approx\varepsilon_s$, where $\varepsilon_0=n_0^2$ and $\varepsilon_s=n_s^2$. To calculate the reflection and transmission in other cases we need to use Eq. (40) with $\sqrt{\varepsilon_{av}}$ instead of $n(L)$ and $n(0)$ in Eq. (41).

As we shall see in the next section, all these drawbacks of the conventional coupled-wave theory lead to obviously incorrect results in cases where the first approximation of our semiclassical theory already gives reasonable results. The second approximation of the semiclassical theory will give us a good agreement (within 10%) with exact numerical results even in the most unfavorable situations.

III. SOME APPLICATIONS OF THE MODIFIED THEORY

A. Bilayer photonic crystal

To illustrate the semiclassical coupled-wave theory, we consider a two-layered periodic medium with real refractive indices n_a and n_b and layer thicknesses a and b such that $d=a+b$, as shown in Fig. 1. From the results of the previous section, for such a structure we have

$$n_{av,\beta}=\frac{n_{a\beta}a+n_{b\beta}b}{d},$$

$$s_m d=i\ln\left(\frac{n_{b\beta}}{n_{a\beta}}\right)e^{-i\pi m}\sin\left(\frac{b}{d}[\pi m+ka(n_{b\beta}-n_{a\beta})]\right), \tag{42}$$

where $n_{a,b\beta}=\sqrt{n_{a,b}^2-\beta^2}$ are the effective refractive indices of the layers n_a and n_b. As a result, at a given angle of incidence θ_0 ($\beta=n_0\sin\theta_0$) the relative width of the forbidden band around the Bragg resonance at k_q in the first approximation can be expressed as

$$\frac{w_q}{k_q}=\frac{2}{\pi q}\left|\ln\left(\frac{n_{b\beta}}{n_{a\beta}}\right)\sin\left(\frac{\pi q}{1+n_{a\beta}a/n_{b\beta}b}\right)\right|. \tag{43}$$

From the transfer matrix method the relative width of the same forbidden band can be obtained only numerically (albeit accurately) by solving the well-known exact dispersion relation

$$\cos\phi=\cos(kn_{a\beta}a)\cos(kn_{b\beta}b)-\frac{n_{a\beta}^2+n_{b\beta}^2}{2n_{a\beta}n_{b\beta}}\sin(kn_{a\beta}a)\sin(kn_{b\beta}b) \tag{44}$$

for $|\cos\phi|>1$ (the Bloch phase ϕ is complex in forbidden bands).

In Fig. 2 we show the reflection coefficient for a two-layered periodic structure of $N=8$ periods whose layers have refractive indices $n_a=2.0$ and $n_b=1.5$ and thicknesses $a=100$ nm and $b=250$ nm. The structure is surrounded by a homogeneous medium with refractive index $n_0=n_s\approx\sqrt{\varepsilon_{av}}=\sqrt{(n_a^2a+n_b^2b)/d}$. A TE polarized plane monochromatic wave impinges on the structure at angle $\theta_0=10°$. We see that for this set of parameters all three approaches are in good agreement with the results of exact numerical calculations.

In Fig. 3 we consider a more demanding situation: a bilayer photonic crystal of $N=4$ periods whose layers have refractive indices $n_a=1.34$ (Na_3AlF_6) and $n_b=2.6$ (ZnSe) and thicknesses $a=b=90$ nm, placed on a substrate with $n_s=n_a=1.34$. These parameters correspond to those in an experiment of Chigrin *et al.* [3]. A TE polarized plane monochromatic wave impinges on the crystal from the air $n_0=1$ at angle $\theta_0=45°$. We see that conventional coupled-wave theory fails completely in the second zone along the k axis, $\frac{3}{2}\pi/(n_{av}d)<k<\frac{5}{2}\pi/(n_{av}d)$, while the first and especially the second approximation of the semiclassical theory work well for all frequencies of the incoming waves.

In Fig. 4 we further increase the refractive index contrast, with a bilayer photonic crystal of $N=4$ periods whose layers have refractive indices $n_a=4.6$ (tellurium) and $n_b=1.6$ (polystyrene) and thicknesses $a=800$ nm and $b=1650$ nm, placed on a substrate with $n_s=n_a=4.6$. These parameters correspond to those in an experiment of Fink *et al.* [2]. A TE polarized monochromatic plane wave impinges on the crystal from the air $n_0=1$ at angle $\theta_0=80°$. Here, only the second approximation of the semiclassical coupled-wave theory is in good agreement with the exact numerical calculations over the entire frequency range. However, the first approximation gives reasonable results within the forbidden bands. Therefore, formula (43) for the widths of forbidden bands remains a good approximation.

The above figures illustrate the fact that conventional coupled-wave theory gives reasonable results only for small angles and small modulation depths ($\delta n=n_b-n_a\approx0.5$) (see Fig. 1). The first approximation of the semiclassical coupled-wave theory works well in forbidden bands for a broad range of incident angles and modulation depths, but it fails in allowed bands for high angles and large modulation depths ($\delta n\approx2.0,\ldots,3.0$) (see Fig. 4). The second approxima-

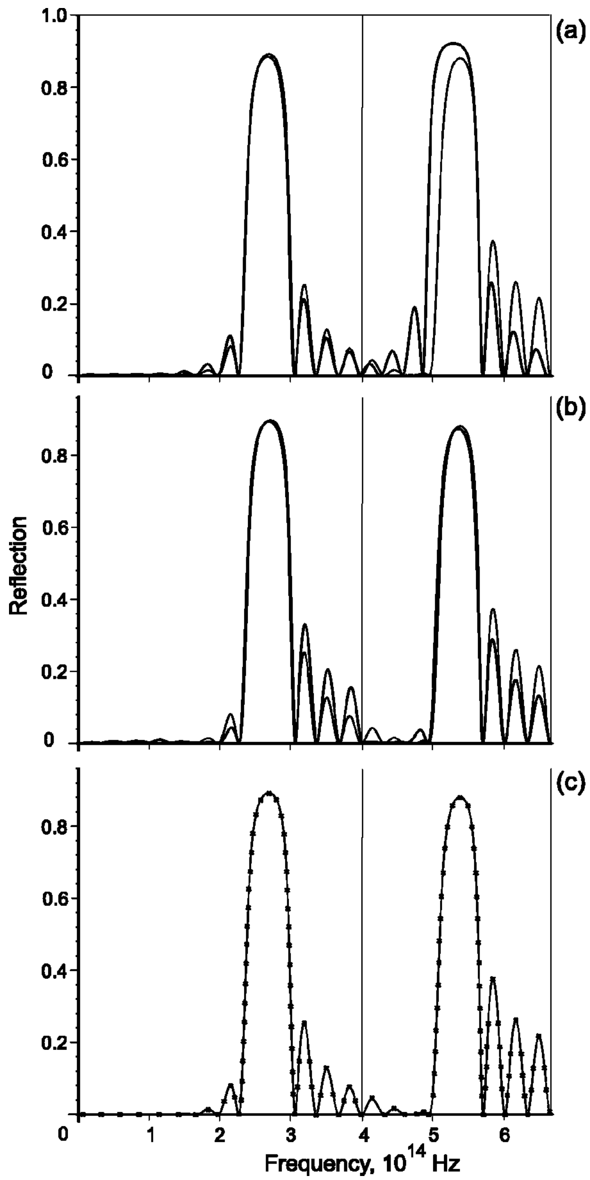

FIG. 2. Reflection vs frequency for a small angle of incidence in the first two zones along the k axis, $0<k<5\pi/2(n_{av,\beta}d)$, of the two-layered periodic structure with small refractive index modulation. The parameters of the structure are as described in text. (a) Conventional coupled-wave theory (thick solid line); (b) first approximation of the semiclassical theory (thick solid line); (c) second approximation of the semiclassical theory (squares). The exact numerical results are shown in all cases by a thin line.

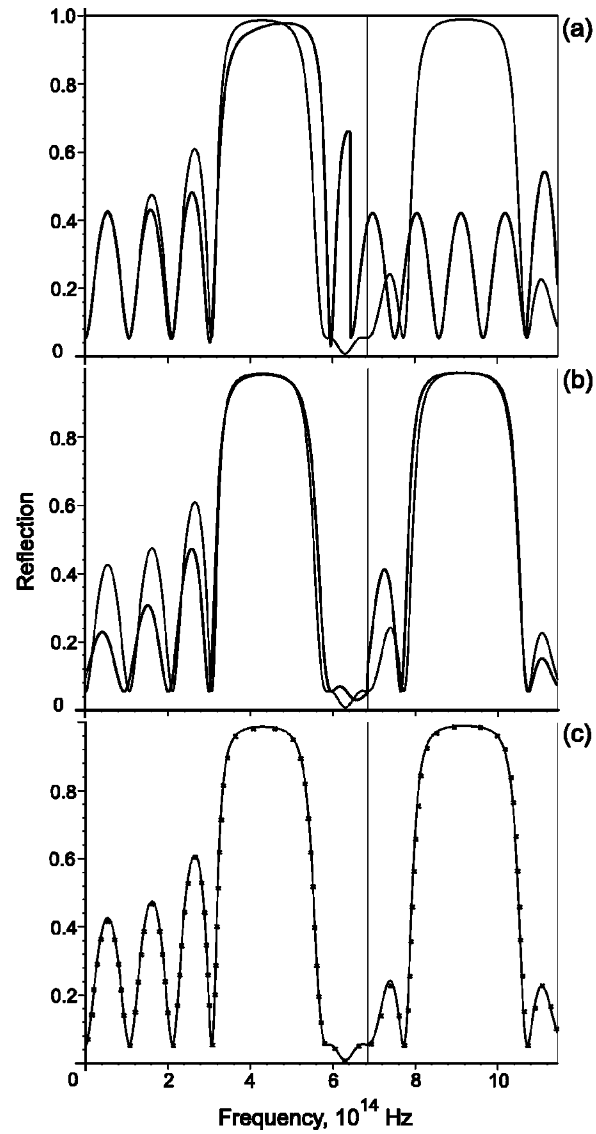

FIG. 3. Reflection vs frequency for a moderate angle of incidence in the first two zones along the k axis, $0<k<5\pi/2(n_{av,\beta}d)$, of the bilayer photonic crystal with moderate refractive index modulation. The parameters of the structure are as described in the text. The lines are as in Fig. 2.

tion developed in this paper is essentially exact for any practically achievable modulation depth and angle of incidence.

B. Periodic structure with triangular profile of refractive index

As a second application of our theory, we consider a periodic structure with a (symmetric) triangular refractive index profile. As sketched in Fig. 5, the index of refraction increases linearly from n_a to n_b along the first half of the period d, and then returns to n_a. An electromagnetic wave is normally ($\theta_0=0°$) incident upon the structure from the region $z<0$. In the case of normal incidence, light polarization does not play a role, and the results given below are valid for TM as well as TE waves. In accordance with Eqs. (10) and (12), for such a structure we have

$$n_{av}=\frac{n_a+n_b}{2},$$

$$s_m d=\frac{I_1+I_2}{2}, \tag{45}$$

where

$$I_1=\int_0^{d/2}\frac{e^{i[k(n_b-n_a)(d-2z)-2\pi m]z/d}}{z+n_a d/[2(n_b-n_a)]}dz,$$

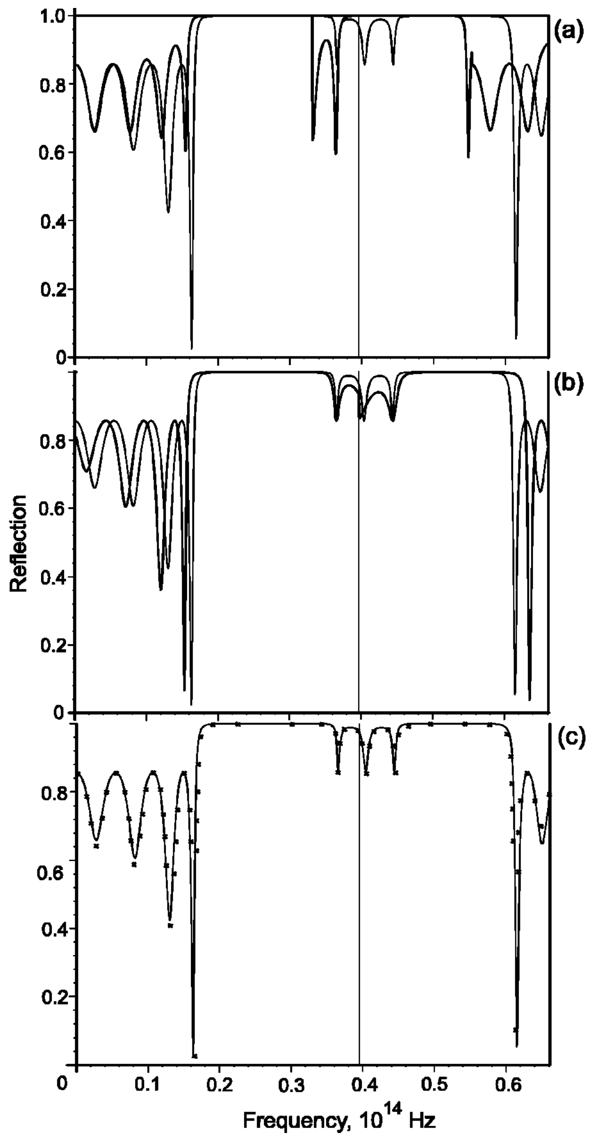

FIG. 4. Reflection vs frequency for a large angle of incidence in the first two zones along the k axis, $0<k<5\pi/2(n_{av,\beta}d)$, of the bilayer photonic crystal with large refractive index modulation. The parameters of the structure are as described in text. The lines are as in Fig. 2.

$$I_2=e^{-i\pi m}\int_0^{d/2}\frac{e^{i[k(n_a-n_b)(d-2z)-2\pi m]z/d}}{z+n_b d/[2(n_a-n_b)]}\,dz. \tag{46}$$

To illustrate the advantages of our theory, we take a structure of $N=5$ periods with a huge modulation depth $n_a=1.3$ and $n_b=4.8$, on a period of $d=500$ nm, surrounded by a homogeneous medium with refractive index $n_0=n_s=1$. In Fig. 6 we see that, as before, only the second approximation of the semiclassical coupled-wave theory is in good agreement with exact numerical calculations over the entire frequency range.

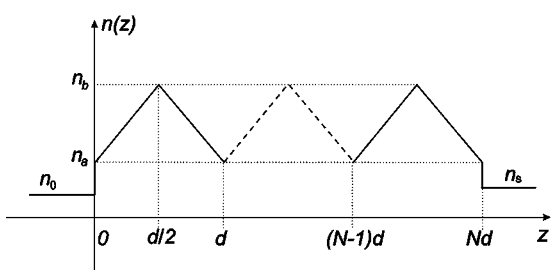

FIG. 5. Periodic dielectric structure with triangular profile of the refractive index.

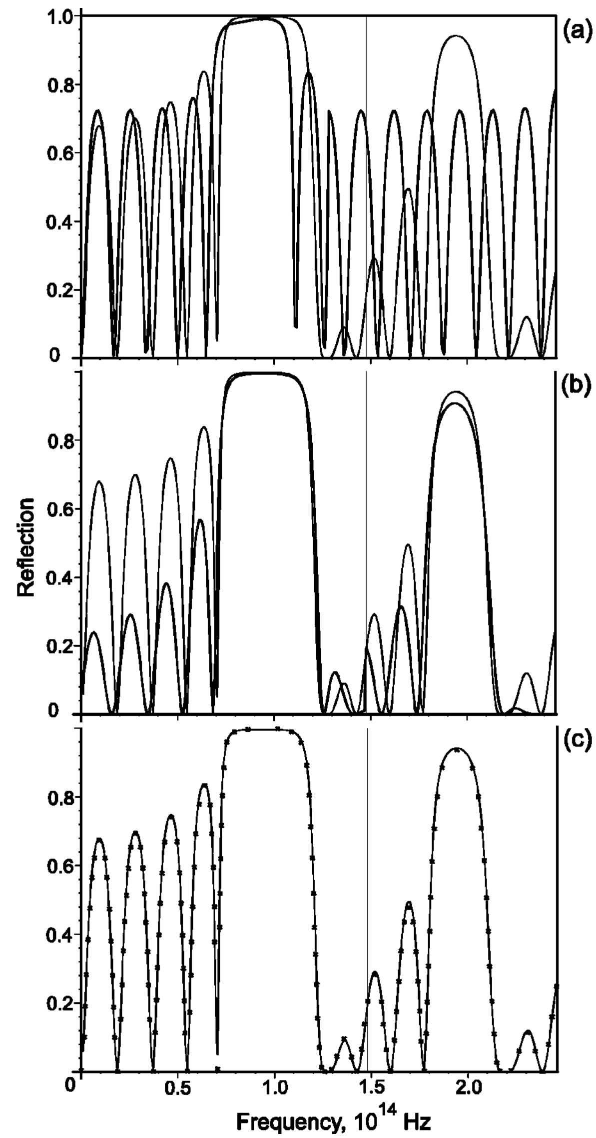

FIG. 6. Reflection vs frequency for normal incidence in the first two zones along the k axis, $0<k<5\pi/2(n_{av,\beta}d)$, of the dielectric periodic structure with a symmetric triangular profile of the refractive index with large modulation. The parameters of the structure are as described in the text. The lines are as in the Fig. 2.

IV. CONCLUSIONS

The semiclassical coupled-wave theory has been extended to the case of oblique incidence for TE waves. The theory was also extended to second order; it turns out to be essentially exact for any achievable refractive index contrast in 1D photonic crystals. Expressions for the reflection and transmission coefficients as well as for the bandwidths in the first and second approximations were obtained for one-dimensional finite periodic structures. The analytical relation between solutions in terms of Bloch waves and in terms of semiclassical coupled waves has been established. Applications to two types of cells illustrate how the theory can be used.

The theory presented here provides a convenient way to derive analytic solutions for waves propagating in one-dimensional periodic structures, solutions that are both relatively simple and essentially exact. The remaining task is to extend the work to the case of TM waves.

ACKNOWLEDGMENTS

We are grateful to NSERC-Canada for Discovery Grant No. SAPIN-3198 (D.W.L.S. and G.V.M.) and to DGES-Spain for continued support through Grant No. BFM2001-3710 (J.M.). This work was carried out as part of CERION-2, EU thematic network IST-2001-39059.

APPENDIX: DERIVATION OF THE SECOND APPROXIMATION

As was stated in the main text, in accordance with the method of averaging (see Ref. [22]), we seek a solution of the exact system (15), as a superposition of slowly varying terms $\overline{B}^{(\pm)}(z)$ plus a sum of small oscillatory terms (16). Further, according to this method, there is a simpler system (17) for the slowly varying terms only.

Let us substitute the solutions (16) into the system (15). This gives

$$\begin{aligned}\frac{d\overline{B}^{(+)}}{dz}+\frac{dv_1}{dz}\overline{B}^{(-)}+v_1\frac{d\overline{B}^{(-)}}{dz}+\frac{dv_2}{dz}\overline{B}^{(+)}+v_2\frac{d\overline{B}^{(+)}}{dz}+\cdots\\=i\delta_q(\overline{B}^{(+)}+v_1\overline{B}^{(-)}+v_2\overline{B}^{(+)}+\cdots)\\+\sum_m s_m e^{i2\pi(m-q)z/d}(\overline{B}^{(-)}+v_1^*\overline{B}^{(+)}+\cdots),\end{aligned}$$

$$\begin{aligned}\frac{d\overline{B}^{(-)}}{dz}+\frac{dv_1^*}{dz}\overline{B}^{(+)}+v_1^*\frac{d\overline{B}^{(+)}}{dz}+\frac{dv_2^*}{dz}\overline{B}^{(-)}+v_2^*\frac{d\overline{B}^{(-)}}{dz}+\cdots\\=-i\delta_q(\overline{B}^{(-)}+v_1^*\overline{B}^{(+)}+v_2^*\overline{B}^{(-)}+\cdots)\\+\sum_m s_m^* e^{-i2\pi(m-q)z/d}(\overline{B}^{(+)}+v_1\overline{B}^{(-)}+\cdots).\end{aligned} \tag{A1}$$

Corresponding expressions for $d\overline{B}^{(+)}/dz$ and $d\overline{B}^{(-)}/dz$ can be taken from the system (17). Then, after some algebra, the relations (A1) take the form

$$\begin{aligned}&\left(c_1+\frac{dv_1(z)}{dz}-2i\delta_q v_1(z)\right)\overline{B}^{(-)}(z)\\&\quad+\left(c_2+\frac{dv_2(z)}{dz}+c_1^*v_1(z)\right)\overline{B}^{(+)}(z)+\cdots\\&\quad=\left(s_q+\sum_{m\neq q}s_m e^{i2\pi(m-q)z/d}\right)\\&\qquad\times[\overline{B}^{(-)}(z)+v_1^*(z)\overline{B}^{(+)}(z)+\cdots],\end{aligned}$$

$$\begin{aligned}&\left(c_1^*+\frac{dv_1^*(z)}{dz}+2i\delta_q v_1^*(z)\right)\overline{B}^{(+)}(z)\\&\quad+\left(c_2^*+\frac{dv_2^*(z)}{dz}+c_1v_1^*(z)\right)\overline{B}^{(-)}(z)+\cdots\\&\quad=\left(s_q^*+\sum_{m\neq q}s_m^* e^{-i2\pi(m-q)z/d}\right)\\&\qquad\times[\overline{B}^{(+)}(z)+v_1(z)\overline{B}^{(-)}(z)+\cdots].\end{aligned} \tag{A2}$$

Extracting from this system those terms which are linear in the small quantities $s_m d$ and $\delta_q d$, we obtain

$$c_1+\frac{dv_1}{dz}-2i\delta_q v_1(z)=s_q+\sum_{m\neq q}s_m e^{i2\pi(m-q)z/d},$$

$$c_1^*+\frac{dv_1^*}{dz}+2i\delta_q v_1^*(z)=s_q^*+\sum_{m\neq q}s_m^* e^{-i2\pi(m-q)z/d}. \tag{A3}$$

The coefficient c_1 does not depend on z. Therefore, the first of the relations (18) and the relation (19) follow immediately from Eq. (A3). Similarly, extracting the terms that are bilinear in the small quantities $s_m d$ and $\delta_q d$, and taking into account the fact that the coefficient c_2 also does not depend on z, we obtain the second of the relations (18).

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