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MODIFIED RAYLEIGH CONJECTURE FOR SCATTERING BY PERIODIC STRUCTURES

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Abstract. This paper contains a self-contained brief presentation of the scattering theory for periodic structures. Its main result is a theorem (the Modified Rayleigh Conjecture, or MRC), which gives a rigorous foundation for a numerical method for solving the direct scattering problem for periodic structures. A numerical example illustrating the procedure is presented.

1. Introduction

For simplicity we consider a 2-D setting, but our arguments can be as easily applied to n-dimensional problems, $n \geq 2$. Let $f : \mathbb{R} \to \mathbb{R},\ f(x+L) = f(x)$ be an L-periodic Lipschitz continuous function, and let D be the domain

$$D = \{(x, y)\ :\ y \geq f(x),\ x \in \mathbb{R}\}.$$

Without loss of generality we assume that $f \geq 0$. If it is not, one can choose the origin so that this assumption is satisfied, because $M := \sup_{0 \leq x \leq L} |f(x)| < \infty$.

Let $\mathbf{x} = (x, y)$ and $u(\mathbf{x})$ be the total field satisfying

$$(\Delta + k^2)u = 0, \quad \mathbf{x} \in D, \quad k = const > 0 \tag{1.1}$$

$$u = 0 \quad \text{on} \quad S := \partial D, \tag{1.2}$$

$$u = u_0 + v, \quad u_0 := e^{ik\alpha\cdot\mathbf{x}}, \tag{1.3}$$

where the unit vector $\alpha = (\cos\theta, -\sin\theta),\ 0 < \theta < \pi/2$, and $v(\mathbf{x})$ is the scattered field, whose asymptotic behavior as $y \to \infty$ will be specified below, and

$$u(x + L, y) = \nu u(x, y), \quad u_x(x + L, y) = \nu u_x(x, y) \text{ in } D, \quad \nu := e^{ikL\cos\theta}\,. \tag{1.4}$$

Conditions (1.4) are the *qp* (**quasiperiodicity**) conditions. To find the proper radiation condition for the scattered field $v(\mathbf{x})$ consider the spectral problem

$$\varphi'' + \lambda^2\varphi = 0, \quad 0 < x < L, \tag{1.5}$$

$$\varphi(L) = \nu\varphi(0), \quad \varphi'(L) = \nu\varphi'(0) \tag{1.6}$$

arising from the separation of variables in (1.1)-(1.4). This problem has a discrete spectrum, and its eigenfunctions form a basis in $L^2(0, L)$. One has

$$\varphi = Ae^{i\lambda x} + Be^{-i\lambda x}, \quad A, B = const,$$
$$Ae^{i\lambda L} + Be^{-i\lambda L} = \nu(A + B), \quad i\lambda Ae^{i\lambda L} - i\lambda Be^{-i\lambda L} = i\lambda\nu(A - B).$$

Thus

$$\begin{vmatrix} e^{i\lambda L} - \nu & e^{-i\lambda L} - \nu \\ i\lambda(e^{i\lambda L} - \nu) & -i\lambda(e^{-i\lambda L} - \nu) \end{vmatrix} = 0.$$

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So, $i\lambda(e^{i\lambda L}-\nu)(e^{-i\lambda L}-\nu)=0$. If $\lambda=0$, then $\varphi=A+Bx,\ A+BL=\nu A,\ B=\nu B$. Since $\nu=e^{ikL\cos\theta}$, one has no eigenvalue $\lambda=0$ unless $kL\sin\theta=2\pi m,\ m>0$ is an integer. Let us assume that $kL\cos\theta\neq 2\pi m$. Then

$$e^{i\lambda L}=e^{ikL\cos\theta} \quad \text{or} \quad e^{-i\lambda L}=e^{ikL\cos\theta},$$

that is

$$\lambda_j^+=k\cos\theta+\frac{2\pi j}{L}, \quad \text{or} \quad \lambda_j^-=-k\cos\theta+\frac{2\pi j}{L}, \quad j=0,\pm1,\pm2,\dots$$

The corresponding eigenfunctions are $e^{i\lambda_j^+x}$ and $e^{-i\lambda_j^-x}$. We will use the system $e^{i\lambda_j^+x}$, which forms an orthogonal bais in $L^2(0,L)$. One has:

$$\int_0^L e^{i\lambda_j^+x}e^{-i\lambda_m^+x}\,dx=\int_0^L e^{\frac{2\pi i}{L}(j-m)}\,dx=0, \quad j\neq m.$$

The normalized eigenfunctions are

$$\varphi_j(x)=\frac{e^{i\lambda_j^+x}}{\sqrt{L}}, \quad j=0,\pm1,\pm2,\dots$$

These functions form an orthonormal basis of $L^2(0,L)$. Let us look for $v(\mathbf{x})=v(x,y)$ of the form

$$v(x,y)=\sum_{j=-\infty}^{\infty}c_jv_j(y)\varphi_j(x), \quad y>M, \quad c_j=const. \tag{1.7}$$

For $y>M$, equation (1.1) implies

$$v_j''+(k^2-\lambda_j^2)v_j=0. \tag{1.8}$$

Let us assume that $\lambda_j^2\neq k^2$ for all j. Then

$$v_j(y)=e^{i\mu_jy}, \tag{1.9}$$

where, for finitely many j, the set of which is denoted by J, one has:

$$\mu_j=(k^2-\lambda_j^2)^{1/2}>0, \quad \text{if} \quad \lambda_j^2<k^2,\ j\in J, \tag{1.10}$$

and

$$\mu_j=i(\lambda_j^2-k^2)^{1/2}, \quad \text{if} \quad \lambda_j^2>k^2,\ j\notin J. \tag{1.11}$$

The **radiation condition** at infinity requires that the scattered field $v(x,y)$ be representable in the form (1.7) with $v_j(y)$ defined by (1.9)-(1.11).

The **Periodic Scattering Problem** consists of finding the solution to (1.1)-(1.4) satisfying the radiation condition (1.7), (1.9)-(1.11).

The existence and uniqueness for such a scattering problem is established in Section 2. Our presentation is essentially self-contained. In [1] the scattering by a periodic structure was considered earlier, and was based on a uniqueness theorem from [7]. Our proofs differ from the proofs in [1]. There are many papers on scattering by periodic structures, of which we mention a few [1], [2], [4], [5], [6], [10],[11], [12], [13], [15], [25]. The Rayleigh conjecture is discussed in several of the above papers. It was shown (e.g. [15], [3]) that this conjecture is incorrect, in general. The modified Rayleigh conjecture is a theorem proved in [18] for scattering by bounded obstacles. A numerical method for solving obstacle scattering problems, based on the modified Rayleigh conjecture is developed in [8]. The main results of our paper are: the modified Rayleigh conjecture for periodic structures (Theorem 4.4) and a rigorous numerical method for solving scattering problems by periodic structures, based on the modified Rayleigh conjecture (Section 4). The proof of the limiting absorption principle (LAP) and the rigorous and self-contained development of the plane wave scattering theory by periodic structures is also of interest for broad audience. This theory is based partly on the ideas developed in [17], [21], [22], [19]. The proof of the key lemma 2.2 is based on a version of Ramm's identity (2.16). Numerical implementation of the method for solving scattering problems by periodic structures, based on the modified Rayleigh conjecture, is constructed using the approach developed in [8] and in [23]. Applications to inverse problems are discussed in [18] and [24].

2. Periodic Scattering Problem

Existence and uniqueness of solutions of the Periodic Scattering Problem can be proved easily, if one establishes first the existence and uniqueness of the resolvent kernel $G(x, y, \xi, \eta, k)$ of the Dirichlet Laplacian in D:

$$(\Delta + k^2)G(x, y, \xi, \eta, k) = -\delta(x - \xi)\delta(y - \eta), \quad G = 0 \quad \text{on} \quad S, \tag{2.1}$$

$$G(x + L, y, \xi, \eta, k) = \nu G(x, y, \xi, \eta, k), \quad G(x, y, \xi + L, \eta, k) = \overline{\nu} G(x, y, \xi, \eta, k), \tag{2.2}$$

$$G_x(x + L, y, \xi, \eta, k) = \nu G_x(x, y, \xi, \eta, k), \quad G_x(x, y, \xi + L, \eta, k) = \overline{\nu} G_x(x, y, \xi, \eta, k), \tag{2.3}$$

and G satisfies the LAP, see (2.5) below. The overbar here and below stands for the complex conjugation.

Indeed, if such a function G exists, then v can be found by the Green's formula

$$v(x, y) = -\int_{S_L} u_0(\xi, \eta) G_N(x, y, \xi, \eta, k)\, ds, \tag{2.4}$$

where N is the unit normal vector to S pointing into D.

To prove the existence and uniqueness of $G(x, y, \xi, \eta, k)$ define

$$\ell_0 = -\Delta$$

to be the Laplacian on the set of $C^2(D)$ quasiperiodic functions vanishing on the boundary S, and vanishing near infinity. Let

$$D_L := \{(x, y) \ : \ 0 \le x \le L, \quad (x, y) \in D\}.$$

Then D_L is a section of D, and ℓ_0 is a symmetric operator in $L^2(D_L)$. This operator is nonnegative , and therefore [9] there exists its unique selfadjoint Friedrichs' extension, which will be denoted by ℓ.

Let $Im(k^2) > 0$. Then there exists a unique resolvent operator $(\ell - k^2)^{-1}$. Thus its kernel $G(x, y, \xi, \eta, k)$ also exists and it is unique. To establish the existence and uniqueness of the kernel for $k > 0$ we are going to prove the following

Limiting Absorption Principle (LAP). Let $k > 0, \ \epsilon > 0$ and assume that k^2 is not equal to λ_j^2. Then the limit

$$\lim_{\epsilon \to 0+} G(x, y, \xi, \eta, k + i\epsilon) = G(x, y, \xi, \eta, k), \tag{2.5}$$

exists for all $(x, y) \in D, \ x \ne y$. The proof is based on the following two lemmas.

Lemma 2.1. *Let* $0 < \epsilon < 1$, *and* $a > 2$. *Then*

$$\int_{D_L} \frac{|G(x, y, \xi, \eta, k + i\epsilon)|^2}{(1 + \xi^2 + \eta^2)^{a/2}}\, d\xi d\eta \le c, \tag{2.6}$$

where $c = const > 0$ *does not depend on* ϵ, *and* (x, y) *is running on compact sets.*

Proof of Lemma 2.1. It is sufficient to prove that the solution to the problem

$$(\Delta + k^2 + i\epsilon) w_\epsilon = F, \ \text{in } D_L, \ w_\epsilon \in L^2(D_L), \ w_\epsilon = 0 \text{ on } S_L \tag{2.7}$$

$$w_\epsilon(x + L, y) = \nu w_\epsilon(x, y), \quad w_{\epsilon x}(x + L, y) = \nu w_{\epsilon x}(x, y), \tag{2.8}$$

satisfies the estimate

$$N_\epsilon^2 := \sup_{0<\epsilon<1} \int_{D_L} \frac{|w_\epsilon(x, y)|^2}{(1 + x^2 + y^2)^{a/2}}\, dxdy := N^2(w_\epsilon) \le c, \tag{2.9}$$

where $F \in C_0^\infty(D_L)$ is arbitrary, and $c = const > 0$ is independent of $\epsilon > 0$.

If (2.9) fails, then $N_{\epsilon_n} \to \infty$, $\epsilon_n \to 0$. Define $\psi_\epsilon := w_\epsilon/N_\epsilon$, where $\epsilon := \epsilon_n$. Then $N(\psi_\epsilon) = 1$, ψ_ϵ solves (2.7) (with F replaced by $F_\epsilon := F/N_\epsilon$), and satisfies (2.8). From $N(\psi_\epsilon) = 1$ it follows that $\psi_\epsilon \rightharpoonup \psi$ as $\epsilon \to 0$, where $\rightharpoonup$ denotes the weak convergence in $L^2(D_L, 1/(1+x^2+y^2)^{a/2}) := L_a^2$. By elliptic estimates, $\psi_\epsilon \rightharpoonup \psi$ in $H^2_{loc}(D_L)$, and therefore $\psi_\epsilon \to \psi$ in $L^2_{loc}(D_L)$. This and (2.7)-(2.8) imply $\psi_\epsilon \to \psi$ in $H^2_{loc}(D_L)$. Thus ψ solves the homogeneous ($F = 0$) problem (2.7)-(2.8). If we prove that $\psi = 0$, then we get a contradiction, which shows that (2.9) holds. The contradiction comes from the relationship $0 = N(\psi) = \lim_{\epsilon\to 0} N(\psi_\epsilon) = 1$. One proves that

$$\lim_{\epsilon\to 0} N(\psi_\epsilon) = N(\psi) \tag{2.10}$$

as follows. If

$$(x, y) \in D_R := \{(x, y) \ : \ f(x) \le y \le R, \ 0 \le x \le L\},$$

where $R > M$ is an arbitrary large fixed number, then $\lim_{\epsilon\to 0} N(\psi_\epsilon \eta_R) = N(\psi\eta_R)$, where

$$\eta_R := \begin{cases} 1, & f(x) < y < R, \\ 0, & y > R. \end{cases}$$

In the region $D'_R = \{(x, y) \ : \ y > R, \ 0 \le x \le L\}$, one has $|\psi_\epsilon(x, y)| \le c, \ (x, y) \in D'_R$. Thus

$$\sup_{0<\epsilon<1} N(\psi_\epsilon(\chi_L - \eta_R)) \le O\left(\frac{1}{R^\gamma}\right), \ 0 < \gamma < a - 2.$$

The desired result (2.10) follows.

To complete the proof let us show that the problem (2.7)-(2.8), with $F = 0$, and $\epsilon = 0$, has only the trivial solution w, provided that w is "outgoing" in the sense

$$w_{jy} - i\mu_j w_j = o(1), \text{ as } y \to \infty, \ w_j := \int_0^L w\overline{\varphi_j}\, dx.$$

One has

$$\lim_{R\to\infty} \int_{S_R} (w\overline{w_y} - w_y\overline{w})\, ds = 0, \tag{2.11}$$

where $S_R := \{(x, y) \ : \ y = R, \ 0 \le x \le L\}$, $ds = dx$ is the element of the arclength of S_R, and the overbar stands for the complex conjugate.

Let us outline the steps of the further argument.

Step 1: we prove that (2.11) implies

$$w \in L^2(D_L), \ |w| + |\nabla w| \le ce^{-\gamma|y|}, \ \gamma = const > 0, \tag{2.12}$$

if w is outgoing.

Step 2: we prove that if $w \in L^2(D_L)$ solves (2.7)-(2.8), with $F = \epsilon = 0$, then $w = 0$. Then we conclude that (2.9) (and (2.6)) holds, and, therefore, (2.5) holds.

Let us prove (2.12). One has

$$\begin{aligned} 0 &= \int_{D_{LR}} [\bar{w}(\Delta + k^2)w - w(\Delta + k^2)\bar{w}]\, dxdy \\ &= -\int_{S_L} (\bar{w}w_N - w\bar{w}_N)\, ds + \int_{S_R} (\bar{w}w_N - w\bar{w}_N)\, ds \\ &= \int_{S_R} (\bar{w}w_N - w\bar{w}_N)\, ds, \end{aligned} \tag{2.13}$$

where the Dirichlet condition (2.7) was used, and the integrals over the lines $x = 0$ and $x = L$ are cancelled due to the *qp* conditions (2.8):

$$\begin{aligned}&\int_{x=0}(-\bar{w}w_x + w\bar{w}_x)\ dy + \int_{x=L}(\bar{w}w_x - w\bar{w}_x)\ dy\\ &= \int_{x=0}(w\bar{w}_x - \bar{w}w_x)\ dy - \int_{x=0}\nu\bar{\nu}(w\bar{w}_x - \bar{w}w_x)\ dy = 0.\end{aligned}$$

Here we have used the relation $\nu\bar{\nu} = 1$. Thus (2.13) implies

$$0 = \int_{S_R}(\bar{w}w_y - w\bar{w}_y)\ dx,\ \forall R > M. \tag{2.14}$$

If w is outgoing, then (2.14) implies $w_j(y) = 0$ for $j \in J$, and $|w_j(y)| \le e^{-\gamma|y|}$, $\gamma = const > 0$, so (2.12) holds. ☐

Lemma 2.2. *Assume that $w \in L^2(D_L)$, w solves (2.7) with $\epsilon = 0$ and $F = 0$, and w satisfies (2.8). Then $w = 0$.*

Proof of Lemma 2.2. If w solves equation (2.7) with $\epsilon = 0$ and $F = 0$, then $w = \sum_j w_j(y)\varphi_j(x)$. Since $\{\varphi_j(x)\}$ is an orthonormal basis and $w \in L^2(D_L)$, it follows that $w_j(y) = 0$ for all $j \in J$, and (2.12) holds. Let us use a version of Ramm's identity ([19], p. 92), which is valid for any solution w of equation (1.1) which is outgoing in the sense that

$$w = \sum_j c_j v_j(y)\varphi_j(x),\ c_j = const,\ j \notin J. \tag{2.15}$$

Note, that $v_j(y) = \overline{v_j(y)}$ for $j \notin J$. The identity is:

$$0 = (x_2\bar{w}_{,2}w_{,j})_{,j} + \frac{(k^2|w|^2x_2 - |\nabla w|^2x_2)_{,2}}{2} + \frac{|\nabla w|^2 - k^2|w|^2}{2} - |w_{,2}|^2, \tag{2.16}$$

where $w_{,j} := \partial w/\partial x_j,\ j = 1, 2,\ x_1 = x,\ x_2 = y$, over the repeated indices one sums up, $|w|^2 := w\bar{w}$. The right-hand side of (2.16) equals to

$$\frac{1}{2}[x_2(\bar{w}_{,2j}w_{,j} - w_{,2j}\bar{w}_{,j}) + k^2x_2(w_{,2}\bar{w} - \bar{w}_{,2}w)] = 0,$$

because $w_{,2}\bar{w} = \bar{w}_{,2}w$ for outgoing w.

One has

$$|w| + |\nabla w| \le ce^{-\gamma|y|},\ \gamma = const > 0,\ c = const > 0. \tag{2.17}$$

Let $R > \max f(x)$. Integrate (2.16) over $D_{LR} := \{(x, y)\ :\ (x, y) \in D_L,\ y \le R\}$ and use Green's formula to get:

$$\begin{aligned}0 = &-\lim_{R\to\infty}\int_{S_L\cup S_R}[x_2\bar{w}_{,2}w_{,j}N_j + \frac{(k^2|w|^2x_2 - |\nabla w|^2x_2)N_2}{2}]\ ds\\ &-\lim_{R\to\infty}\int_{D_{LR}}|w_{,2}|^2\ dx_1dx_2,\end{aligned} \tag{2.18}$$

where N is the normal pointing into D_{LR}, and we have used the relation

$$\lim_{R\to\infty}\int_{D_{LR}}|\nabla w|^2\ dx_1dx_2 = k^2\lim_{R\to\infty}\int_{D_{LR}}|w|^2\ dx_1dx_2, \tag{2.19}$$

which follows from the equation $\Delta w + k^2w = 0$, boundary condition $w = 0$ on S, quasiperiodicity of w, and from (2.17). We have also used the relation $\bar{w}_{,2}w_{,j}N_j = x_2|\nabla w|^2N_2$, which follows from the condition $u = 0$ on S. From (2.18) one gets:

$$\lim_{R\to\infty}\int_{D_{LR}}|w_{,2}|^2\ dx_1dx_2 = -\frac{1}{2}\int_{S_L}x_2N_2|\nabla w|^2\ ds. \tag{2.20}$$

Since $f(x)$ is a graph, one has $N_2x_2 \geq 0$, and it follows from (2.20) that $w_{,2} = 0$, so $w = const$, and $const = 0$ because $w|_S = 0$. Lemma 2.2 is proved. □

Remark 2.3. Condition of the type

$$N_2x_2 \geq 0 \text{ on } S_L \tag{2.21}$$

was also used in [19].

The proof of Lemma 2.2 *is not valid if the Neumann boundary condition is imposed on S.*

3. INTEGRAL EQUATIONS METHOD

In this Section we present another proof of the existence and uniqueness of the resolvent kernel G. We want to construct a scattering theory quite similar to the one for the exterior of a bounded obstacle [17]. The *first step* is to construct an analog to the half-space Dirichlet Green's function. The function $g = g(\mathbf{x}, \xi, k)$ can be constructed analytically ($\mathbf{x} = (x_1, x_2), \xi = (\xi_1, \xi_2)$):

$$g(\mathbf{x}, \xi) = \sum_j \varphi_j(x_1)\overline{\varphi_j(\xi_1)} g_j(x_2, \xi_2, k), \tag{3.1}$$

$$g_j := g_j(x_2, \xi_2, k) = \begin{cases} v_j(x_2)\psi_j(\xi_2), & x_2 > \xi_2 \\ v_j(\xi_2)\psi_j(x_2), & x_2 < \xi_2 \end{cases}$$

$$\psi_j = (\mu_j)^{-1} e^{i\mu_j b} \sin[\mu_j(\xi_2 + b)], \ \mu_j = [k^2 - \lambda_j^2]^{1/2}, \quad v_j(x_2) = e^{i\mu_j x_2},$$

where

$$\psi_j'' + (k^2 - \lambda_j^2)\psi_j = 0, \ \psi_j(-b) = 0, \ W[v_j, \psi_j] = 1, \ \lambda_j = k\cos(\theta) + \frac{2\pi j}{L},$$

and $W[v, \psi]$ is the Wronskian.

The function g is analytic with respect to k on the complex plain with cuts along the rays $\lambda_j - i\tau$, $0 \leq \tau < \infty, j = 0, \pm 1, \pm 2, ...$, in particular, in the region $\Im k > 0$, up to the real positive half-axis except for the set $\{\lambda_j\}_{j=0,\pm1,\pm2,..}$.

Choose $b > 0$ such that $k^2 > 0$ is not an eigenvalue of the problem:

$$(\Delta + k^2)\psi = 0, \quad \text{in } D_{-b} := \{(x, y) \ : \ -b \leq y \leq f(x), \quad 0 \leq x \leq L\}. \tag{3.2}$$

$$\begin{aligned} &\psi|_{y=-b} = 0, \quad \psi_N = 0 \text{ on } S, \\ &\psi(x + L, y) = \nu\psi(x, y), \quad \psi_x(x + L, y) = \nu\psi_x(x, y). \end{aligned} \tag{3.3}$$

One has

$$\begin{aligned} &(\Delta + k^2)g = -\delta(\mathbf{x} - \xi), \ \mathbf{x} = (x_1, x_2), \ \xi = (\xi_1, \xi_2), \\ &\mathbf{x} \in \{(x, y) \ : \ -b < y < \infty, \quad 0 \leq x \leq L\}, \end{aligned} \tag{3.4}$$

$$g|_{y=-b} = 0, \tag{3.5}$$

and

$$(\Delta + k^2)G = -\delta(\mathbf{x} - \xi), G = 0 \text{ on } S, \tag{3.6}$$

G satisfies the *qp* condition and the radiation condition (it is outgoing at infinity).

Multiply (3.4) by G, (3.6) by g, subtract from the second equation the first one, integrate over D_{LR}, and take $R \to \infty$, to get

$$G = g + \int_{S_L} (Gg_N - G_N g) ds = g - \int_{S_L} g\mu \ ds, \ \mu := G_N|_{S_L}. \tag{3.7}$$

The *qp* condition allows one to cancel the integrals over the lateral boundary ($x = 0$ and $x = L$), and the radiation condition allows one to have

$$\lim_{R\to\infty} \int_{S_R} (Gg_N - G_N g) ds = 0.$$

Differentiate (3.7) to get

$$\mu = -A\mu + 2\frac{\partial g}{\partial N} \text{ on } S_L,\ A\mu := 2\int_{S_L} \frac{\partial g(s,\sigma)}{\partial N_s}\mu(\sigma)\, d\sigma. \tag{3.8}$$

This is a Fredholm equation for μ in $L^2(S_L)$, if S_L is $C^{1,m},\ m > 0$. The homogeneous equation (3.8) has only the trivial solution: if $\mu + A\mu = 0$, then the function $\psi := \int_{S_L} g\mu\, ds$ satisfies $\psi_N^+|_{S_L} = 0$, where $\psi_N^+(\psi_N^-)$ is the normal derivative of ψ from $D_{-b}(D_L)$, and we use the known formula for the normal derivative of the single layer potential at the boundary. The ψ satisfies also (3.2) and (3.3), and, by the choice of b, one has $\psi = 0$ in D_{-b}. Also $\psi = 0$ in D_L, because $(\Delta + k^2)\psi = 0$ in D_L, $\psi|_{S_L} = 0$ (by the continuity of the single layer potential), ψ satisfies the *qp* condition (because g satisfies it), and ψ is outgoing (because g is).

Since $\psi = 0$ in D_{-b} and in D_L, one concludes that $\mu = \psi_N^+ - \psi_N^-$, where $\psi_N^+(\psi_N^-)$ is the normal derivative of ψ from $D_{-b}(D_L)$, and we use the jump relation for the normal derivative of the single layer potential.

Thus, we have proved the existence and uniqueness of μ, and, therefore, of G, and got a representation formula

$$G = g - \int_{S_L} g\mu\, ds. \tag{3.9}$$

This representation shows that the rate of decay of G as $y \to \infty$ is essentially the same as that of g.

The G is analytic with respect to k on the complex plain with cuts along the rays $\lambda_j - i\tau$, $0 \le \tau < \infty, j = 0, \pm1, \pm2, ...$, in particular, in the region $\Im k > 0$, up to the real positive half-axis except for the set $\{\lambda_j\}_{j=0,\pm1,\pm2,..}$. This follows from (3.8), (3.9), and the general result [17], p. 57, [20], concerning analyticity of the solution to a Fredholm equation with respect to a parameter.

Suppose a bounded obstacle D_0 is placed inside D_L, $u = 0$ on $S_0 = \partial D_0$, S_0 is a Lipschitz boundary. If *qp* condition is imposed, then Green's function G_0 in the presence of the obstacle satisfies equations similar to (3.9) and (3.8):

$$G_0(x,y) = G(x,y) - \int_{S_0} G(x,s)\mu_0(s,y)\, ds, \quad \mu_0 = G_{0N}, \tag{3.10}$$

where N is the unit normal to S_0 pointing into D_L, and

$$\mu_0 = -A_0\mu_0 + 2\frac{\partial G}{\partial N} \text{ on } S_0,\ A_0\mu_0 := 2\int_{S_0} \frac{\partial G(s,\sigma)}{\partial N_s}\mu_0(\sigma)\, d\sigma. \tag{3.11}$$

This is a Fredholm equation (with index zero). If k^2 is not an eigenvalue of the Neumann Laplacian in D_0 (=not exceptional), then equation (3.11) is uniqueley solvable and, by (3.10), G_0 exists and is unique for this $k > 0$. It is not known what are nontrivial sufficient conditions for $k > 0$ to be not exceptional. The exceptional k form a discrete countable set on the positive semi-axis $k > 0$. If the Neumann boundary condition is imposed on S_L, then, even in the absence of the obstacle D_0, it is not known if LAP holds, because the proof of Lemma 2.2 *is not valid for the Neumann boundary condition on* S_L.

4. MODIFIED RAYLEIGH CONJECTURE (MRC)

Rayleigh conjectured [25] ("Rayleigh hypothesis") that the series (1.7) converges up to the boundary S_L. This conjecture is wrong ([15]) for some $f(x)$. Since the Rayleigh hypothesis has been widely used for numerical solution of the scattering problem by physicists and engineers, and because these practitioners reported high instability of the numerical solution, and there are no error estimates, we propose a modification of the Rayleigh conjecture, which is a Theorem. This MRC (Modified Rayleigh Conjecture) can be used for a numerical solution of the scattering problem, and it gives an error estimate for this solution. Our arguments are very similar to the ones in [18].

Rewrite the scattering problem (1.1)-(1.4) as

$$(\Delta + k^2)v = 0 \text{ in } D,\ v = -u_0 \text{ on } S_L, \tag{4.1}$$

where v satisfies (1.4), and v has representation (1.7), that is, v is "outgoing", it satisfies the radiation condition. Fix an arbitrarily small $\epsilon > 0$, and assume that

$$\|u_0 + \sum_{|j|\le j(\epsilon)} c_j(\epsilon)v_j(y)\varphi_j(x)\| \le \epsilon,\ 0 \le x \le L,\ y = f(x), \tag{4.2}$$

where $\|\cdot\| = \|\cdot\|_{L^2(S_L)}$.

Lemma 4.1. *For any $\epsilon > 0$, however small, and for any $u_0 \in L^2(S_L)$, there exists $j(\epsilon)$ and $c_j(\epsilon)$ such that (4.2) holds.*

Proof. Lemma 4.1 follows from the completeness of the system $\{\varphi_j(x)v_j(f(x))\}_{j=0,\pm1,\pm2,\dots}$ in $L^2(S_L)$. Let us prove this completeness. Assume that there is an $h \in L^2(S_L),\ h \not\equiv 0$ such that

$$\int_{S_L} h\overline{\varphi_j(x)}v_j(f(x))\, ds = 0 \tag{4.3}$$

for any j. From (4.3) one derives (cf. [17], p.162-163)

$$\psi(\mathbf{x}) := \int_{S_L} hg(\mathbf{x}, \xi)d\xi = 0,\ \mathbf{x} \in D_{-b}. \tag{4.4}$$

Thus $\psi = 0$ in D_L, and $h = \psi_N^+ - \psi_N^- = 0$. Lemma 4.1 is proved. □

Lemma 4.2. *If (4.2) holds, then*

$$|||v(\mathbf{x}) - \sum_{|j|\le j(\epsilon)} c_j(\epsilon)v_j(y)\varphi_j(x)||| \le c\epsilon,\ \forall x, y \in D_L,\ 0 \le x \le L,\ y \ge f(x),$$

where $c = const > 0$ does not depend on ϵ, x, y, and R; $R > M$ is an arbitrary fixed number, and $|||w||| = \sup_{\mathbf{x}\in D\setminus D_{LR}} |w(\mathbf{x})| + ||w||_{H^{1/2}(D_{LR})}$.

Proof. Let $w := v - \sum_{|j|\le j(\epsilon)} c_j(\epsilon)v_j(y)\varphi_j(x)$. Then w solves equation (1.1), w satisfies (1.4), w is outgoing, and $\|w\|_{L^2(S_L)} \le \epsilon$. One has (cf. (2.4))

$$w(\mathbf{x}) = -\int_{S_L} wG_N(\mathbf{x}, \xi)\, ds. \tag{4.5}$$

Thus (4.2), i.e. $\|w\| := \|w\|_{L^2(S_L)} \le \epsilon$, implies

$$|w(\mathbf{x})|_{y=R} \le \|w\|_{L^2(S_L)}\|G_N(\mathbf{x}, \xi)\|_{L^2(S_L)} \le c\epsilon,\ c = const > 0, \tag{4.6}$$

where c is independent of ϵ, and $R > \max f(x)$ is arbitrary. Now let us use the elliptic inequality

$$\|w\|_{H^m(D_{LR})} \le c\left(\|w\|_{H^{m-0.5}(S_L)} + \|w\|_{H^{m-0.5}(S_R)}\right), \tag{4.7}$$

where we have used the equation $\Delta w + k^2 w = 0$, and assumed that k^2 is not a Dirichlet eigenvalue of the Laplacian in D_{LR}, which can be done without loss of generality, because one can vary R. The integer $m \geq 0$ is arbitrary if S_L is sufficiently smooth, and $m \leq 1$ if S_L is Lipschitz. Taking $m = 0.5$ and using (4.2) and (4.6) one gets

$$\|w\|_{H^{1/2}(D_{LR})} \leq c\epsilon. \tag{4.8}$$

Thus, in a neighborhood of S_L, we have proved estimate (4.8), and in a complement of this neighborhood in D_L we have proved estimate (4.6). Lemma 4.2 is proved. □

Remark 4.3. In (4.7) there are no terms with boundary norms over the lateral boundary (lines $x = 0$ and $x = L$) because of the quasiperiodicity condition.

From Lemma 4.2 the basic result, Theorem 4.4, follows immediately:

Theorem 4.4. MRC-Modified Rayleigh Conjecture. *Fix $\epsilon > 0$, however small, and choose a positive integer p. Find*

$$\min_{c_j} \|u_0 + \sum_{|j| \leq p} c_j \varphi_j(x) v_j(y)\| := m(p). \tag{4.9}$$

Let $\{c_j(p)\}$ be the minimizer of (4.9). If $m(p) \leq \epsilon$, then

$$v(p) = \sum_{|j| \leq p} c_j(p) \varphi_j(x) v_j(y) \tag{4.10}$$

satisfies the inequality

$$|||v - v(p)||| \leq c\epsilon, \tag{4.11}$$

where $c = const > 0$ does not depend on ϵ. If $m(p) > \epsilon$, then there exists $j = j(\epsilon) > p$ such that $m(j(\epsilon)) < \epsilon$. Denote $c_j(j(\epsilon)) := c_j(\epsilon)$ and $v(j(\epsilon)) := v_\epsilon$. Then

$$|||v - v_\epsilon||| \leq c\epsilon. \tag{4.12}$$

5. Numerical solution of the scattering problem

According to the MRC method (Theorem 4.4), if the restriction of the incident field $-u_0(x, y)$ to S_L is approximated as in (4.9), then the series (4.10) approximates the scattered field in the entire region above the profile $y = f(x)$. However, a numerical method that uses (4.9) does not produce satisfactory results as reported in [15] and elsewhere. Our own numerical experiments confirm this observation. A way to overcome this difficulty is to realize that the numerical approximation of the field $-u_0|_{S_L}$ can be carried out by using outgoing solutions described below.

Let $\xi = (\xi_1, \xi_2) \in D_{-b}$, where $b > 0$,

$$D_{-b} := \{(\xi_1, \xi_2) \ : \ -b \leq \xi_2 \leq f(x), \quad 0 \leq \xi_1 \leq L\},$$

and $g(\mathbf{x}, \xi)$ be defined as in Section 3. Then $g(\mathbf{x}, \xi)$ is an outgoing solution satisfying $\Delta g + k^2 g = 0$ in D_L, according to (3.4).

To implement the MRC method numerically one proceeds as follows:

1. Choose the nodes $\mathbf{x}_i, \ i = 1, 2, ..., N$ on the profile S_L. These points are used to approximate L^2 norms on S_L.
2. Choose points $\xi^{(1)}, \xi^{(2)}, ..., \xi^{(M)}$ in $D_{-b}, \ M < N$.
3. Form the vectors $\mathbf{b} = (u_0(\mathbf{x}_i))$, and $\mathbf{a}^{(m)} = (g(\mathbf{x}_i, \xi^{(m)})), \ i = 1, 2, ..., N, \ m = 1, 2, ..., M$. Let $\mathbf{A}$ be the $N \times M$ matrix containing vectors $\mathbf{a}^{(m)}$ as its columns.
4. Find the Singular Value Decomposition of $\mathbf{A}$. Use a predetermined $w_{min} > 0$ to eliminate its small singular values. Use the decomposition to compute

   $$r^{min} = \min\{\|\mathbf{b} + \mathbf{A}\mathbf{c}\|, \ \mathbf{c} \in \mathbb{C}^M\},$$

   where

   $$\|\mathbf{a}\|^2 = \frac{1}{N} \sum_{i=1}^{N} |a_i|^2.$$

(5) **Stopping criterion.** Let $\epsilon > 0$.
   (a) If $r^{min} \le \epsilon$, then stop. Use the coefficients $\mathbf{c} = \{c_1, c_2, ..., c_M\}$ obtained in the above minimization step to compute the scattered field by

$$v(x,y) = \sum_{m=1}^{M} c_m g(x, y, \xi^{(m)}).$$

   (b) If $r^{min} > \epsilon$, then increase N, M by the order of 2, readjust the location of points $\xi^{(m)} \in D_{-b}$ as needed, and repeat the procedure.

We have conducted numerical experiments for four different profiles. In each case we used $L = \pi, k = 1.0$ and three values for the angle θ. Table 1 shows the resulting residuals r^{min}. Note that $\|\mathbf{b}\| = 1$. Thus, in all the considered cases, the MRC method achieved 0.04% to 2% accuracy of the approximation. Other parameters used in the experiments were chosen as follows: $N = 256,\ M = 64,\ w_{min} = 10^{-8},\ b = 1.2$. The value of $b > 0$, used in the definition of g, was chosen experimentally, but the dependency of r^{min} on b was slight. The Singular Value Decomposition (SVD) is used in Step 4 since the vectors $\mathbf{a}^{(m)},\ m = 1, 2, ..., M$ may be nearly linearly dependent, which leads to an instability in the determination of the minimizer $\mathbf{c}$. According to the SVD method this instability is eliminated by cutting off small singular values of the matrix $\mathbf{A}$, see e.g. [16] for details. The cut-off value $w_{min} > 0$ was chosen experimentally. We used the truncated series (3.1) with $|j| \le 120$ to compute functions $g(x, y, \xi)$. A typical run time on a 333 MHz PC was about $40s$ for each experiment.

The following is a description of the profiles $y = f(x)$, the nodes $\mathbf{x}_i \in S_L$, and the poles $\xi^{(m)} \in D_{-b}$ used in the computation of $g(\mathbf{x}_i, \xi^{(m)})$ in Step 3. For example, in profile I the x-coordinates of the N nodes $\mathbf{x}_i \in S_L$ are uniformly distributed on the interval $0 \le x \le L$. The poles $\xi^{(m)} \in D_{-b}$ were chosen as follows: every fourth node $\mathbf{x}_i$ was moved by a fixed amount -0.1 parallel to the y axis, so it would be within the region D_{-b}. The location of the poles was chosen experimentally to give the smallest value of the residual r^{min}.

Profile I. $f(x) = sin(2x)$ for $0 \le x \le L,\ t_i = iL/N,\ \mathbf{x}_i = (t_i, f(t_i)),\ i = 1, 2, ..., N,\ \xi^{(m)} = (x_{4m}, y_{4m} - 0.1),\ m = 1, 2, ..., M$.

Profile II. $f(x) = sin(0.2x)$ for $0 \le x \le L,\ t_i = iL/N,\ \mathbf{x}_i = (t_i, f(t_i)),\ i = 1, 2, ..., N,\ \xi^{(m)} = (x_{4m}, y_{4m} - 0.1),\ m = 1, 2, ..., M$.

Profile III. $f(x) = x$ for $0 \le x \le L/2,\ f(x) = L - x$ for $L/2 \le x \le L,\ t_i = iL/N,\ \mathbf{x}_i = (t_i, f(t_i)),\ i = 1, 2, ..., N,\ \xi^{(m)} = (x_{4m}, y_{4m} - 0.1),\ m = 1, 2, ..., M$.

Profile IV. $f(x) = x$ for $0 \le x \le L,\ t_i = 2iL/N,\ \mathbf{x}_i = (t_i, f(t_i),\ i = 1, ..., N/2,\ \mathbf{x}_i = (L, f(2(i - N/2)L/N)),\ i = N/2 + 1, ..., N, \xi^{(m)} = (x_{4m} - 0.03, y_{4m} - 0.05),\ m = 1, 2, ..., M$. In this profile $N/2$ nodes $\mathbf{x}_i$ are uniformly distributed on its slant part, and $N/2$ nodes are uniformly distributed on its vertical portion $x = L$.

The experiments show that the MRC method provides a competitive alternative to other methods for the computation of fields scattered from periodic structures. It is fast and inexpensive. The results depend on the number of the internal points $\xi^{(m)}$ and on their location. A similar MRC method for the computation of fields scattered by a bounded obstacle was presented in [8].

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Table 1. Residuals attained in the numerical experiments.

Profile	θ	r^{min}
I	$\pi/4$	0.000424
	$\pi/3$	0.000407
	$\pi/2$	0.000371
II	$\pi/4$	0.001491
	$\pi/3$	0.001815
	$\pi/2$	0.002089
III	$\pi/4$	0.009623
	$\pi/3$	0.011903
	$\pi/2$	0.013828
IV	$\pi/4$	0.014398
	$\pi/3$	0.017648
	$\pi/2$	0.020451

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