On Surface Waves in Diffraction Gratings

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Abstract

We discuss the existence criterion of surface waves based on the augmented scattering matrices. Such matrices arise if one takes into account not only oscillating waves but also those which grow (attenuate) in amplitude far from the grating.

A family of planar dielectric gratings with periodic modulation of the refraction index is considered. Asymptotic and numerical analysis of the model are given. We represent various examples of gratings which support (or do not support) surface waves.

Keywords: existence criterion for surface waves, asymptotic and numerical analysis

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1 Introduction

In this paper we discuss the existence of surface waves for a family of diffraction gratings. The asymptotic and numerical analysis is based on using the 'augmented' scattering matrices (ASM) that take into account not only oscillating waves but also waves which grow (attenuate) in amplitude far from the grating.

In terms of the scattering matrices there has been formulated an existence criterion for a surface wave with given order of attenuation. The criterion was obtained in the theory of elliptic boundary value problems in domains with singularities on the boundary [6, 7]. The definition itself of the (augmented) scattering matrices requires some generalizations of the initial notions (of incoming and outgoing waves, etc.). Such generalizations are related to auxiliary boundary value problems (operator pencils) that polynomially depend on a spectral parameter. The spectrum of a pencil can be rather complicated; generally, there are not only eigenvectors but associated vectors as well. The structure of spectrum reflects on the definition of waves. The necessity of the mentioned generalizations manifests itself in full measure, for instance, in problems of elasticity theory (see [8, 7]). All the generalizations were thoroughly discussed in the paper [8] devoted to the development of mathematical tools for the rigorous treatment of Wood's anomalies [14] in electromagnetics and elasticity (see also [7]). The new technique turned out to be of use in the general theory of elliptic boundary value problems in domains with singularities, too. In particular, it provided new statements of the problems with radiation conditions at the singularities [7].

In [1, 2] the aforementioned criterion was put to prove the existence of surface waves for the Helmholtz equation in some domains with periodic boundaries.

In this paper we consider a family of diffraction gratings. For the motivation see discussion of physicists and engineers (for instance, [11, 12, 9, 4, 5, 13, 10]). Dealing with asymptotic analysis, we provide the model with a small positive parameter. The asymptotic and numerical analysis is given to prove the existence (or nonexistence) of surface waves, i.e., nontrivial solutions to the homogeneous problem which exponentially decay far from the grating.

The paper is organized as follows. In Section 2 we give the statement of the problem and formulate the existence criterion for surface waves. The asymptotic analysis is presented in Section 3. Here we use an approach similar to that in [2]. The numerical results are collected in Section 4. Besides, some details are explained in Appendices A and B.

2 Statement of the problem and basic conceptions

2.1 Statement of the problem

First consider a planar dielectric-layer modulated grating (Fig. 2.1).

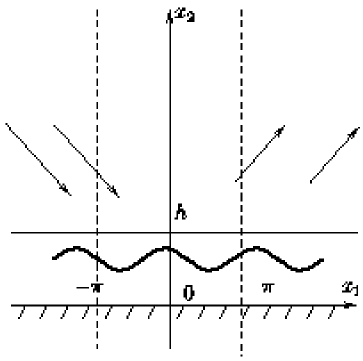

Figure 2.1: Diffraction by a planar dielectric-layer grating.

A wave field w satisfies the Helmholtz equation

$$(\nabla^2 + k^2\chi(x_1, x_2))w(x_1, x_2) = 0 \tag{2.1}$$

for $x_2 > 0$, $x_2 \neq h$; the quasi-periodicity condition

$$\partial^j_{x_1} w(x_1, x_2) = e^{2\pi i\alpha}\partial^j_{x_1} w(x_1 - 2\pi, x_2), \quad j = 0, 1 \tag{2.2}$$

with a constant $\alpha \in (-1/2, 0)$; the contact conditions

$$\begin{aligned} w(x_1, h+0) &= w(x_1, h-0), \\ \partial_{x_2} w(x_1, h+0) &= æ\partial_{x_2} w(x_1, h-0) \end{aligned} \tag{2.3}$$

with constant æ, and the boundary condition

$$\partial_{x_2} w\big|_{x_2=0} = 0 \quad (\text{or } \; w|_{x_2=0} = 0). \tag{2.4}$$

Here k is a wave number, χ is a refraction index such that

$$\chi(x_1, x_2) = \begin{cases} 1, & x_2 > h, \\ \chi_0(x_1, x_2), & 0 < x_2 < h, \end{cases} \tag{2.5}$$

χ_0 being $2\pi-$periodic in x_1. We refer to (2.1)–(2.4) as $\mathcal{N}$-problem (or $\mathcal{D}$-problem).

Let us comment on the statement of the problem. The quasi-periodicity condition (2.2) originates from the corresponding nonhomogeneous problem containing the incident plane wave $u(x_1, x_2) = \exp ik(-x_1 \sin\theta - x_2 \cos\theta)$. Since u satisfies the quasi-periodicity condition with $\alpha = -k\sin\theta$ and the rest characteristics of the problem are 2π-periodic with respect to x_1, it is natural to look for solutions subject to the condition (2.2). To avoid going into nonessential details we consider $\alpha \in (-1/2, 0)$.

2.2 The scattering matrices and the existence criterion for surface waves

In this section we give some results extracted from the general theory (see [6, 7, 8]) and adapted for the problem (2.1)–(2.5).

2.2.1 Waves. The outgoing and incoming subspaces

In view of the quasi-periodicity condition (2.2), the problem can be restricted to the half-strip $\Pi_+ = \{(x_1, x_2) : -\pi < x_1 < \pi,\ 0 < x_2\}$. To describe the behavior of solutions as $x_2 \to \infty$ we need some auxiliary notions. We introduce the equation with spectral parameter λ (that plays the role of the operator pencil mentioned at the beginning of paper):

$$\mathbf{A}(\lambda)v(x_1) := d^2v(x_1)/dx_1^2 + (k^2 - \lambda^2)v(x_1) = 0, \quad -\pi < x_1 < \pi, \tag{2.6}$$

while v is subject to the condition (2.2). The spectrum of the problem (2.6) consists of the eigenvalues $\lambda_n^\pm = \pm(k^2 - (n+\alpha)^2)^{1/2}$, where $n = 0, \pm1, \dots$. To the simple eigenvalue $\lambda_n^\pm \neq 0$ there corresponds the eigenfunction $v_n(x_1) = \exp(i(n+\alpha)x_1)$, i.e., $\mathbf{A}(\lambda_n^\pm)v_n = 0$. If $\lambda_m^\pm = 0$ for some m, then there arises not only the eigenfunction v_m but also the associated function $v_{m,1} = 0$ (i.e., $\mathbf{A}(\lambda_m^\pm)v_m = 0$ and $\mathbf{A}(\lambda_m^\pm)v_{m,1} + \partial_\lambda \mathbf{A}(\lambda_m^\pm)v_m = 0$).

Consider the equation

$$(\nabla^2 + k^2)u(x) = 0 \tag{2.7}$$

in the strip $\Pi = \{x = (x_1, x_2) : -\pi < x_1 < \pi,\ -\infty < x_2 < +\infty\}$ with u subject to the condition (2.2). The eigenvalues of problem (2.6) generate the solutions to the equation (2.7):

$$\mathbf{u}_n^{\pm}(x_1, x_2) = \exp(i\lambda_n^{\pm} x_2) v_n(x_1) \quad \text{for } \lambda_n^{\pm} \neq 0$$

and the two solutions

$$\mathbf{u}_m(x) = v_m(x_1), \quad \mathbf{u}_{m,1}(x) = x_2 v_m(x_1) \quad \text{for } \lambda_m = 0.$$

Denote by $\mathcal{W}_\beta$ the class of functions in Π_+ satisfying (2.2)–(2.4) that admit the estimate $|\partial_x^\sigma u(x)| = O\left(\exp(-\beta x_2)\right)$ as $x_2 \to +\infty$; here β is a real number, $|\sigma| \leqslant 2$, σ being a multi-index (σ_1, σ_2). We choose a positive β so that only the real eigenvalues of the problem (2.6) belong to the strip $\{\lambda : |\mathrm{Im}\lambda| < \beta\}$.

The functions in $\mathcal{W}_{-\beta}$ that satisfy the homogeneous problem (2.1)–(2.5) in the half-strip Π_+ up to a term of order $O\left(\exp(-\beta x_2)\right)$ are called waves. By definition, two waves w and w' are equivalent, if $w - w' \in \mathcal{W}_\beta$. It turns out that any wave w admits the representation

$$w = \eta \left(\sum c_n^{\pm} \mathbf{u}_n^{\pm} + c_m \mathbf{u}_m + c_{m,1} \mathbf{u}_{m,1} \right) + u', \tag{2.8}$$

where $u' \in \mathcal{W}_\beta$, η is a cut-off function (i.e., smooth function such that $0 \leqslant \eta \leqslant 1$, $\eta = 0$ for $x_2 < h + 1$, and $\eta = 1$ for $x_2 \geqslant h + 2$); in the braces, the summation is over all real nonzero eigenvalues of the problem (2.6) while the two last terms arise if zero is an eigenvalue; finally, $c_n^{\pm}$, c_m, and $c_{m,1}$ are some constant coefficients (depending on w). Thus, waves are equivalent if and only if there coincide the corresponding expressions in braces in (2.8). In what follows we do not discriminate equivalent waves and by a "wave" we mean any of them. Then the space of waves becomes finite dimensional (in other words, we deal with the quotient space of waves modulo $\mathcal{W}_\beta$). Its dimension is always even and equal to the total multiplicity $2T$ of all real eigenvalues of the problem (2.6).

We now choose a basis in the space of waves subject to some orthogonality and normalization conditions. To this end it is convenient to use the Green formula

$$\begin{aligned} &æ \int_{\{x \in \Pi_+ : 0 < x_2 < h\}} (\Delta u \overline{v} - u \Delta \overline{v})\, dx + \int_{\{x \in \Pi_+ : h < x_2 < R\}} (\Delta u \overline{v} - u \Delta \overline{v})\, dx = \\ &\quad = \int_{-\pi}^{\pi} \left([æ\partial_{x_2} u]|_{x_2 = h} \overline{v}(x_1, h) - u(x_1, h) [æ\partial_{x_2} \overline{v}]|_{x_2 = h} \right) dx_1 + \\ &\quad\quad + \int_{-\pi}^{\pi} (\partial_{x_2} u \overline{v} - u \partial_{x_2} \overline{v})|_{x_2 = R}\, dx_1 - æ \int_{-\pi}^{\pi} (\partial_{x_2} u \overline{v} - u \partial_{x_2} \overline{v})|_{x_2 = 0}\, dx_1. \end{aligned}$$

(We supposed that u and v satisfy (2.2) and (2.3).) Let u and v be waves. By virtue of the conditions (2.3) and (2.4) we have

$$\begin{aligned} &æ \int_{\{x \in \Pi_+ : 0 < x_2 < h\}} (\Delta u \overline{v} - u \Delta \overline{v})\, dx + \int_{\{x \in \Pi_+ : h < x_2 < R\}} (\Delta u \overline{v} - u \Delta \overline{v})\, dx = \\ &\qquad = \int_{-\pi}^{\pi} (\partial_{x_2} u \overline{v} - u \partial_{x_2} \overline{v})|_{x_2 = R}\, dx_1. \end{aligned} \tag{2.9}$$

In view of (2.8) the right-hand side of (2.9) has a finite limit as $R \to \infty$. The limit can be explicitly calculated in terms of the coefficients of u and v in (2.8). Denote by $q(u, v)$ the left-hand side in (2.9) with $R = +\infty$. It is invariant under changes of the waves u and v for equivalent ones.

For the eigenvalues $\mu^{\pm} = \pm(k^2 - (n+\alpha)^2)^{1/2} \neq 0$ of the problem (2.6) we introduce the solutions to the equation (2.7) in the strip Π

$$w^{\pm} = (4\pi|\mu^{\pm}|)^{-1/2} e^{i\mu^{\pm} x_2} \exp(i(n+\alpha)x_1). \tag{2.10}$$

For $\mu^{\pm} = 0$, i.e., in the case $k^2 = (n+\alpha)^2$ we introduce solutions

$$w^0(x) = (2\pi)^{-1/2} \exp\left(i(n+\alpha)x_1\right),$$
$$\tilde{w}^0(x) = (2\pi)^{-1/2} x_2 \exp\left(i(n+\alpha)x_1\right).$$

We now provide the eigenvalues with new numbers in order to simplify notations in what follows. Let $\lambda_1 < \cdots < \lambda_T \leqslant \lambda_{T+1} < \cdots < \lambda_{2T}$ be all the real eigenvalues of the problem (2.6). If 0 is an eigenvalue, then $\lambda_T = \lambda_{T+1}$, otherwise $\lambda_T < 0 < \lambda_{T+1}$. By w_j we denote the function (2.10) corresponding to the eigenvalue $\mu = \lambda_j \neq 0$. If zero is an eigenvalue we put

$$\begin{aligned} w_T(x) &= w^0(x), \\ w_{T+1}(x) &= \tilde{w}^0(x). \end{aligned} \tag{2.11}$$

Let us write $u \sim w$ for a wave u with asymptotics w (i.e., w is the expression in braces in the representation (2.8) for u). We define the waves

$$\begin{aligned} u_j^+ &\sim w_j, & j &= 1, \ldots, T, \\ u_j^- &\sim w_{2T-j+1}, & j &= 1, \ldots, T, \end{aligned} \tag{2.12}$$

provided zero is not an eigenvalue of (2.6). Otherwise, j runs from 1 to $T-1$ and

$$u_T^{\pm} \sim \frac{1}{\sqrt{2}}(w_T \mp i w_{T+1}). \tag{2.13}$$

It is easy to verify the equalities

$$\begin{aligned} q(u_j^-, u_l^-) &= +i\delta_{j\,l}, \\ q(u_j^+, u_l^+) &= -i\delta_{j\,l}, \\ q(u_j^-, u_l^+) &= 0. \end{aligned} \tag{2.14}$$

The subspace of waves spanned by u_j^+ (u_j^-) we call the incoming (outgoing) subspace. Its elements are called incoming (outgoing) waves.

2.2.2 The scattering matrix

Considering solutions that belong to the class $\mathcal{W}_\beta$, we denote the problem (2.1)–(2.4) by $A(\beta)$ (for any real β). Let $\ker A(\beta)$ stand for the space of all solutions to the homogeneous problem (2.1)–(2.4). As before, we assume that a positive β is small so that the strip $\{\lambda : |\text{Im}\lambda| < \beta\}$ may contain only the real eigenvalues of the problem (2.6). As was shown in [6] (see also [7]) dim ker$A(-\beta)/\mathcal{W}_\beta = T$. In other words, there exist T solutions to the problem linearly independent modulo $\mathcal{W}_\beta$. Moreover, one can choose $Y_1, \dots, Y_T$ in ker$A(-\beta)$ such that

$$Y_m \sim u_m^+ + \sum_{n=1}^{T} s_{mn} u_n^- \quad \text{for } m = 1, \dots, T. \tag{2.15}$$

The matrix s is unitary and is called the scattering matrix.

A few words on the definitions of waves and the scattering matrix. We emphasize that the waves $u_T^\pm$ in (2.13), too, are considered as incoming or outgoing. Therefore, one can state the problems with radiation conditions and define the scattering matrix even at the threshold values of the parameter k. In particular, such a "threshold" scattering matrix was used in [1] to describe the asymptotic behavior of the scattering matrix near the threshold. It will be of use in what follows (for the same purpose).

2.2.3 The augmented scattering matrix

To define the matrix we introduce into consideration the waves corresponding to the imaginary eigenvalues of problem (2.6). Let $\lambda_{T+1}^\pm, \lambda_{T+2}^\pm, \dots$ stand for these eigenvalues numbered so that $\text{Im}\lambda_j^+ > 0$, $\text{Im}\lambda_{T+1}^+ < \text{Im}\lambda_{T+2}^+ < \dots$, and $\lambda_j^+ = -\lambda_j^-$. To every $\lambda_j^\pm$ we associate the solution $w_j^\pm$ of the problem (2.7) defined by (2.2.1). Let γ be a positive number different from $\text{Im}\lambda_j^\pm$, $j = T+1, T+2, \dots$, and such that $0 < \beta < \gamma$, β being chosen above. Assume that $\lambda_j^\pm$ for $j = T+1, \dots, M$ are all the eigenvalues of problem (2.6) that satisfy $\beta < |\text{Im}\lambda_j^\pm| < \gamma$.

A function $u \in \mathcal{W}_{-\gamma}$ is called a wave if

$$u = \eta \left[\sum_{j=1}^{2T} c_j w_j + \sum_{j=T+1}^{M} (c_j^+ w_j^+ + c_j^- w_j^-) \right] + u', \tag{2.16}$$

where $u' \in \mathcal{W}_\gamma$, $c_j, c_j^\pm$ are some constant coefficients, and η is the same cut-off function as in (2.8). By definition, waves u, v are equivalent, i.e., $u \sim v$, if $u - v \in \mathcal{W}_\gamma$. We do not distinguish equivalent waves. The dimension of the space of waves is equal to $2M$. Put

$$u_j^\pm \sim 2^{-1/2}(w_j^+ \mp i w_j^-), \quad j = T+1, \dots, M. \tag{2.17}$$

The waves $u_j^\pm$, $j = 1, \dots, M$, defined by (2.12), (2.13), and (2.17) satisfy the relation (2.14). The u_j^+ and u_j^- are called incoming and outgoing waves, respectively. There holds the equality dim ker$A(-\gamma) = M$. One can choose elements $Y_1, \dots, Y_M$ in the space ker$A(-\gamma)$ such that

$$Y_m \sim u_m^+ + \sum_{n=1}^{M} S_{mn} u_n^-, \quad m = 1, \dots, M. \tag{2.18}$$

The matrix S depending on γ is called the augmented scattering matrix (ASM).

2.2.4 The existence criterion of surface waves

Any function $u \in \ker A(\gamma)$ with positive γ is said to be a surface wave. In other words, u satisfies the problem (2.1)–(2.4) and admits the estimate $u = O(\exp(-\gamma x_2))$ as $x_2 \to +\infty$.

Let $0 < \gamma^1 < \gamma^2$ and let γ^j differ from $\mathrm{Im}\lambda^+_{T+q}$, $q = 1, 2, \ldots$. The ASM defined for $A(-\gamma^j)$ will be denoted by S_{γ^j}. Assume that S_{γ^j} is of size $M_j \times M_j$. It is obvious that $M_2 \geq M_1$.

We write S_{γ^2} in the form

$$S_{\gamma^2} = \|S_{(ij)}\|_{i,j=1,2},$$

where the block $S_{(22)}$ is of size $(M_2 - M_1) \times (M_2 - M_1)$.

The existence criterion for surface waves reads

$$\dim\,\ker A(\gamma^1) - \dim\,\ker A(\gamma^2) = \dim\,\ker(S_{(22)} - 1). \tag{2.19}$$

We comment on (2.19). If $\dim\,\ker(S_{(22)} - 1) > 0$, then there exists $u \in \ker A(\gamma^1) \setminus \ker A(\gamma^2)$. Thus u is a surface wave that admits the estimate $u = O(\exp(-\gamma^1 x_2))$ and does not satisfy $u = O(\exp(-\gamma^2 x_2))$. In particular, put $\gamma^1 = \beta > 0$, where β is the sufficiently small number chosen above. If one can take $\gamma^2 > \beta$ such that

$$\dim\,\ker(S_{(22)} - 1) \neq 0, \tag{2.20}$$

then one proves the existence of a surface wave.

3 Asymptotic analysis of the problem

3.1 Model with a small parameter

In order to make the problem (2.1)–(2.4) available for asymptotic analysis we introduce a small parameter ε into the model. We assume that a wave field satisfies the equation

$$\left(\nabla^2 + k^2(\varepsilon)\chi(x_1, x_2, \varepsilon)\right) w(x_1, x_2, \varepsilon) = 0 \tag{3.1}$$

for $x_2 > 0$, $x_2 \neq h(\varepsilon)$; the quasi-periodicity condition (2.2); the contact conditions

$$\begin{gathered} w(x_1, h(\varepsilon) + 0, \varepsilon) = w(x_1, h(\varepsilon) - 0, \varepsilon), \\ \frac{\partial w(x_1, h(\varepsilon) + 0, \varepsilon)}{\partial x_2} = æ\frac{\partial w(x_1, h(\varepsilon) - 0, \varepsilon)}{\partial x_2}, \end{gathered} \tag{3.2}$$

and the boundary condition (2.4). Furthermore,

$$\chi(x_1, x_2, \varepsilon) = \begin{cases} 1, & x_2 > h(\varepsilon), \\ N(\varepsilon) + a\cos(x_1) + b\cos(2x_1), & 0 < x_2 < h(\varepsilon)\,, \end{cases} \tag{3.3}$$
$$|a| + |b| \leqslant 1\,.$$

We suppose that

$$\begin{aligned} k^2(\varepsilon) &= (n + \alpha)^2 - \Lambda^2\varepsilon^4 + \ldots, \\ h(\varepsilon) &= h_1\varepsilon + \ldots, \\ N(\varepsilon) &= 1 + N_1\varepsilon + \ldots, \end{aligned} \tag{3.4}$$

where $n = 0, \pm 1, \pm 2, \dots$. The first asymptotic expansion (for k^2) is in powers of ε^4 while the two other expansions are in powers of ε.

We now explain the expansion (3.4) for $k^2(\varepsilon)$. The asymptotics of solutions to the problem (2.1)–(2.4) (as $x_2 \to \infty$) changes its form at the points $k^2 = (n+\alpha)^2$ which are called the thresholds. So it is convenient to consider $k^2(\varepsilon)$ as a perturbation of a threshold value. The scattering matrices will be defined in terms of solutions to the problem (2.1)–(2.4) subject to some orthogonality and normalization conditions. Such solutions depend on the parameter $(k^2 - (n+\alpha)^2)^{1/4}$ that can be taken as a natural small parameter in the problem, i.e., we assume that $(k^2(\varepsilon) - (n+\alpha)^2)^{1/4} = O(\varepsilon)$.

There is another hint at the expansions (3.4). It is known that if $a = 0$, $b = 0$ in (2.5) and the dispersion relation

$$\sqrt{\alpha^2 - k^2} = æ \begin{cases} -\sqrt{k^2N - \alpha^2}(\tan h\sqrt{k^2N - \alpha^2})^{-1} & \text{for } \mathcal{D}\text{-problem at } x_2 = 0, \\ \sqrt{k^2N - \alpha^2}\, \tan h\sqrt{k^2N - \alpha^2} & \text{for } \mathcal{N}\text{-problem at } x_2 = 0 \end{cases} \tag{3.5}$$

holds then, generally, there can exist surface waves. (They always exist for the $\mathcal{N}$-problem and arise for the $\mathcal{D}$-problem, too, under some additional condition.) Near the threshold $k = |\alpha|$ the relation (3.5) admits a solution of the form $k = |\alpha| - k_4\varepsilon^4 + \dots$ with $k_4 = |\alpha|(\alpha N_1 h_1)^2/2$ for any N_1 and h_1.

In what follows we restrict ourselves to considering the case $k^2(\varepsilon) = (1+\alpha)^2 - \Lambda^2\varepsilon^4$ with small positive ε. In other words, we deal with $k^2(\varepsilon)$ close to the threshold value $k^2(0) = (1+\alpha)^2$.

Moreover, we look for a surface wave in $\ker A(\beta) \setminus \ker A(\gamma)$ with a positive β and γ such that $\beta < \gamma$ while the strip $0 \le \mathrm{Im}\lambda < \beta$ contains two eigenvalues of the problem (2.6), and only one eigenvalue belongs to the strip $\beta \le \mathrm{Im}\lambda < \gamma$. Thus, the augmented scattering matrix is of size 2×2 and the existence criterion reads

$$S_{22}(\varepsilon) = 1. \tag{3.6}$$

Since $S(\varepsilon)$ is unitary, this is equivalent to the equations

$$S_{12}(\varepsilon) = 0, \;\; \mathrm{Im} S_{22}(\varepsilon) = 0\,. \tag{3.7}$$

3.2 Contrast dielectric grating

First we consider the case of a contrast dielectric grating under the assumptions that in (3.3) we have $b = 0$, $N(\varepsilon)$ is equal to N and is independent of ε while $N \neq 1$ (which is contrary to the last expansion (3.4)). One can show that in the $\mathcal{N}-$problem

$$\begin{aligned} S_{12}(\varepsilon) &= \varepsilon \frac{(i-1)\sqrt{\Lambda/2}\, a}{(1+2\alpha)^{1/4}(N-1)} + O(\varepsilon^2), \\ S_{22}(\varepsilon) &= i + \varepsilon \frac{2\Lambda}{h_1 æ(1+\alpha)^2(N-1)} + O(\varepsilon^2). \end{aligned} \tag{3.8}$$

It means that $S_{22}(\varepsilon) \neq 1$, and there is no surface wave. We dropped details of the analysis because they are similar to the reasons given below.

Note that in the $\mathcal{D}-$problem we have

$$S_{12}(\varepsilon) = O(\varepsilon^2),$$
$$S_{22}(\varepsilon) = i + O(\varepsilon^3),$$

which leads to the same conclusion.

3.3 Weakly contrast grating

The formulae (3.8) are valid provided $N - 1 \neq 0$. In the case $N(\varepsilon) - 1 = O(\varepsilon)$ as $\varepsilon \to 0$, the grating is called weakly contrast. We now assume there hold the expansions (3.4) and seek the asymptotics of $S_{22}(\varepsilon)$ as $\varepsilon \to 0$.

For the same γ as in Section 2.1 we consider two problems $A_0(\gamma)$ and $A(\gamma)$. Here $A_0(\gamma)$ stands for the problem (3.1)–(3.3), where $k^2 = (1+\alpha)^2$. Emphasize that $A_0(\gamma)$, too, depends on ε in accordance with (3.1)–(3.3).

Let $S(\varepsilon)$ be the augmented scattering matrix for $A(\gamma)$ and $s(\varepsilon)$ is the scattering matrix for $A_0(\gamma)$. The asymptotics of $S(\varepsilon)$ as $\varepsilon \to 0$ will be found in two steps. First we describe the connection between $S(\varepsilon)$ and $s(\varepsilon)$. After that we derive the asymptotics of $s(\varepsilon)$. To compare $S(\varepsilon)$ and $s(\varepsilon)$ we consider the basis $\{Y_1, Y_2\}$ in $\ker A(-\gamma)$ (see 2.15). Then we express the basis waves $u_j^{\pm}$ corresponding to $A(-\gamma)$ by means of those corresponding to $A_0(-\gamma)$.

We need some new notation. Let $U_j^{\pm}$, $j = 1, 2$, denote the solutions to the equation (2.7) with $k^2 = (1+\alpha)^2 - \Lambda^2\varepsilon^4$ defined by

$$U_1^{\pm}(x_1, x_2) = \frac{1}{\sqrt{4\pi|\lambda_0^{\pm}|}} \exp\{i\alpha x_1 \mp i(1 + 2\alpha - \Lambda^2\varepsilon^4)^{1/2} x_2\} \tag{3.9}$$

with $\lambda_0^{\pm}(\varepsilon) = \pm\sqrt{k^2(\varepsilon) - \alpha^2}$ and

$$U_2^{\pm}(x_1, x_2) = \frac{1}{\sqrt{4\pi|\lambda_1^{\pm}|}} \exp\{i(1+\alpha)x_1\}[e^{-\Lambda\varepsilon^2 x_2} \mp i e^{\Lambda\varepsilon^2 x_2}] \tag{3.10}$$

with $\lambda_1^{\pm}(\varepsilon) = \pm\sqrt{k^2(\varepsilon) - (1+\alpha)^2}$. From now on by $u_j^{\pm}$, $j = 1, 2$, we denote the solutions of equation (2.7) with $k^2 = (1+\alpha)^2$ defined by

$$\begin{aligned} u_1^{\pm}(x_1, x_2) &= \frac{1}{\sqrt{4\pi|\lambda_0^{\pm}(0)|}} \exp\{i\alpha x_1 \mp i(1+2\alpha)^{1/2} x_2\}, \\ u_2^{\pm}(x_1, x_2) &= \frac{1}{\sqrt{4\pi}} \exp\{i(1+\alpha)x_1\}(1 \mp i x_2). \end{aligned} \tag{3.11}$$

We have

$$\begin{aligned} (2\Lambda)^{1/2}\varepsilon(1 \pm i)U_2^{\pm}(x_1, x_2, \varepsilon) &= u_2^{+}(x_1, x_2) + u_2^{-}(x_1, x_2) \pm \\ &\pm \Lambda\varepsilon^2(u_2^{+}(x_1, x_2) - u_2^{-}(x_1, x_2)) + O(\varepsilon^4 x_2^2), \\ U_1^{\pm}(x_1, x_2, \varepsilon) &= u_1^{\pm}(x_1, x_2) + O(\varepsilon^4 x_2^2). \end{aligned} \tag{3.12}$$

The element Y_2 in the basis of $\ker A(-\gamma)$ takes the form

$$Y_2(x_1,x_2,\varepsilon) = \frac{u_2^+}{\varepsilon}\left[\frac{1+\Lambda\varepsilon^2}{(2\Lambda)^{1/2}(1+i)} + S_{22}(\varepsilon)\frac{1-\Lambda\varepsilon^2}{(2\Lambda)^{1/2}(1-i)}\right] + \\ + \frac{u_1^-}{\varepsilon}\varepsilon S_{12}(\varepsilon) + \frac{u_2^-}{\varepsilon}\left[\frac{1-\Lambda\varepsilon^2}{(2\Lambda)^{1/2}(1+i)} + S_{22}(\varepsilon)\frac{1+\Lambda\varepsilon^2}{(2\Lambda)^{1/2}(1-i)}\right] + \dots, \quad (3.13)$$

where the dots stand for a term that is $O\left(e^{-\gamma x_2}\right)$ uniformly with respect to ε. This expression hints that we should compare Y_2 with an element in $\ker A_0(-\gamma)$ of the form

$$\eta(x_1,x_2,\varepsilon) = \varepsilon^{-1}u_2^+(x_1,x_2) + \varepsilon^{-1}u_1^-(x_1,x_2)s_{12}(\varepsilon) + \\ + \varepsilon^{-1}u_2^-(x_1,x_2)s_{22}(\varepsilon) + \dots, \quad (3.14)$$

where the dots are of the same sense as in (3.13). Combining (3.13) and (3.14), we obtain the equalities

$$\frac{\varepsilon S_{12}(\varepsilon)}{\left(\frac{1+\Lambda\varepsilon^2}{(2\Lambda)^{1/2}(1+i)} + S_{22}(\varepsilon)\frac{1-\Lambda\varepsilon^2}{(2\Lambda)^{1/2}(1-i)}\right)} = s_{12}(\varepsilon) + O(\varepsilon^4\log^2\varepsilon) \quad (3.15)$$

and

$$\frac{\left(\frac{1-\Lambda\varepsilon^2}{(2\Lambda)^{1/2}(1+i)} + S_{22}(\varepsilon)\frac{1+\Lambda\varepsilon^2}{(2\Lambda)^{1/2}(1-i)}\right)}{\left(\frac{1+\Lambda\varepsilon^2}{(2\Lambda)^{1/2}(1+i)} + S_{22}(\varepsilon)\frac{1-\Lambda\varepsilon^2}{(2\Lambda)^{1/2}(1-i)}\right)} = s_{22}(\varepsilon) + O(\varepsilon^4\log^2\varepsilon). \quad (3.16)$$

We now turn to the asymptotics of $s_{12}(\varepsilon)$ and $s_{22}(\varepsilon)$ as $\varepsilon\to 0$. We seek it in the form

$$s_{12}(\varepsilon) = s_{12}^0 + \varepsilon s_{12}^1 + \varepsilon^2 s_{12}^2 + \dots, \qquad s_{22}(\varepsilon) = s_{22}^0 + \varepsilon s_{22}^1 + \varepsilon^2 s_{22}^2 + \dots. \quad (3.17)$$

Represent η as the asymptotic series

$$\eta(x_1,x_2,\varepsilon) = \varepsilon^{-1}\sum_{m=0}^{\infty}\zeta_m\left(x_1,\frac{x_2}{\varepsilon}\right)\varepsilon^m \quad \text{for } 0\le x_2\le\varepsilon h \\ \eta(x_1,x_2,\varepsilon) = \varepsilon^{-1}\sum_{m=0}^{\infty}\eta_m(x_1,x_2)\,\varepsilon^m \quad \text{for } x_2\ge\varepsilon h \quad (3.18)$$

Using the procedure of matched asymptotic expansions (see Appendix A), we arrive at the relations

$$s_{12}(\varepsilon) = -2i\varepsilon Q + O(\varepsilon^2), \\ s_{22}(\varepsilon) = 1 - 2\varepsilon^2 P + O(\varepsilon^3), \quad (3.19)$$

where

$$Q = -h_1\text{æ}\frac{(1+\alpha)^2}{(1+2\alpha)^{1/4}}\frac{a}{2}, \\ P = |Q|^2 - ih_1\text{æ}(1+\alpha)^2\left(h_1\text{æ}\frac{(1+\alpha)^2}{(3+2\alpha)^{1/2}}\frac{a^2}{4} + N_1 + \right. \\ \left. + h_1\text{æ}(1+\alpha)^2\frac{b^2}{4}\left(\frac{1}{(4|\alpha|)^{1/2}} + \frac{1}{(8+4\alpha)^{1/2}}\right)\right). \quad (3.20)$$

Taking into account (3.19) and (3.15), (3.16),

$$
\begin{aligned}
S_{12}(\varepsilon) &= \frac{(8\Lambda)^{1/2}}{i-1}\frac{Q}{\Lambda+P} + O(\varepsilon),\\
S_{22}(\varepsilon) &= (-i)\frac{\Lambda-P}{\Lambda+P} + O(\varepsilon).
\end{aligned}
\tag{3.21}
$$

3.4 Verification of the equality $S_{22} = 1$

Since $\mathrm{Re}S_{22} > 0$ due to $\Lambda \mathrm{Im} P < 0$, it is sufficient to check the solvability of the system consisting of the two equations in (3.7). We rewrite the system in the form

$$
\begin{aligned}
Q &= \Phi_1(Q, \Lambda, \varepsilon),\\
\Lambda &= \Phi_2(Q, \Lambda, \varepsilon)
\end{aligned}
\tag{3.22}
$$

with

$$
\begin{aligned}
\Phi_1(Q, \Lambda, \varepsilon) &= Q - \frac{i-1}{(8\Lambda)^{1/2}}(\Lambda+P)S_{12}(\varepsilon),\\
\Phi_2(Q, \Lambda, \varepsilon) &= \Lambda + \frac{\mathrm{Im}\{S_{22}(\varepsilon)\}}{2|P|}((\Lambda+|Q|^2)^2 + |\mathrm{Im}P|^2).
\end{aligned}
$$

The asymptotics of $S(\varepsilon)$ as $\varepsilon \to 0$ enables us to show the mapping $(Q, \Lambda) \to \Phi(Q, \Lambda, \varepsilon)$ is a contraction (uniformly with respect to ε) in a neighborhood of the point $(0, |P|)$. Moreover, the disk centered at $(0, |P|)$ with radius of $O(\varepsilon)$ is sent into itself by the mapping Φ. Hence there exists a fixed point (Q^*, Λ^*) of the mapping. It is clear that

$$
|Q^*| + |\Lambda^* - |P|| = O(\varepsilon). \tag{3.23}
$$

The existence of the fixed point implies the existence of a surface wave. From the relations (3.20) and (3.23) it follows that the surface wave arises for the grating with coefficient a in (3.3) vanishing as $\varepsilon \to 0$. The coefficient b in (3.3) may be chosen arbitrarily; the point $(0, |P|)$ depends on b in accordance with (3.20).

4 Rigorous coupled wave approach: analysis and numerical results

In this section we discuss a numerical implementation of the existence criterion. We examine numerically the function

$$
\det(S_{(22)} - 1) \tag{4.1}
$$

depending on all parameters of the problem. Recall that the block $S_{(22)}$ is of size $(M-T) \times (M-T)$, where $2T$ is the number of real eigenvalues of the problem (2.6) and $2M$ is the total number of eigenvalues of the same problem in the strip $|\mathrm{Im}\lambda| < \gamma$ (see Section 2.2.4).

The manifold(s) in the parameter's space at which the function (4.1) vanishes for some M corresponds to surface waves. The trivial case of such a manifold arises if the function χ_0 in (2.5) is a constant and the rest parameters are constrained by the dispersion relation (3.5).

In what follows we present some numerical results concerning non-trivial cases of arising of surface waves. We examine the planar grating model (2.1)–(2.5) with the periodic modulation which admits the rigorous coupled wave approach (see Appendix B.1).

The function (4.1) can also have local minima which are close to zero. The waves whose asymptotics as $x_2 \to \infty$ contain growing exponents with small coefficients arise if the parameters belong to a neighborhood of such a minimum. Such waves are called "quasi-surface waves". Apparently, in applications these waves are of the same importance as the "pure" surface waves. We also discuss the example of such kind.

To be specific, we consider the $\mathcal{N}$-problem only and assume that the constant æ is equal to one.

4.1 Numerical results related to the model (3.3)–(3.4)

First consider ASM corresponding to the same numbers $0 < \gamma < \beta$ as in Section 3, i.e., $S_{(12)}$ and $S_{(22)}$ are scalars. Fig. 4.1 shows comparison of the asymptotic results (3.21) with the numerics.

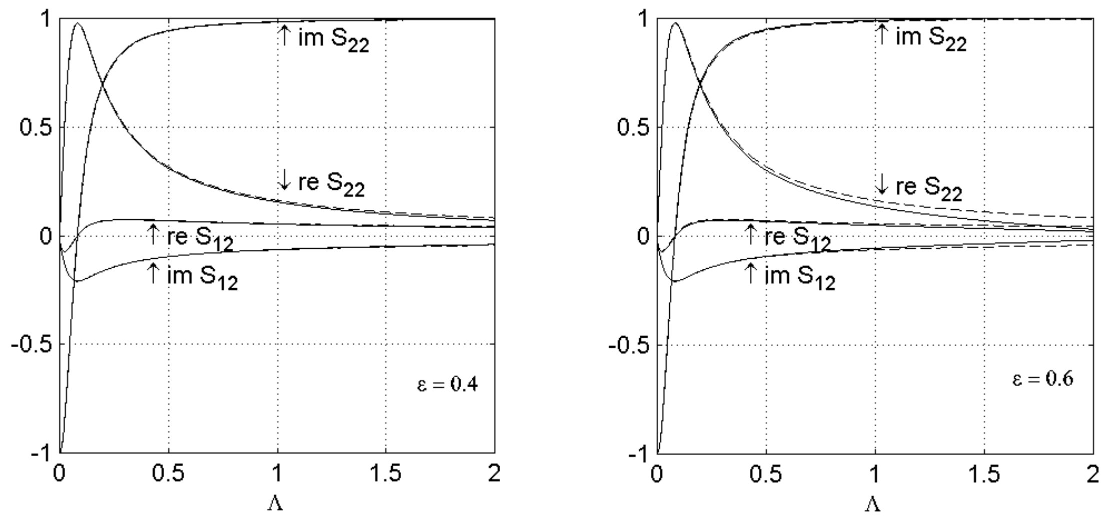

Figure 4.1: Entries of ASM as functions of Λ for the model (3.3)–(3.4): comparison of numerical results (solid lines) with the asymptotic formulas (3.21) (dashed lines) for different ε-s. *Other parameters:* $a = 1$, $b = 1$, $N_1 = 1$, $h_1 = 0.1$, $\alpha = -0.1$.

Figure 4.2 shows the function (4.1) depending on a and Λ while $b = 0$. The rest parameters are fixed.

It is seen that the function (4.1) is close to zero in a neighborhood of the point $(0, |P|)$ (see (3.20) and Section 3.4). This coincides with the results of the asymptotic analysis of Section 3. However, the fixed point of the contraction (3.22) is $(0, P^*)$: the function (4.1) has no zeros if $a \neq 0$ (see the right-hand part of Fig. 4.2). Therefore, only the trivial case of the existence of surface waves is observed in this example.

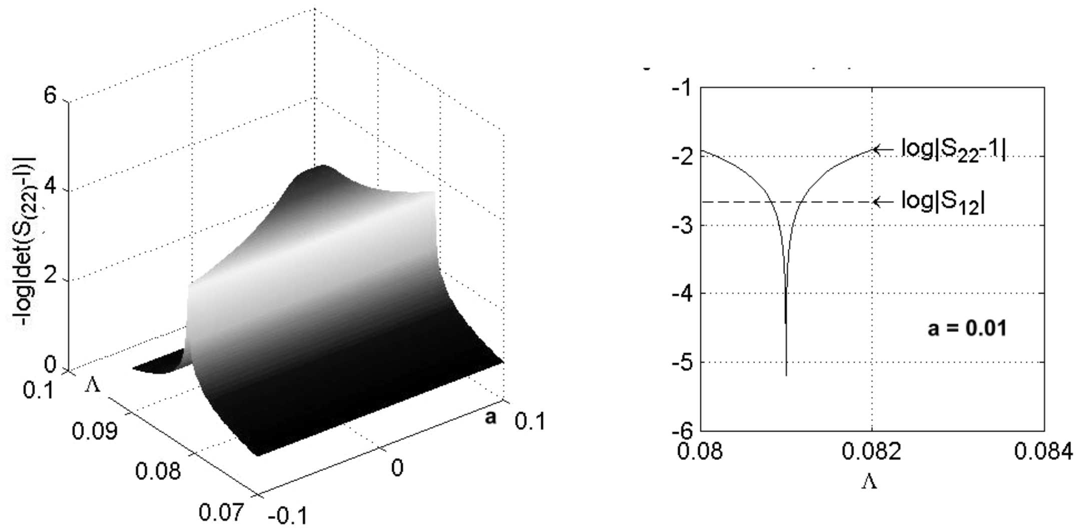

Figure 4.2: *Left:* The surface of logarithm (with the minus sign) of the module of function (4.1) for the model (3.3)–(3.4) depending on a and Λ; *Right:* The cross-section of this surface by the plane $a = 0.01$ (solid line), dashed line shows $\log|S_{12}(\Lambda)||_{a=0.01}$. *Other parameters:* $b = 0$, $\varepsilon = 0.01$, $N_1 = 1$, $h_1 = 0.1$, $\alpha = -0.1$.

Now apply the numerical approach to the problem more general then (3.3)–(3.4). Namely, let in (3.3)

$$\chi(x_1, x_2, \varepsilon) = N(\varepsilon) + a\cos(x_1) + b\cos(2x_1) + \sum_{j=3}^{6} c_j \cos(jx_1) \tag{4.2}$$

for $0 < x_2 < h(\varepsilon)$. Fig. 4.3 shows numerical evidences of the existence of surface waves for $a = 0$ provided one of the Fourier coefficients b, c_3, c_4 differs from zero. It is seen that the real and imaginary parts of the function (4.1) vanish simultaneously. This implies the existence of a surface wave.

Fig. 4.4 shows the location of curves in the plane of parameters which correspond to zeros of the function (4.1), i.e., to surface waves. In the left-hand part of this figure the parabolic line in the plane (b, Λ) is seen. This parabolic line is in agreement with the formula (3.20) of the asymptotic analysis in Section 3.3. The right-hand part of the same figure shows that a surface wave arises under a similar dependence between Λ and one of the other Fourier coefficients (say, c_4) in (4.2).

In Section 3 we did not work with the situation where the block $S_{(11)}$ of ASM was of size T greater than one. Now we discuss numerical results related to certain cases with $T > 1$ (see Fig. 4.5 and Fig. 4.6).

In Fig. 4.5 a few examples showing the non-vanishing behaviour of the function (4.1) depending on Λ are listed. In all these examples the size T of the block $S_{(11)}$ of ASM is greater than or equal to the number R of the first non-zero coefficient in the Fourier expansion of the periodic modulation. The natural hypothesis is there are no surface waves in this case. Fig. 4.6 shows two examples corresponding to the inequality $T < R$: every of them manifests the existence of surface waves.

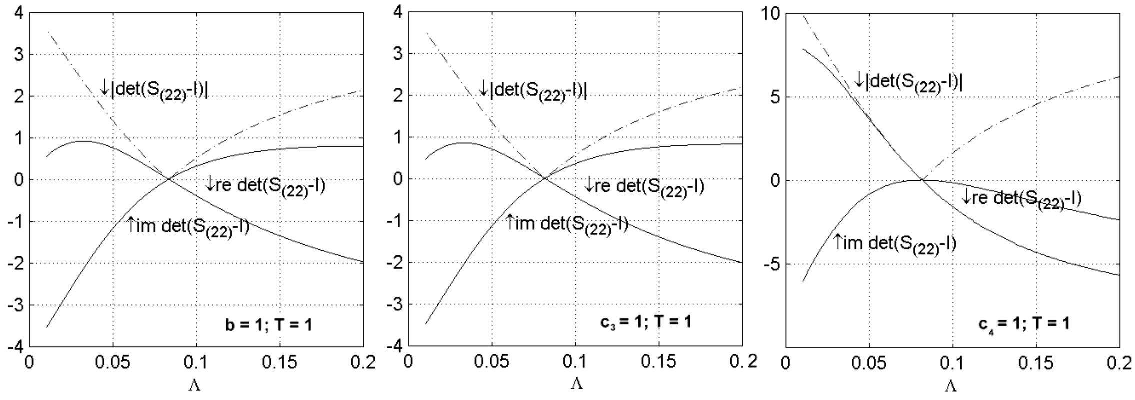

Figure 4.3: The function (4.1) for the model (3.4), (4.2) depending on Λ; the solid lines are used for the real and imaginary parts of this function, the dashed line shows its module. *Left:* $b = 1$, $c_j = 0$, $j = 3, \dots, 6$; *Middle:* $b = 0$, $c_3 = 1$, $c_j = 0$, $j = 4, 5, 6$; *Right:* $b = 0$, $c_4 = 1$, $c_j = 0$, $j = 3, 5, 6$; *Other parameters:* $\varepsilon = 0.01$, $N_1 = 1$, $h_1 = 0.1$, $\alpha = -0.1$, $a = 0$, $T = 1$, $M - T = 4$.

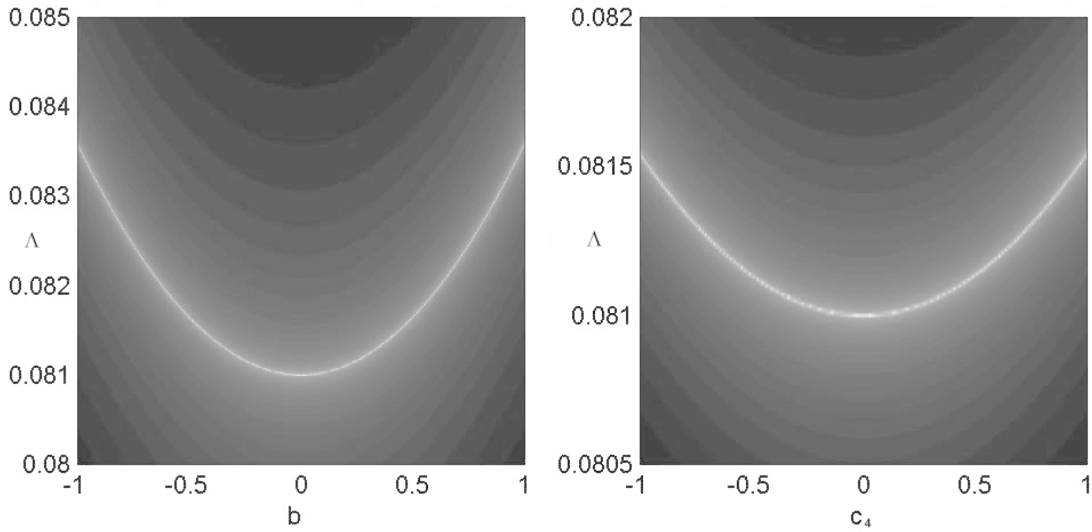

Figure 4.4: The function $\Xi \equiv -\log\left|\det\left(S_{(22)} - 1\right)\right|$ for the model (3.4), (4.2): the brighter point the larger Ξ is. *Left:* The function Ξ depending on b and Λ provided $c_j = 0$, $j = 3, \dots, 6$; *Right:* The function Ξ depending on c_4 and Λ provided $b = 0$, $c_j = 0$, $j = 3, 5, 6$; *Other parameters:* $\varepsilon = 0.01$, $N_1 = 1$, $h_1 = 0.1$, $\alpha = -0.1$, $a = 0$, $T = 1$, $M - T = 4$.

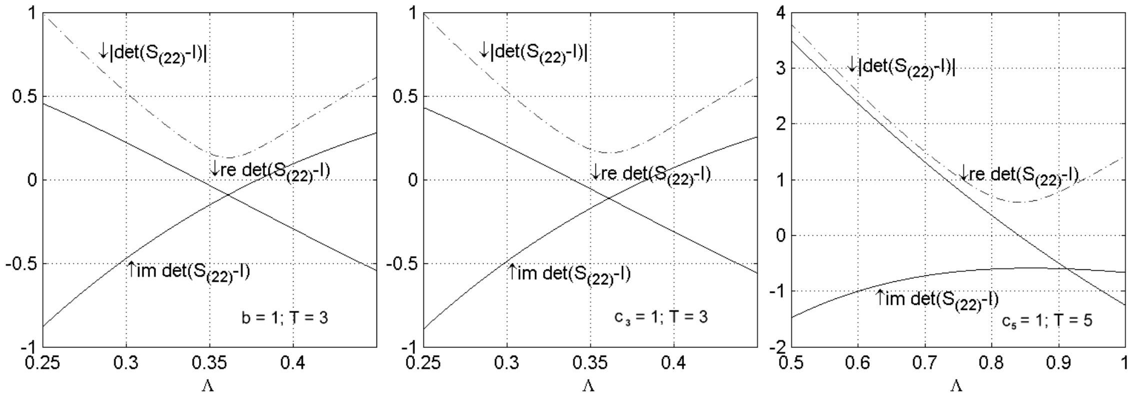

Figure 4.5: The function (4.1) for the model (3.4), (4.2) depending on Λ; the solid lines are used for the real and imaginary parts of this function, the dashed line shows its module. *Left:* $b = 1$, $c_j = 0$, $j = 3, \ldots, 6$; $T = 3$, $M - T = 4$; *Middle:* $b = 0$, $c_3 = 1$, $c_j = 0$, $j = 4, 5, 6$; $T = 3$, $M - T = 4$; *Right:* $b = 0$, $c_4 = 1$, $c_j = 0$, $j = 3, 5, 6$; $T = 5$, $M - T = 7$; *Other parameters:* $\varepsilon = 0.01$, $N_1 = 1$, $h_1 = 0.1$, $\alpha = -0.1$, $a = 0$.

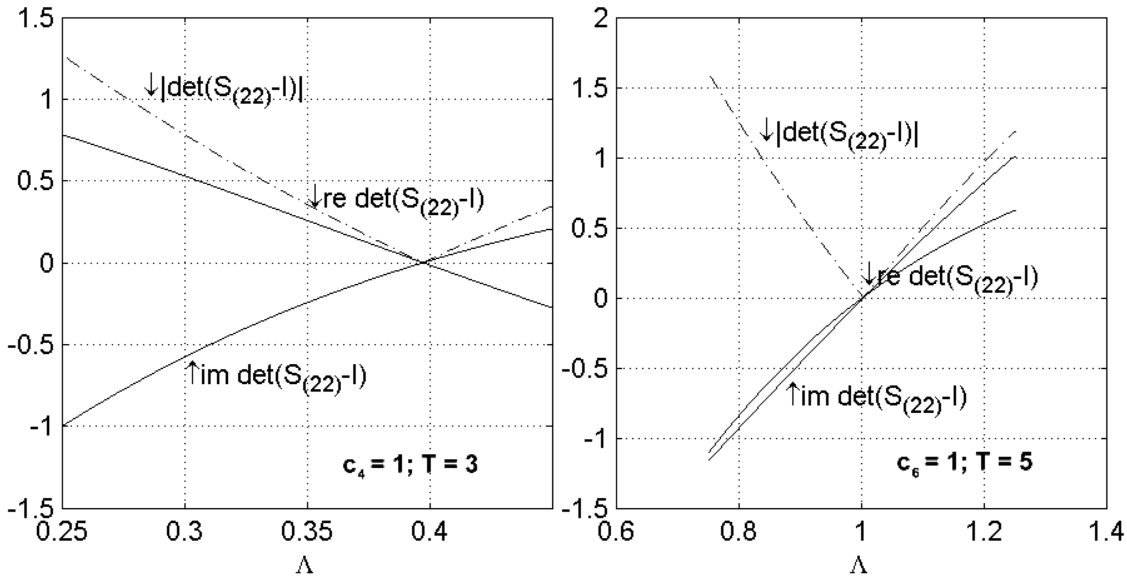

Figure 4.6: The function (4.1) for the model (3.4), (4.2) depending on Λ; the solid lines are used for the real and imaginary parts of this function, the dashed line shows its module. *Left:* $b = 0$, $c_3 = 1$, $c_j = 0$, $j = 3, 5, 6$; $T = 3$, $M - T = 4$; *Right:* $b = 0$, $c_6 = 1$, $c_j = 0$, $j = 3, 4, 5$; $T = 5$, $M - T = 7$; *Other parameters:* $\varepsilon = 0.01$, $N_1 = 1$, $h_1 = 0.1$, $\alpha = -0.1$, $a = 0$, $T = 1$, $M - T = 4$.

We formulate the following conjecture based on the above observations.

Conjecture: let in the model (3.1), (3.2) and (3.4) the periodic modulation be given by

$$\chi(x_1, x_2, \varepsilon) = \begin{cases} 1, & x_2 > h(\varepsilon), \\ N(\varepsilon) + \sum_{j\neq 0} \nu_j e^{ijx_1}, & 0 < x_2 < h(\varepsilon) \end{cases}$$

and let the total multiplicity of real eigenvalues of the problem (2.6) be equal to $2T$. Then a surface wave arises for such a grating if $\nu_{\pm 1} = \dots \nu_{\pm T} = 0$.

4.2 Grating with characteristics oscillating in x_2

We now turn to the analysis of the grating (2.1)–(2.5) with the refraction index (2.5) of the form

$$\chi_0(x_1, x_2) = 1 + N + a\cos(x_1 + \omega x_2) + b\cos 2(x_1 + \omega x_2)\,, \quad |a| + |b| < 1 + N\,, \tag{4.3}$$

provided some grating parameters are constrained by some an additional (dispersion) relation. The motivation for introducing of this additional relation is based on the analysis in Appendix B.2.

In Appendix B.2 a more general model is examined under assumption of smallness of the Fourier coefficients of periodic modulation. As a result, the entries of ASM are given as $S^{(0)}_{mn} + \epsilon S^{(1)}_{mn} + \dots$ with explicit formulas (B.11) and (B.12) for $S^{(0)}_{mn}$ and $S^{(1)}_{mn}$. To verify the existence criterion one has

$$S^{(0)}_{Mn} = \delta_{Mn}\,, \quad S^{(1)}_{Mn} = 0\,, \dots, \quad n = 1, \dots M \tag{4.4}$$

(we assume here $M = T + 1$). The first equation in (4.4) yields the dispersion relation

$$|\lambda_M| = æ\sigma_M \tan(\sigma_M h)\,. \tag{4.5}$$

Note that the analysis of Appendix B.2 is also motivated if $\omega \gg 1$ since $S^{(1)}_{mn} = O(1/\omega)$ as $\omega \to \infty$. Therefore, the assumption of smallness of Fourier coefficients is irrelevant for the motivation.

The numerical results for the model (4.3) with parameters constrained by the dispersion relation (4.5) are presented in Fig. 4.7. The entries $|S_{22} - 1|$ and $|S_{21}|$ are shown depending on ωh in the right-hand part of Fig. 4.7. It is seen that these entries display synchronized oscillations in ωh independently of a. The appearance of oscillations in ωh is explained by the analysis in Appendix B.2. The left-hand part of the same figure shows that these oscillations correspond to relative minima of the function (4.1) in neighborhoods of the points $\omega h = 2\pi l$, $l \neq 0$. Thus, the model with characteristics oscillating in x_2 exhibits the existence of quasi-surface waves in the the non-trivial case $a \neq 0$.

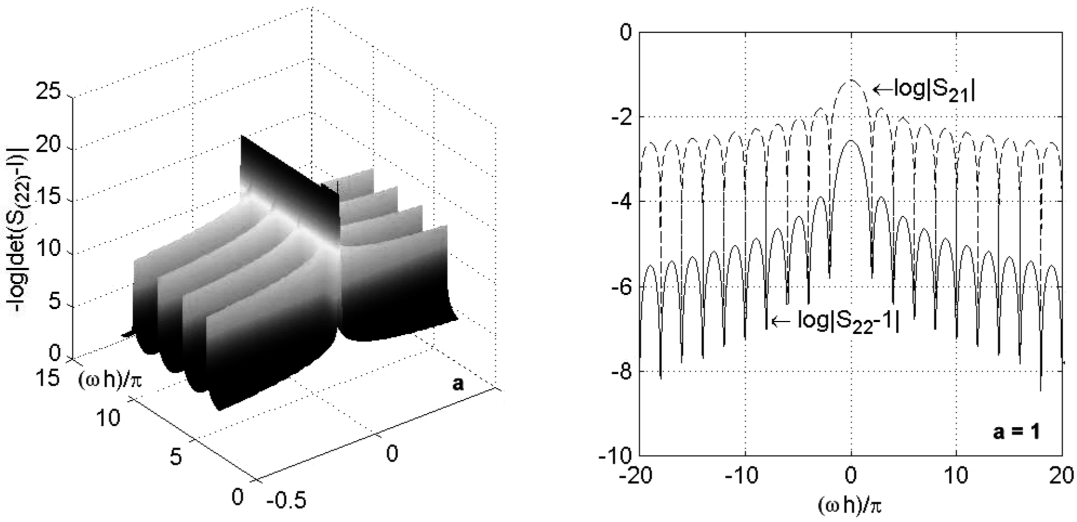

Figure 4.7: *Left:* The surface of logarithm (with the minus sign) of the module of function (4.1) for the model (2.1)–(2.5), (4.3), (4.5) depending on a and ωh; *Right:* The cross-section of this surface by the plane $a = 1$ (solid line), dashed line shows $\log|S_{12}(\omega h/\pi)||_{a=1}$. *Other parameters:* $b = 0$, $N = 1$, $\alpha = -0.1$, $T = 1$, $M = T + 1$.

5 Conclusion

In the paper we dealt with the periodically modulated planar diffraction grating and concentrated on the problem of existence of surface waves whose amplitudes vanish exponentially apart from the grating. The universal existence criterion was formulated. It was applied to the asymptotic analysis of a model with small parameter and to numerical investigation of planar gratings. Evidences of the existence of surface waves have been given.

6 Acknowledgment

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A Construction of asymptotic expansion for $s(\varepsilon)$

We substitute series (3.18) into the problem (3.1)–(3.2) with $k^2(\varepsilon) \equiv k_0^2 = (1+\alpha)^2$ and obtain the sequence of problems ($m = 0, 1, 2 \dots$)

$$\frac{\partial^2 \zeta_m}{\partial y^2} = -(\partial_{x_1}^2 + k_0^2[1 + a\cos(x_1) + b\cos(2x_1)])\zeta_{m-2} - \\ - k_0^2 N_1 \zeta_{m-3} - k_0^2 N_2 \zeta_{m-4}, \quad 0 < y < h_1,\ \zeta_{-1} = \zeta_{-2} = \zeta_{-3} \equiv 0, \quad \text{(A.1)}$$

where ζ_m satisfies the quasi-periodicity conditions (2.2); N_1, N_2 are the coefficients in (3.4),

$$\left.\frac{\partial\zeta_m}{\partial y}\right|_{y=0} = 0, \tag{A.2}$$

$$\left.\frac{\partial\zeta_m}{\partial y}\right|_{y=h_1} = æ \left.\frac{\partial\eta_{m-1}}{\partial x_2}\right|_{x_2=0} + F_{m-2}(\eta_{m-2},\dots,\eta_0), \tag{A.3}$$

$$\eta_{-1} = \eta_{-2} = 0,\ F_{-1} = F_{-2} = 0$$

with

$$F_0(\eta_0) = h_1 æ \left.\frac{\partial^2\eta_0}{\partial x_2^2}\right|_{x_2=0},$$

$$F_1(\eta_0,\eta_1) = h_1 æ \left.\frac{\partial^2\eta_1}{\partial x_2^2}\right|_{x_2=0} + h_1^2 æ/2 \left.\frac{\partial^3\eta_0}{\partial x_2^3}\right|_{x_2=0},$$

etc. The function η_m satisfies

$$(\nabla^2 + k_0^2)\eta_m = 0, \tag{A.4}$$

the condition (2.2), and

$$\begin{gathered}\left.\frac{\partial\eta_m}{\partial x_2}\right|_{x_2=0} = \frac{1}{æ}\left.\frac{\partial\zeta_{m+1}}{\partial y}\right|_{y=h} - f_{m-1}(\eta_{m-1},\dots,\eta_0)\\ f_{-1} = 0,\end{gathered} \tag{A.5}$$

with

$$f_0(\eta_0) = h_1 \left.\frac{\partial^2\eta_0}{\partial x_2^2}\right|_{x_2=0},$$

$$f_1(\eta_1,\eta_0) = h_1 \left.\frac{\partial^2\eta_1}{\partial x_2^2}\right|_{x_2=0} + \frac{h_1^2}{2}\left.\frac{\partial^3\eta_0}{\partial x_2^3}\right|_{x_2=0},$$

$$f_2(\eta_2,\eta_1,\eta_0) = h_1 \left.\frac{\partial^2\eta_2}{\partial x_2^2}\right|_{x_2=0} + \frac{h_1^2}{2}\left.\frac{\partial^3\eta_1}{\partial x_2^3}\right|_{x_2=0} + \frac{h_1^3}{6}\left.\frac{\partial^4\eta_0}{\partial x_2^4}\right|_{x_2=0},$$

and so on. Besides, for large $x_2 \sim M|\log\varepsilon|$ we have the matching condition

$$\begin{aligned}\eta_0(x_1,x_2) &\sim u_2^+(x_1,x_2) + u_1^-(x_1,x_2)s_{12}^0 + u_2^-(x_1,x_2)s_{22}^0,\\ \eta_m(x_1,x_2) &\sim u_1^-(x_1,x_2)s_{12}^m + u_2^-(x_1,x_2)s_{22}^m, \quad m \ge 1,\end{aligned} \tag{A.6}$$

which follows from (3.14).

From the contact condition $[\eta]|_{x_2=h_1\varepsilon} = 0$ we deduce

$$\zeta_m(x_1,h_1) = \eta_m(x_1,0) + \Psi_{m-1}(\eta_{m-1},\dots,\eta_0) \tag{A.7}$$

with

$$\Psi_{-1} = 0, \quad \Psi_0(\eta_0) = h_1 \left.\frac{\partial\eta_0}{\partial x_2}\right|_{x_2=0},$$

$$\Psi_1(\eta_1,\eta_0) = h_1 \left.\frac{\partial\eta_1}{\partial x_2}\right|_{x_2=0} + \frac{h_1^2}{2}\left.\frac{\partial^2\eta_0}{\partial x_2^2}\right|_{x_2=0},$$

$$\Psi_2(\eta_2,\eta_1,\eta_0) = h_1 \left.\frac{\partial\eta_2}{\partial x_2}\right|_{x_2=0} + \frac{h_1^2}{2}\left.\frac{\partial^2\eta_1}{\partial x_2^2}\right|_{x_2=0} + \frac{h_1^3}{6}\left.\frac{\partial^3\eta_0}{\partial x_2^3}\right|_{x_2=0},$$

and so on.

The homogeneous problem corresponding to (A.1)–(A.3) always has a nontrivial solution which is an arbitrary function in x_1 subject to (2.2). The solvability condition for the problem (A.1)–(A.3)

$$\left.\frac{\partial \zeta_{m+1}}{\partial y}\right|_{y=h_1} = -\int\limits_0^{h_1} \{(\partial_{x_1}^2 + k_0^2[1 + a\cos(x_1) + b\cos(2x_1)])\zeta_{m-1}(x_1,t) + \\ + k_0^2 N_1 \zeta_{m-2}(x_1,t) + k_0^2 N_2 \zeta_{m-3}(x_1,t)\}\, dt. \quad (A.8)$$

Thus, we obtain the boundary condition for η_m combining (A.5)–(A.8). The procedure of finding ζ_m and η_m is as follows. We first obtain ζ_m from (A.1)–(A.3) up to a solution of the homogeneous problem. Then we use (A.4)–(A.6) to find η_m. Finally, with the help of (A.7) we eliminate the arbitrariness in the choice of ζ_m. Let us implement this plan for the three first terms.

For the leading term we find

$$\left.\frac{\partial \eta_0}{\partial x_2}\right|_{x_2=0} = 0, \eta_0(x_1,x_2) = \frac{\exp[i(1+\alpha)x_1]}{\sqrt{\pi}}, \zeta_0(x_1,y) = \frac{\exp[i(1+\alpha)x_1]}{\sqrt{\pi}},$$

$$s_{12}^0 = 0, \quad s_{22}^0 = 1. \quad (A.9)$$

For $m = 1$ we obtain

$$\begin{aligned} \left.\frac{\partial \eta_1}{\partial x_2}\right|_{x_2=0} &= -h_1 æ \frac{(1+\alpha)^2}{2\sqrt{\pi}}[e^{i(2+\alpha)x_1}a + e^{i\alpha x_1}a + e^{i(\alpha-1)x_1}b + e^{i(\alpha+3)x_1}b], \\ \eta_1(x_1,x_2) &= b_{-1}w_{-1}^+(x_1,x_2) + b_1^- u_1^-(x_1,x_2) + b_2^- u_2^-(x_1,x_2) \\ &\quad + b_2 w_2^+(x_1,x_2) + b_3 w_3^+(x_1,x_2), \\ \zeta_1(x_1,y) &= \eta_1(x_1,0), \end{aligned}$$

where $u_j^\pm$, $j = 1,2$, are defined in (3.11) while $w_n^\pm$ satisfies (2.10) with $\mu^\pm = \pm(k^2 - (n+\alpha)^2)^{1/2}$. Besides

$$b_1^- = ih_1 æ \frac{(1+\alpha)^2}{(1+2\alpha)^{1/4}}a, \quad b_2^- = 0, \quad b_2 = h_1 æ \frac{(1+\alpha)^2}{(3+2\alpha)^{1/4}}a,$$
$$b_{-1} = h_1 æ \frac{(1+\alpha)^2}{(4|\alpha|)^{1/4}}b, b_3 = h_1 æ \frac{(1+\alpha)^2}{(8+4\alpha)^{1/4}}b,$$

$$s_{12}^1 = b_1^-, s_{22}^1 = b_2^- = 0. \quad (A.10)$$

For $m = 2$ a bit more tedious calculation leads to

$$\left.\frac{\partial \eta_2}{\partial x_2}\right|_{x_2=0} = \frac{e^{i(\alpha+1)x_1}}{\sqrt{4\pi}}(-h_1 æ)\left[\frac{(1+\alpha)^2}{(3+2\alpha)^{1/4}}\frac{a}{2}b_2 + \frac{(1+\alpha)^2}{(1+2\alpha)^{1/4}}\frac{a}{2}b_1^- + \right. \\ \left. + 2(1+\alpha)^2 N_1 + \frac{(1+\alpha)^2}{(4|\alpha|)^{1/4}}\frac{b}{2}b_{-1} + \frac{(1+\alpha)^2}{(8+4\alpha)^{1/4}}\frac{b}{2}b_3\right] + \dots,$$

where the dots stands for the terms not needed for computing s_{12}^2, s_{22}^2,

$$\eta_2(x_1,x_2) = c_{-1}w_{-1}^+(x_1,x_2) + c_{-3}w_{-3}^+(x_1,x_2) \\ + c_{-2}w_{-2}^+(x_1,x_2) + c_1^- u_1^-(x_1,x_2) + c_2^- u_2^-(x_1,x_2) + \\ + c_2 w_2^+(x_1,x_2) + c_3 w_3^+(x_1,x_2) + c_4 w_4^+(x_1,x_2) + c_5 w_5^+(x_1,x_2)$$

with

$$c_2^- = h_1 æ(1+\alpha)^2 \left[-h_1 æ \frac{(1+\alpha)^2}{(1+2\alpha)^{1/2}} \frac{a^2}{2} + i \left(h_1 æ \frac{(1+\alpha)^2}{(3+2\alpha)^{1/2}} \frac{a^2}{2} + 2N_1 + \right.\right. \\ \left.\left. + h_1 æ (1+\alpha)^2 \frac{b^2}{2} \left(\frac{1}{(4|\alpha|)^{1/2}} + \frac{1}{(8+4\alpha)^{1/2}} \right) \right) \right],$$

$$s_{12}^2 = c_1^-, \quad s_{22}^2 = c_2^-. \tag{A.11}$$

B Rigorous coupled-wave approach for planar grating

B.1 General algorithm

Consider the planar grating (2.1)–(2.5) whose periodic refraction index $\chi_0(x_1 + \omega x_2)$ in (2.5) is expanded into the Fourier series

$$\chi_0(y) = 1 + N + \sum_{l \neq 0} \nu_l e^{ily}. \tag{B.1}$$

Inside the layer $0 < x_2 < h$, we seek a solution of the form

$$u(x_1,x_2) = \sum_{n=-\infty}^{\infty} e^{i(n+\alpha)x_1} u_n(x_2). \tag{B.2}$$

Note that the quasi-periodicity condition (2.2) is automatically satisfied by the series (B.2). Substitution of (B.2) and (B.1) into the Helmholtz equation inside the layer leads to the system of ordinary differential equations

$$u_n''(x_2) + + \left[k^2(1+N) - (n+\alpha)^2\right] u_n(x_2) + k^2 \sum_{l \neq n} \nu_{n-l} e^{i(n-l)\omega x_2} u_l(x_2) = 0, \tag{B.3}$$

$n = 0, \pm 1, \ldots$, for the unknown functions u_n in (B.2).

By the substitution $u_n(x_2) = e^{i\omega(n+\alpha)x_2} v_n(x_2)$ system (B.3) is reduced to the system with constant coefficients

$$v_n''(x_2) + 2i\omega(n+\alpha)v_n'(x_2) + \\ + \left[k^2(1+N) - (1+\omega^2)(n+\alpha)^2\right] v_n(x_2) + k^2 \sum_{l \neq n} \nu_{n-l} v_l(x_2) = 0, \tag{B.4}$$

whose solution is of the form

$$u_n(x_2) = \sum_l c_l e^{i\mu_l x_2} v_{nl}, \tag{B.5}$$

where $\left(i\mu_l; \{v_{nl}\}|_{n=-\infty}^{\infty}\right)$ are eigenpairs of the matrix

$$\left(\begin{array}{cc} 0 & E \\ A & B \end{array}\right), \quad \begin{array}{ll} A = \|a_{nl}\|, & a_{nl} = -k^2\nu_{n-l} - [k^2(1+N) - (1+\omega^2)(n+\alpha)^2]\delta_{nl}, \\ B = \|b_{nl}\|, & b_{nl} = -2i\omega(n+\alpha)\delta_{nl}, \end{array}$$

E is the identity matrix and δ_{nl} is the Kronecker symbol.

The coefficients c_l are to be found by matching the solution (B.5) with the boundary conditions (2.4) and with the solution outside the grating.

The series (B.2) must be truncated in order to keep into consideration only those Floquet waves which correspond to the eigenvalues in the strip $\beta < \mathrm{Im}\lambda < \gamma$. Let as before M stand for the size of ASM. Thus, the m-th row of the ASM ($1 \leqslant m \leqslant M$), together with $2M$ unknown coefficients $c_l^{(m)}$, is determined by the following linear algebraic system of size $3M \times 3M$:

$$\begin{cases} \displaystyle\sum_{l=1}^{2M} c_l^{(m)} e^{i(\omega(n+\alpha)+\mu_l)x_2} v_{nl}\Big|_{x_2=0} = 0 \quad \text{or} \quad \frac{d}{dx_2}\sum_{l=1}^{2M} c_l^{(m)} e^{i(\omega(n+\alpha)+\mu_l)x_2} v_{nl}\Big|_{x_2=0} = 0 \\ \displaystyle\sum_{l=1}^{2M} c_l^{(m)} e^{i(\omega(n+\alpha)+\mu_l)x_2} v_{nl}\Big|_{x_2=h} = \left(V_m^{(+)}\delta_{mn} + S_{mn}V_n^{(-)}\right)\Big|_{x_2=h} \\ \displaystyle\frac{d}{dx_2}\sum_{l=1}^{2M} c_l^{(m)} e^{i(\omega(n+\alpha)+\mu_l)x_2} v_{nl}\Big|_{x_2=h} = \frac{1}{æ}\frac{d}{dx_2}\left(V_m^{(+)}\delta_{mn} + S_{mn}V_n^{(-)}\right)\Big|_{x_2=h}, \end{cases}$$

$$n = 1, \dots, M, \tag{B.6}$$

where the functions $V_n^{\pm}(x_2)$ are the Floquet waves without factors $e^{i(n+\alpha)x_1}$.

B.2 Analysis of weakly–modulated grating

Now suppose that the Fourier coefficients in (B.1) are small:

$$\chi_0(y) = 1 + N + \epsilon\sum_{l\neq 0}\nu_l e^{ily}, \quad \epsilon \ll 1. \tag{B.7}$$

Then the matrix corresponding to system (B.3) is

$$\left(\begin{array}{cc} 0 & E \\ A_0 & 0 \end{array}\right) + \epsilon\left(\begin{array}{cc} 0 & E \\ A_1(x_2) & 0 \end{array}\right), \tag{B.8}$$

where $A_0 = \|-\sigma_{nl}^2\delta_{nl}\|$, $\sigma_n^2 \equiv k^2(1+N) - (\alpha+n)^2$ and $A_1(x_2) = \|a_{nl}(x_2)\|$, $a_{nl}(x_2) = -k^2\nu_{n-l}e^{i\omega(n-l)x_2}$. Application of the standard perturbation technique to system (B.3) shows that the spectrum of the unperturbed matrix in (B.8) does not change in the first order of perturbation, and

$$u_n(x_2) = A_n^{(0)}e^{i\sigma_n x_2} + B_n^{(0)}e^{-i\sigma_n x_2} + \tag{B.9}$$
$$+k^2\epsilon\sum_{j\neq n}\nu_{n-j}e^{i\omega(n-l)x_2}\left[\frac{A_n^{(1)}e^{i\sigma_n x_2}}{(\sigma_j+\omega(n-j))^2-\sigma_n^2} + \frac{B_n^{(1)}e^{i\sigma_n x_2}}{(\sigma_j-\omega(n-j))^2-\sigma_n^2}\right] + O(\epsilon^2)$$

with unknown coefficients $A_n^{(0,1)}$, $B_n^{(0,1)}$.

Outside the grating the solution is $V_m^{(+)} + \sum_{n=1}^{M} S_{mn} V_n^{(-)}$, where $\exp\{i(n+\alpha)x_1\} V_n^{(\pm)}$ are Floquet waves. Let us seek the entries of ASM as series

$$S_{mn} = \sum_{j\geqslant 0} S_{mn}^{(j)} \epsilon^j \,. \tag{B.10}$$

Now one can satisfy the contact and the boundary conditions (2.3) and (2.4) in powers of ϵ. To shorten, we discuss the procedure for the $\mathcal{N}$-problem only.

In the leading approximation $S_{mn}^{(0)}$ and $A_n^{(0)} = B_n^{(0)} \equiv C_{mn}^{(0)}$ are obtained from the system

$$\begin{aligned} C_{mn}^{(0)} \cos(\sigma_n h) &= \left(\delta_{mn} V_n^{(+)} + S_{mn}^{(0)}\right)\Big|_{x_2=h} \,, \\ -æ\sigma_n C_{mn}^{(0)} \sin(\sigma_n h) &= \frac{d}{dx_2} \left(\delta_{mn} V_n^{(+)} + S_{mn}^{(0)}\right)\Big|_{x_2=h} \,. \end{aligned}$$

Therefore, in this approximation the scattering matrix is diagonal

$$\begin{aligned} S_{mn}^{(0)} &= \delta_{mn} e^{-2i\lambda_n h} \frac{i\lambda_n - æ\sigma_n \tan(\sigma_n h)}{i\lambda_n + æ\sigma_n \tan(\sigma_n h)} \qquad \text{for} \quad \lambda_n^2 \geqslant 0 \,, \\ S_{mn}^{(0)} &= \delta_{mn} \frac{ie^{|\lambda_n|h}\left[|\lambda_n| + æ\sigma_n \tan(\sigma_n h)\right] + e^{-|\lambda_n|h}\left[|\lambda_n| - æ\sigma_n \tan(\sigma_n h)\right]}{ie^{|\lambda_n|h}\left[|\lambda_n| + æ\sigma_n \tan(\sigma_n h)\right] - e^{-|\lambda_n|h}\left[|\lambda_n| - æ\sigma_n \tan(\sigma_n h)\right]} \quad \text{for} \quad \lambda_n^2 < 0 \,, \end{aligned} \tag{B.11}$$

where $\lambda_n^2 \equiv k^2 - (\alpha+n)^2$ are eigenvalues of the problem (2.6).

We also have

$$\begin{aligned} S_{mn}^{(1)} &= 4æk^2 D_n^{-1} \sum_{j\neq n} \frac{\nu_{n-j} C_{mj}^{(0)}}{\left[(\sigma_j + \omega(n-j))^2 - \sigma_n^2\right]\left[(\sigma_j - \omega(n-j))^2 - \sigma_n^2\right]} \times \\ &\times \Big\{ e^{i\omega(n-j)h} \cos(\sigma_j h) \times \\ &\times \left(\left[\sigma_j^2 - \sigma_n^2 + \omega^2(n-j)^2\right]\left[\sigma_n \tan(\sigma_j h) - \sigma_j \tan(\sigma_n h) + i\omega(n-j)\right] + \right. \\ &+ \left. i\omega\sigma_j[\sigma_j - \sigma_n \tan(\sigma_n h)\tan(\sigma_j h)]\right) + \\ &+ \omega(n-j)\sigma_j^2/\cos(\sigma_n h) \Big\} \,, \end{aligned} \tag{B.12}$$

where D_n is the same denominator as in (B.11).

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