

Photonic Crystals: from Theory to Practice

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Abstract: In this paper we develop a numerical algorithm that computes the Green's function for a 2D finite-size photonic crystal, composed of rods of arbitrary shape. The method is based on boundary integral equation, and a Nyström discretization is used for the numerical solution. We derive multipole expansions for circular cylinders using our integral equation approach. Its numerical solution is used for validating our numerical method. We also show computation for nontrivial boundaries and discuss the convergence.

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References and links

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Introduction

A photonic crystal is a periodic dielectric structure that has the feature that there are prohibited frequencies of propagation of electromagnetic waves inside. The range of these frequencies is called the (complete) bandgap. If designed, such crystals would have an enormous technological applications (cf. [3] and the references therein). The existence of bandgaps means that the spectrum of the Maxwell operator for such media is expected to consist of a finite union of intervals. This is in contrast with a half line which is known to characterize the spectrum of the Maxwell operator for dielectrics with constant coefficients. Another property of photonic bandgap (PBG) is the changes in the local density of states (LDOS). In particular, for infinite structures, the LDOS vanishes inside a complete band gap.

Since their introduction [12], the study of photonic crystals has increased significantly in the past decade and many techniques were used in the computation of the spectra ([7], [2]) and the analysis of the LDOS [3].

For both the spectra analysis and computation of LDOS a key element is the computation of the Green's function. Two groups of methods have emerged: semi-analytical and numerical algorithms. For the former group, the exact formalism of multipole expansions is extensively used. In particular, in [7] the method was used for transmission calculations. This was extended in [3] to construct the two-dimensional Green's function and LDOS for finite-sized two-dimensional photonic crystals composed of circular cylinders of infinite length. Numerical methods are based on boundary element and finite element methods.

In this paper we discuss a boundary element method (BEM) to compute the two dimensional (2D) electromagnetic Green's function for a source at location \mathbf{x}_s and observation point at \mathbf{x} . The source, a line antenna of infinite length parallel to the cylinder axes, radiates with harmonic time dependence. The clusters we consider consist of parallel, disjoint dielectric cylinders of arbitrary smooth shapes.

The BEM technique is known to have many attractions: It reduces the 2D problem to 1D; the bounded integrals use the free source Green's function and inherits from its properties. Integral equation techniques were used for the study of photonic crystals [8] where a system of two integral equations with two unknown functions on the boundary of each rod was obtained by applying Green's theorems to a periodic problem. Here we choose an alternate route. In particular, we use a hybrid of Green's theorem and layer potentials to derive one equation with only one unknown on each rod. Our method is expected to have several advantages since, for N rods, it reduces the $2N$ equations with $2N$ unknowns to N equations with N unknowns; the use of the Nyström method that enjoys the exponential convergence for analytic boundaries; and fast multiple methods are available for the matrix vector multiplications for layer potentials. Our method has several advantages. The first advantage, for the problem with N rods, it reduces the $2N$ equations with $2N$ unknowns to N equations with N unknowns. The second, it employs the Nystrom method that has the advantage of exponential convergence for analytic boundaries. The third, fast multipole methods can be readily used for the matrix vector multiplications for layer potentials.

For the two-dimensional problem, the polarizations of the electromagnetic waves decouple to TM and TE polarizations. Here we only consider the TM case, the derivation for TE polarization being similar.

To validate our integral equation method, we derive a multipole expansion for circular cylinders, based on our boundary integral equation method. This will lead to the same formulae obtained in [7], [3] and [1]. Our results show an excellent match of the two methods.

The paper is organized as follows. In the first section we derive the equations and then state the problem. The second section is devoted to the integral equation formulation of the problem, the multipole expansion methods, and the numerical results. Finally, in the conclusion, we summarize the results and state our future interest.

1 Statement of the problem

The 2D photonic crystal under consideration is a mixed dielectric structure that is (without loss of generality) non magnetic. It consists of a finite number of rods of arbitrary shapes Ω_l , $l = 1, 2, \dots, M$, transverse to the $\mathbf{x} = (x_1, x_2)$ plane. The region outside of the rods is denoted by $\Omega_0 = \mathbf{R}^2 \setminus \cup_{l=1}^M (\overline{\Omega}_l)$ and the medium is characterized by the dielectric permittivity $\epsilon(x_1, x_2)$.

The Green's function $v(\mathbf{x}) = G(\mathbf{x}, \mathbf{x}_s, \omega)$, with frequency ω , satisfies the following equation.

$$\nabla^2 v + \omega^2 \epsilon v = \delta(\mathbf{x} - \mathbf{x}_s), \quad (1)$$

where δ is the Dirac delta function. We assume further that the permittivity ϵ is given by

$$\epsilon(\mathbf{x}) = \begin{cases} \epsilon_l, & \mathbf{x} \in \Omega_l, \quad l = 1, 2, \dots, M, \\ \epsilon_0, & \mathbf{x} \in \Omega_0, \end{cases}$$

where ϵ_l and ϵ_0 are real positive constants, and $\epsilon_l > 1$. This means that the equation in (1) is satisfied in the outer region Ω_0 (resp. inner rods Ω_l , $l = 1, 2, \dots, M$) with ϵ replaced by ϵ_0 (resp. ϵ_l). The solution in Ω_0 (resp. Ω_l , $l = 1, 2, \dots, M$) will be denoted by v_0 (resp. v_l). We have matching conditions on the interface between Ω_0

and each rod Ω_l, Γ_l (the boundary of Ω_l), $l = 1, 2, \dots, M$. This latter requires, due to the non-magnetic nature of the problem, the continuity of v and its normal derivative on the interface Γ_l .

Let us introduce the fundamental solution to the Helmholtz equations (the free-space source) by

$$\Phi_l(\mathbf{x}, \mathbf{x}') = -\frac{i}{2} H_0^{(1)}(\kappa_l |\mathbf{x} - \mathbf{x}'|), \quad l = 0, 1, \dots, M,$$

where $\kappa_l = \omega \sqrt{\epsilon_l}$ and $H_0^{(1)}$ is the Hankel function of the first kind and order zero. Now, for $l = 0, \dots, M$, define $u_l(\mathbf{x}) = v_l(\mathbf{x}) - \xi_l \Phi_l(\mathbf{x}, \mathbf{x}_s)$, where $\xi_l = 1$ (resp. $\xi_l = 0$) if \mathbf{x}_s lies in Ω_l (resp. outside of Ω_l). Since Φ_l satisfies equation (1) with \mathbf{x}' replaced by \mathbf{x}_s we have,

$$\nabla^2 u_l + \omega^2 \epsilon_l u_l = 0 \quad \text{in } \Omega_l, \quad l = 1, 2, \dots, M, \quad (2)$$

$$\nabla^2 u_0 + \omega^2 \epsilon_0 u_0 = 0 \quad \text{in } \Omega_0, \quad (3)$$

$$u = u_l \quad \text{and} \quad \frac{\partial}{\partial \mathbf{N}} u = \frac{\partial}{\partial \mathbf{N}} u_l \quad \text{on } \Gamma_l, \quad l = 1, 2, \dots, M, \quad (4)$$

$$u(\mathbf{x}) = u_0(\mathbf{x}) - \xi_l \Phi_l(\mathbf{x}, \mathbf{x}_s), \quad (5)$$

where \mathbf{N} is the normal derivative which is assumed to be directed to the exterior.

So, to obtain the Green's function in (1), we solve the problem (2)-(5) to obtain u_l and get $v_l = u_l + \xi_l \Phi_l$.

2 The Numerical methods

Let us define the single and double layer potentials, for $l = 1, 2, \dots, M$,

$$S_k^l \phi_l(\mathbf{x}) = \int_{\Gamma_l} \Phi_k(\mathbf{x}, \mathbf{x}') \phi_l(\mathbf{x}') ds(\mathbf{x}'), \quad \mathbf{x} \in \mathbf{R}^2 \setminus \Gamma_l,$$

and

$$D_k^l \psi_l(\mathbf{x}) = \int_{\Gamma_l} \frac{\partial}{\partial \mathbf{N}_l(\mathbf{x}')} \Phi_k(\mathbf{x}, \mathbf{x}') \psi_l(\mathbf{x}') ds(\mathbf{x}'), \quad \mathbf{x} \in \mathbf{R}^2 \setminus \Gamma_l, \quad (6)$$

respectively, for $k = 0, 1, \dots, M$. where the functions ϕ_l and ψ_l are the density functions. We also denote by P_k^l and Q_k^l the normal derivatives of S_k^l and D_k^l , respectively.

Applying Green's theorem we obtain

$$-2u_l(\mathbf{x}) = S_l^l \frac{\partial}{\partial \nu} u(\mathbf{x}) - D_l^l u(\mathbf{x}), \quad \mathbf{x} \in \Omega_l \quad (7)$$

and

$$0 = S_l^l \frac{\partial}{\partial \nu} u(\mathbf{x}) - D_l^l u(\mathbf{x}), \quad \mathbf{x} \in \Omega_0. \quad (8)$$

So, we obtain the field inside the rods by (7). For the exterior domain Ω_0 , we represent the field as a sum of double layer potentials, i.e.

$$u_0 = \sum_{l=1}^M D_0^l \phi_l, \quad (9)$$

2.1 The integral equation approach (IEM)

To obtain the desired integral equations, we let \mathbf{x} tend to the boundary in (8), using the boundary conditions, continuity and jump properties of layer potentials [5]. We then have on every boundary Γ_l , $l = 1, 2, \dots, M$

$$\left((I - \hat{D}_l^l)(\hat{D}_0^l - I) + \hat{S}_l^l \hat{Q}_0^l \right) \phi_l + \sum_{m \neq l}^l \left((I - \hat{D}_l^l) D_0^{m,l} + \hat{S}_l^l Q_0^{m,l} \right) \phi_m = f \quad (10)$$

where the hats on the operators means their limit as \mathbf{x} tends to the boundary, the superscripts m, l on the operators is the evaluation of the integral on Γ_l for a point that belongs to Γ_m , and

$$f = \xi_l(I - \hat{D}_l^l)\Phi_l + \xi_l \hat{S}_l^l \frac{\partial}{\partial \nu} \Phi_l, \quad (\text{resp. } f = (I - \hat{D}_l^l)\Phi_0 + \hat{S}_l^l \frac{\partial}{\partial \nu} \Phi_0)$$

for x_s in Ω_l (resp. Ω_0).

We can write the system of equation in a simplified form as

$$f = \hat{A}_0^l \phi_l - \sum_{m=1, m \neq l}^M A_0^{m,l} \phi_m \quad \text{on } \Gamma_l, \quad l = 1, 2, \dots, M. \quad (11)$$

We discretize this problem by the Nyström method [9] and the resulted matrix equation is solved by a multigrid method. The numerous matrix-vector multiplication can be done quickly by the fast multipole method [11].

2.2 The multipole expansions method (MEM)

Now, suppose the finite-size photonic crystal is composed of circular cylinders. We would like to derive a closed form of the solution using (7) and (9). The main tool is the following Graf formula [4].

$$H_0^{(1)}(\kappa_l |\mathbf{x} - \mathbf{x}'|) = \sum_{m=-\infty}^{\infty} e^{im\theta(\mathbf{x})} J_m[\kappa_l r(\mathbf{x})] H_m^{(1)}[\kappa_l r(\mathbf{x}')] e^{-im\theta(\mathbf{x}')} \quad \text{if } r(\mathbf{x}') \geq r(\mathbf{x})$$

and

$$H_0^{(1)}(\kappa_l |\mathbf{x} - \mathbf{x}'|) = \sum_{m=-\infty}^{\infty} e^{im\theta(\mathbf{x})} H_m^{(1)}[\kappa_l r(\mathbf{x})] J_m[\kappa_l r(\mathbf{x}')] e^{-im\theta(\mathbf{x}')} \quad \text{if } r(\mathbf{x}') < r(\mathbf{x}),$$

where $r(\mathbf{x})$ and $\theta(\mathbf{x})$ are the polar coordinates of \mathbf{x} . For a point \mathbf{x} inside the circular cylinder Ω_l we represent the polar coordinates of the cross section by $r_l(\mathbf{x})$ and $\theta_l(\mathbf{x})$. Clearly for \mathbf{x}' on the boundary we have $r(\mathbf{x}') \geq r(\mathbf{x})$. If we substitute the above expansion in (7) we obtain

$$u_l = \sum_{m=-\infty}^{\infty} a_m^l J_m(\kappa_l r_l(\mathbf{x})) e^{im\theta_l(\mathbf{x})}, \quad (12)$$

where

$$a_m^l = \int_{\Gamma_l} \left(H_m^{(1)}[\kappa_l r_l(\mathbf{x}')] e^{-im\theta_l(\mathbf{x}')} \frac{\partial}{\partial \mathbf{N}_l(\mathbf{x}')} u_l(\mathbf{x}') + \frac{\partial}{\partial \mathbf{N}_l(\mathbf{x}')} [H_m^{(1)}[\kappa_l r_l(\mathbf{x}')] e^{-im\theta_l(\mathbf{x}')} u_l(\mathbf{x}') \right) ds(\mathbf{x}').$$

Similarly, substitution in (9) and replacing k by zero in the graf formula, gives

$$u_0 = \sum_{l=1}^M \sum_{m=-\infty}^{\infty} b_m^l H_m^{(1)}(\kappa_0 r_l(\mathbf{x})) e^{im\theta_l(\mathbf{x})}, \quad (13)$$

where

$$b_m^l = \int_{\Gamma_l} \frac{\partial}{\partial \mathbf{N}(\mathbf{x}')} \left(H_m^{(1)}[\kappa_0 r_l(\mathbf{x}')] e^{-im\theta_l(\mathbf{x}')} \right) \phi_l(\mathbf{x}') ds(\mathbf{x}').$$

Now, using the boundary conditions (4) and the graf formula for translating the coordinates in (13) we obtain the same infinite system as given in formula (5) in [3]. This system is truncated and a multigrid method is used for approximating the solution.

2.3 Numerical results

For the numerical examples we first use a photonic crystal composed of 33 uniform circular cylinders with radius $r = 0.35d$, where the constant d is the cylinder spacing (distance between the centers of the closest cylinders). We have used, for $l = 1, \dots, M$, $\omega = 2\pi/\lambda$, $\epsilon_l = 2.9$ and $\epsilon_0 = 1$. In this case we see that the boundary integrals \hat{S}_l^l and \hat{D}_l^l need to be computed only once. The same argument holds for the scattering matrix that results from the boundary condition in the multipole method. This makes the computation much quicker. For a source point placed just above the photonic crystal we try and plot the absolute value of the Green's function on the line $x_1 = -5$. The result, for two different wave lengths, $\lambda = 2.25d$ and $\lambda = 3d$, is reported in Figure 2. An exact match of the two methods is observed.

Next, we consider a more complex geometry since in practical situations we do not have circular cylinders. We analyze a crystal where the circular cylinders are replaced by moon-like cylinders (Figure 3). In this case we can not apply MEM. We have used 16 Nyström points (the number of grids in the discretized version of the integral equation). The result is in Figure 4. Finally we tested the convergence for this problem, by plotting the absolute value of the Green's function against the Nyström points (Figure 5). We see a clear convergence.

3 Conclusion:

We have derived a new integral equation method for computing the Green's function for 2D Electromagnetic wave propagation in a finite size photonic crystal. The method is also used for deriving the multipole expansions for the case of circular cylinders. This derivation is different from the ones in the literature. Our numerical results show an excellent agreement of the two algorithms. We have also shown computation for a crystal where MEM can not be applied and we showed the convergence in this case. In the future we would like to expand the method to the numerical solution of the three-dimensional electromagnetic problem.

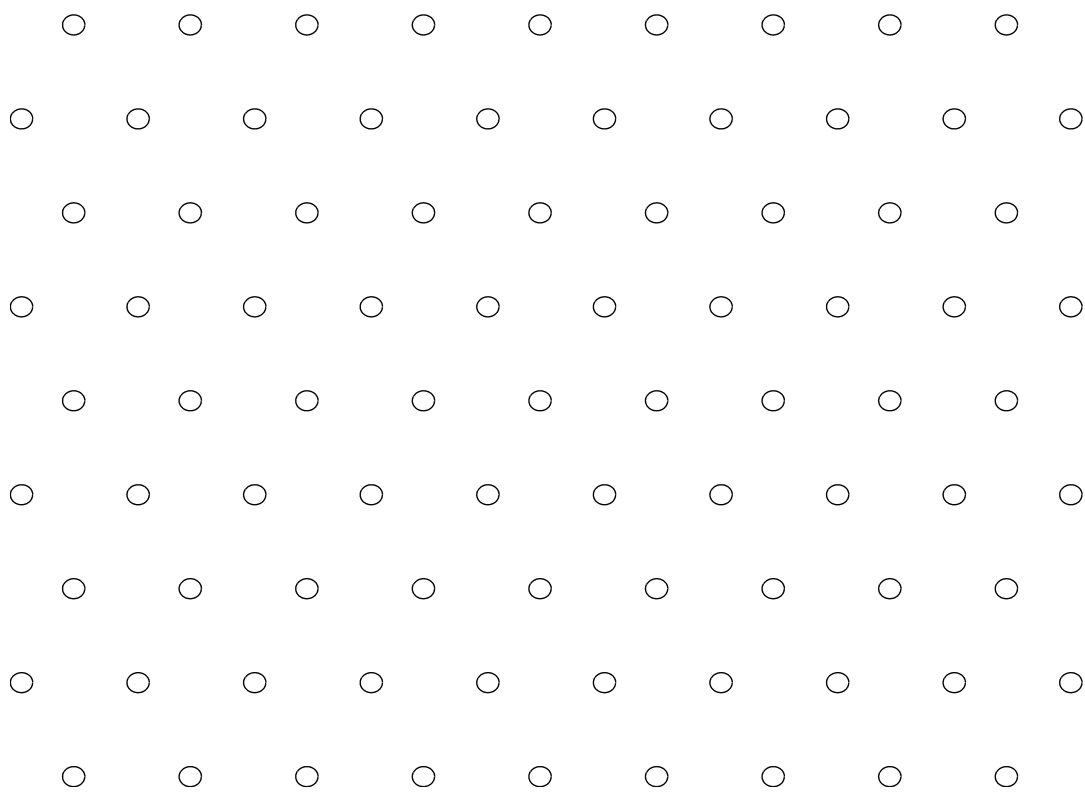


Fig. 1. A finite size photonic crystal consisting of 31 circular cylinders

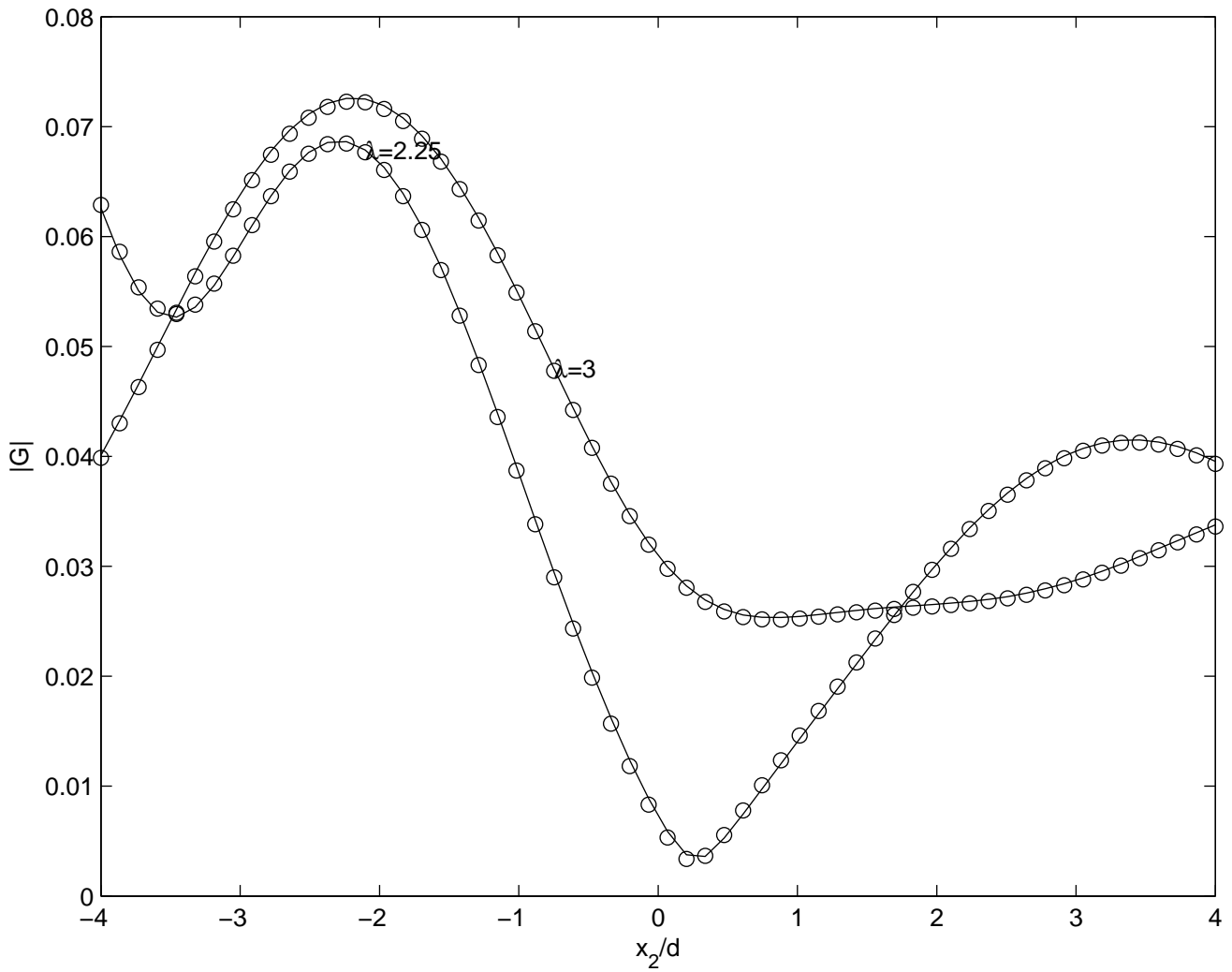


Fig. 2. The absolute value of the Green's function on the line $x_1 = -5$ for a finite-size photonic crystal consisting of 33 circular cylinders, for $\lambda = 2.25d$ and $\lambda = 3d$, using the integral equation method (solid line) and MEM 'o'.

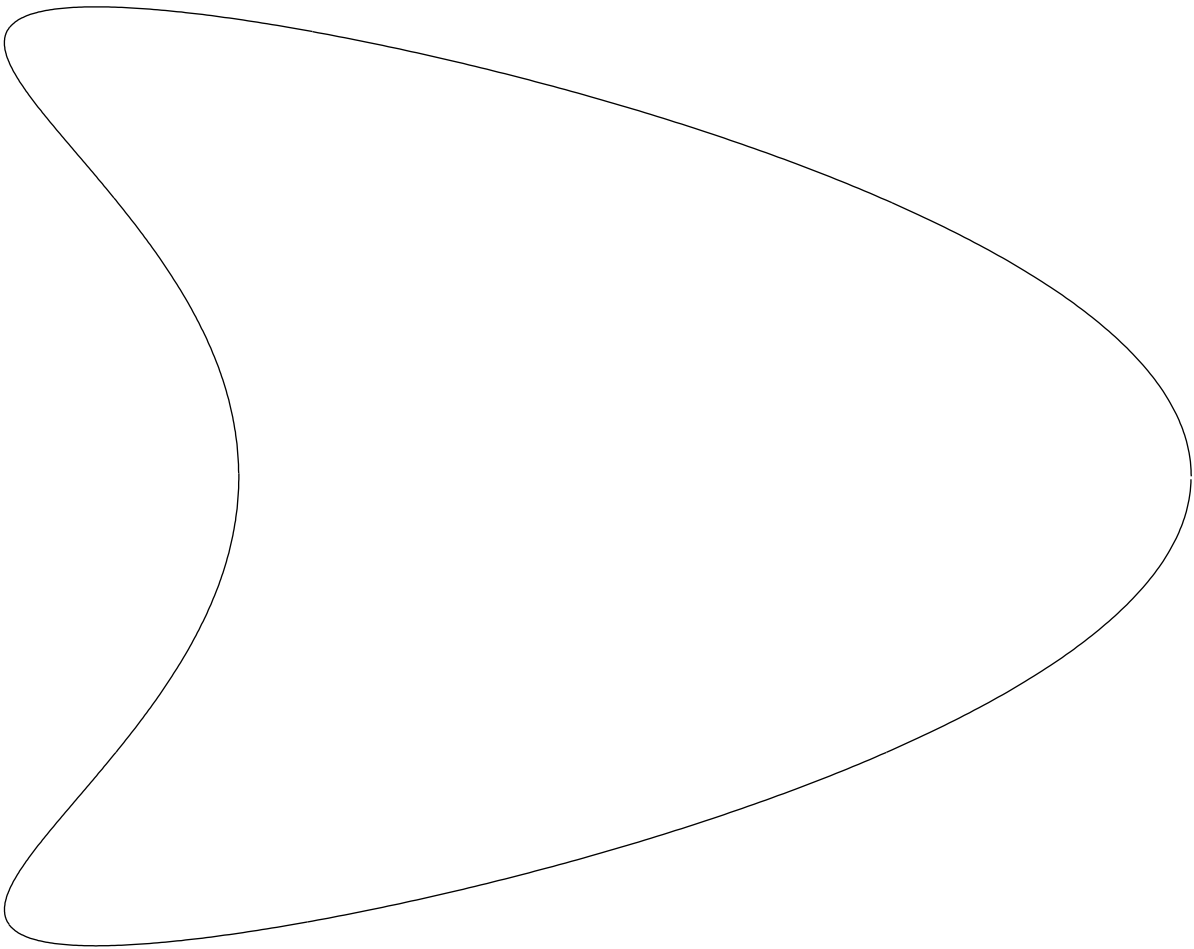


Fig. 3. A moon-like domain for which analytical methods can not be derived.

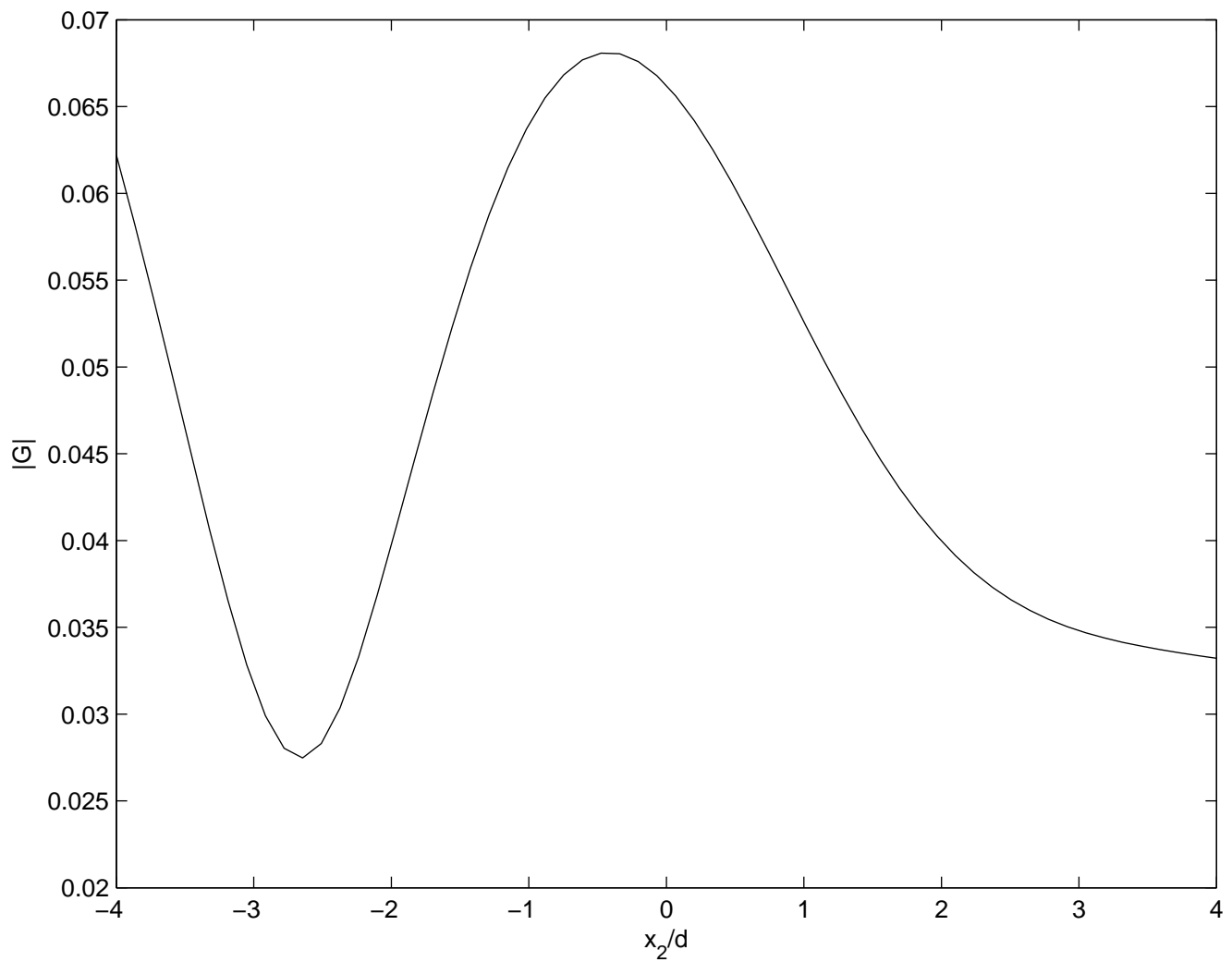


Fig. 4. The absolute value of the Green's function on the line $x_1 = -5$ for a finite-size photonic crystal consisting of 33 moon-like cylinders, for $\lambda = 3d$, using the integral equation method.

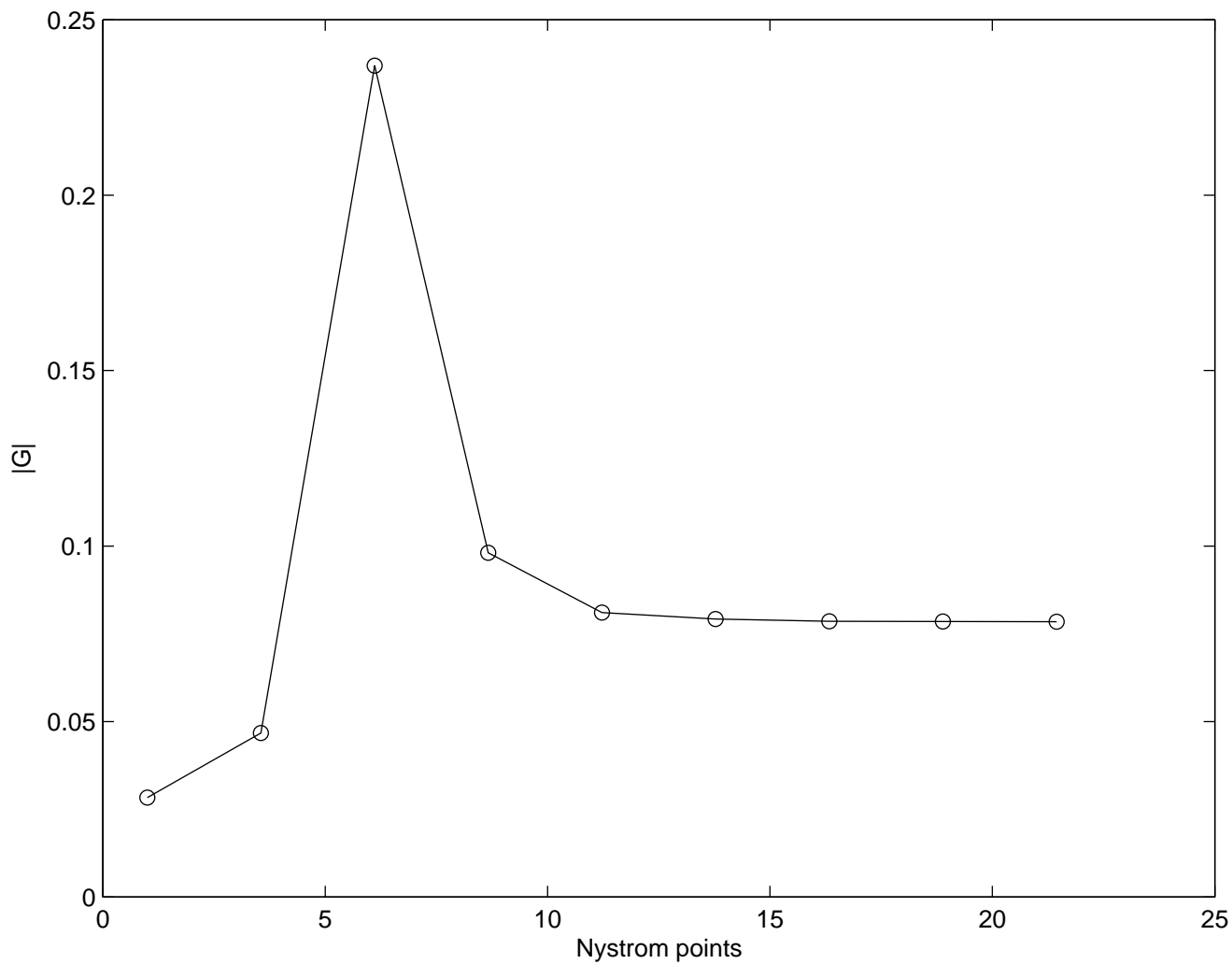


Fig. 5. Convergence test. The absolute value of the Green's function against Nyström points, at the point $(-5, 5)$, for a finite-size photonic crystal consisting of 33 moon-like cylinders. Here $\lambda = 3d$, using the integral equation method.