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DIRECT CHARACTERIZATION OF STATES AND MODES IN DEFECT GRATING STRUCTURES

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For one-dimensional optical structures consisting of gratings surrounding a defect region, optical field solutions inside the bandgap are investigated that are steady states or fully transmitted modes. The observation that a mode is a suitable combination of two states, and that each state is a resonant phenomenon, implies that an accidental degeneracy condition has to be satisfied in order that two states occur at the same frequency. Finding the conditions, and thereby the required design-parameters of the structure, makes it possible to characterize the modes without the necessity to scan the whole bandgap for transmission properties. The mathematical formulation is based on the optical transfer map and leads to a non-standard, not well-studied, eigenvalue problem on the defect region with effective boundary conditions that simulate the surrounding gratings.

Keywords: Optical defect grating structures; bandgap states and modes; optical transfer map; non-standard eigenvalue problem.

1. Introduction

In this paper we consider the transmission through one-dimensional grating structures that consist of a "defect" region that is positioned between two infinite gratings or between two finite gratings placed in an exterior uniform medium. In particular we will address the problem of the direct characterization of so-called defect modes (DM) that can be observed to appear for specific defect frequencies (DF) in the bandgap (BG) of certain finite defect grating structures; see Figs. 1 and 2. This appearance is remarkable since in a uniform grating without defect the bandgap is the interval of wavelengths for which the structure acts like an almost perfect mirror.

For several applications and for fundamental understanding of the resonance phenomenon, it is desirable to characterize the DF and DM in a direct way, avoiding the necessity to scan with transmittance experiments the whole frequency range in the BG. Except when transfer matrix techniques (TMT) can be used, which is

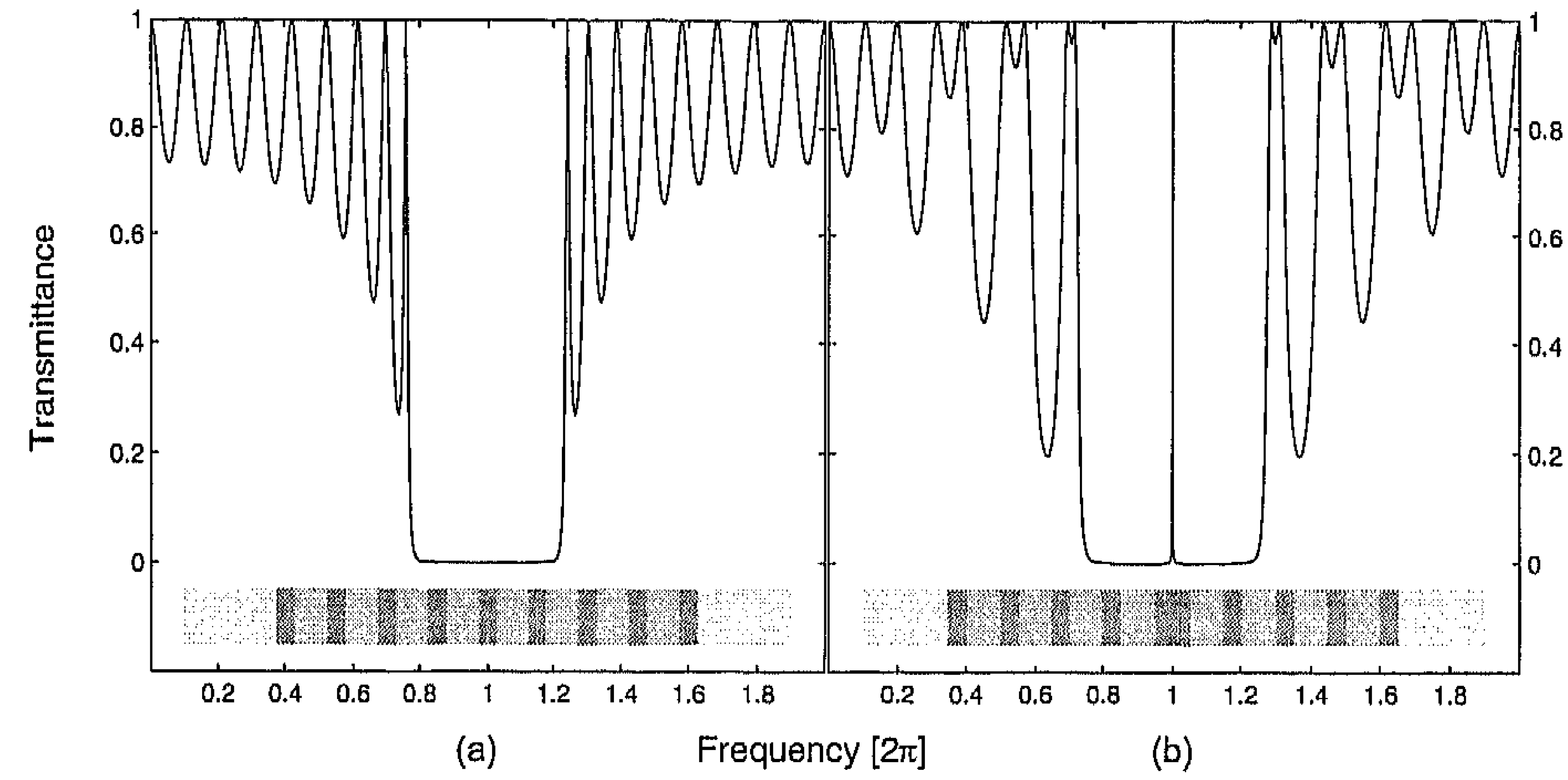

Fig. 1. (a) Relative optical transmission $|T|^2$ versus the frequency, for perpendicular plane wave incidence on a multilayer stack of transparent dielectric materials. The symmetric, finite periodic grating consists of 17 inner layers, alternating with low refractive index $n_1 = 1.25$ and high refractive index $n_2 = 2.5$, with their thicknesses satisfying $n_1 l_1 = n_2 l_2 = 1/4$ (quarter-wavelength stack). The outermost layers are of the high index material; we assume the structure to be surrounded by air (refractive index $n_0 = 1.0$). (b) Analogous to the one in (a), for a grating, where the central, high refractive index layer is twice as thick as the neighboring layers with high refractive index. Observe the additional transmission maximum at the design frequency $\omega = 1 \cdot 2\pi$.

restricted to linear materials with step-wise index structures, no analytic way to tackle this problem seems to exist. This will be the aim and contribution of this paper: to characterize in a direct way the DF and DM. The formulation will in principle be applicable for arbitrary material properties within the defect region, even if it is inhomogeneous or nonlinear. Further it is possible, to design simple numerical programs, Finite Element for instance, that use only the defect region as calculational domain. First the problem for defect states (DS) will be addressed. This DS is the solution of an eigenvalue problem in the frequency ω, which problem is, for Kerr-type of nonlinear materials, of the form

$$\begin{aligned} &\partial_z^2 u + \omega^2 \left[n_d^2(z) + \chi |u|^2 \right] u = 0, \quad \text{for } z \in (-L, L) \\ &\partial_z u = \kappa_{\pm}(\omega) u \quad \text{at } z = \pm L \,. \end{aligned} \tag{1}$$

Note that the (possibly nonlinear) Helmholtz equation is dressed up with so-called "effective" boundary conditions at the boundary $\pm L$ of the defect region; these boundary conditions replace the optical effect of the surrounding gratings. The fact that these effective boundary conditions depend on the frequency itself makes this a *non-standard* eigenvalue problem: even when the field equation is linear ($\chi = 0$) the eigenvalue appears in a nonlinear (and non-polynomial) way in the functions $\kappa(\omega)$. Not much is known yet about such eigenvalue problems in its generality; we will restrict therefore to special cases in the following, leaving a more complete investigation for later.

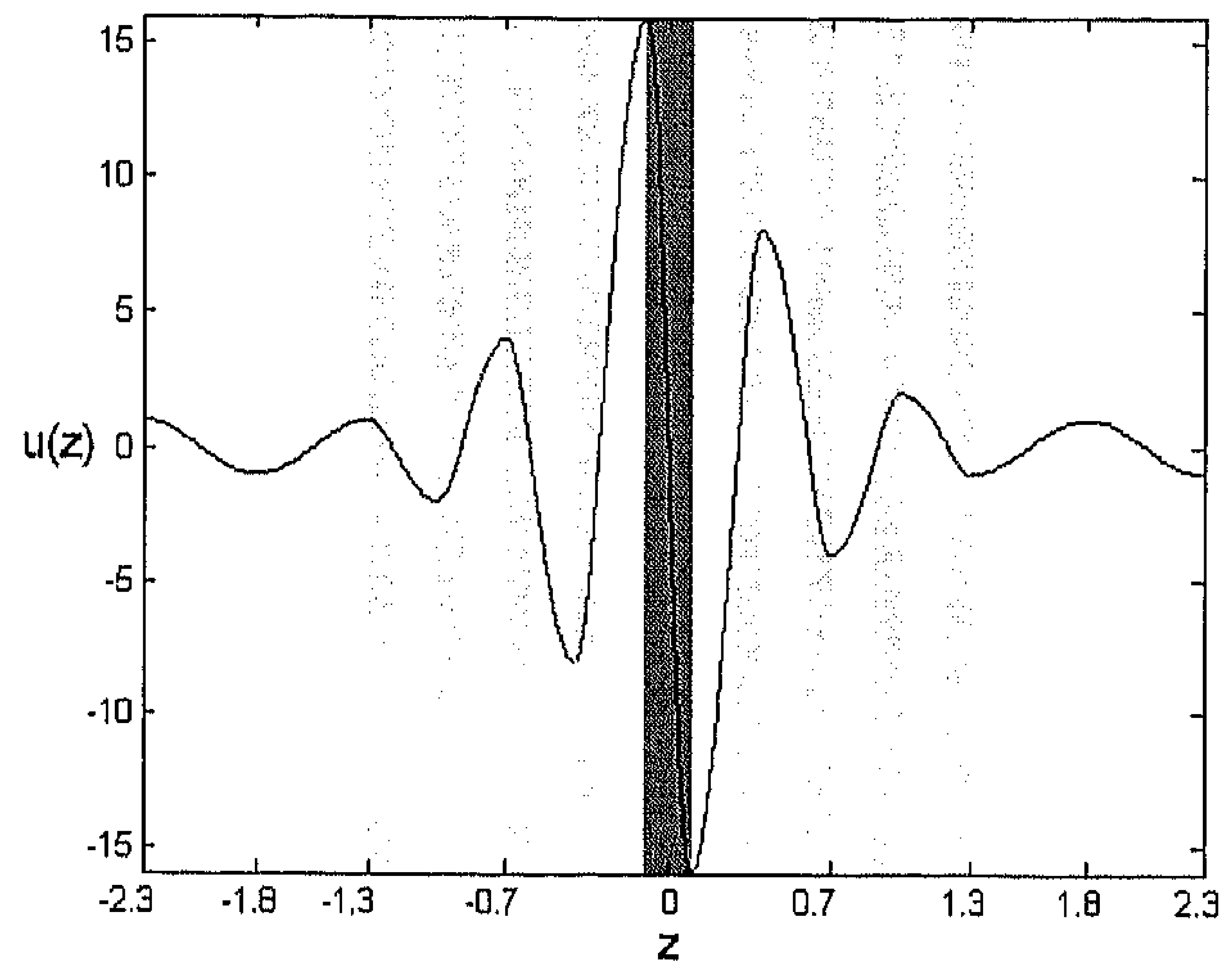

Fig. 2. Defect mode profile of the defect grating structure in Fig. 1(b).

Having found DSs in finite gratings, defect modes will then be investigated. Different from DSs, which are non-translating states with vanishing Poynting quantity, a DM is a fully transmitted solution, and hence has nonzero Poynting quantity. Such DM will be obtained from a superposition of DSs at the same frequency. In fact, in the structures that we consider, there exists one so-called amplified DS with largely amplified field in the defect which closely resembles a DM. However, the non-translating property of a DS, and the translating property of a DM, also in the exterior uniform medium, make them very different, and a relation seems difficult to establish. The explanation for this apparent discrepancy is the coexistence of an attenuated DS at the same frequency which, when suitably superimposed with the amplified one, leads to the correct influx and transmittance properties while hardly changing the field profile in the defect region. This attenuated DS may be easily overlooked as being uninteresting in itself. Yet its contribution to the DM is essential: in exterior regions it is of the same order as the amplified state and together they can constitute a traveling wave; in the defect region, despite its small amplitude, the combination with the amplified state produces the correct value of the Poynting quantity.

Bragg gratings that have step-wise index changes caused by a periodic succession of materials with different index has been studied extensively.[1,2] In all cases the gratings can be viewed as one-dimensional versions of photonic bandgap materials or photonic crystals.[3,4] When in such a grating the periodicity is broken either in a geometric way, or by index changes, a "cavity" is created in between two nearly completely reflecting mirrors. A Fabry–Perot cavity as described for e.g. in Refs. 2, 5–7 can be viewed as a result of such a "defect" in a Bragg grating. The appearance of defect modes and the building up of a high intensity in the defect (growing with the number of periods in the supporting Bragg reflectors), has been investigated for linear and nonlinear structures by means of finite-element techniques.[8,9] The wavelength (frequency) of the defect mode depends sensitively on the refractive index in the cavity. Furthermore, according to systematic studies in Refs. 8 and 9, the width of the resonances can be narrowed — and the steepness of the transmission curve increased — by extending the length of the cavity segment or by increasing the number of periods in the reflectors. These two properties of a DM explain the interest in structures which support DMs to design optical devices with various functionality. For instance, for sensor applications, the property is used that external influences on the defect region (temperature, stress, light) will effect the defect index; measuring the resulting change in the DF will correspond to the external effect. Another application is to exploit the amplified intensity to enhance the small nonlinear effects of nonlinear materials[9].

In Sec. 2 we introduce a slightly novel way to characterize the optical properties of gratings; this will make it easier in the following to optically connect the gratings to the defect and surrounding regions by effective boundary conditions. Then in Sec. 3 we construct DSs for various defect grating structures. In Sec. 4, for symmetric structures consisting of two finite gratings surrounding a linear defect region, it is shown that a superposition of two coexisting DSs can produce a DM. In Sec. 5 we will make several remarks about possible extensions of the methods.

2. Optical Characterization of Gratings

In this section we study the gratings that constitute important building blocks of the considered structures. We will introduce a slightly novel way of describing the optical properties of gratings, or of any layered structure for that matter, which will allow us to express the optical effect of the grating directly into a form, through effective boundary conditions, that allows a direct optical adjustment to surrounding media. We will only consider the TE-case, but the same method can be applied for TM polarization.

2.1. *The optical transfer matrix*

The optical properties of any inhomogeneous interval $[0, L]$ are, for TE-polarization, completely determined by the connection of the field and its derivative at the end and at the beginning of the interval:

$$\begin{pmatrix} u \\ \partial_z u \end{pmatrix}_{z=L} = T(\omega) \begin{pmatrix} u \\ \partial_z u \end{pmatrix}_{z=0}$$

where the optical transfer map (or matrix) (OTM) T depends on ω. Since for linear materials there are precisely two independent solutions, the two boundary values at each of the two endpoints, and the observation that the amplitude of a solution is arbitrary, lead to the conclusion that three (real-valued) quantities are needed for a full characterization.

Although the OTM is closely related to the usual transfer matrix technique (TMT) for layered structures, see e.g. Refs. 10 and 11, and can be found for such structures from such TMT calculations, the OTM does not depend on the choice of base functions, and therefore makes it possible to describe in a direct way the connection between adjacent regions by continuity conditions at the endpoints, irrespective of which method or base functions are used to calculate the OTM of the separate regions. This turns out to be very efficient and convenient in dealing with gratings in composite structures, as we shall see.

Restricting to frequencies inside the first BG of a linear grating, we will show that two of the basic quantities, denoted in the following by $\kappa^{\pm}(\omega)$, are the value of the quotient $\partial_z u/u$ at the edge (facet) of one (and any) period for the real-valued attenuated and amplified independent solutions $G^{\pm}$; the notation $\kappa = \infty$ is used to denote the case when u vanishes at the period facet. The gain factor per period, denoted by g, is the third basic variable. The optical transfer properties of a grating with N periods are determined by the OTM which is then given by

$$T(\omega)_{N\text{-periods}} = \frac{(-1)^N}{\kappa^- - \kappa^+} \begin{pmatrix} \kappa^- g^N - \kappa^+/g^N & -g^N + 1/g^N \\ \kappa^+\kappa^- \left(g^N - 1/g^N\right) & -\kappa^+ g^N + \kappa^-/g^N \end{pmatrix}.$$

Note that $\det(T) = (-1)^N$, expressing area conservation in phase space.

For frequencies inside the first BG we will give explicit formulas for the example of a linear grating with two layers; extension of the number of layers, or for arbitrary layered structures, composition of the matrices can be invoked. For smoothly varying index changes and/or nonlinear materials, results of characterization of this OTM, and of the basic quantities by explicit variational expressions, will be published elsewhere.

2.2. *Grating properties*

Let n be the index of reflection that is periodic with period p. Then, according to Bloch's (Floquet) theorem for periodic structures, each solution of

$$\partial_z^2 u + \omega^2 n^2(z) u = 0\,, \qquad u(z+p) = u(z)$$

can be written as a combination of two independent solutions that are of the form

$$u(z) = v(z) e^{iK(\omega)z}\,, \qquad v(z) = v(z+p)$$

where $K(\omega)$ describes the Bragg dispersion properties of the grating. For frequencies within the first BG, the value of K is given by $K(\omega) = \pi/p \pm i\rho(\omega)z$, and the two corresponding real-valued solutions are given by

$$G^{\pm}(\omega; z) = w^{\pm}(z) e^{\pm\rho z}\,, \qquad w(z+p) = -w(z)\,, \qquad \rho > 0\,.$$

Since the quotient $\partial_z G/G$ is p-periodic, the value of this quotient is the same at each period-facet. Hence we can define real-valued numbers associated with these solutions by

$$\kappa^{\pm}(\omega) := \frac{\partial_z G^{\pm}}{G^{\pm}} \text{ evaluated at (any) period-facet}\,.$$

Denoting by $g(\omega) := \exp(\rho(\omega)p)$ the "gain-factor" per period (Floquet multiplier), we have $G^+(z+p) = -gG^+(z)$ and $G^-(z+p) = -G^-(z)/g$. The three quantities $g, \kappa^\pm$ can now be used to determine the OTM as follows. Any solution within the grating can be written as a superposition: $u = AG^+ + BG^-$. At the left facet of a period, say at $z = 0$, the solution and its derivative are given by

$$u(0) = AG^+(0) + BG^-(0)$$
$$\partial_z u(0) = \kappa^+ AG^+(0) + \kappa^- BG^-(0)\,,$$

while after N periods, $z = Np$, these quantities are given by

$$u(Np) = (-g)^N AG^+(0) + (-g)^{-N} BG^-(0)$$
$$\partial_z u(Np) = \kappa^+(-g)^N AG^+(0) + \kappa^-(-g)^{-N} BG^-(0)\,.$$

Eliminating the amplitude factors $AG^+(0), BG^-(0)$ leads to the OTM given above.

2.2.1. *Calculation of the optical quantities*

Consider as an example the case of a grating consisting of two layers with indices $n_{1,2}$ and width $\ell_{1,2}$, so that the period is given by $p = \ell_1 + \ell_2$; for notational convenience we use $k_{1,2} = \omega n_{1,2}$. Introducing phase parameters α, β, the solutions can be written down explicitly. For the "amplified" solution we find:

$$G^+ = \begin{cases} \cos(k_1 z - \alpha) & \text{for } 0 \le z \le \ell_1 \\ \dfrac{\cos(k_1\ell_1 - \alpha)}{\cos\beta}\cos(k_2(z-\ell_1) - \beta) & \text{for } \ell_1 \le z \le p \end{cases}$$

which is a solution provided

$$k_1 \tan(k_1\ell_1 - \alpha) = -k_2 \tan\beta$$
$$k_2 \tan(k_2\ell_2 - \beta) = -k_1 \tan\alpha\,.$$

Having solved for α and β, the basic quantities can then be expressed in the geometric and material properties of the grating through the values of α and β as follows:

$$g = -\frac{\cos(k_1\ell_1 - \alpha)\cdot\cos(k_2\ell_2 - \beta)}{\cos\alpha\cdot\cos\beta}$$

$$\kappa^+ = k_1 \tan\alpha\,, \qquad \kappa^- = -k_2\tan\beta\,.$$

Then an independent attenuated solution follows from reversibility:

$$G^- = \begin{cases} g\cos(k_1(\ell_1 - z) - \alpha) & \text{for } 0 \le z \le \ell_1 \\ -\dfrac{\cos(k_1\ell_1 - \alpha)}{\cos\beta}\cos(k_2(p-z) - \beta) & \text{for } \ell_1 \le z \le p \end{cases}.$$

2.2.2. *Quarter wave stack example*

We present some graphical information about the relevant quantities for the case of a so-called quarter wave stack structure with two layers in Fig. 3. Such a structure has the same optical path length in each layer since by design $n_1\ell_1 = n_2\ell_2 = 1/4$.

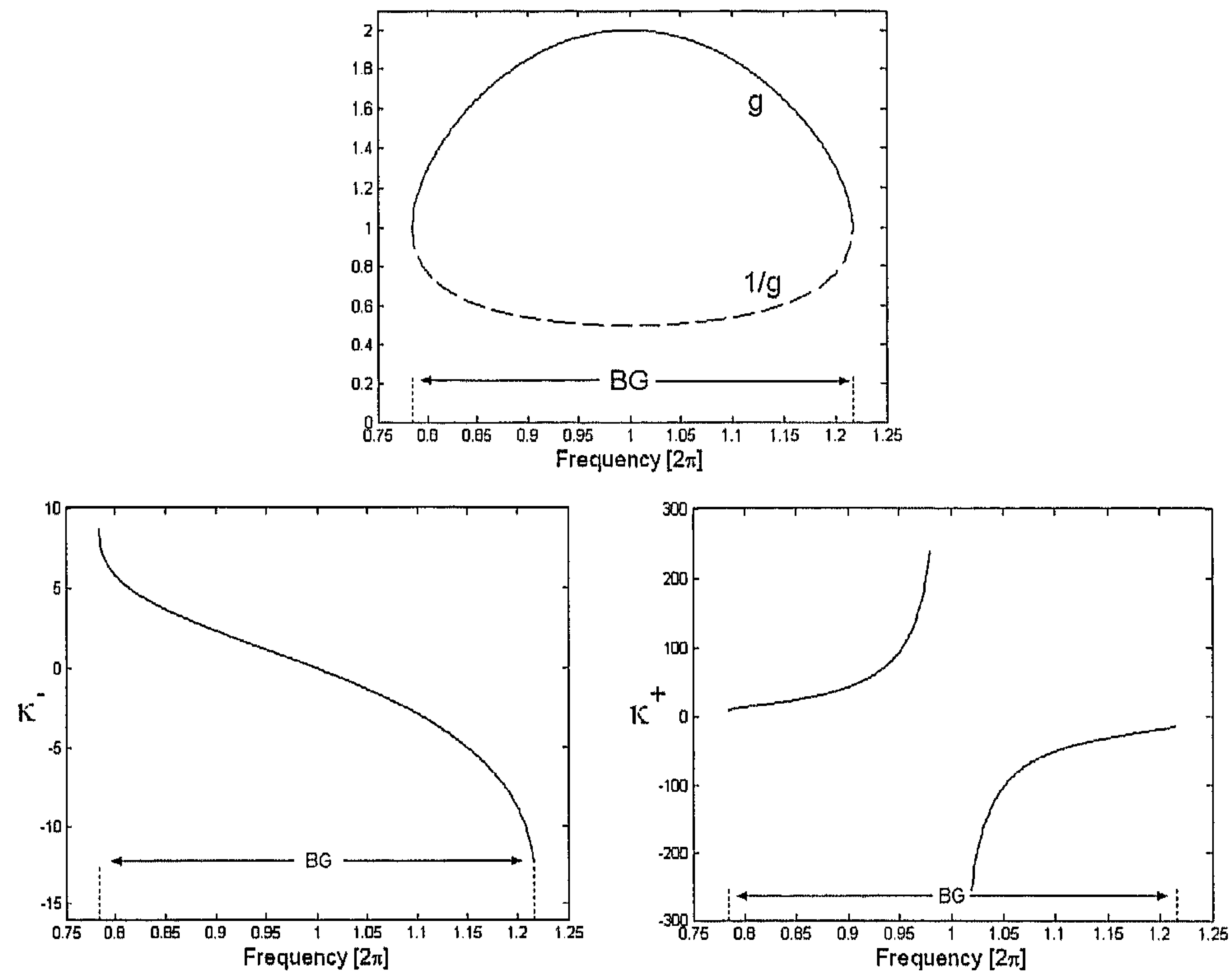

Fig. 3. Plot of the gain factor $g(\omega)$, $\kappa^+(\omega)$ and $\kappa^-(\omega)$.

For indices $n_1 = 1.25$ and $n_2 = 2.5$, the band gap, determined by values ω for which $g > 1$, is the interval $2\pi \cdot [0.7836, 1.2163]$. Then, for the special ("design") frequency ω_0 such that $\omega_0 n_1 \ell_1 = \pi/2$, a quarter "wavelength", it follows that the two basic solutions have at a period-facet the boundary values

$$G^+(0) = 0, \partial_z G^+(0) = 1 \quad \text{and} \quad G^-(0) = 1, \partial_z G^-(0) = 0$$

(when the low index layer is the first layer; else the signs are interchanged) corresponding to $\kappa^+(\omega_0) = 0$, $\kappa^-(\omega_0) = \infty$, while the gain factor is maximal $g = 2$.

For the design frequency, plots of the solutions G^+ and G^- are depicted over a distance of four periods, in which a gain of $2^{\pm 4}$ is visible, in Fig. 4.

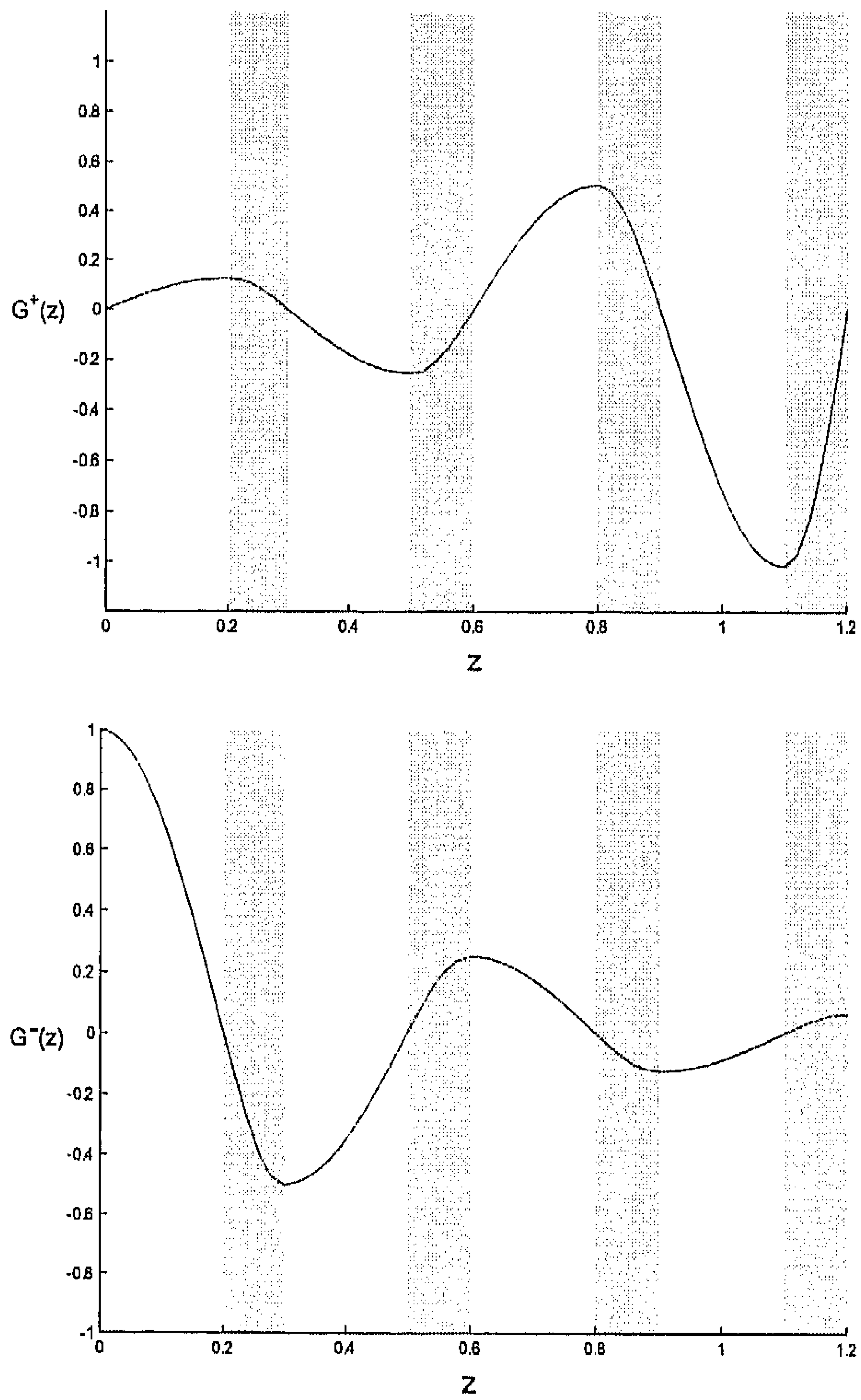

Fig. 4. Plots of G^+ and G^- over four periods.

2.3. *Effective boundary conditions*

The two basic solutions $G^\pm$ considered above are of no relevance for infinitely long gratings since then both are unbounded, and the only bounded solution is the vanishing field, the characteristic property of an infinitely long grating. When the grating is half-infinite, one solution is bounded inside the grating. Take as an example the half-infinite grating at the left, say $(-\infty, -L)$; then only the amplified solution G^+, that decays to zero at $-\infty$, is nontrivial and bounded. The optical effect of this half-infinite grating is then completely determined by the value κ^+. Stated differently, any field at the right should satisfy the boundary condition

$$\partial_z u = \kappa^+ u \text{ at } z = -L\,;$$

for obvious reasons we will call this an "effective boundary condition" (EBC).

Remark 1. The above formulation makes it possible to give a somewhat different interpretation to the value κ^+ which may also be more constructive in the case when no explicit analytical solutions can be found, for instance for nonlinear gratings. In fact, the value of the coefficient κ^+ can be described in a variational way using the Helmholtz functional on the half-infinite interval. Specifying the amplitude at the end point, arbitrary for linear gratings, the characterization is:

$$\kappa^+(\omega) = \inf\left\{\int_{-L}^{\infty}\{(\partial_z u)^2 - \omega^2 n^2 u^2\}dz | u(-L) = 1\right\},$$

i.e. the value function of the Helmholtz functional is $\kappa^+ u(-L)$, see Ref. 12. For nonlinear gratings the value of the amplitude has to be taken into account and appears nonlinearly in the result. This formulation makes it feasible to calculate the coefficient κ^+ numerically.

When the grating is finite, both basic solutions are bounded, and for optical communication with the two exterior sides the OTM-approach can be applied. For instance, consider the configuration of a uniform medium at the left with index n_{left} and a finite grating of N periods between $[-M, -L]$. When we consider the transmission problem with a given influx from the left, the solution for $z < -M$ is given by

$$u(z) = Ae^{ik_{\text{left}}(z+M)} + re^{-ik_{\text{left}}(z+M)}$$

with A the influx amplitude and r the amplitude of the reflected wave. Then

$$\begin{pmatrix} u \\ \partial_z u \end{pmatrix}_{z=-L} = T_N(\omega)\begin{pmatrix} u \\ \partial_z u \end{pmatrix}_{z=-M} = T_N(\omega)\begin{pmatrix} 1 & 1 \\ ik_{\text{left}} & -ik_{\text{left}} \end{pmatrix}\begin{pmatrix} A \\ r \end{pmatrix}$$

from which we can solve $\partial_z u(-L)$ as function of A and $u(-L)$, leading to the effective boundary condition at $z = -L$.

A somewhat different interpretation is to look at the effect of influx from the left-most uniform exterior on the basic solutions in the finite grating. Taking the field in the uniform medium at the left that is consistent with the basic (amplified or attenuated) state in the grating, the state will be a standing wave $C\cos(k_0(z + M) + \theta)$ with $k_0\tan(\theta) = \kappa$, and so will the state in the uniform medium to the right of the grating. The attenuated state will correspond to a very small amplitude state at the right. However, for the grating placed in air at both sides, an influxed wave $e^{ik_0 z}$ only from the left (no incoming wave from the right) will not be a standing wave: it will not be totally reflected and there is a small transmittance. Related to this is a slightly different effective boundary condition at the grating end at $z = -L$. This will depend on the number of gratings: for increasing number of periods the presence of the uniform exterior becomes rapidly very small, see Fig. 5 for the effective boundary value κ_N of the transmittance problem through the grating with N periods compared to the value κ^- for the half-infinite grating.

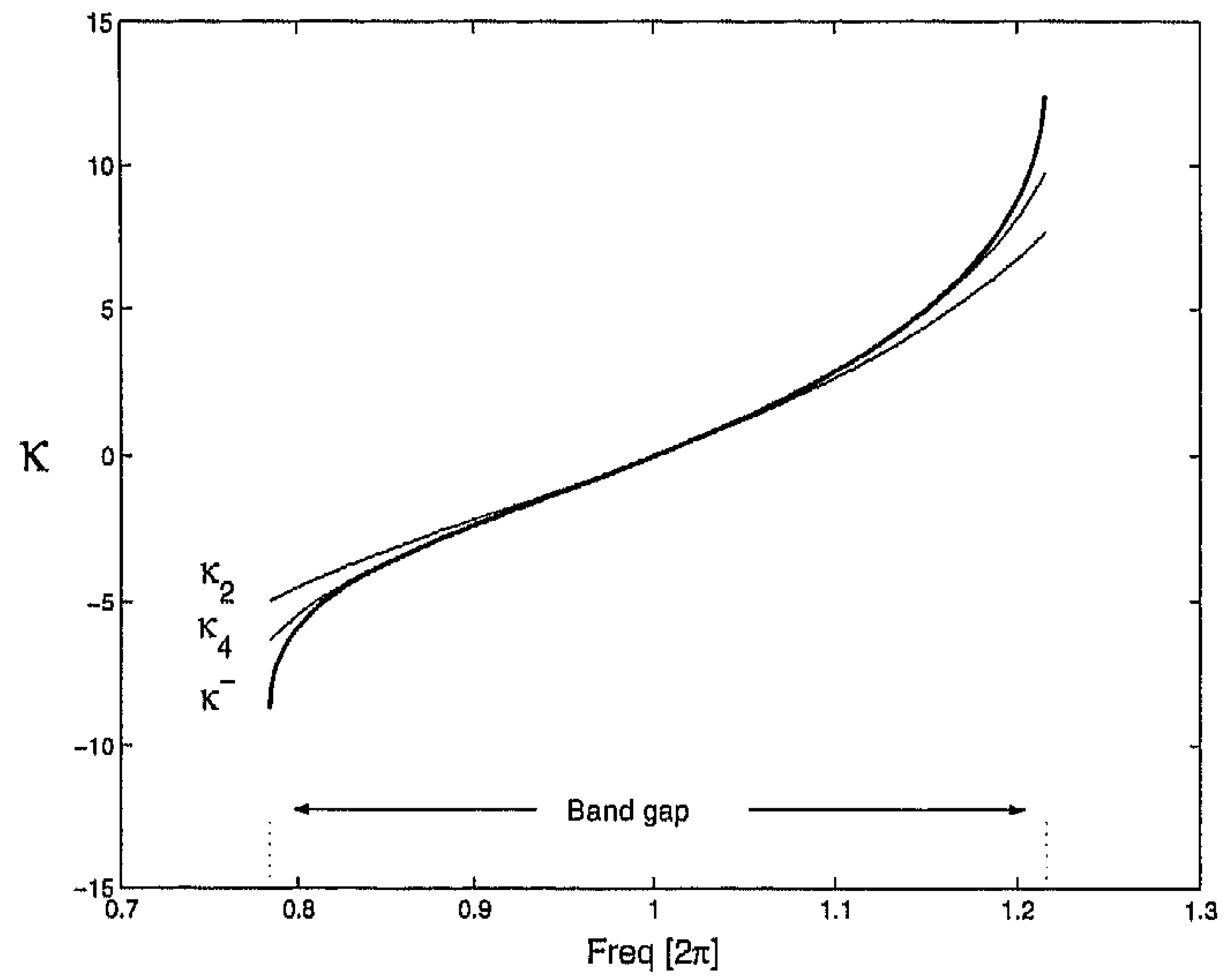

Fig. 5. Graph of κ_N for $N = 2, 4$ and κ^-.

2.4. *States and modes*

In the following sections we will characterize special field distributions that may exist in defect grating structures. In Sec. 3 we will investigate defect states DS, and in Sec. 4 defect modes DM. The difference between the two is that a DS is a "standing wave" while a DM is a traveling wave that is completely transmitted through the structure.

As is well known, the Poynting vector can be used to distinguish clearly between standing waves and traveling (not necessarily completely transmitted) solutions.

In the one-dimensional case considered here, we will use the Poynting quantity which is related to the Poynting vector as being *the powerflow in the z-direction of the electromagnetic field.* For any solution u of the Helmholtz equation, the Poynting quantity is given by $P(z) := \mathrm{Im}[\bar{u}\partial_z u]$, and is independent of z:

$$P(z) := \mathrm{Im}[\bar{u}\partial_z u]\,, \qquad \partial_z P(z) = 0\,. \tag{2}$$

The relevance of these quantities becomes clear when we investigate them for a uniform medium, say index n_0; with $k_0 = \omega n_0$, any solution consists of a superposition of a right and a left traveling wave $u = Ae^{ik_0 z} + Be^{-ik_0 z}$ and we find that at any position z:

$$P = k_0[|A|^2 - |B|^2]\,.$$

In general, P measures the net flow of the power transported to the right and the left; our interest is that it clearly identifies a state as a solution for which $P = 0$ (then $|A| = |B|$ and the solution is a standing wave: $u = |A|\cos(k_0 z + \psi)$ for some

ψ). A traveling wave, possibly superimposed by a standing wave, will have $P \neq 0$, and so, in particular, any DM will have $P \neq 0$.

When investigating the so-called transmittance problem for an optical structure, one looks at a wave influxed from a uniform medium at the left, say, and investigates its transmittance through the structure into a uniform medium at the right, where no influx from the right into the structure is supposed. A DS cannot be obtained in that manner, since it has standing wave in the left region (meaning that an incoming wave $e^{ik_0 z}$ is compensated with a reflected wave of the same amplitude, forming together a standing wave) and just as well a standing wave in the "outflux"-region at the right. This means that there is not only an outgoing wave to the right, but just as well a wave coming in from the right and hence a defect state cannot be "produced" by light influxed from one side only.

3. Defect States in Grating Structures

In this section we consider various grating structures with defects; in each case we will employ effective boundary conditions for the defect region to replace the optical properties of the surrounding gratings. The interest is to find defect states, i.e. solutions with vanishing Poynting quantity P. In structures that contain at least one half-infinite grating, any nontrivial solution will have vanishing Poynting quantity and so any solution is a state.

3.1. *Defect states between half-infinite gratings*

When a defect region is introduced in an infinite grating, the defect separates a left and a right half infinite grating. The amplified state in the left grating can possibly be connected in the defect region to the attenuated state in the right one for suitable frequencies. Such "resonant" frequencies will depend on properties of the gratings and of the defect region. The problem can be formulated as an eigenvalue problem on the defect region, say $[-L, L]$, when we use effective boundary conditions at the defect boundaries:

$$\partial_z u = \kappa^+_{\text{left}}(\omega) u \text{ at } z = -L\,, \quad \partial_z u = \kappa^-_{\text{right}}(\omega) u \text{ at } z = L \tag{3}$$

where we use obvious notation for the amplified/attenuated state in the left/right grating. If for some defect frequency there exists a field distribution inside the defect region that satisfies these two boundary conditions, a defect state is obtained.

Note that for this formulation it is not necessary that left and right gratings are the same. But it should be remarked that, even when the problem is linear, the eigenvalue problem is non-standard since the eigenvalue (ω) appears in a nonlinear way so that even methods for "polynomial" eigenvalue problems[13,14] cannot be applied directly. Existence of a solution is therefore a nontrivial matter. When, in addition, the Helmholtz equation is nonlinear, bistable solutions can be expected to exist under certain circumstances.[9] We will show here that for some specific cases we can directly find the solution; more general results will be published elsewhere.

Consider the case of a linear defect region with constant index n_d. Then the general solution in the defect region is of the form

$$u = A\cos(\omega n_d z + \theta)\,.$$

Satisfying the boundary conditions leads to the condition for ω

$$\omega n_d \tan(\omega n_d L - \theta) = \kappa^+_{\text{left}}(\omega) \text{ and } \omega n_d \tan(\omega n_d L + \theta) = -\kappa^-_{\text{right}}(\omega)\,.$$

Eliminating θ leads to the equation for ω for arbitrary integer m:

$$2\omega n_d L = \arctan(\kappa^+_{\text{left}}(\omega)/\omega n_d) - \arctan(\kappa^-_{\text{right}}(\omega)/\omega n_d) + m\pi\,.$$

Since the right-hand side is bounded, while the left-hand side is linear in ω, for suitable m there exists at least one solution that belongs to the band gap; the corresponding value of θ is then found from

$$2\theta = -\arctan(\kappa^+_{\text{left}}(\omega)/\omega n_d) - \arctan(\kappa^-_{\text{right}}(\omega)/\omega n_d) + m\pi\,.$$

Hence we conclude that for a uniform defect region between arbitrary half-infinite gratings there always exists at least one DS.

In Fig. 6 we show an example for a quarter wave stack defect grating with low refractive index $n_1 = 1.25$ and high refractive index $n_2 = 2.5$. The defect layer between the two half infinite gratings has index $n_d = 2.5$ and is twice as thick as the high index layer. The intersection between the function $f_1(\omega) = \arctan(\kappa^+_{\text{left}}(\omega)/\omega n_d) - \arctan(\kappa^-_{\text{right}}(\omega)/\omega n_d) + 2\pi$ and $f_2(\omega) = 2\omega n_d L$ gives the defect frequency $\omega = 1 \cdot 2\pi$.

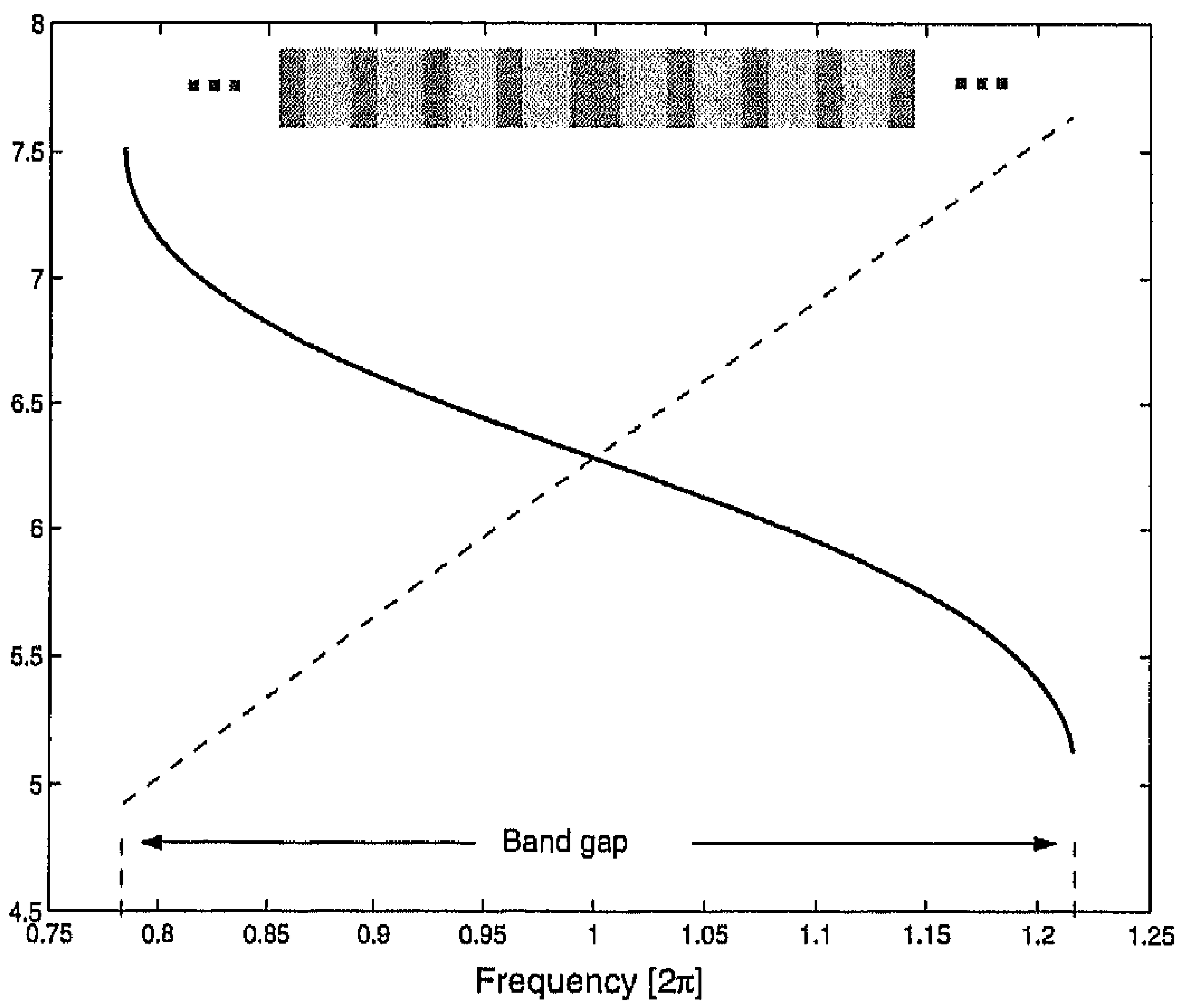

Fig. 6. The graph of $f_1(\omega) = \arctan(\kappa^+_{\text{left}}(\omega)/\omega n_d) - \arctan(\kappa^-_{\text{right}}(\omega)/\omega n_d) + 2\pi$ (solid curve), and $f_2(\omega) = 2\omega n_d L$ (dashed line).

3.2. *States for a single finite grating*

Consider a finite grating, of N periods in the interval say $[-M, M]$; let $\kappa^{\pm}(\omega), g(\omega)$ be given, and take a uniform medium at both sides, index n_{left} for $z < -M$, n_{right} for $z > M$.

Then, for *each* ω in BG there is an increasing and a decreasing state which connect standing waves in the exteriors through the respective increasing and decreasing grating solutions $G^{\pm}$. Indeed, the total solution is of the form

$$u = \begin{cases} A\cos(\omega n_{\text{left}}(z+M) + \psi_{\text{left}}) & \text{for } z < -M \\ aG(z) & \text{for } -M < z < M \\ B\cos(\omega n_{\text{right}}(z-M) + \psi_{\text{right}}) & \text{for } z > M \end{cases} .$$

Continuity of the field derivative leads to the two equations

$$\kappa(\omega) = -\omega n_{\text{left}} \tan(\psi_{\text{left}}) = -\omega n_{\text{right}} \tan(\psi_{\text{right}})$$

from which the values of ψ follow. For the amplitudes we then find

$$A\cos(\psi_{\text{left}}) = aG(-M)\,, \qquad B\cos(\psi_{\text{right}}) = aG(M)$$

with $G(M) = (-g)^{\pm N} G(-M)$ corresponding to an amplitude amplification/attenuation g^N. In particular, when exteriors are identical, $B = (-g)^N A$ for the amplified solution and $B = A/(-g)^N$ for the attenuated solution.

3.3. *States in a defect grating*

The above result for a single finite grating can now be used to investigate states in structures with a succession of possibly different finite gratings placed in air by composition of the OTMs. We will consider the case of one defect region $[-L, L]$ with two adjacent gratings in $[-M_{\text{left}}, -L]$ and $[L, M_{\text{right}}]$ only; for more defect regions between gratings, additional degeneracy conditions will have to be satisfied for a state to exist.

A defect state of the whole structure will couple in the defect region a decreasing or increasing state in the left grating to an increasing or decreasing state in the right grating. Suppose the left and right gratings are characterized by their values $\kappa^{\pm}$ and the gain factor g per period. Then with each possible combination of states in the separate gratings, a defect state of the whole structure is found for the frequency that solves an eigenvalue problem of the form shown in (1) on the defect region $[-L, L]$. Using obvious notation for the state S that corresponds to the different possible choices of the behavior in the constituent gratings, we obtain the following four different possible states:

- S^{++}: the state that is amplified in both gratings;
- S^{+-}: the state that is amplified in the left grating and attenuated in the right grating;
- S^{-+}: the state that is attenuated in the left grating and amplified in the right grating;
- S^{--}: the state that is attenuated in both gratings.

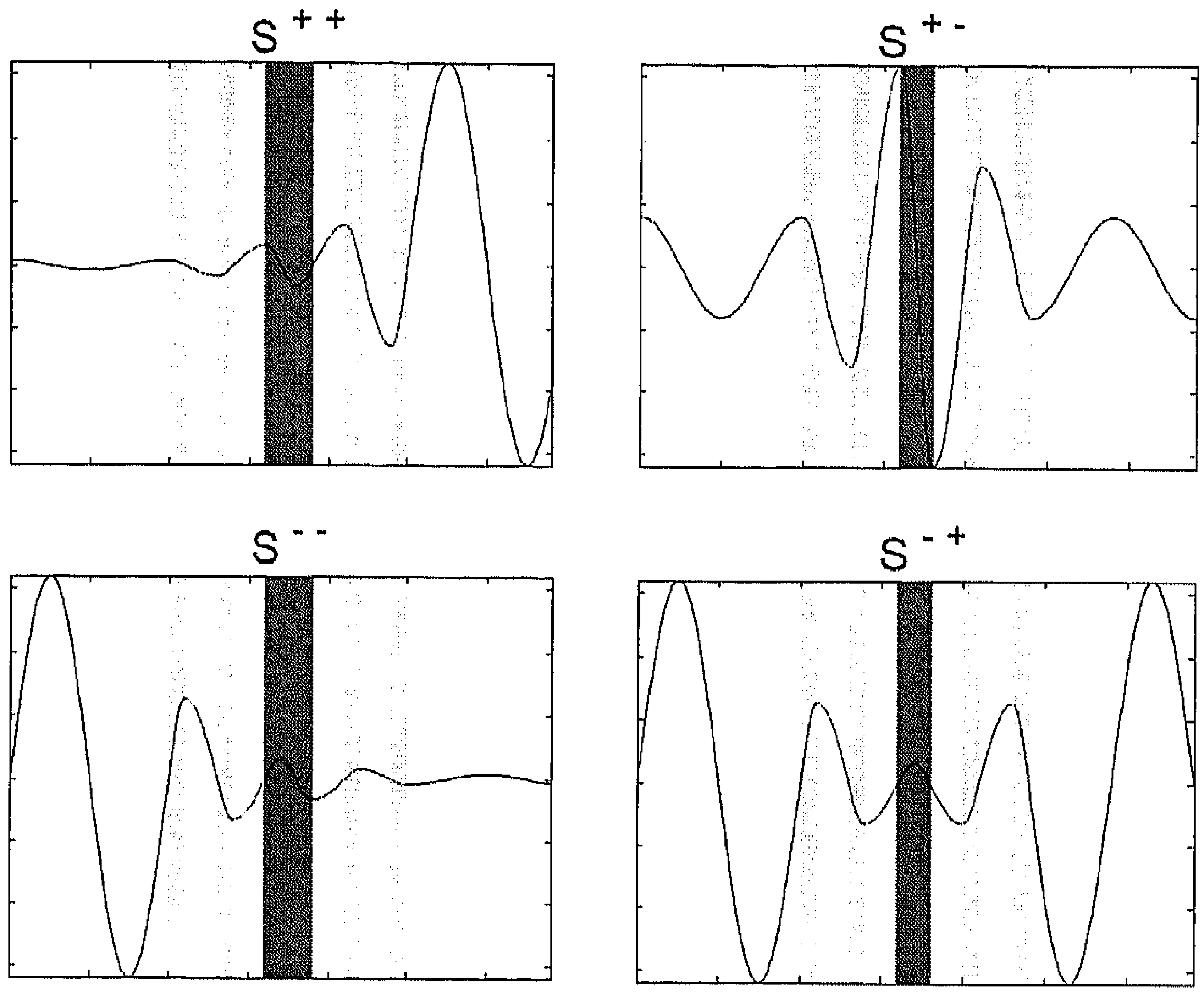

Fig. 7. Illustration of four different possible states in a defect grating.

We will denote the state S^{+-} by S^{+} in the following and call this the "amplified" state since it has large amplitude inside the cavity compared to the exterior; likewise we will denote S^{-+} by S^{-} and call it the attenuated state since it has small amplitude in the defect region compared to the exterior. We will see in the next section that these two states can, under specific conditions, form a defect mode. The states S^{+} and S^{-} are solutions of the eigenvalue problem on the defect region with boundary values

$$\text{for } S^{+}: \partial_z u = \kappa^{+}_{\text{left}}(\omega)u \text{ at } z=-L\,, \quad \partial_z u = \kappa^{-}_{\text{right}}(\omega)u \text{ at } z = L\,, \tag{4}$$

$$\text{for } S^{-}: \partial_z u = \kappa^{-}_{\text{left}}(\omega)u \text{ at } z=-L\,, \quad \partial_z u = \kappa^{+}_{\text{right}}(\omega)u \text{ at } z = L\,. \tag{5}$$

In general a defect frequency ω_{+} of the amplified state will not coincide with a defect frequency ω_{-} of the attenuated state. For further use in the next section, we observe the phase difference of the solution over the defect-grating structure as follows. The amplified/attenuated state can be represented in the uniform exterior regions as (for $s = +$ or $s = -$)

$$S^s = \begin{cases} a_s \cos(\omega_s n_{\text{left}}(z + M_{\text{left}}) + \alpha_s) & \text{for } z < -M_{\text{left}} \\ b_s \cos(\omega_s n_{\text{right}}(z - M_{\text{right}}) + \beta_s) & \text{for } z > M_{\text{right}} \end{cases}$$

corresponding to a phase change of $\beta_s - \alpha_s$ over the complete structure; this phase change can also be found from the value of the Helmholtz functional.

4. Defect Modes

We will now study the transmittance problem, and in particular solutions that are completely transmitted: defect modes.

The general transmittance problem is often studied by numerical methods, and by scanning the frequency range inside a band gap it is then observed that defect modes can exist for certain resonant frequencies. Such a DM looks very similar to a defect state S^+ as characterized above. This is remarkable because the behavior in the influx and outflux regions is completely different, and a defect mode can be created by one-sided influx, while a defect state cannot.

4.1. *Defect mode decomposed into defect states*

Consider a linear grating structure with one defect as considered above. If a defect mode exists for some defect frequency ω_d, its behavior in the exterior regions is given by

$$M_d = \begin{cases} a_d \exp i(\omega_d n_{\text{left}}(z + M_{\text{left}}) + \alpha_d) & \text{for } z < -M_{\text{left}} \\ b_d \exp i(\omega_d n_{\text{right}}(z - M_{\text{right}}) + \beta_d) & \text{for } z > M_{\text{right}} \end{cases}$$

with real amplitudes a_d (which can be taken arbitrarily) and b_d which satisfy (from Poynting conservation)

$$n_{\text{left}} a_d^2 = n_{\text{right}} b_d^2 .$$

Now observe that, given a DM, the real and imaginary parts of this mode are also solutions. Since these solutions are real, each has vanishing Poynting quantity. $\text{Re}(M_d)$ and $\text{Im}(M_d)$ are therefore two different defect states of the structure that exist at the same defect frequency ω_d. Moreover, each of these states has the same phase difference $\beta_d - \alpha_d$ over the total defect grating structure.

4.2. *Defect mode as superposition of defect states*

Now consider a defect grating structure for which we have identified four different DSs in Sec. 3.3. We want to investigate under which conditions a DM exists in such a structure and how it can be obtained from a superposition of the two identified DSs S^+ and S^-; for definiteness, we normalize the amplitude of these waves at the left uniform exterior region and take $\alpha_+ = 0, \alpha_- = -\pi/2$, so that

$$S^+ = \cos(\omega n_{\text{left}}(z + M_{\text{left}})) \text{ for } z < -M_{\text{left}} ,$$

$$S^- = \sin(\omega n_{\text{left}}(z + M_{\text{left}})) \text{ for } z < -M_{\text{left}} .$$

For later reference, we note that $S^+\partial_z S^- - S^-\partial_z S^+ = \gamma$ is a nonzero constant over the whole structure, in fact $\gamma = \omega n_{\text{left}}$.

In view of the results in the previous subsection, at least two accidental degeneracy conditions should be satisfied in order that a defect mode can exist. Restricting the further investigation to symmetric structures only, for which $n(z) = n(-z)$, we will now investigate the possibilities. For a symmetric structure it holds that

$$\kappa^+_{\text{left}} = -\kappa^-_{\text{right}} \text{ and } \kappa^-_{\text{left}} = -\kappa^+_{\text{right}} ,$$

and hence the boundary conditions are:

$$\text{for } S^+: \ \partial_z u = -\kappa^-_{\text{right}}(\omega) u \text{ at } z = -L\,, \quad \partial_z u = \kappa^-_{\text{right}}(\omega) u \text{ at } z = L\,,$$
$$\text{for } S^-: \ \partial_z u = -\kappa^+_{\text{right}}(\omega) u \text{ at } z = -L\,, \quad \partial_z u = \kappa^+_{\text{right}}(\omega) u \text{ at } z = L\,.$$

Any solution in the defect region is of the form $u_d = A\cos(\omega n_d z + \theta)$, and hence

$$\left.\frac{\partial_z u_d}{u_d}\right|_{z=-L} = -\omega n_d \tan(-\omega n_d L + \theta),\ \left.\frac{\partial_z u_d}{u_d}\right|_{z=L} = -\omega n_d \tan(\omega n_d L + \theta)\,.$$

In view of the boundary conditions for $S^\pm$ a first condition follows from the requirement that

$$\omega n_d \tan(-\omega n_d L + \theta) = -\omega n_d \tan(\omega n_d L + \theta)$$
$$\tan(\omega n_d L - \theta) = \tan(\omega n_d L + \theta)$$

from which we conclude that necessarily $\theta = 0$ or $\theta = \pi/2$. The two possible solutions in the defect region are therefore the symmetric and the skew-symmetric functions $\cos(\omega n_d z)$ and $\sin(\omega n_d z)$.

This leads to two cases depending on which defect solution will connect which state: for a solution with skew-symmetric amplified, and symmetric attenuated state we find the two conditions

$$\omega n_d \cot(\omega n_d L) = \kappa^-_{\text{right}}$$
$$-\omega n_d \tan(\omega n_d L) = \kappa^+_{\text{right}}$$

and for a solution with symmetric amplified, and skew-symmetric attenuated state the conditions are:

$$-\omega n_d \tan(\omega n_d L) = \kappa^-_{\text{right}}$$
$$\omega n_d \cot(\omega n_d L) = \kappa^+_{\text{right}}\,.$$

It is clear that for arbitrary grating the two conditions cannot be satisfied for the same ω, which means that only specific gratings can support a DM.

The case of a QWS is an example that can satisfy these conditions, at the design frequency ω_0 with $\omega_0 n_1 \ell_1 = \pi/2$, $\kappa^+_{\text{right}} = 0$, $\kappa^-_{\text{right}} = \infty$. Hence if the optical length of the defect region satisfies $\omega_0 n_d L = m\pi/2$ for some integer m, then for $m = odd$ we get a skew-symmetric state S^+ and a symmetric state S^-, while for $m = even$ we get a symmetric state S^+ and a skew-symmetric state S^-.

Each state has a standing wave at the influx region, but the phases of each will be different. Therefore a suitable complex combination will produce a pure influx wave from the left. Because of the normalization for the states chosen above, we get for the specific complex superposition a purely incoming wave at the left:

$$u_M := S^+ + iS^- = \exp i(\omega_0 n_{\text{left}}(z+M)) \text{ for } z < -M\,.$$

The (skew-) symmetry of the states $S^\pm$ guarantee that their phase difference over the total structure is the same for both. Hence, the same superposition produces a pure outflux wave at the right:

$$S^+ + iS^- = \exp i(\omega_0 n_{\text{right}}(z-M)) \text{ for } z > M\,.$$

It is interesting to see the importance of the attenuated state in the construction of this mode. In the exterior regions both constituent states have the same amplitude while in the defect region between gratings of N layers, the attenuated state has amplitude g^{-N} while the amplified state has amplitude g^N. Consequently, for large N, the contribution to the field profile of the attenuated state is hardly visible and the mode profile resembles the profile of the amplified state. Yet for the propagating property of the mode the contribution of the attenuated mode is essential, as seen by considering the Poynting quantity:

$$\begin{aligned} P\left(S^+ + iS^-\right) &= P(S^+) + P(S^-) + \operatorname{Im}\left(iS^+\partial_z S^- - iS^-\partial_z S^+\right) \\ &= 0 + 0 + \left[S^+\partial_z S^- - S^-\partial_z S^+\right] = \omega n_{\text{left}} \end{aligned}$$

since $P\left(S^\pm\right) = 0$ and $S^+\partial_z S^- - S^-\partial_z S^+ = \omega n_{\text{left}}$ constant over the whole structure. See Fig. 8 for the illustration.

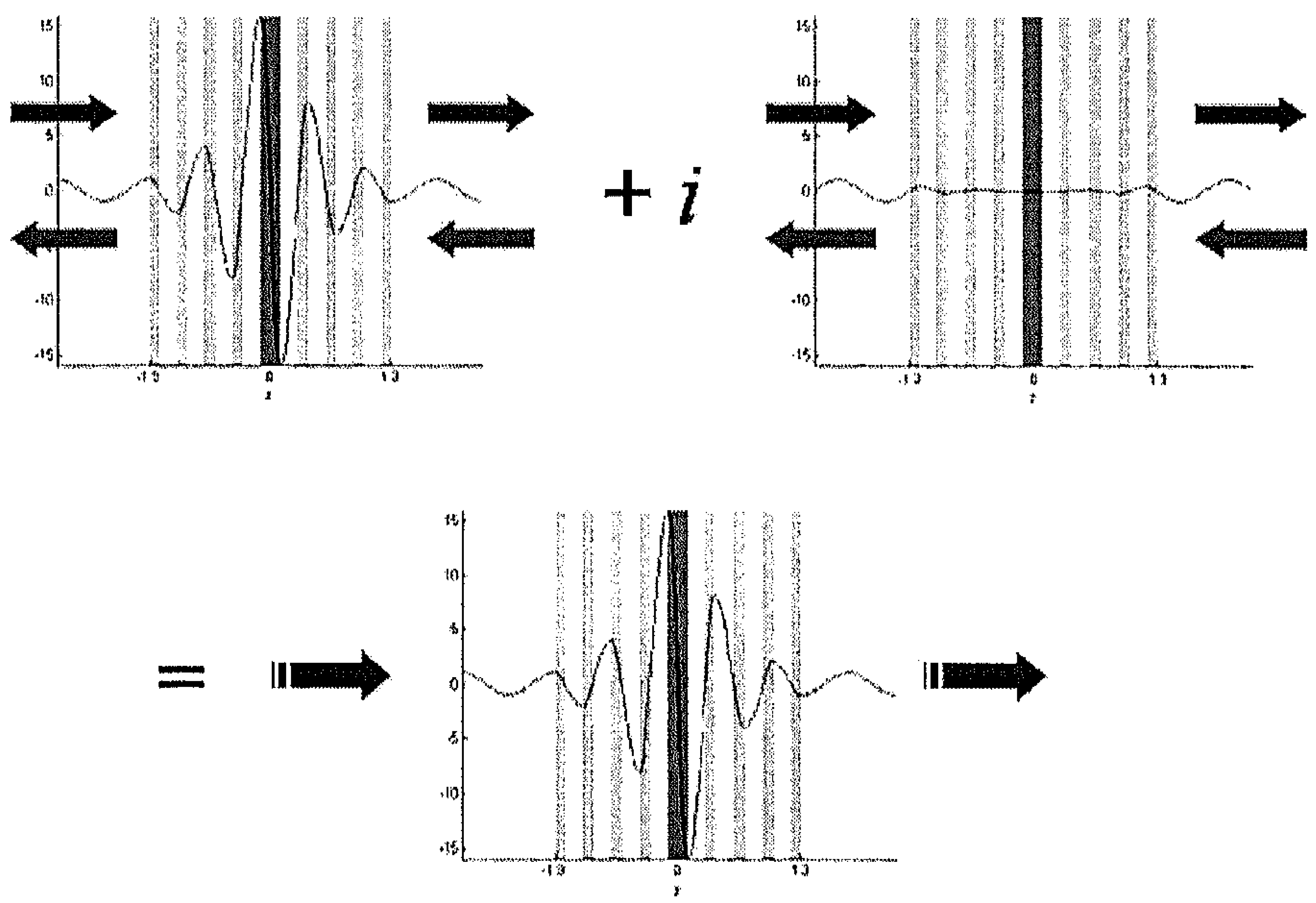

Fig. 8. Construction of the defect mode from complex superposition of the "amplified" and "attenuated" states.

5. Remarks and Conclusions

One-dimensional grating structures as investigated in this paper are simple cases of two and three dimensional photonic structures. The mathematical methods, and the observed phenomena in this paper should therefore be helpful for a further investigation and understanding of these more-dimensional cases.

Concerning the mathematical methods, the use of the optical transfer matrix has proven to be fruitful to decompose the structure and to investigate the problems on successive intervals with effective boundary conditions replacing the optical effect of the adjacent intervals. However, the resulting boundary-value problem, and in particular the eigenvalue problem, is non-standard since the eigenvalue (frequency) to be found appears in a nonlinear, non-algebraic way. Solving such problems is not easy since both *a priori* existence statements, as well as effective (iterative) solution methods, have still to be developed.

The optical phenomena found show an essential difference between the appearance of states and modes. In Sec. 3 it is shown that states can be found as solutions of an eigenvalue problem. For the relatively simple cases to which we restricted ourselves, this eigenvalue problem could be solved by finding a solution of a transcendental equation for the frequency. No specific grating properties are required for their existence. However, in Sec. 4 we showed that a mode, a full-transmitted traveling wave through the structure, corresponds to the existence of two different states, which requires the frequency to satisfy two such equations. Even for symmetric structures, these equations can only be satisfied simultaneously if an accidental degeneracy condition is satisfied, which means that the grating properties should be chosen appropriately. A quarter wavelength stack was shown to be an example that has the desired degeneracy properties, and defect modes were identified.

The findings in this paper can be useful for some applications of optical grating structures. For instance for the design of sensors, when the critical dependence of the defect frequency for a mode is to be used to detect changes in the optical properties in the structure. The existence of multiple states in a defect finite grating could have applications, for instance to construct an optical memory when light influx from both sides can control the change of the state.

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