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ON HELMHOLTZ PROBLEM FOR PLANE PERIODICAL STRUCTURES

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1. Introduction

The Helmholtz problem for the plane periodical structures is arising in investigations of quantum motion of a free particle on periodical system of reflecting discs [1]-[4]. In the recent paper [4] this problem is reduced to solving the system of the boundary integral equations for the potentials of simple and double layers of the Hankel function on the boundary of the complex domain consisting of the forth arcs of the discs and the forth pieces of the sides of the hexagonal cell.

In the present paper we consider another approach of reducing the Helmholtz problem to the boundary integral equations for the simple layer potentials of the special Green function of the periodical lattice on the boundary of one disc only .

We consider the formulation of the Helmholtz problem. Let $\{e_j, \quad j = 1,2\}$ be a system of the noncollinear basis vectors in plane $\mathbf{R}^2$, which defines the fundamental domain Ω ($\Omega : x = \alpha\, e_1 + \beta\, e_2, \quad 0 \leq \alpha \leq 1, \quad 0 \leq \beta \leq 1$), see fig. 1. We define the cell $\hat{\Omega}$ of the reflection structure by means of arrangement of the disc S of the radius R in the fundamental domain Ω: $\hat{\Omega} = \Omega \setminus S$, see fig. 2.

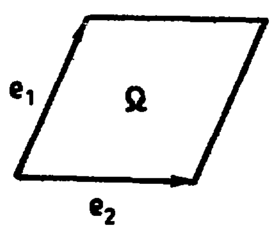

*Fig.*1

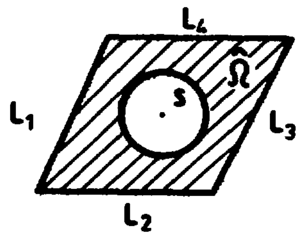

*Fig.*2

The wave function $u(x)$ in the domain $\hat{\Omega}$ satisfies the Helmholtz equation:

$$\Delta u + \lambda u = 0 \tag{0.1}$$

with Direchlet condition on the boundary ∂S of the disc S

$$u(x) = 0, \quad x \in \partial S.$$

The wave function is expanded on all the cells of the periodical structure with the help of the following conditions:

$$u(x+e_j)=e^{ip_j}u(x), \quad j=1,2, \tag{0.2}$$

$$\nabla u(x+e_j)=e^{ip_j}\nabla u(x), \quad j=1,2. \tag{0.3}$$

The problem is to find the spectral parameter λ and the wave function $u(x)$ with fixed values of the parameters p_1, p_2.

In Section 2 we construct the special Green function of the periodical lattice.

In Section 3 the Helmholtz problem is reduced to the boundary integral equations for the simple layer potentials of this Green function.

In Section 4,5 two methods of discretization of arising the boundary integral equations are discussed. The former is based on the piece-wise approximation of the density. The latter uses the Fourier series of the density and the explicit analytical form of matrix elements of the secular equation is obtained. The reality of the nonlinear spectral parameter of the boundary equations is proved.

2. Green function of the periodical lattice

Let $\{e_j, \quad j=1,2\}$ be the system of the noncollinear basis vectors in plane $\mathbf{R}^2$, determined early. We define the Green function $G(x,x_0) = G(x,x_0,p_1,p_2,\lambda)$ as the solution of the Helmholtz equation in the fundamental domain Ω:

$$\Delta G+\lambda G=\delta(x-x_0), \tag{1}$$

where λ does not belong to the spectrum of the homogeneous problem. The function G is expanded on all plane $\mathbf{R}^2$ by means of the quasiperiodical conditions:

$$G(x+e_j)=e^{-ip_j}G(x) \tag{2}$$

with the parameters $\{p_j, \quad j=1,2\}$. Using the continuity of the function G and its derivatives, one can link the corresponding values on the oppositive sides L_j and L_{j+2} of the boundary $\partial\Omega$ of the fundamental domain Ω (fig.1):

$$G(x)|_{L_{j+2}}=e^{-ip_j}G(x)|_{L_j}, \tag{3}$$

$$\frac{\partial}{\partial n_x} G(x)|_{L_{j+2}} = -\epsilon^{-ip_j} \frac{\partial}{\partial n_x} G(x)|_{L_j}, \tag{4}$$

where $\frac{\partial}{\partial n_x}$ is the normal derivative of the function G in the point x.

Let $\{f_j, \quad j = 1,2\}$ be the attendant system of vectors connected with $\{e_j, \quad j = 1,2\}$ by the following relation

$$(f_i, e_j) = \delta_{i,j}. \tag{5}$$

We introduce the new variables $\{y_j, \quad j = 1,2\}$ defined as

$$y_1 = (x, f_1), \quad y_2 = (x, f_2). \tag{6}$$

After this change of the variables the domain Ω is transformed to the unit square $[0,1]$x$[0,1]$, and the boundary conditions may be written in the form

$$G(1, y_2) = e^{-ip_1} G(0, y_2), \quad G(y_1, 1) = e^{-ip_2} G(y_1, 0),$$

$$\partial_{y_1} G(1, y_2) = e^{-ip_1} \partial_{y_1} G(0, y_2),$$
$$\partial_{y_2} G(y_1, 1) = e^{-ip_2} \partial_{y_2} G(y_1, 0). \tag{7}$$

In the new variables the Laplacian Δ has the form

$$\Delta = ||f_1||^2 \frac{\partial^2}{\partial y_1^2} + ||f_2||^2 \frac{\partial^2}{\partial y_2^2} + 2(f_1, f_2) \frac{\partial^2}{\partial y_1 y_2}, \tag{8}$$

and δ-function is defined by the relation [5]

$$\delta(x - x_0) = |A|^{-1} \delta(y - y_0),$$

where $|A|$ is the Jacobian of the transformation from y to x. The set of functions $\{e^{-i(p+2k\pi)y}, \quad -\infty \le k \le \infty\}$ forms the basis in the space of one-dimensional functions $\{\phi(y)\}$ which satisfy the quasiperiodical relation

$$\phi(y+1) = e^{-ip} \phi(y). \tag{9}$$

We find the Green function in the form

$$G(y_1, y_2) = \sum_{k,l=-\infty}^{\infty} C_{kl} e^{-i(p_1 + 2k\pi)y_1} e^{-i(p_2 + 2l\pi)y_2}. \tag{10}$$

Using the orthogonality of functions $\phi_{kl}(y)$:

$$\phi_{kl}(y) = e^{-i(p_1+2k\pi)y_1}e^{-i(p_2+2l\pi)y_2}, \tag{11}$$

we have coefficients C_{kl} being defined as

$$C_{kl} = |A|^{-1}\overline{\phi_{kl}(y_0)}/(\lambda - ||u_k + v_l||^2), \tag{12}$$

where

$$u_k = (p_1 + 2k\pi)f_1, \quad v_l = (p_2 + 2l\pi)f_2. \tag{13}$$

Applying the inverse transformation, we obtain that $G(x, x_0)$ is defined by the following relation

$$G(x, x_0) = |A|^{-1} \sum_{k,l=-\infty}^{\infty} \frac{e^{-i(p_1+2k\pi)(x-x_0,f_1)}e^{-i(p_2+2l\pi)(x-x_0,f_2)}}{(\lambda - ||(p_1+2k\pi)f_1 + (p_2+2l\pi)f_2||^2)}. \tag{14}$$

3. Boundary integral equations

Now we multiply the equation (1) by the solution of the initial problem $u(x)$, subtract the equation (0.1) multiplying by G, and integrate over the domain $\Omega \setminus S$ containing the disc S (see fig.2.), and obtain

$$\int_{\Omega\setminus S}(\Delta G u - \Delta u G)ds_x = u(x_0). \tag{15}$$

From the equation (15) it follows, that

$$u(x_0) = \int_{\partial\Omega}(\frac{\partial G}{\partial n_x}u - \frac{\partial u}{\partial n_x}G)dl_x + \int_{\partial S}(\frac{\partial u}{\partial n_x}G - \frac{\partial G}{\partial n_x}u)dl_x. \tag{16}$$

Here $\frac{\partial G}{\partial n_x}$ and $\frac{\partial u}{\partial n_x}$ are the limit of the normal derivative when point x tends to the boundaries of domains Ω and S, correspondingly, for the first and second integrals in equation (16). We show that first integral with respect to $\partial\Omega$ equals zero. Indeed this integral is the sum of fourth integrals

$$\int_{\partial\Omega} = \sum_{j=1}^{4}\int_{L_j}. \tag{17}$$

Using the property of the Green function G and solution $u(x)$ from (0.2) we obtain that

$$\int_{L_j} = -\int_{L_{j+2}}, \quad j = 1,2.$$

In result the equation (16) reduces to the following integral equation with respect to the boundary ∂S only:

$$u(x_0) = \int_{\partial S} (\frac{\partial u}{\partial n_x} G - \frac{\partial G}{\partial n_x} u) dl_x. \tag{18}$$

Taking into account that on the boundary ∂S of the disc S the solution $u(x) = 0$, we have

$$u(x_0) = \int_{\partial S} \frac{\partial u(x)}{\partial n_x} G(x, x_0, \lambda) dl_x. \tag{19}$$

Thus, one can find the solution $u(x)$ in the form of the potential of single layer for the Green function $G(x, x_0)$ from the previous section. For determining λ the following integral equation on the boundary ∂S of the disc S takes place:

$$\int_{\partial S} \sigma(x) G(x, x_0, \lambda) dl_x = 0, \quad x_0 \in \partial S. \tag{20}$$

were $\sigma(x) = \frac{\partial u(x)}{\partial n_x}$.

It should be noted that only real values of the spectral parameter λ correspond to the solution of this problem. Multiplying the eq.(20) by $\overline{\sigma(x)}$, integrating over the boundary ∂S and substituting the explicit representation of the Green function (14), we have

$$\sum_{k,l} \int_{\partial S} \int_{\partial S} \exp(-i(p_1 + 2k\pi)(x - x_0, f_1) - i(p_2 + 2l\pi)(x - x_0, f_2)) \times$$

$$\times \sigma(x) \overline{\sigma(x_0)} dl_x dl_{x_0} / (\lambda - \|u_k + v_l\|^2) = 0. \tag{21}$$

Then the following equation takes place

$$\sum_{k,l} \frac{|\int_{\partial S} \exp(-i(p_1 + 2k\pi)(x, f_1) - i(p_2 + 2l\pi)(x, f_2)) \sigma(x) dl_x|^2}{(\lambda - \|u_k + v_l\|^2)} = 0. \tag{22}$$

Taking the complex conjugation of the eq.(22), we obtain the same equation

$$\sum_{k,l} \frac{|\int_{\partial S} \exp(-i(p_1 + 2k\pi)(x, f_1) - i(p_2 + 2l\pi)(x, f_2))\sigma(x) dl_x|^2}{(\overline{\lambda} - \|u_k + v_l\|^2)} = 0. \quad (23)$$

After subtraction of the eq.(22) from the eq.(23) we have

$$(\lambda - \overline{\lambda})[\sum_{k,l} \frac{|\int_{\partial S} \exp(-i(p_1 + 2k\pi)(x, f_1) - i(p_2 + 2l\pi)(x, f_2))\sigma(x) dl_x|^2}{|\lambda - \|u_k + v_l\|^2|^2}] = 0. \quad (24)$$

Taking into account that the expression in the square brackets is more than zero we have $\overline{\lambda} = \lambda$. It means that the spectral parameter λ satisfying nonlinear equation (20), is real.

It should be noted that the equation (20) has the additional solutions which are not solutions of initial problem (0.1)-(0.3). Let $u^*(x)$ be the solution of the Helmholtz equation (0.1) inside the disc S with the Dirichlet boundary condition:

$$u^*(x) = 0, \quad x \in \partial S.$$

We multiply the equation (0.1) by the Green function G, subtract the equation (1) multiplying by $u^*(x)$ and integrate over the domain S. After this we obtain

$$\int_S (\Delta u^* G \quad \Delta G u^*) ds_x = u^*(x_0).$$

From this equation it follows, that

$$u^*(x_0) = \int_{\partial S} (\frac{\partial u^*}{\partial n_x} G - \frac{\partial G}{\partial n_x} u^*) dl_x.$$

Taking into account that $u^*(x) = 0, \quad x \in \partial S$, we obtain that λ and $u^*(x)$ satisfy the eq.(20).

The eigenfunctions $u^*(x)$ and eigenvalues λ^* of the internal Helmholtz problem for the disc S may be expressed through of the Bessel functions and these nodes and found analytically.

4. Discretization of the boundary integral equations

In the papers [6, 7] the procedure of discretization of the boundary integral equations and algorithms of the determining eigenvalues of the arising nonlinear problems based on the Newton method with the extraction on founded roots were described. For discretization of the the boundary integral equations the collocation method with the piece-wise approximation of the density $\sigma(x)$ was applied. The main difficulty of using the collocation method for integral equations (20) consists in the fact that the Green function (14) is a complex valued function. It means that solutions of the problem λ may go out from the real axis to the complex plane as a result of the discretization errors of the boundary integral equations. That is why we use the momentum method for discretization of the problem. The boundary ∂S is approximated by right N-polygons. Let $\{S_i\}$ be sides of the inscribed N-polygon and σ_i be approximation of $\sigma(x)$ on the sides S_i. Then the discretized system of equations has the form

$$\sum_{j=1}^{N} \int_{S_i} \int_{S_j} G(x, x_0, \lambda)\sigma_j dl_x dl_{x_0} = 0, \quad i = \overline{1, N}. \tag{25}$$

This system may be written in the matrix form:

$$A(\lambda)\hat{\sigma} = 0, \tag{26}$$

where $\hat{\sigma} = (\sigma_1, \sigma_2, \cdots, \sigma_N)^T$ and elements of the matrix $A(\lambda)$ are corresponding double integrals from eq.(25). The equation (26) has a nontrivial solution when the determinant of matrix equals zero:

$$det[A(\lambda)] = 0. \tag{27}$$

As a consequence of the chosen method of the discretization (the moment method) the elements of matrix $A(\lambda)$ satisfy the following relations

$$a_{ij} = a^*_{ji}. \tag{28}$$

This means that this matrix is complex Hermitian. The reality of λ may be proved by using the method from Section 3 .

Thus, we constructed the approximative equations (26,27) for determining egenvalue λ of the problem (0.1) - (0.3).

5. Explicit form of the secular equation

In the previous section the discretization of the boundary integral equations based on piecewise-polynomial approximation of the density $\sigma(x)$ has been proposed. The matrix elements were expressed by means of double integrals of the Green function. In this section we improve the method of reduction of the boundary integral equations to algebraic system using the expansion of the density $\sigma(x)$ in the Fourier series.

The vectors x ($x \in \partial S$) belonging to the circle of the radius R with center in origin of coordinates may be written in the parametric form

$$x(\phi) = (R\cos\phi, R\sin\phi)^T, \tag{29}$$

where $0 \leq \phi \leq 2\pi$. Let the function $\sigma(x)$ be expressed in the Fourier series

$$\sigma(x) = \sum_{m=-\infty}^{\infty} \sigma_m e^{-im\phi}. \tag{30}$$

From the eqs.(20),(30) it follows

$$\sum_{m=-\infty}^{\infty} \sigma_m \int_0^{2\pi} G(x(\phi), x_0(\phi'), \lambda) e^{-im\phi} R d\phi = 0. \tag{31}$$

Substituting the Green function from the eq. (14) in the eq. (31), we obtain

$$\sum_{m=-\infty}^{\infty} \sigma_m \sum_{k,l=-\infty}^{\infty} \int_0^{2\pi} \frac{\exp\{-iR((u_k + v_l),(e(\phi) - e(\phi'))\}}{\lambda - ||u_k + v_l||^2} e^{-im\phi} R d\phi = 0, \tag{32}$$

where $e(\phi) = (\cos\phi, \sin\phi)^T$. The expression $((u_k + v_l), e(\phi))$ may be transformed to the form

$$((u_k + v_l), e(\phi)) = ||u_k + v_l|| \cos(\phi + \psi_{kl}), \tag{33}$$

where

$$\psi_{kl} = \arctan \frac{(u_k + v_l, a_1)}{(u_k + v_l, a_2)},$$

a_1 and a_2 are the orthogonal system of unit vectors in the Cartesian system of coordinates. Then the eq.(32) may be written in the form

$$\sum_{m=-\infty}^{\infty} \sigma_m \sum_{k,l=-\infty}^{\infty} \frac{\exp\{i[||u_k+v_l||R\cos(\phi'+\psi_{kl})]\}}{\lambda-||u_k+v_l||^2} A_{klm} = 0. \qquad (34)$$

where

$$A_{klm} = \int_0^{2\pi} \exp\{-i(||u_k+v_l||R\cos(\phi+\psi_{kl})+m\phi)\}Rd\phi. \qquad (35)$$

Using the integral representation of the Bessel functions [8]

$$J_m(z) = (2\pi i^m)^{-1} \int_0^{2\pi} exp(iz\cos u)\cos(mu)du,$$

we obtain the analytical expression for the coefficients A_{klm}

$$A_{klm} = (2\pi i^m)^{-1} J_m(-R||u_k+v_k||)\exp(im\psi_{kl}). \qquad (36)$$

Multipiying the eq.(34) by $\exp(in\phi')$ and integrating over the interval $[0, 2\pi]$, we have

$$\sum_{m=-\infty}^{\infty} \sigma_m \sum_{k,l=-\infty}^{\infty} A_{klm}\overline{A_{kln}}/(\lambda-||u_k+v_l||)^2 = 0, \qquad (37)$$

where n is variating from $-\infty$ to ∞. It should be noted that the coefficients A_{klm} fast decrease as k, l, m tend to infinity. Taking a finite number of members in (37), we obtain the approximative system of equations for determining σ_m and λ :

$$\sum_{m=-M}^{M} \sigma_m \sum_{k,l=-K,L}^{K,L} A_{klm}\overline{A_{kln}}/(\lambda-||u_k+v_l||)^2 = 0. \qquad (38)$$

Let B be the complex matrix with elements b_{nm}:

$$b_{nm} = \sum_{k,l=-K,L}^{k,l=K,L} A_{klm}A_{kln}/(\lambda-||u_k+v_l||^2). \qquad (39)$$

The system (38) has a nontrivial solution when the determinant of the matrix B equals zero. Note that the error of reduction in (38) may be majorized by the value of the order

$$\sum_{|m|>M} \sum_{|k|>K} \sum_{|l|>L} \frac{C}{\|u_k + v_l\|^3 |m|^J}. \tag{40}$$

Here C is the maximum of module of the J-th derivative of the density $\sigma(\phi)$ with respect to ϕ. It means that the error fast decreases if K, L, M tend to infinity.

Thus, for the fixed values of the parameters p_1, p_2 of the periodical structure we obtained the approximative equation for determining λ and $\sigma(\phi)$. Note that truncated matrix B is complex Hermitian and using the techniques developed earlier, one can show that the roots λ^* of the secular equation

$$det\|B(\lambda^*)\| = 0$$

are real. Using the integral representation for $u(x)$ from (19), the founded values of the spectral parameter λ, and the density $\sigma(\phi)$, one can recalculate the values of the wave function $u(x)$ in an arbitrary point of the plane $\mathbf{R}^2$.

6. Conclusion

We have reduced the Helmholtz problem to the boundary integral equations for the simple layer potentials of the constructed Green function on the boundary of one disc only. Two methods of discretization of boundary integral equations have been developed. The first one is more universal. It may be used for wide type of domains. But this method needs creation of fast algorithms of calculation of the Green function and its derivatives with respect to spectral parameter. The second approach allows one to evaluate the elements of the discretized matrix analytically, but it may be used for discs only. Both the methods of the discretization of the boundary integral equations preserve the Hermiticy of the discretized matrices and the reality of spectrum of the approximated problems.

It should be noted, that the proposed approaches lead to the necessity of calculations with the completely filled complex matrices. For good approximation of the initial problem it is necessary to increase the dimension of the solved problem. It leads to high requests to operative and virtual memory and productivity of computers used for calculations.

The boundary integral equation method admits to apply the parallel algorithms and, as consequence, to use computers with the vector-parallel architecture, that allows one to make more qualitative calculations.

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