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On Computation of Scattering Matrices and on Surface Waves for Diffraction Gratings

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Summary. A method for the numerical computation of the so-called augmented scattering matrices (ASM) is suggested for diffraction gratings. To construct such (unitary) matrices one has to take into account not only the oscillating modes but also those which exponentially grow (attenuate) in amplitude away from the grating. The method uses an optimization procedure to identify the coefficients in the asymptotics of such modes. A justification of the approach is given and its numerical implementation is discussed. Reliable numerical results allow us to study the occurrences of surface waves by means of a general existence criterion based on the properties of ASM. To illustrate the method we give some examples of surface waves in gratings.

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1 Introduction

In this paper, we consider a boundary value problem for the Helmholtz equation in a “half-plane” with periodic boundary; in other words, we are dealing with diffraction gratings. As it usually is, the problem reduces to the quasiperiodic boundary value problem for the Helmholtz equation in a semi-infinite “strip”. The nontrivial solutions of the latter (homogeneous) problem with exponential decay at infinity are called surface waves.[1] There is an existence

[1] Sometimes in the literature (e.g.,[14]) such waves are called Rayleigh-Bloch surface waves.

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criterion of surface waves related to the spectrum of an augmented scattering matrix (ASM). The unitary matrix takes into account not only oscillating modes but also finitely many of those which grow (attenuate) in amplitude at infinity.

Phenomena connected with surface waves have attracted much attention in engineering and physics (see, e.g., [17, 16] and references there). Related questions have been discussed by mathematicians as well. We shall indicate a few recent works.

The mentioned ASM and the existence criterion were introduced by Nazarov and Plamenevskii in the theory of elliptic problems in domains with singularities [11–13]. Kamotsky and Nazarov used the criterion to prove the existence of surface waves for some diffraction gratings by means of a subtle asymptotic analysis of the problem [6, 7]. The existence of trapped modes in a waveguide was proved by Evans, Levitin and Vasiliev in [3]. Trapped modes in a waveguide and surface waves in diffraction gratings were discussed in [10]. Some surface waves were found by various numerical methods [2, 14, 5]; besides, an asymptotic analysis was given in [5]. The methods in [2, 14, 5] essentially used specific features of the problems (the structure of gratings, etc).

As was already mentioned, to construct ASM we have to deal with some exponentially growing solutions. This causes new difficulties for numerical analysis. We introduce a method which reduces the computation of a row of ASM to minimization of a quadratic functional. The main idea is to truncate the "semi-strip" of the original problem at a finite distance R and to use the optimization of a functional J^R to match a solution in the truncated strip to a predetermined asymptotic expansion at the truncation boundary. To obtain the functional we have to solve auxiliary boundary value problems in the truncated strip. We prove that the minimizer of the functional J^R tends exponentially to the row of actual ASM as R goes to infinity. The procedure can be applied to gratings of rather general structure.

Of course, there is a long tradition of using truncated domains in numerical analysis of wave guides and diffraction gratings (see, e.g., Goldstein [4]). However, our special purpose requires to consider some growing modes which cannot be handled by the traditional methods. Moreover, we are interested only in the asymptotics of the modes which participate in an ASM. That is why we avoid the numerical computation of the growing modes; instead we develop the mentioned optimization procedure to find the needed part of their asymptotics.

Apparently, the basic difficulty for the numerical implementation of the method is related to the fact that the functional J^R can degenerate at infinity (as $R \to \infty$). Therefore for ASM of "large" size, the numerical results are not reliable. Nevertheless, a wealth of information about surface waves can be gained with ASM of even “moderate” size. Here we restrict ourselves to some examples illustrating the method. We plan to give a closer examination of surface waves in another paper.

Preliminaries and statement of the problem are given in Section 2. We describe and justify the method of calculation of ASM in Section 3. Numerical implementation is discussed in Section 4. Section 5 is devoted to surface waves, while in Section 6 we describe some details of the finite element implementation.

2 Preliminaries

2.1 Statement of the problem

Let $\mathcal{P}$ be an open subset of $\mathbb{R}^2$ such that $\{(x, y) \in \mathbb{R}^2 : y > c\} \subset \mathcal{P} \subset \{(x, y) \in \mathbb{R}^2 : y > -c\}$. Moreover, let $\mathcal{P}$ be 2π-periodic with respect to x, i.e., $(x, y) \in \mathcal{P} \Leftrightarrow (x + 2\pi, y) \in \mathcal{P}$. The boundary $\partial\mathcal{P}$ of $\mathcal{P}$ is supposed to be piecewise smooth; the strip $\{(x, y) : -\pi \le x \le +\pi\}$ intersects finitely many components of $\partial\mathcal{P}$.

We consider the “strip” $\Pi = \{(x, y) \in \mathcal{P} : -\pi < x < \pi\}$, denote by $\Gamma_\pm$ the parts of $\partial\Pi$ that are parallel to the axis y, $\Gamma_\pm = \{(x, y) : x = \pm\pi\}$, and put $\Gamma_0 = \partial\Pi \cap \partial\mathcal{P}$. Clearly, $\partial\Pi = \Gamma_0 \cup \Gamma_+ \cup \Gamma_-$. The sketch of the domain Π is shown in Fig.1.

We search a solution of the equation

$$(1) \qquad \left(\Delta + k^2\right) w(x, y) = 0\,, \quad (x, y) \in \mathcal{P}\,,$$

satisfying the quasi-periodicity conditions

$$(2) \qquad \partial_x^j\, w(x + 2\pi, y) = e^{2\pi i\alpha} \partial_x^j\, w(x, y)\,, \quad j = 0, 1\,,$$

and the boundary condition

$$(3) \qquad (\mathcal{B}w)\,(x, y) = 0\,, \quad (x, y) \in \Gamma_0\,,$$

where by $\mathcal{B}$ is meant any elliptic boundary condition (of order ≤ 1) such that (1) – (3) is a formally self-adjoint problem. The quasi-periodicity conditions originate from the corresponding nonhomogeneous problem containing an incident wave

$$(4) \qquad u^{in}(x, y) = \exp\{-ik(x \sin\theta + y \cos\theta)\}.$$

Since u^{in} satisfies (2) with $\alpha = -k \sin\theta$ and all the other characteristics of the problem are 2π-periodic, it is natural to search a solution of the problem

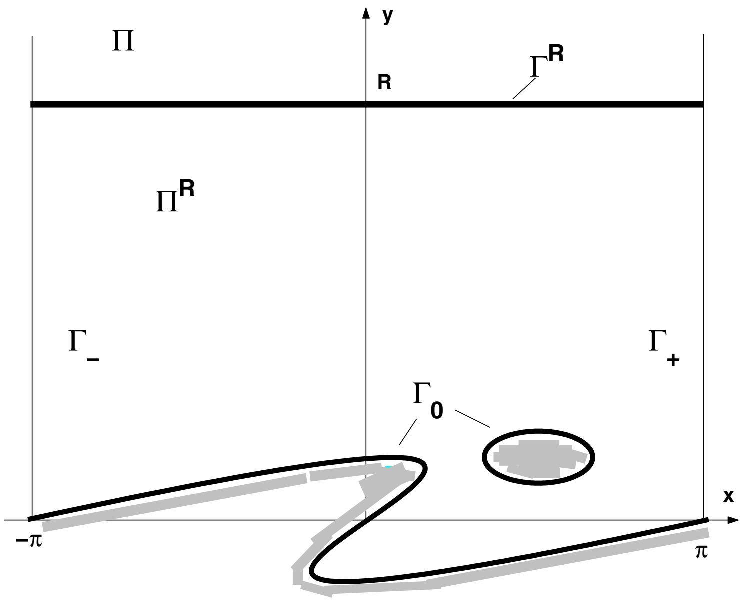

Fig. 1. Geometry of the problem

(1), (3) subject to (2). Then problem (1) – (3) turns out to be equivalent to the following problem in the strip Π:

(5) $\left(\Delta + k^2\right) w(x, y) = 0, \quad (x, y) \in \Pi\,,$

(6) $\partial_x^j\, w(\pi, y) = e^{2\pi i\alpha} \partial_x^j\, w(-\pi, y), \quad (\pm\pi, y) \in \Gamma_\pm, \;\; j = 0, 1,$

(7) $(\mathcal{B}w)\,(x, y) = 0, \quad (x, y) \in \Gamma_0.$

2.2 An existence criterion of surface waves

By definition, a surface wave is a solution w to the problem (5) – (7) satisfying $w(x, y) = O(\exp(-\gamma y))$ with $\gamma > 0$ as $y \to +\infty$. The existence criterion of such waves used in the paper can be formulated in terms of an "augmented" scattering matrix. To construct such a matrix one has to take into account not only the oscillating solutions of the problem (5) – (7) but also finitely many of those which exponentially grow (attenuate) in amplitude at infinity.

Let us recall some necessary definitions. Consider the boundary value problem

(8) $$\frac{d^2 v}{dx^2}(x) + (k^2 - \lambda^2)\, v(x) = 0\,, \quad -\pi < x < \pi\,,$$

$$\frac{d^j v}{dx^j}(\pi) = e^{2\pi i\alpha}\frac{d^j v}{dx^j}(-\pi)\,, \quad j = 0, 1\,, \tag{9}$$

with spectral parameter λ. The spectrum of the problem (8), (9) consists of the eigenvalues $\pm(k^2 - (n+\alpha)^2)^{1/2}$, where $n = 0, \pm 1, \dots$. For the eigenvalues $\mu^\pm = \pm(k^2 - (n+\alpha)^2)^{1/2} \neq 0$ we introduce the functions

$$w^\pm(x, y) = \left(4\pi|\mu^\pm|\right)^{-1/2} \exp\{i\mu^\pm y\} e^{i(n+\alpha)x}\,, \tag{10}$$

and for $\mu^\pm = 0$ (in the case $k^2 = (n+\alpha)^2$) we define

$$w^0(x, y) = (2\pi)^{-1/2} e^{i(n+\alpha)x}\,, \quad \tilde{w}^0(x, y) = (2\pi)^{-1/2} y\, e^{i(n+\alpha)x}\,. \tag{11}$$

Functions (10) and (11) satisfy the homogeneous Helmholtz equation in the strip $\{(x, y) : -\pi < x < \pi\,, -\infty < y < \infty\}$ and the quasi-periodicity conditions (2) on the boundary of the strip.

Let $\lambda_1 < \cdots < \lambda_T \leq \lambda_{T+1} < \cdots < \lambda_{2T}$ be all the real eigenvalues of the problem (8), (9). If 0 is an eigenvalue, then $\lambda_T = \lambda_{T+1} = 0$, otherwise $\lambda_T < \lambda_{T+1}$. By $\lambda^\pm_{T+1}\,, \lambda^\pm_{T+2}\,, \dots$ we denote the imaginary eigenvalues of the same problem numbered so that $\operatorname{Im}\lambda^+_{T+1} < \operatorname{Im}\lambda^+_{T+2} < \dots$ and $\lambda^+_j = -\lambda^-_j$. To every real eigenvalue λ_j we associate the function w_j defined by (10) or (11) and set

$$u^+_j = w_j\,, \quad u^-_j = w_{2T-j+1}\,, \quad j = 1, \dots, T\,, \tag{12}$$

under the condition that 0 is not in the spectrum of the problem (8), (9). In the case $\lambda_T = \lambda_{T+1} = 0$ we replace the definition (12) of $u^\pm_T$ by

$$u^\pm_T = 2^{-1/2}\,(w_T \mp i w_{T+1})\,. \tag{13}$$

To the imaginary eigenvalues $\lambda^\pm_j$ we associate the functions $w^\pm_j$ defined by (10) and set

$$u^\pm_j = 2^{-1/2}\left(w^+_j \mp i w^-_j\right)\,. \tag{14}$$

It is known (see [11]–[13]) that for any $M = 0, 1, \dots$ there exist solutions $Y_1, \dots, Y_{T+M}$ to the homogeneous problem (5)–(7) with asymptotics

$$Y_m(x, y) = u^+_m(x, y) + \sum_{n=1}^{T+M} S_{mn} u^-_n(x, y) + O\left(e^{-\gamma y}\right)\,, \tag{15}$$

where $\gamma = |\operatorname{Im}\lambda^+_{T+M+1}|$, $m = 1, \dots, T+M$, and the matrix $S = \|S_{mn}\|^{T+M}_{m,n=1}$ is unitary. Generally, problem (5)–(7) may have nontrivial solutions u such that $u(x, y) = O(e^{-\gamma y})$ as $y \to \infty$, however, the arbitrariness in defining Y_m does not affect the matrix S. The "asymptotics" u^+_j are called incoming waves and the u^-_j outgoing. The matrix S is called an augmented scattering matrix. If $M = 0$ and $\lambda_T < \lambda_{T+1}$ (0 is not an eigenvalue of the problem (8), (9)) then the matrix S coincides with the "classical" scattering matrix. However, even in the case $M = 0$ and $\lambda_T = \lambda_{T+1}$ our definition differs from the classical one because the asymptotics u_T^+ and u_T^- are classified as incoming and outgoing waves. Let us emphasize that, generally, the AMS S_M of size $(T + M) \times (T + M)$ is not a block of the matrix S_N for $N > M$.

We are now in a position to formulate the existence criterion of surface waves. Let us take integers M and M' such that $0 \le M < M'$ and put $\gamma = |\mathrm{Im}\,\lambda^+_{T+M+1}|$ and $\gamma' = |\mathrm{Im}\,\lambda^+_{T+M'+1}|$. We denote by $N(\gamma)$ $(N(\gamma'))$ the dimension of the space of solutions u to the homogeneous problem (5)–(7) such that $u(x, y) = O(e^{-\gamma y})$ $(u(x, y) = O(e^{-\gamma' y}))$ as $y \to \infty$. Write down the AMS $S_{M'}$ in the form $S_{M'} = \|S_{(ij)}\|_{i,j=1,2}$, where the block $S_{(22)}$ is of size $(M' - M) \times (M' - M)$. The existence criterion reads

$$N(\gamma) - N(\gamma') = \dim\ker\left(S_{(22)} - 1\right) . \tag{16}$$

Thus, the right-hand side is equal to the dimension of the eigenspace of $S_{(22)}$ corresponding to the eigenvalue 1.

Let us explain the equality (16). Assume that there exist M and M' such that $N(\gamma) - N(\gamma') > 0$. It means there is a solution u of the problem (5)–(7) that admits the estimate $u(x, y) = O(e^{-\gamma y})$ and does not satisfy $u(x, y) = O(e^{-\gamma' y})$. We see that the u is a surface wave; moreover, we have a more detailed information on the behaviour of u at infinity.

3 On calculation of the scattering matrix

3.1 Description of the method

We search the m-th row $S_{m,1}, \dots, S_{m,T+M}$ of an augmented scattering matrix S, $1 \le m \le T + M$. As approximation, let us take the minimizer of some functional. To construct the functional we consider an auxiliary boundary value problem in the "truncated" strip $\Pi^R = \{(x, y) \in \Pi : y < R\}$, $R > c$ (see Fig.1). Namely, we introduce the problem

$$(\Delta + k^2) X_m^R(x, y) = 0\,, \quad (x, y) \in \Pi^R, \tag{17}$$

$$\partial_x^j\ X_m^R\big|_{\Gamma_+^R} = e^{2\pi i\alpha}\partial_x^j\ X_m^R\big|_{\Gamma_-^R}\,,\ j = 0, 1, \tag{18}$$

$$\mathcal{B}\, X_m^R\big|_{\Gamma_0} = 0, \tag{19}$$

$$\mathcal{N}_\zeta X_m^R\big|_{\Gamma^R} = \mathcal{N}_\zeta \left(u_m^+ + \sum_{n=1}^{T+M} a_n u_n^- \right)\Bigg|_{\Gamma^R}\,, \tag{20}$$

where $\Gamma_\pm^R = \{(x, y) \in \Gamma_\pm : y < R\}$, $\Gamma^R = \{(x, y) \in \Pi : y = R\}$, and $\mathcal{N}_\zeta = \partial_y + i\zeta$ with some $\zeta > 0$. The numbers a_n are arbitrary.

As in Section 2, let Y_m be a solution to the problem (5)–(7) with asymptotics (15). We temporarily put $X_m^R = Y_m|_{\Pi^R}$. It is obvious that the function X_m^R satisfies (17)–(19). Consider the condition (20). Since the asymptotic equality (15) can be differentiated, we obtain

$$X_m^R\big|_{\Gamma^R} = \left(u_m^+ + \sum_{n=1}^{T+M} S_{mn} u_n^- \right)\bigg|_{\Gamma^R} + O\left(e^{-\gamma R}\right) , \tag{21}$$

$$\mathcal{N}_\zeta \; X_m^R\big|_{\Gamma^R} = \mathcal{N}_\zeta \left(u_m^+ + \sum_{n=1}^{T+M} S_{mn} u_n^- \right)\bigg|_{\Gamma^R} + O\left(e^{-\gamma R}\right) . \tag{22}$$

Therefore, it is reasonable to take an approximation $a(R)$ for S_{mj}, $j = 1, \dots, T+M$, so that the vector $a(R) = (a_1(R), \dots, a_{T+M}(R))$ be the minimizer of the functional

$$\begin{aligned} &J_m^R\left(a_1, \dots, a_{T+M}\right) \\ &= \left\| X_m^R(\cdot, R) - \left(u_m^+(\cdot, R) + \sum_{n=1}^{T+M} a_n u_n^-(\cdot, R) \right) ; L_2(-\pi, \pi) \right\|^2 , \end{aligned} \tag{23}$$

where $X_m^R(\cdot, R)$ stands for the solution to the problem (17)–(20) calculated at $y = R$. Then one can expect that $a_n(R) \underset{R\to\infty}{\to} S_{mn}$ for any fixed $\zeta > 0$. In (20) we take $\mathcal{N}_\zeta$ instead of ∂_y in order to provide the unique solvability of the problem (17)–(20) for any real k and for any $R > c$.

Let us describe a simple formal reduction of the minimization problem of the functional (23). Denote by $v_n^\pm$ $\left(v_{n;R}^\pm\right)$ a function satisfying the equations (17)–(19) and the boundary condition

$$\mathcal{N}_\zeta v_n^\pm\big|_{\Gamma^R} = \mathcal{N}_\zeta u_n^\pm\big|_{\Gamma^R} . \tag{24}$$

Then X_m^R admits the representation $X_m^R = v_{m;R}^+ + \sum_{n=1}^{T+M} a_n \, v_{n;R}^-$.

Introduce the two matrices of size $(T+M) \times (T+M)$

$$\begin{aligned} \mathcal{E}^R &= \|\mathcal{E}_{jk}^R\| = \left\| \left\langle v_k^-(\cdot, R) - u_k^-(\cdot, R), v_j^-(\cdot, R) - u_j^-(\cdot, R) \right\rangle \right\| , \\ \mathcal{F}^R &= \|\mathcal{F}_{jk}^R\| = \left\| \left\langle v_k^-(\cdot, R) - u_k^-(\cdot, R), v_j^+(\cdot, R) - u_j^+(\cdot, R) \right\rangle \right\| , \end{aligned} \tag{25}$$

and the scalar

$$\mathcal{G}_m^R = \left\langle v_m^+(\cdot, R) - u_m^+(\cdot, R), v_m^+(\cdot, R) - u_m^+(\cdot, R) \right\rangle , \tag{26}$$

where $\langle\, ,\, \rangle$ stands for the inner product on $L_2(-\pi, +\pi)$ and $\|\ \|^t$ is the transposed matrix of $\|\ \|$. Then the functional (23) can be written as

$$J_m^R(a) = \left(\mathcal{E}^R\, a, a\right) + 2\,\mathrm{Re}\,\left(\mathcal{F}_m^R, a\right) + \mathcal{G}_m^R,\ \mathcal{F}_m^R = \left\|\mathcal{F}_{jm}^R\right\|_{j=1}^{T+M}. \tag{27}$$

To justify the above algorithm we will show that: *1)* the boundary value problems for $v^{\pm}_{n;R}$ are uniquely solvable for all $R > c$ and any fixed $\zeta > 0$; *2)* the matrix $\mathcal{E}^R$ is nonsingular; *3)* the minimizer $\{a_n(R)\}_{n=1}^{T+M}$ of the functional J_m^R tends to $\{S_{mn}\}_{n=1}^{T+M}$ with exponential rate as $R \to \infty$ (for any fixed $\zeta > 0$).

3.2 Justification of the algorithm

We consider the problem

$$(\Delta + k^2)w(x, y) = f(x, y), \quad (x, y) \in \Pi^R, \tag{28}$$

$$\partial_x^j\, w(\pi, y) = e^{2\pi i\alpha}\partial_x^j\, w(-\pi, y), \quad (\pm\pi, y) \in \Gamma_{\pm}^R,\ j = 0, 1, \tag{29}$$

$$\mathcal{B}w(x, y) = 0, \quad (x, y) \in \Gamma_0, \tag{30}$$

$$\mathcal{N}_\zeta\, w(x, y) = g(x, y), \quad (x, y) \in \Gamma^R, \tag{31}$$

where $R > c$ and $\zeta > 0$. In the section we assume that the boundary $\partial\mathcal{P}$ of $\mathcal{P}$ is smooth (see Section 2). This additional requirement is not essential for the method and is introduced only to simplify description.

Proposition 1 *Let ζ be a fixed positive number, $f \in L_2(\Pi^R)$, and $g \in H^{1/2}(\Gamma^R)$. Then, there exists a unique solution $w \in H^2(\Pi^R)$ to the problem (28)–(31), and the estimate*

$$\left\|w; H^2(\Pi^R)\right\| \le C(R)\left(\left\|f; L_2(\Pi^R)\right\| + \left\|g; H^{1/2}(\Gamma^R)\right\|\right) \tag{32}$$

holds with constant $C(R)$ independent of f and g.

Proof. As usual (see, e.g. [8]), one can prove that the uniqueness of a solution implies its existence and the estimate (32). Let us check the uniqueness. Assume that $v \in H^2(\Pi^R)$ satisfies the homogeneous problem (28)–(31). Using the Green formula, we obtain

$$\zeta \int_{-\pi}^{+\pi} |v(x, R)|^2\, dx = 0, \tag{33}$$

hence $v(x, R) = 0$. In accordance with (31) for $g = 0$ we have $\frac{\partial v}{\partial y}(x, R) \equiv 0$. Taking into account (28), we see that all derivatives of v vanish on Γ^R. Since the function v is analytic on Π^R, it follows that $v = 0$ on Π^R. □

Now we turn to the matrix $\mathcal{E}^R$ given by (25). Proposition 1 provides the existence of the matrix for any $R > c$.

Proposition 2 *For all $R > c$, the matrix $\mathcal{E}^R$ is nonsingular, i.e.,* $\det \mathcal{E}^R \neq 0$.

Proof. Suppose the assertion is not true, and matrix $\mathcal{E}^R$ degenerates for certain $R_0 > c$. Then there exists a nonzero vector $(c_1, \dots, c_{T+M})$ such that the functions $\mathcal{U}^-(x, y) := \sum c_j u_j^-(x, y)$ and $\mathcal{V}^-(x, y) := \sum c_j v_j^-(x, y)$ satisfy the equality

$$\mathcal{U}^-(x, R_0) = \mathcal{V}^-(x, R_0) \tag{34}$$

for all $x \in (-\pi, +\pi)$. Moreover, $\mathcal{U}^-$ and $\mathcal{V}^-$ satisfy the homogeneous Helmholtz equation (5) in a neighborhood of the interval

$$\Gamma^{R_0} = \{(x, y) : -\pi < x < \pi , y = R_0\} \tag{35}$$

in the closure $\overline{\Pi^{R_0}}$. In view of (24),

$$\partial_y \mathcal{U}^-(x, y) = \partial_y \mathcal{V}^-(x, y) , \quad (x, y) \in \Gamma^{R_0} . \tag{36}$$

From (5), (34) and (36) it follows that all derivatives of $\mathcal{U}^-$ and $\mathcal{V}^-$ coincide on the interval Γ^{R_0}. We extend $\mathcal{V}^-$ to the whole domain Π putting $\mathcal{V}^- = \mathcal{U}^-$ outside Π^R. Then the "new" $\mathcal{V}^-$ satisfies the homogeneous problem (5)–(7) in the domain Π. Besides, $\mathcal{V}^-$ is subject to the intrinsic radiation condition at infinity, which means that the asymptotics of $\mathcal{V}^-$ consists of outgoing waves. It follows that $c_1 = \dots = c_{T+M} = 0$ (see, e.g., [13]). This contradiction completes the proof. □

For later use, we now give some information on the behavior of the constant $C(R)$ in (32).

Proposition 3 *1) If there are no real eigenvalues of problem (8)–(9), then the $C(R)$ can be subject to the estimate*

$$C(R) \leq C_0 = \text{const} \quad \textit{for all} \quad R \geq R_0 > c . \tag{37}$$

2) If the real axis contains some eigenvalues of problem (8)–(9), then

$$C(R) \leq C_0 R^\nu \quad \textit{for all} \quad R \geq R_0 > c \tag{38}$$

with some $\nu > 0$.

The first part of Proposition 3 is a special case of Theorem 5.6.3 in [9]. The second part can be verified by an argument similar to that in Section 4.4 of [9]. We shall discuss in detail estimates of such kind for much more general situation in another paper.

Proposition 4 *Let $a(R) = (a_1(R), \dots, a_{T+M}(R))$ be the minimizer of the functional J_m^R in (23) and let γ be the same number as in (15). Then $J_m^R\,(a(R)) = O\left(\exp(-2\gamma' R)\right)$ as $R \to \infty$, where γ' is any number such that $\gamma' < \gamma$; if (37) holds, one can take $\gamma' = \gamma$.*

Proof. As before, let $S_m = \left(S_{m1}, \dots, S_{m,T+M}\right)$ be the m-th row of the augmented scattering matrix S. We substitute S_{mn} for a_n, $n = 1, \dots, T+M$, in (20) and denote the corresponding solution to the problem (17)–(20) by Y_m^R. Since the asymptotics (15) can be differentiated, we have $\mathcal{N}_\zeta\,\left(Y_m^R - Y_m\right)\big|_{\Gamma^R} = O\left(e^{-\gamma R}\right)$. This and Proposition 3 lead to

$$\begin{aligned} \left\| Y_m^R(\cdot, R) - Y_m(\cdot, R); L_2(-\pi, \pi)\right\| &\le C\,\left\| Y_m^R - Y_m;\, H^2(\Pi^R)\right\| \\ &\le\; C(R)\, e^{-\gamma R} \le C_0\, e^{-\gamma' R} \end{aligned} \tag{39}$$

(if (37) holds, one can put $\gamma' = \gamma$). From (39) and (15) it follows that

$$\begin{aligned} J_m^R\,(S_m) &= \left\| Y_m^R(\cdot, R) - \left(u_m^+(\cdot, R) + \sum_{n=1}^{M} S_{mn} u_n^-(\cdot, R)\right); L_2(-\pi, \pi)\right\|^2 \\ &\le C e^{-2\gamma' R}\,. \end{aligned}$$

It remains to note that $J_m^R\,(a(R)) \le J_m^R(S_m)$. □

Now we are directly studying the behaviour of $a(R)$ as $R \to \infty$.

Lemma 1 *For all $R \ge R_0 > c$ there hold the inequalities*

$$\left|a_j(R)\right| \le A\,, \quad j = 1, \dots, T+M\,, \tag{40}$$

with a constant $A < \infty$.

Proof. Let Z_m^R stand for the solution of problem (17)–(20) that corresponds to the vector $a(R) = (a_1(R), \dots, a_{T+M}(R))$. Using the Green formula, we obtain

$$\begin{aligned} &\int\limits_{\Pi^R} \left(\left(\Delta + k^2\right) Z_m^R(x, y)\overline{Z_m^R(x, y)} - \overline{\left(\Delta + k^2\right) Z_m^R(x, y)} Z_m^R(x, y)\right) dx dy \\ &\quad = \int\limits_{-\pi}^{+\pi} \left(\left(\mathcal{N}_\zeta Z_m^R\right)(x, R)\overline{Z_m^R(x, R)} - \overline{\left(\mathcal{N}_{-\zeta} Z_m^R\right)(x, R)} Z_m^R(x, R)\right) dx. \end{aligned} \tag{41}$$

The left-hand side vanishes by virtue of (17). Consider the right-hand side. We take account of (20) (with $a(R) = (a_1(R), \ldots, a_{T+M}(R))$) and substitute

$$\mathcal{N}_\zeta \left(u_m^+ + \sum_n a_n(R)\, u_n^- \right) \tag{42}$$

for $\mathcal{N}_\zeta Z_m^R$. The second factor $Z_m^R(x, R)$ on the right in (41) can be rewritten as

$$Z_m^R(x, R) = u_m^+(x, R) + \sum_n a_n(R)\, u_n^-(x, R) + O\left(\exp(-\gamma' R)\right) \tag{43}$$

(according to Proposition 4). Now the formulas (10)–(13) enable us to calculate the right-hand side of (41) up to an exponentially decaying term. As a result, from (41) we obtain $0 = 1 - \sum_n |a_n(R)|^2 + O\left(\exp(-\varepsilon R)\right)$ with some $\varepsilon > 0$. Thus

$$\sum_{n=1}^{T+M} |a_n(R)|^2 = 1 + O\left(e^{-\varepsilon R}\right) , \tag{44}$$

which concludes the proof. □

Remark 1 The number ε in (44) can be estimated precisely: one can take any number satisfying $\varepsilon < \left|\lambda_{T+M}^+ - \lambda_{T+M+1}^+\right|$.

We are ready to prove the main result of the section.

Theorem 1 *Let $a(R) = (a_1(R), \ldots, a_{T+M}(R))$ be the minimizer of the functional $J_m^R(a)$ given by (23). Let $\left(S_{m1}, \ldots, S_{m,T+M}\right)$ be the m-th row of the augmented scattering matrix S with $M \geq 0$. Then, for $R \geq R_0 > c$ the estimates*

$$|a_n(R) - S_{mn}| \leq A_\varepsilon e^{-\varepsilon R} , \quad n = 1, \ldots, T + M , \tag{45}$$

hold with constant A_ε independent of R, and ε can be any positive number verifying $\varepsilon < \left|\lambda_{T+M}^+ - \lambda_{T+M+1}^+\right|$.

Proof. As before, denote by $Z_m^R(x, y)$ the solution to the problem (17)–(20) with $(a_1(R), \ldots, a_{T+M}(R))$. Recall that $Y_m(x, y)$ satisfies the homogeneous problem (5)–(7) having the asymptotics (15). We write down the Green formula (41) changing Z_m^R for the difference $D_m = Y_m - Z_m^R$. Since the left-hand side vanishes, we obtain

$$0 = \int_{-\pi}^{+\pi} \left(\left(\mathcal{N}_\zeta D_m\right)(\cdot, R)\overline{D_m(\cdot, R)} - \overline{\left(\mathcal{N}_{-\zeta} D_m\right)(\cdot, R)} D_m(\cdot, R)\right) dx . \tag{46}$$

Introduce

$$\Phi_m(x,y) = u_m^+(x,y) + \sum_{n=1}^{T+M} S_{mn}\, u_m^-(x,y), \tag{47}$$
$$\Psi_m(x,y) = u_m^+(x,y) + \sum_{n=1}^{T+M} a_n(R)\, u_m^-(x,y)$$

and represent D_m in the form

$$D_m = Y_m - Z_m^R = (Y_m - \Phi_m) + (\Phi_m - \Psi_m) + (\Psi_m - Z_m^R)\,. \tag{48}$$

From (15) it follows that $Y_m(x,R) - \Phi_m(x,R) = O\left(e^{-\gamma R}\right)$. According to Proposition 4, $\Psi_m - Z_m^R = O(e^{-\gamma' R})$. This and Lemma 1 enable us to rewrite (46) in the form

$$\int_{-\pi}^{+\pi} \Big(\left(\mathcal{N}_\zeta \Phi_m - \mathcal{N}_\zeta \Psi_m\right)(x,R)\overline{(\Phi_m - \Psi_m)(x,R)} - \overline{\left(\mathcal{N}_{-\zeta}\Phi_m - \mathcal{N}_{-\zeta}\Psi_m\right)(x,R)}\,(\Phi_m - \Psi_m)(x,R)\Big) dx = O\left(e^{-\varepsilon R}\right) \tag{49}$$

with the same ε as in (44) (see Remark 1). In view of (10)–(13), the left-hand side of (49) admits straightforward calculation. As a result, we obtain

$$\sum_{n=1}^{T+M} |a_n(R) - S_{mn}|^2 = O\left(e^{-2\varepsilon R}\right)\,, \tag{50}$$

which concludes the proof. □

4 Numerical implementation of the algorithm

To obtain a numerical approximation S^R of an augmented scattering matrix S by the method given in Section 3 one has:

1. to find $2(T+M)$ functions $v_n^\pm\left(v_{n,R}^\pm\right)$, $n = 1, \ldots, T+M$, by solving the boundary value problem (17), (18), (19), and (24) in the domain Π^R (for sufficiently large R);
2. to compute the matrices (25) using the solutions $v_n^\pm(\cdot, R)$;
3. to minimize the functionals J_m^R (given by (23)) for $m = 1, \ldots, T+M$.

Clearly, the last step is equivalent to solving the linear equations

$$\mathcal{E}^R\left(S^R\right)^t + \mathcal{F}^R = 0\,. \tag{51}$$

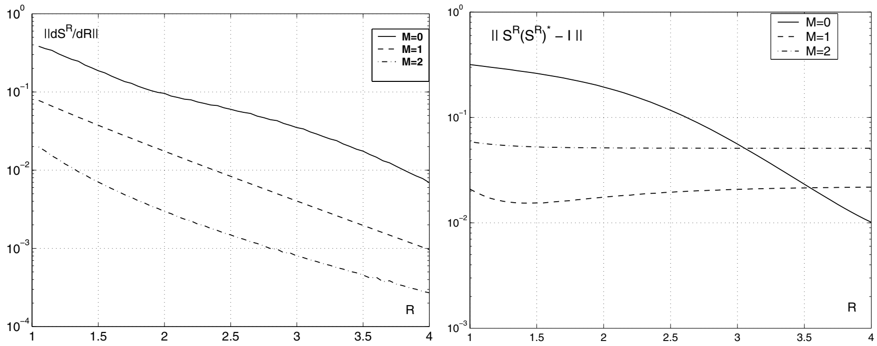

Fig. 2. The convergence of the procedure for "moderate" values of M and R: *left:* difference approximation of $\left\|dS^R/dR\right\|$, *right:* $\|S^R(S^R)^* - I\|$ for RGA model with $a/2\pi = 0.3$, $b/2\pi = 0.6$; other parameters: $k = 1$, $\alpha = 0.25$ $(T = 2)$; Neumann boundary condition imposed on Γ_0

At step **1,** any numerical procedure to solve the elliptic boundary value problems could be applied. We use a finite element technique; some details are collected in Section 6.

We mainly consider a *rectangular grating array* (RGA). In this model, the grating profile Γ_0 is the broken line with segments $y = 0$, $x = -b/2$, $y = -a$, and $x = b/2$ (a, b being given parameters, see Fig. 3). Other grating models are examined in Section 5.

First of all, we are interested in observing the numerical convergence of the procedure as $R \to \infty$. To this end it is convenient to consider the norm of derivative $\left\|dS^R/dR\right\|$ (actually, we deal with a difference approximation of this derivative) and the norm $\|S^R(S^R)^* - I\|$. It is expected that these norms are exponentially decaying as $R \to \infty$.

Let us first discuss scattering matrices of a "moderate" size of augmentation ($M \leq 2$) and restrict our consideration to "moderate" R ($1 \leq R \leq 4$). The results are shown in Fig. 2. The picture on the left demonstrates a convincing convergence $\left\|dS^R/dR\right\| \to 0$. Moreover, this convergence is of exponential character. The right-hand part of the same figure shows that the approximation S^R is close to a unitary matrix (moreover, in the case $M = 0$, the norm $\|S^R(S^R)^* - I\|$ is decaying).

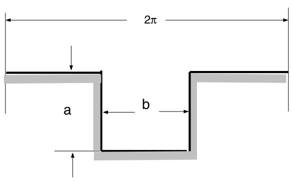

Fig. 3. Rectangular grating array

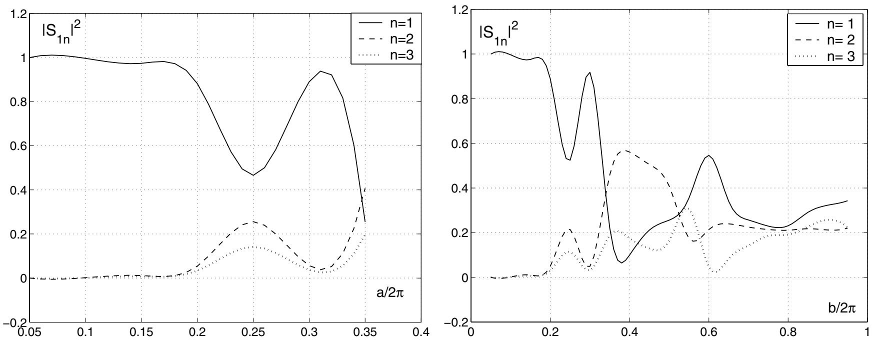

Fig. 4. Scattering of a plane wave by RGA: $\alpha = -0.5$ (incidence angle equals the so-called 1-st Bregg's angle), $k = 2$ (there are $T = 4$ propagating waves). The curves refer to the intensities (diffraction coefficients) of the principle ($n = 1$) and two adjacent ($n = 2$ and $n = 3$) scattered waves depending on: *(left)* grating depth a and *(right)* groove's width b; the Dirichlet boundary condition imposed on Γ_0

These observations allows us to conclude that, using the method, one can reliably compute scattering matrices for "moderate" M (in particular, classical scattering matrices). To achieve an appropriate accuracy it is sufficient to deal with "moderate" values of R. An immediate application is given in Fig. 4 (other results are discussed in Section 5).

However, it appears to be impossible to observe numerically the exponential convergence of the procedure for augmented scattering matrices S_M with sufficiently large M. Indeed, for $M > 0$ the matrix $\mathcal{E}^R$, although being nonsingular for any finite $R > c$ (Proposition 2), can degenerate as $R \to \infty$. In view of unavoidable numerical errors, the solution of equations (51) becomes unreliable for large R. This effect is demonstrated in Fig. 5: it is seen that the approximation S^R of a scattering matrix with "large" augmentation ($M \geq 3$) does not tend to a unitary matrix as R increases. Moreover, the behaviour of $\|dS^R/dR\|$ becomes oscillating with respect to R and loses the features of convergence (not shown).[2]

5 Numerical detection of surface waves

In the section we discuss numerical examples of detection and computation of surface waves in diffraction gratings by means of the optimization approach given in Section 3. Let us fix all parameters of the problem (5)–(7) except for α and k and introduce $D(\alpha, k) = \det\big(S_{(22)} - 1\big)$. According to the existence criterion, to every point of the set

(52) $$\Xi = \big\{(\alpha, k) \in \mathbb{R}^2 \,:\, D(\alpha, k) = 0\big\}$$

[2] It is worth to note that the results given in Fig. 5 correspond to a shallow-depth grating profile ($a/2\pi = 0.01$); the same effect is observed even for uniform ($a = 0$) grating.

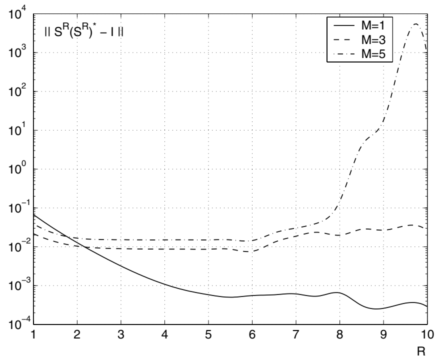

Fig. 5. The convergence of the procedure for "large" values of M and R for RGA model with $a/2\pi = 0.01$, $b/2\pi = 0.6$; other parameters: $k = 0.245$, $\alpha = 0.25$ ($T = 0$); the Neumann boundary condition is imposed on Γ_0

there corresponds a surface wave. Suppose that the Neumann condition is imposed on Γ_0. We restrict our consideration to the subset

$$\Xi_0 = \Xi \bigcap \{(\alpha, k) \ : 0 \leq \alpha \leq k \leq 1/2\}\,. \tag{53}$$

In this case $T = 0$ and the matrix S consists only of the block $S_{(22)}$ of size $M \times M$.

It turns out in all our examples, that a surface wave can be detected already for $M = 1$. In this case the block $S_{(22)}$ coincides with the only entry S_{11} of the matrix S so that $S = S_{(22)} = S_{11}$.

We choose the subset Ξ_0 to compare our results with those in [2]. That paper was devoted to an RGA model; by means of a different approach (based on a separation of variables), there were found points (α, k) corresponding to surface waves. Comparison of our results with those in [2] is shown in the left-hand part of Fig. 6.

A numerical approximation of a part of the trajectory of the point

$$D(\alpha, k) = S_{11}(\alpha, k) - 1 \tag{54}$$

in the complex plane for a fixed α and varying k is shown in Fig. 6 on the right. For $k = k_*$ the trajectory meets the real axis; the point (α, k_*) is taken as approximation to a point in Ξ_0.

Results related to a grating with a more complicated geometry are given in Fig. 7. Moreover, it turns out that even for gratings having essentially different geometry (see, e.g., Fig. 8) the structure of the sets Ξ_0 is similar to that in Figures 6 and 7.

In applications, it is of interest to know not only the sets Ξ but the intensity distribution of the corresponding surface waves as well (see, e.g., [17, 16]). Let us now discuss how the approach can be adapted to obtain a specific

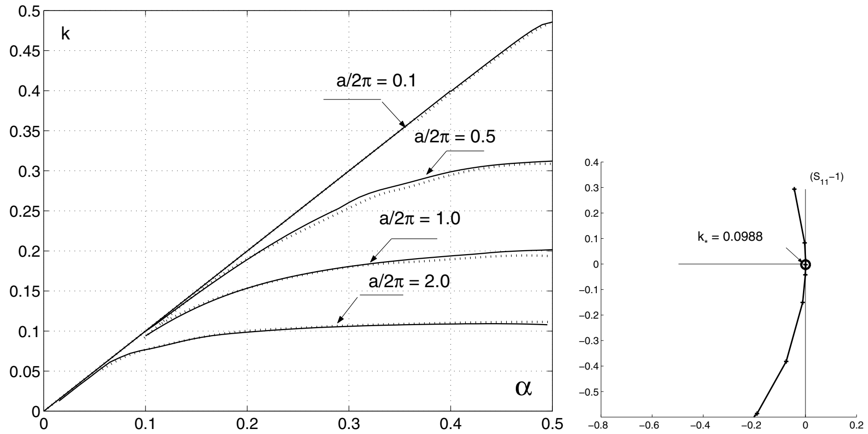

Fig. 6. *Left:* Sets Ξ_0 (given in solid) for various values of the grating depth a of RGA model with $b/2\pi$=0.6; plots are shown in comparison with the results of [2] (dotted lines). *Right:* The trajectory of $S_{11}-1$ when k runs over the interval [0.0898,0.0993] and $\alpha = 0.1$, $a/2\pi = 0.5$ are fixed; the center of the circle indicates the point $k_* = 0.0988$

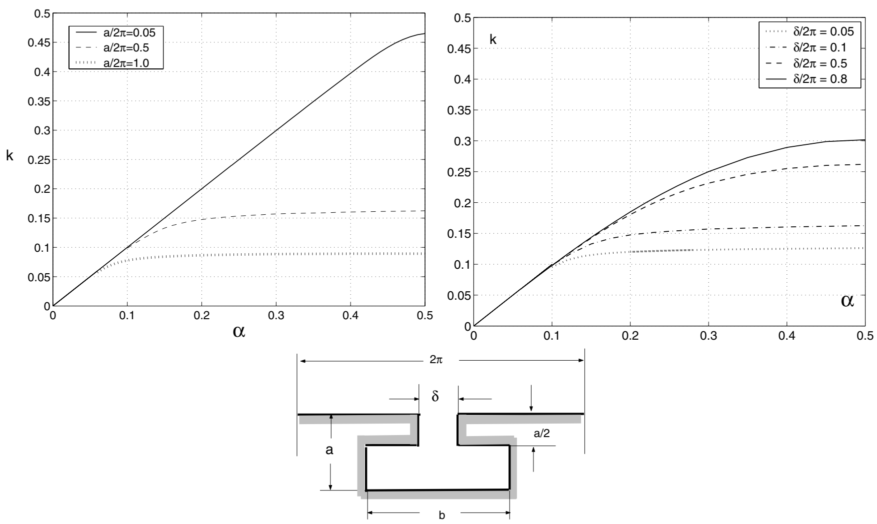

Fig. 7. Sets Ξ_0 for various values of parameters of the grating model shown at the *bottom* part of the figure. *Left* fixed parameters: $\delta/2\pi = 0.1$, $b/2\pi$=0.6; *Right* fixed parameters: $a/2\pi = 0.5$, $b/2\pi$=0.6

solution (in particular, a surface wave) in the domain Π^R. It is clear from the proof of Lemma 1 that the solution Z_m^R of problem (17)–(20), corresponding to the minimizer $(S_{m1}^R, \ldots, S_{m,T+M}^R)$ of functional J_m^R, is a good approximation to the solution Y_m (15), $m = 1, \ldots, T+M$. Note that after the steps mentioned in Section 4 both

$$Z_m^R = v_m^+ + \sum_{n=1}^{T+M} S_{mn}^R\, v_n^- \tag{55}$$

and $S^R = \|S_{mn}^R\|$ are at our disposal.

Suppose that 1 is an eigenvalue of $S_{(22)}$. Let $h_{(2)} = (h_{T+1}, \dots, h_{T+M})$ be a left eigenvector of the matrix $S_{(22)}$ corresponding to the eigenvalue 1. It can be easily shown that such an eigenvector satisfies $h_{(2)} S_{(21)} = 0$. Take $h_1 = \dots = h_T = 0$, then the asymptotics (as $R \to \infty$) of the linear combination

$$u = \sum_{m=1}^{T+M} h_m Y_m \tag{56}$$

contains only decaying exponents, i.e., u is a surface wave. Therefore, a numerical approximation of a surface wave can be obtained by substituting Z_m^R for Y_m.

However, having only approximate values for the coefficients, we can not expect that the growing exponents cancel one another in the combination (56). To avoid the difficulty we substitute for Y_m not Z_m^R but the function

$$\tilde{Z}_m^R = \tilde{v}_m^+ + \sum_{n=1}^{T+M} S_{mn}^R\, \tilde{v}_n^-, \tag{57}$$

where $\tilde{v}_m^\pm$ satisfies the equations (17)–(19) and the condition

$$\mathcal{N}_\zeta \tilde{v}_m^\pm = \mathcal{N}_\zeta \left(\frac{\exp\left(-\,|\lambda_m|\, y\right)}{\sqrt{8\pi\, |\lambda_m|}} \exp\left(i(m+\alpha)x\right) \right), \tag{58}$$

$m = T+1, \dots, T+M$, on Γ^R instead of (20). Then the functions $\tilde{Z}_m^R$ do not contain the growing exponents from the very beginning.

The intensity distributions obtained in this way are shown in Fig. 8.

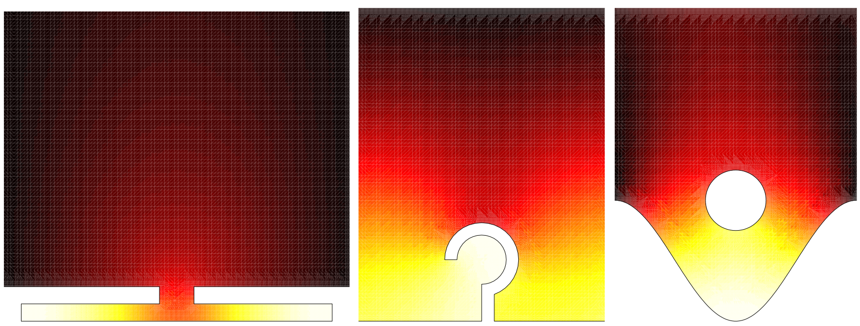

Fig. 8. Distribution of the intensity of normalized surface waves for various grating models (numerous parameters of the corresponding problems are not specified)

6 Details of the finite element implementation

First, we rewrite the problem (17), (18), (19), and (24) for the function $v_n^{\pm}(x, y)$ as:

(59)
$$(\Delta + k^2)w(x, y) = 0\,, \quad (x, y) \in \Pi^R\,,$$

(60) $$\partial_x^j\, w(\pi, y) = e^{2\pi i\alpha}\partial_x^j\, w(-\pi, y)\,, \quad (\pm\pi, y) \in \Gamma_{\pm}^R\,, \quad j = 0, 1\,,$$

(61) $$\mathcal{B}w(x, y) = g(x, y)\,, \quad (x, y) \in \Gamma_0\,,$$

(62) $$\mathcal{N}_\zeta\, w(x, y) = 0\,, \quad (x, y) \in \Gamma^R\,,$$

where $w(x, y) := v_n^{\pm}(x, y) - u_n^{\pm}(x, y)$ and $g(x, y) = -\,\mathcal{B}u_n^{\pm}\big|_{\Gamma_0}$.

Introduce the function space

(63) $$\mathcal{W} = \left\{w(x, y) \in H^1(\Pi^R) :\ w \text{ satisfies condition (60)}\right\}\,.$$

Then the problem (59)–(62) admits the following "weak" formulation: to find $w \in \mathcal{W}$ such that

(64) $$\mathcal{A}(w, \tilde{w}) = f(\tilde{w})\,, \quad \forall\, \tilde{w} \in \mathcal{W}\,.$$

The representation of the forms $\mathcal{A}(\cdot, \cdot)$ and $f(\tilde{w})$ depend on the boundary operator $\mathcal{B}$; for example, in the case of Neumann condition (that is assumed in what follows)

(65)
$$\mathcal{A}(w, \tilde{w}) = \int\limits_{\Pi^R} \left(\nabla w \cdot \overline{\nabla\tilde{w}} - k^2 w\overline{\tilde{w}}\right) dxdy - i\zeta \int\limits_{\Gamma^R} w\overline{\tilde{w}}\, ds\,,$$
$$f(\tilde{w}) = \int\limits_{\Gamma_0} g\overline{\tilde{w}}\, ds\,.$$

We describe a finite elements discretization of the problem (64). Let $\{\tau_k\}_{k=1}^{k=N}$ be a triangular mesh approximating the domain Π^R, and let h denote the maximal diameter of the triangles τ_k.[3] Introduce the function space

(66)
$$\mathcal{W}_h = \left\{w_h \in C(\Pi^R)\ :\ w_h|_{\tau_k} \in \mathcal{P}^1(\tau_k)\ \forall\, k\,,\ w_h \text{ satisfies condition (60)}\right\}\,,$$

where $\mathcal{P}^1$ denotes the space of linear polynomials. Then the following finite element problem corresponds to (66): find $w_h \in \mathcal{W}_h$ such that

(67) $$\mathcal{A}(w_h, \tilde{w}_h) = f(\tilde{w}_h), \quad \forall\, \tilde{w}_h \in \mathcal{W}_h.$$

[3] We use triangulation package [15] to construct the mesh; the range of mesh size h is $0.05 < h < 0.2$ for all numerical results that are presented in the paper; further decreasing of h does not affect the results under the chosen tolerance 10^{-3}.

The solvability of the finite element problem (67) and the approximation error $w - w_h$ were analyzed, for example, in [1]. In particular, it can be shown that the finite element problem is uniquely solvable for sufficiently small h provided the problem (64) is uniquely solvable.

In the space $\mathcal{W}_h$ we introduce the standard Courant basis functions ϕ_m corresponding to the nodal points p_m by the conditions

$$\phi_m(p_l) = \delta_{m,l} \text{ and } \phi_m|_{\tau_k} \in P^1(\tau_k)\ \forall k. \tag{68}$$

Let us denote by $I_\pm$ those indices in $I = \{1, \dots, N\}$ which correspond to the nodal points at the boundaries $\Gamma^R_\pm$. We assume that the mesh is constructed in such a way that each node p_m on the boundary Γ^R_- has a corresponding node $p_{p(m)}$ on the boundary Γ^R_+ such that their $y-$coordinates are the same. Furthermore, we define $\tilde{I} = I \setminus (I_- \cup I_+)$. Then, the functions ψ_m given by

$$\psi_m = \begin{cases} \phi_m, & m \in \tilde{I}, \\ \phi_m + e^{2\pi i\alpha}\phi_{p(m)}, & m \in I_-, \end{cases} \tag{69}$$

span the space $\mathcal{W}_h$, i.e. $\forall\, w_h \in \mathcal{W}_h$

$$w_h = \sum_{m \in \tilde{I} \cup I_-} \nu_m \psi_m\,, \tag{70}$$

with some $\vec{\nu} = \{\nu_m\}$. Finally, the finite element problem is equivalent to the linear system

$$\hat{A}\vec{\nu} = \vec{f}\,, \quad \hat{A} = \left\| \mathcal{A}(\psi_i, \psi_j) \right\|_{i,j \in \tilde{I} \cup I_-}\,, \quad \vec{f} = \left\| f(\psi_j) \right\|_{j \in \tilde{I} \cup I_-}\,. \tag{71}$$

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