Exact Nonlocal Boundary Conditions in the Theory of Dielectric Waveguides

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Abstract— The original problem in an unbounded domain is reduced to a linear parametric eigenvalue problem in a circle, which is convenient for numerical solution. The examination of the solvability of this problem is based on the spectral theory of compact self-adjoint operators. The existence of surface guided waves is proved, and properties of the dispersion curves are investigated. An algorithm for the numerical solution of the problem based on the finite element method is proposed. The convergence of the numerical method is proved. Numerical results are discussed.

1. INTRODUCTION

Optical waveguides are dielectric cylindrical structures that can conduct electromagnetic energy in the visible and infrared parts of the spectrum. The waveguides used in optical communication are flexible fibers made of transparent dielectrics. The cross section of a waveguide usually consists of three regions: the central region (core) is surrounded by a cladding which, in turn, is surrounded by a protective coating. The dielectric permittivity ε of the core can be constant or can vary over the cross section; the dielectric permittivity of the cladding is usually positive constant (denote it by ε_∞). The coating is optically isolated from the core; for this reason, it is usually neglected in mathematical models, and it is assumed that the cladding is unbounded from the outside.

We use the classical model (see [1]), in which the waveguide is assumed to be unbounded and linearly isotropic. A mathematical analysis of surface waves based on the theory of unbounded self-adjoint operators can be found in [2]. In that paper, the original problem is considered as a problem of the form $A(\beta)\mathrm{H} = k^2\mathrm{H}$ with respect to the spectral parameter k^2, and the dependence $k = k(\beta)$ is studied (H is the magnetic vector amplitude, k is the wavenumber, β is the propagation constant). In [3], a similar technique is used to extend the results obtained in [2] to the case of waveguides with a variable magnetic permeability.

The results obtained in [2, 3] give a complete understanding of the qualitative properties of the spectrum of surface guided waves; however, in order to calculate the spectral characteristics of waveguides, numerical methods are needed (see survey [4]). The formulations of the problems used in [2, 3] are not quite convenient for obtaining numerical solutions. This is due to two specific features of those statements.

1. The problems are formulated for the entire plane $\mathbb{R}^2$. For a numerical solution, special measures must be taken to restrict the integration domain and to formulate additional boundary conditions.

2. Spectral problems (except for a point spectrum) have a continuous part of the spectrum. Although the location of this part is known exactly, a numerical solution requires that false approximate solutions be detected and discarded.

Statements of problems suggested in [5, 6] are free of those drawbacks. In those papers, exact nonlocal boundary conditions (see [7, 8]) are used to reduce the problems that were originally formulated for the entire plane $\mathbb{R}^2$ to equivalent problems in a circle. In [5, 6] the spectral problems are formulated in a circle Ω which includes waveguide's cross-section domain Ω_i (see Fig. 1); these problems have no continuous spectrum. Moreover, their spectrum is identical to the point part of the spectrum of the original problem. These statements are convenient for the finite element method. The cost of this advantage is that the spectral parameter appears in the equation in a nonlinear fashion; more precisely, the problems have the form $\mathrm{A}(\beta,\lambda)\mathrm{H} = \lambda\mathrm{H}$, where A is a compact self-adjoint operator. The solution of such problems requires the use of special iterative methods.

In this paper, we use a new formulation of the problem proposed in [9]. The original problem by exact nonlocal boundary conditions method is reduced to an equivalent linear self-adjoint eigenvalue problem $A(p)\mathcal{H} = \beta^2 B(p)\mathcal{H}$ in the circle Ω. Here, the parameter p is the transverse wave number $p = \sqrt{\beta^2 - k^2\varepsilon_\infty}$; for each $p \geq 0$ the operators $A(p)$ and $B(p)$ are bounded and $B(p)$ is compact; vector $\mathcal{H} = (\mathrm{H}_1, \mathrm{H}_2)$ represents the first two components of the intensity vector H. We examine the solvability of the problem and investigate some properties of the dispersion curves. Then we

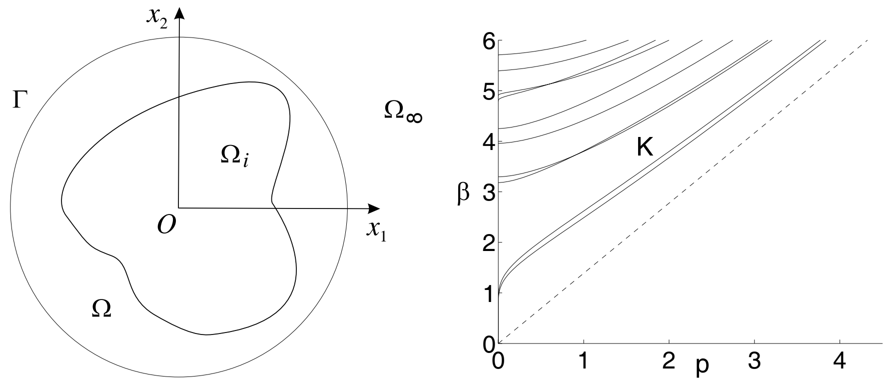

Figure 1: A schematic waveguide's cross-section (on the left) and the dispersion curves for 1.5×1 rectangular waveguide, $\varepsilon(x) = 2.08$, $x \in \Omega_i$, $\varepsilon_\infty = 1$ (on the right).

propose an algorithm for the numerical solution of the problem based on the finite element method. We prove the convergence of the numerical method and discuss some numerical results.

2. SOLVABILITY OF THE PROBLEM

First, we recall the statement of the problem given in [2]. Let $\overline{\mathrm{H}}$ be the complex conjugate of H. For the complex-valued vector fields $\mathrm{H} = (\mathrm{H}_1, \ldots, \mathrm{H}_l)$ and $\mathrm{H}' = (\mathrm{H}'_1, \ldots, \mathrm{H}'_l)$ $(l \geq 1)$, we define

$$\begin{aligned} \mathrm{H} \cdot \mathrm{H}' &= \mathrm{H}_1\mathrm{H}'_1 + \ldots + \mathrm{H}_l\mathrm{H}'_l, \quad |\mathrm{H}|^2 = \mathrm{H} \cdot \overline{\mathrm{H}}, \quad \nabla\mathrm{H} = (\nabla\mathrm{H}_1, \ldots, \nabla\mathrm{H}_l), \\ \nabla\mathrm{H} \cdot \nabla\mathrm{H}' &= \nabla\mathrm{H}_1 \cdot \nabla\mathrm{H}'_1 + \ldots + \nabla\mathrm{H}_l \cdot \nabla\mathrm{H}'_l, \quad |\nabla\mathrm{H}|^2 = \nabla\mathrm{H} \cdot \nabla\overline{\mathrm{H}}. \end{aligned}$$

Let $V(D) = H^1(D)$ be the Sobolev space of complex-valued scalar functions defined on the domain $D \subseteq \mathbb{R}^2$, and $V^l(D) = [H^1(D)]^l$ be the corresponding space of l-dimensional vector-functions. The scalar product and norm in Hilbert space $V^l(D)$ are defined in the conventional way:

$$(\mathrm{H}, \mathrm{H}') = \int_D \left(\nabla\mathrm{H} \cdot \nabla\overline{\mathrm{H}'} + \mathrm{H} \cdot \overline{\mathrm{H}'}\right) dx, \quad \|\mathrm{H}\|_{1,D} = (\mathrm{H}, \mathrm{H})^{1/2}.$$

Consider a weak formulation of the original problem [2]: Find nonzero vectors $\mathrm{H} \in V^3(\mathbb{R}^2)$ and all pairs $(\beta, k) \in \Lambda = \{(\beta, k) : \beta/\sqrt{\varepsilon_+} < k < \beta/\sqrt{\varepsilon_\infty},\ \beta > 0\}$ such that

$$\int_{\mathbb{R}^2} \left(\frac{1}{\varepsilon}\mathrm{rot}_\beta\mathrm{H} \cdot \overline{\mathrm{rot}_\beta\mathrm{H}'} + \frac{1}{\varepsilon_\infty}\mathrm{div}_\beta\mathrm{H}\ \overline{\mathrm{div}_\beta\mathrm{H}'}\right) dx = k^2 \int_{\mathbb{R}^2} \mathrm{H} \cdot \overline{\mathrm{H}'}\, dx, \tag{1}$$

for any $\mathrm{H}' \in V^3(\mathbb{R}^2)$. Here differential operators div_β and rot_β are obtained from usual operators by replacing generating waveguide line derivative with $i\beta$ multiplication; ε_+ is the maximum of the function ε. We suppose that $\varepsilon \geq \varepsilon_\infty$, $x \in \mathbb{R}^2$.

Definition 1. The vector-function $\mathrm{H} \in V^l(\mathbb{R}^2)$ is called metaharmonic in $D \subset \mathbb{R}^2$ if

$$-\triangle\mathrm{H} + p^2\mathrm{H} = 0,\ x \in D, \quad p \neq 0.$$

The vector-function $\mathrm{H}_p \in V^l(\mathbb{R}^2)$ is called metaharmonic extension of $\mathrm{H} \in V^l(\Omega)$ to $\Omega_\infty = \mathbb{R}^2 \setminus \overline{\Omega}$ if H_p is metaharmonic in Ω_∞ and $\mathrm{H}_p\big|_\Omega = \mathrm{H}$.

The dielectric permittivity ε is equal to ε_∞ in the domain Ω_∞. Therefore, if a vector-function H satisfies (1) then it is metaharmonic [2]. This fact let us to obtain (see [9] for technical details) a new formulation of the original problem: For each $p > 0$ find all parameters $\beta > 0$ and nonzero vectors $\mathrm{H} = (\mathcal{H}, i\mathrm{H}_3) \in V^3(\Omega)$, where H_l, $l = 1, 2, 3$, are real-valued functions, such that the following relations are valid:

$$A(p)\mathcal{H} = \beta^2 B(p)\mathcal{H}, \quad \mathrm{H}_3 = \beta T(p)\mathcal{H}. \tag{2}$$

Here $B(p) = D + C^* L^{-1}(p) C$ and $T(p) = L^{-1}(p) C$; by C^* denote the adjoint operator. The linear operators $C : V^2(\Omega) \to V(\Omega)$, $D : V^2(\Omega) \to V^2(\Omega)$, and $L : V(\Omega) \to V(\Omega)$ are defined by the following relations:

$$
\begin{aligned}
(A(p)\mathcal{H},\mathcal{H}') &= \int\limits_\Omega \Big(\frac{1}{\varepsilon}\mathrm{rot}\mathcal{H}\,\mathrm{rot}\mathcal{H}' + \frac{1}{\varepsilon_\infty}\mathrm{div}\mathcal{H}\,\mathrm{div}\mathcal{H}' + \frac{p^2}{\varepsilon_\infty}\mathcal{H}\cdot\mathcal{H}'\Big)\,dx \\
&\quad + \frac{2\pi}{\varepsilon_\infty}\sum_{n=-\infty}^{\infty}\mathbb{K}_n(Rp)\,a_n(\mathcal{H})\cdot\overline{a_n(\mathcal{H}')} + \frac{1}{\varepsilon_\infty}\int\limits_0^{2\pi}\Big(\frac{\partial \mathrm{H}_1}{\partial\varphi}\,\mathrm{H}_2' - \frac{\partial \mathrm{H}_2}{\partial\varphi}\,\mathrm{H}_1'\Big)\Big|_{r=R}\,d\varphi, \\
(D\mathcal{H},\mathcal{H}') &= \int\limits_\Omega \sigma\mathcal{H}\cdot\mathcal{H}'\,dx, \quad (C\mathcal{H},H') = \int\limits_\Omega \sigma\mathcal{H}\cdot\nabla H'\,dx, \quad \sigma = \varepsilon_\infty^{-1} - \varepsilon^{-1}, \\
(L(p)H,H') &= \int\limits_\Omega \Big(\frac{1}{\varepsilon}\nabla H\cdot\nabla H' + \frac{p^2}{\varepsilon_\infty}HH'\Big)dx + \frac{2\pi}{\varepsilon_\infty}\sum_{n=-\infty}^{\infty}\mathbb{K}_n(Rp)\,a_n(H)\,\overline{a_n(H')}. \\
\mathbb{K}_n(z) &= -zK_n'(z)/K_n(z), \quad a_n(H) = \frac{1}{2\pi}\int\limits_0^{2\pi} H|_{r=R}\,e^{-in\varphi}\,d\varphi.
\end{aligned}
$$

Here $\mathrm{rot}\mathcal{H} = \partial\mathrm{H}_2/\partial x_1 - \partial\mathrm{H}_1/\partial x_2$, $\mathrm{div}\mathcal{H} = \partial\mathrm{H}_1/\partial x_1 + \partial\mathrm{H}_2/\partial x_2$, R is the radius of the circle Ω, and $K_n(z)$ is the modified Bessel function of order n. The following theorem states some important properties of the operators of the problem (2).

Theorem 1 (see (9)). *For each $p > 0$ the operator $A(p)$ is self-adjoint and positive definite; for $p = 0$ this operator is self-adjoint and nonnegative. The operator-function $A(p)$ is continuously differentiable and increasing for $p > 0$. For each $p \geq 0$ the operator $B(p)$ is self-adjoint, nonnegative and compact. The operator-function $B(p)$ is continuously differentiable and nonincreasing for $p > 0$. For each $p > 0$ the operator $T(p)$ is compact. For each $p > 0$ the operator $L(p)$ is continuously invertible. All operators mentioned above are real.*

The original problem (1) and problem (2) are equivalent in the sense of the following theorem.

Theorem 2 (see [9]). *Suppose that (β, p, H) is a solution of the problem (2). Then $(\beta, p) \in K$, where $K = \{(\beta, p) : p > 0,\ \beta > p\sqrt{\varepsilon_+/(\varepsilon_+ - \varepsilon_\infty)}\}$. Let H_p be the metaharmonic extension of H to Ω_∞, and let $k = \sqrt{(\beta^2 - p^2)/\varepsilon_\infty}$. Then (β, k, H_p) is the solution of the problem (1). Conversely. Suppose that (β, k, H) is a solution of the problem (1). Let $p = \sqrt{\beta^2 - k^2\varepsilon_\infty}$. Then $(\beta, p, \mathrm{H}|_\Omega)$ is the solution of the problem (2) with $(\beta, p) \in K$.*

The existence and qualitative properties of the spectrum of surface guided waves were investigated in the book [10] using new formulation (2) of the problem.

Theorem 3 (see [10]). *For each $p > 0$ the set of all existing solutions of the problem (2) can be represented as $\{\beta_l(p), \mathrm{H}_l(p),\ l = 1, 2, \ldots\}$. Moreover, the following assertions hold:*

(a) $\beta_1(p) \leq \ldots \leq \beta_l(p) \leq \ldots$, $\beta_l(p) \to \infty$ *as* $l \to \infty$; *any* $\beta_l(p)$ *has a finite multiplicity (i.e.,* $\beta_l(p)$ *can coincide only with a finite number of* $\beta_j(p)$, $j \geq 1$).
(b) $(A(p)\mathcal{H}_l, \mathcal{H}_j) = \delta_{l,j}$.
(c) *The functions* $p \to \beta_l(p)$, $l = 1, 2, \ldots$, *are increasing and have the local Lipschitz property.*
(d) $\beta_l(p)/p \to k_0 = \sqrt{\varepsilon_+/(\varepsilon_+ - \varepsilon_\infty)}$ *as* $p \to \infty$, $l \geq 1$.
(e) $\beta_1(p) \to +0$, $\beta_2(p) \to +0$ *as* $p \to +0$; $\beta_l(0) > 0$, $l \geq 3$.

The dispersion curves $\beta = \beta_l(p)$ for a homogeneous waveguide with a rectangular cross section are shown in Fig. 1 on the right. Setting $p = 0$ in the first Equation (2), we obtain the cut-off equation for finding the squares of the cut-off points $\beta_l(0)$.

3. APPROXIMATE SOLUTION OF THE PROBLEM

For discretization of the problem (2) we use finite element method with numerical integration. Approximation V_h of the real Sobolev space $H^1(\Omega)$ is based on usual conformal Lagrange finite elements of the order m. Thus we obtain the real matrices $A_h^N(p)$, D_h, C_h, and $L_h^N(p)$ which are discrete analogs of the operators $A(p)$, D, C, and $L(p)$, respectively [10]. These approximations depend on two parameters: the real parameter h (the characteristic size of finite elements, $h \to 0$) and the integer parameter N, which specifies the number of the Fourier harmonics taken into account ($N \to \infty$). Since we assume that the circle Ω of radius R is fixed, we do not explicitly indicate the dependence on the third parameter R of the problem here.

The finite-dimensional approximation of the first equation in (2) is naturally described as the generalized algebraic linear eigenvalue problem regarding spectral parameter $(\beta_h^N)^2$:

$$A_h^N(p)\mathcal{H}_h^N = (\beta_h^N)^2 B_h^N(p)\mathcal{H}_h^N, \quad B_h^N(p) = D_h + (C_h)^T (L_h^N(p))^{-1} C_h. \tag{3}$$

Here, $A_h^N(p)$, $L_h^N(p)$, and $B_h^N(p)$ are large symmetric and positive definite matrices for each $p > 0$; matrices $A_h^N(p)$, $L_h^N(p)$), and C_h are sparse; $B_h^N(p)$ is full and such that there is an efficient method for multiplying this matrix by a vector (after an LL^T factorization of the matrix $L_h^N(p)$). For each fixed $p \geq 0$, we have to find all eigenvalues $(\beta_h^N)^2 = (\beta_h^N)^2(p)$ of the problem (3) from the given interval $(p^2/(1-\varepsilon_\infty/\varepsilon_+), \beta_{\max}^2)$ and the corresponding eigenvectors $\mathcal{H}_h^N = \mathcal{H}_h^N(p)$. There are many methods that solve problem (3) subject to the constraints specified above. We used the Lanczos method.

After solution of the problem (3) we can find $\mathrm{H}_{3,h}^N = \beta_h^N (L_h^N(p))^{-1} C_h \mathcal{H}_h^N$. The pair $(\beta_h^N, \mathrm{H}_h^N)$, where $\mathrm{H}_h^N = (\mathcal{H}_h^N, \mathrm{H}_{3,h}^N)$, is the discrete solution of the problem (2). A theorem analogous to the theorem 3 on the existence of the discrete solutions for h small enough was proved in [10]. The convergence of the numerical method is justified by the following theorem.

Theorem 4 (see [10]). *Let for $p \geq 0$ a pair $(\beta(p), \mathrm{H}(p))$ be a solution of the problem (2) and $\beta(p)$ has the multiplicity is equal to one. Let $(\beta_h^N(p), \mathrm{H}_h^N(p))$ be a corresponding solution of discrete problem. Then for h small enough and $N \geq c_0 \ln(1/h)$, $c_0 = m/\ln(R/R_0)$, the following assertions hold:*

$$\|\mathrm{H}(p) - \mathrm{H}_h^N(p)\|_{1,\Omega} \leq c(p)h^m, \quad |\beta(p) - \beta_h^N(p)| \leq c(p)h^{2m}.$$

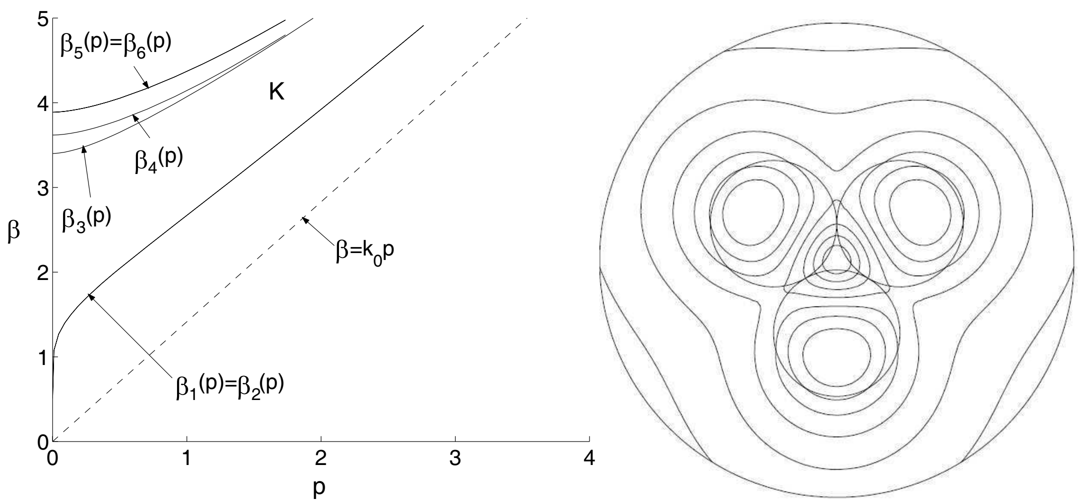

Figure 2: The dispersion curves for the three-circle waveguide (on the left) and the level curves of the function $|\mathrm{H}| = (\mathrm{H} \cdot \mathrm{H})^{1/2}$ corresponding to $\beta_4 = 3.6532$ and $p = 0.2$ (on the right).

Table 1: Calculation error $e = h^{-2}|\beta_4 - \beta_{4,h}^N|/|\beta_4|$ against N and N_h, where β_4 is the approximate value of the propagation constant obtained with 6006 grid nodes.

$N \vert N_h$	78	335	1093
1	0.5	23.3	92.5
3	0.619	1.67	1.56
5	0.62	1.67	1.57
7	0.62	1.67	1.57
15	0.62	1.67	1.57

Here R_0 is the minimal radius of the circumscribed circle Γ (see Fig. 1 on the left).

An analogous result holds for β which has a finite multiplicity [10].

To demonstrate the universality of the proposed method, we numerically solved the problem for the domain Ω_i consisting of three circles of radius 0.4 tangent to each other. The center of the domain Ω_i coincided with the center of the circle Ω of radius 1.5. The dielectric permittivity within Ω_i was $\varepsilon = 2$, and $\varepsilon_\infty = 1$. For each fixed p in the interval from 0 to 3, the first six (with account for the multiplicity) eigenvalues β^2 of problem (3) and the corresponding eigenvectors were found. The calculations were based on the linear triangular finite elements ($m = 1$) and were performed for the number N_h of the grid nodes in Ω in the range from 78 to 6006. Table 1 presents the results for the forth eigenvalue β_4 for $p = 1$. From this table we can conclude that it is enough to use only five of the Fourier harmonics, $N = 5$, at that $|\beta_4 - \beta_{4,h}^N|/|\beta_4| \approx 1.6h^2$.

The dispersion curves for the three-circle waveguide are shown in Fig. 2 on the left. There are only four dispersion curves because the upper and the lower curves are multiple due to the symmetry of the problem: $\beta_1 = \beta_2$ and $\beta_5 = \beta_6$. Fig. 2 on the right shows, for $p = 0.2$, the level curves of the function $|\mathrm{H}| = (\mathrm{H} \cdot \mathrm{H})^{1/2}$ corresponding to $\beta_4 = 3.6532$. The calculations were performed with 3150 grid nodes within Ω.

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