

# Numerical computation of the Green's function for two-dimensional finite-size photonic crystals of infinite length

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**Abstract:** We develop a numerical algorithm that computes the Green's function of Maxwell equation for a 2D finite-size photonic crystal, composed of rods of arbitrary shape. The method is based on the boundary integral equation, and a Nyström discretization is used for the numerical solution. To provide an exact solution that validates our code we derive multipole expansions for circular cylinders using our integral equation approach. The numerical method performs very well on the test case. We then apply it to crystals of arbitrary shape and discuss the convergence.

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## 1. Introduction

A photonic crystal is a periodic dielectric structure that has the feature that there are prohibited frequencies for the propagation of electromagnetic waves inside. The range of these frequencies is called the (complete) bandgap. If they could be designed, such crystals would have an enormous technological applications (cf. [1] 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. Another property of the 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 [2], the study of photonic crystals has increased significantly in the past decade and many techniques have been used for the computation of the spectra ([3], [4]) and the analysis of the LDOS [1].

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. In the former group, the exact formalism of multipole expansions is extensively used. In particular, in [3] and [5] the method was used for transmission calculations. This was extended in [1] to construct the two-dimensional Greens 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 shapes.

The BEM technique is known to have many attractions ([6],[7]) : 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 function on each rod. Our method is expected to have several advantages since, for  $N$  rods, it reduces the  $2N$  equations with  $2N$  unknown functions to  $N$  equations with  $N$  unknown functions; the use of the Nyström method that enjoys the exponential convergence for analytic boundaries; and fast multipole methods are available 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 the multipole expansion for circular cylinders, based on our boundary integral equation method. This will lead to the same formulae obtained in [3], [1] and [9]. Our results show an excellent match between the two methods. Our numerical method is computationally efficient and can be implemented on a laptop with short computation times.

The paper is organized as follows. In the first section we 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 discuss future applications.

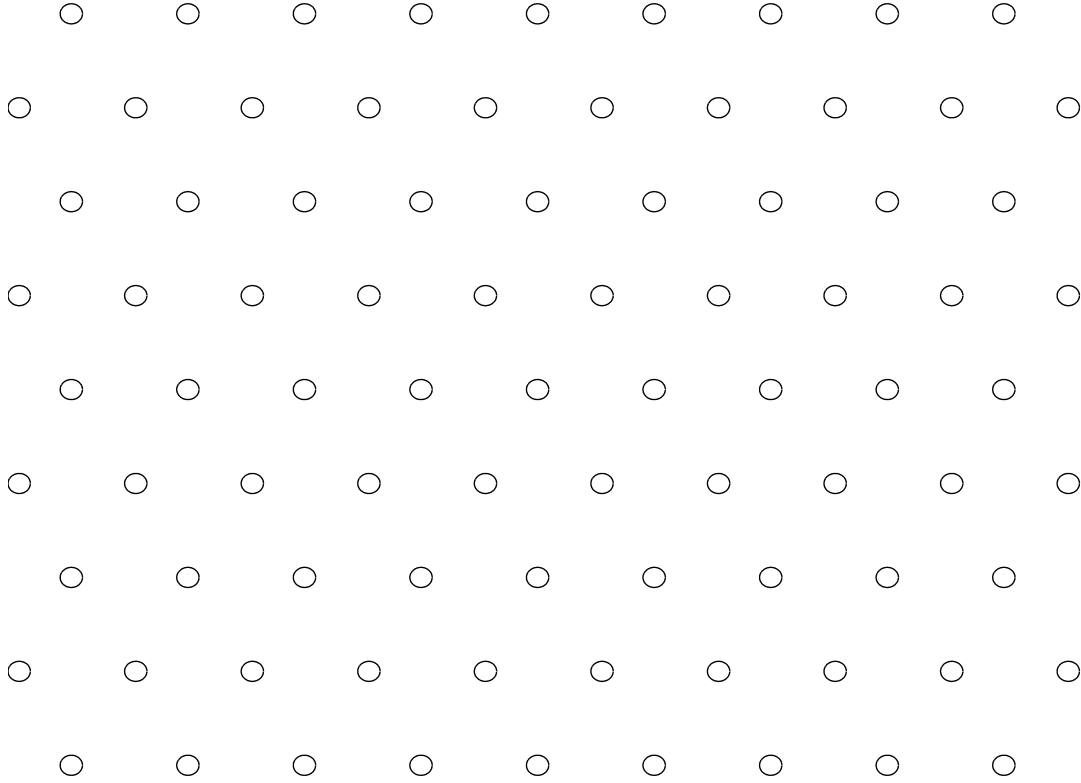


Fig. 1. A finite size photonic crystal consisting of 85 circular cylinders

## 2. 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  $\Omega_l$ ,  $l = 1, 2, \dots, M$ , 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  $\varepsilon(x_1, x_2)$ . In Fig. 1 we represent a finite-size photonic crystal consisting of 85 circular cylinders.

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

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

where  $\delta$  is the Dirac delta function. We assume further that the permittivity  $\varepsilon$  is given by

$$\varepsilon(\mathbf{x}) = \begin{cases} \varepsilon_l, & \mathbf{x} \in \Omega_l, \quad l = 1, 2, \dots, M, \\ \varepsilon_0, & \mathbf{x} \in \Omega_0, \end{cases}$$

where  $\varepsilon_l$  and  $\varepsilon_0$  are real positive constants, and  $\varepsilon_l > 1$ . This means that Eq. (1) is satisfied in the outer region  $\Omega_0$  (resp. inner rods  $\Omega_l$ ,  $l = 1, 2, \dots, M$ ) with  $\varepsilon$  replaced by  $\varepsilon_0$  (resp.  $\varepsilon_l$ ). The solution in  $\Omega_0$  (resp.  $\Omega_l$ ,  $l = 1, 2, \dots, M$ ) will be denoted by  $G_0$  (resp.  $G_l$ ). We have matching

conditions on the interface  $\Gamma_l$  (the boundary of  $\Omega_l$ ) between  $\Omega_0$  and each rod  $\Omega_l, l = 1, 2, \dots, M$ . This latter condition requires, due to the non-magnetic nature of the problem, the continuity of  $G$  and its normal derivative on the interface  $\Gamma_l$ .

Let us introduce the fundamental solution to the Helmholtz equations in free space as

$$\Phi_l(\mathbf{x}, \mathbf{x}') = -\frac{i}{4} H_0^{(1)}(\kappa_l |\mathbf{x} - \mathbf{x}'|), \quad l = 0, 1, \dots, M,$$

where  $\kappa_l = \omega \sqrt{\varepsilon_l}$  and  $H_0^{(1)}$  is the Hankel function of the first kind and order zero. Now, for  $l = 1, \dots, M$ , define in the interior of the rods  $u_l(\mathbf{x}) = G_l(\mathbf{x}) - \xi_l^{int} \Phi_l(\mathbf{x}, \mathbf{x}_s)$ , where  $\xi_l^{int} = 1$  (resp.  $\xi_l^{int} = 0$ ) if  $\mathbf{x}_s$  lies in  $\Omega_l$  (resp. outside of  $\Omega_l$ ). Define in the exterior  $u_0(\mathbf{x}) = G_0(\mathbf{x}) - \xi^{ext} \Phi_0(\mathbf{x}, \mathbf{x}_s)$ , where  $\xi^{ext} = 1$  (resp.  $\xi^{ext} = 0$ ) if  $\mathbf{x}_s$  lies in  $\Omega_0$  (resp. otherwise). Since  $\Phi_l, l = 0, 1, 2, \dots, M$  satisfy Eq. (1) with  $\mathbf{x}'$  replaced by  $\mathbf{x}_s$  we have,

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

$$\nabla^2 u_0 + \omega^2 \varepsilon_0 u_0 = 0 \quad \text{in } \Omega_0, \quad (3)$$

$$u_l + \xi_l^{int} \Phi_l = u_0 + \xi^{ext} \Phi_0 \quad \text{and} \quad \frac{\partial}{\partial \mathbf{N}}(u_l + \xi_l^{int} \Phi_l) = \frac{\partial}{\partial \mathbf{N}}(u_0 + \xi^{ext} \Phi_0) \quad \text{on } \Gamma_l, \quad l = 1, 2, \dots, M, \quad (4)$$

where  $\mathbf{N}$  is the normal derivative which is assumed to be directed to the exterior. In order to obtain uniqueness we must use the Sommerfeld radiation condition [10], i.e.,

$$\lim_{|\mathbf{x}| \rightarrow \infty} |\mathbf{x}|^{1/2} \left( \frac{\partial u_0}{\partial |\mathbf{x}|} - i\omega \varepsilon_0 u_0 \right) = 0. \quad (5)$$

So, to obtain the Green's function in (1), we solve the problem (2)-(5) to obtain  $u_l$ , then  $G_l = u_l + \xi_l^{int} \Phi_l$ , for  $l = 1, 2, \dots, M$ ; and  $u_0$ , then  $G_0 = u_0 + \xi^{ext} \Phi_0$ ,

### 3. The Numerical methods

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

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

and

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

respectively, for  $k = 0, 1, \dots, M$ . where the functions  $\phi_l$  and  $\psi_l$  are the density functions. We also denote by  $P_k^{m,l}$  and  $Q_k^{m,l}$  the normal derivatives of  $S_k^l$  and  $D_k^l$  at some point on a boundary  $\Gamma_m, m \neq l$ , respectively. Accordingly we denote by  $S_k^{m,l} \phi_l(\mathbf{x})$  and  $D_k^{m,l} \psi_l(\mathbf{x})$  the values of  $S_k^l \phi_l(\mathbf{x})$  and  $D_k^l \psi_l(\mathbf{x})$  when  $\mathbf{x}$  belongs to  $\Gamma_m, m \neq l$ .

It is known (cf. ([10], [11])) that the above defined potentials are analytic in  $\mathbf{R}^2 \setminus \Gamma_l$  and, when  $\mathbf{x}$  approaches  $\Gamma_l$ ,  $S_k^l$  and  $Q_k^l$  are continuous whereas  $D_k^l$  and  $P_k^l$  exhibit jumps.

Applying Green's theorem we obtain

$$-2u_l(\mathbf{x}) = S_l^l \frac{\partial}{\partial \mathbf{N}} u_l(\mathbf{x}) - D_l^l u_l(\mathbf{x}), \quad \mathbf{x} \in \Omega_l \quad (6)$$

and

$$0 = S_l^l \frac{\partial}{\partial \mathbf{N}} u_l(\mathbf{x}) - D_l^l u_l(\mathbf{x}), \quad \mathbf{x} \in \Omega_0. \quad (7)$$

So, we obtain the field inside the rods by (6). For the exterior domain  $\Omega_0$ , we represent the field as a sum of double layer potentials, i.e.

$$u_0 = \sum_{l=1}^M D_0^l \phi_l. \quad (8)$$

By straightforward calculations we can see that  $u_0$  given in this form satisfies the Sommerfeld radiation condition.

### 3.1. The integral equation method (IEM)

To obtain the desired integral equations, we let  $\mathbf{x}$  tend to the boundary in (7), using the boundary conditions, continuity and jump properties of layer potentials mentioned above. We then have on every boundary  $\Gamma_l$ ,  $l = 1, 2, \dots, M$

$$\left( (I - \hat{D}_l^l)(\hat{D}_0^l - I) + \hat{S}_l^l \hat{Q}_0^l \right) \phi_l + \sum_{m=1, m \neq l}^M \left( (I - \hat{D}_l^l) D_0^{m,l} + \hat{S}_l^l Q_0^{m,l} \right) \phi_m = f \quad (9)$$

where the hats on the operators mean their limit as  $\mathbf{x}$  approaches the boundary  $\Gamma_l$  where the integrals are being evaluated, and

$$f = \xi_l^{int} (I - \hat{D}_l^l) \Phi_l + \xi_l^{int} \hat{S}_l^l \frac{\partial}{\partial \mathbf{N}} \Phi_l - \xi^{ext} (I - \hat{D}_l^l) \Phi_0 - \xi^{ext} \hat{S}_l^l \frac{\partial}{\partial \mathbf{N}} \Phi_0.$$

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

$$f = \hat{A}_0^l \phi_l - \sum_{m=1, m \neq l}^M A_0^{m,l} \phi_m \quad \text{on } \Gamma_l, \quad l = 1, 2, \dots, M. \quad (10)$$

We discretize this problem by the Nyström method [12] and the resulted matrix equation is solved by a multigrid method ([7] and [13]). The numerous matrix-vector multiplication can be done efficiently by the fast multipole method [14].

### 3.2. The multipole expansions method (MEM)

Now, suppose the finite-size photonic crystal is composed of circular cylinders. A closed form of the solution can be derived using Green's identity [15]. Using Eq. (6), Eq. (8), the boundary conditions (4) and the Graf formula we obtain the same infinite system as given in formula (5) in [1]. This system is truncated and a multigrid method is used for approximating the solution.

### 3.3. Numerical results

Throughout the paper we retain a crystal with a hexagonal symmetry (Fig. 1), wavelength  $\lambda$ , frequency  $\omega = 2\pi/\lambda$  and  $\epsilon_0 = 1$ .

First we consider the photonic crystal in Fig. 1. It is composed of a set of dielectric circular cylinders with radius  $r=0.6$ , spacing constant (distance between the centers of the closest cylinders)  $d = 4$ , and  $\epsilon_l = 2.9$ ,  $l = 1, \dots, M$ . 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 these values of parameters it is known [3] that the gap lies between wavelengths 7.3 and 10.8.

Now for a fixed wavelength  $\lambda = 3.05$  and a source located in the photonic crystal we plot the absolute value of the Green's function on the  $x$ - coordinate for MEM and IEM. The result is

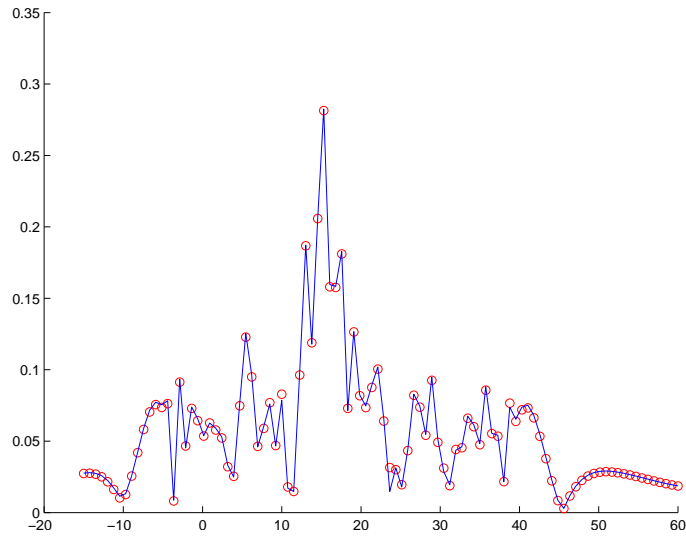


Fig. 2. The absolute value of the Green's function on the  $x$ -coordinate for a finite-size photonic crystal consisting of 85 circular cylinders. Here  $\lambda = 3.05$ , using IEM (solid line) and MEM ('o').

in Fig. 2. A strong agreement between the two methods is observed. The figure is not symmetric since the location of the source is arbitrary in the crystal. In Fig. 3 we do the same plots for different wavelengths. We see, as in [1], that for wavelengths in the gap the absolute value of the Green's function decay exponentially and that is not the case for other wavelengths.

Next, we replace the circular boundaries by squares (Fig. 7) of the same size as the circular cylinders considered above, i.e. the sides are equal to the diameters of the circular boundaries. For  $\lambda = 8.05$  we plot the absolute value of the Green's function on the  $x$ -coordinate for 39 cylinders of square and circular shapes (Fig. 4). We see that the absolute value of the Green's function for the square-shaped cylinders decays faster than for circular cylinders. When we increase the number of cylinders to 49 (Fig. 5) we see more similarity in the decay rate. On the other hand, when we use 85 square-shaped cylinders with the same parameters as in the case of circular boundaries, we observe that the absolute value of the Green's function decay fast for the wavelengths within the gap (Fig. 6). This suggests that with a small deformation in the construction we should not expect a significant difference in the gap.

Finally we consider a more complex geometry since in practical situations we may not have circular cylinders or boundaries that could be approximated as such. We analyze a crystal where the circular cylinders are replaced by cylinders of non-convex boundaries (Fig. 7). In this case we can not apply MEM. We tested the convergence for this problem, by plotting the absolute value of the Green's function against the Nyström points (Fig. 8). We see an exponential convergence.

#### 4. 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. Our numerical results show an excellent agreement of the two algorithms. We have also shown computations for a crystal where MEM can not be applied and we showed convergence in this case. Furthermore,

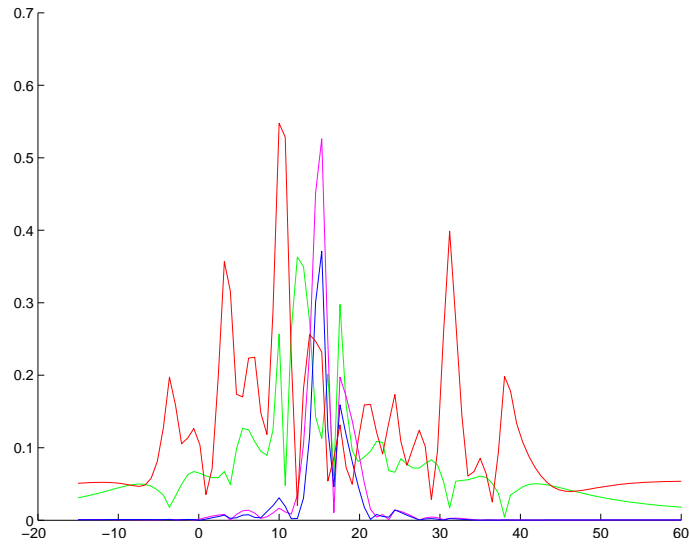


Fig. 3. The absolute value of the Green's function on the  $x$ -coordinate for a finite-size photonic crystal consisting of 85 circular cylinders. Here  $\lambda = 6.05$  (green),  $\lambda = 9.05$  (blue),  $\lambda = 11.25$  (red) and  $\lambda = 8.05$  (magnum) using IEM.

the method can be used to describe the electromagnetic quantities for crystals of finite size, with short computation time and excellent precision. In the future we would like to expand the method to the numerical solution of the three-dimensional electromagnetic problem.

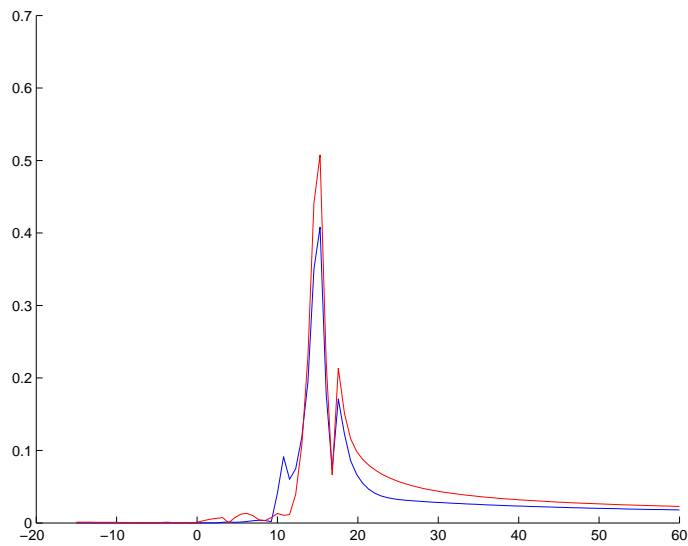


Fig. 4. The absolute value of the Green's function on the  $x$ - coordinate for a finite-size photonic crystal consisting of 38 cylinders of square shape (blue) and circular shape (red). Here  $\lambda = 8.05$  using IEM.

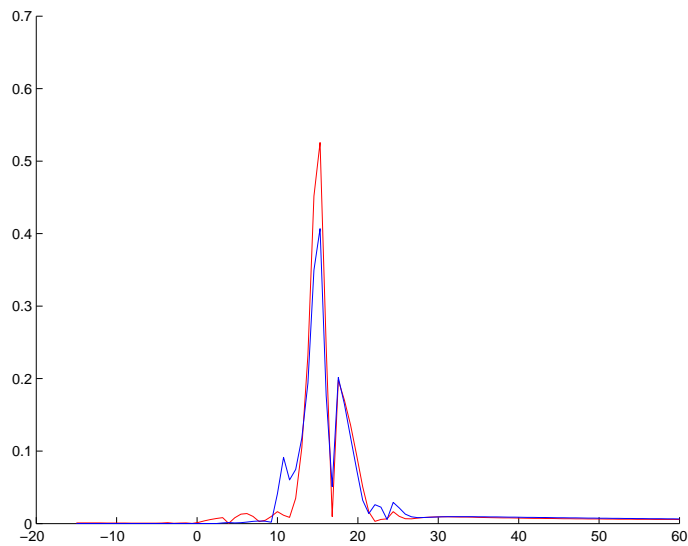


Fig. 5. The absolute value of the Green's function on the  $x$ - coordinate for a finite-size photonic crystal consisting of 49 cylinders of square shape (blue) and circular shape (red). Here  $\lambda = 8.05$  using IEM.

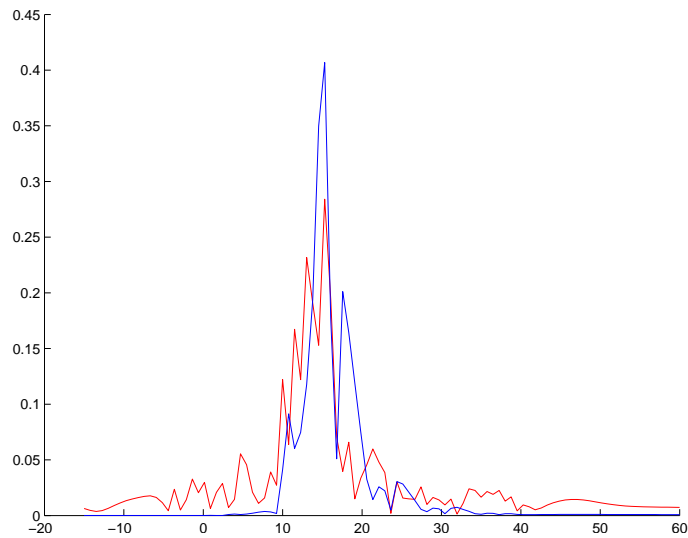


Fig. 6. The absolute value of the Green's function on the  $x$ -coordinate for a finite-size photonic crystal consisting of 85 square-shaped cylinders. Here  $\lambda = 2.25$  (red) and  $\lambda = 8.05$  (blue) using IEM.

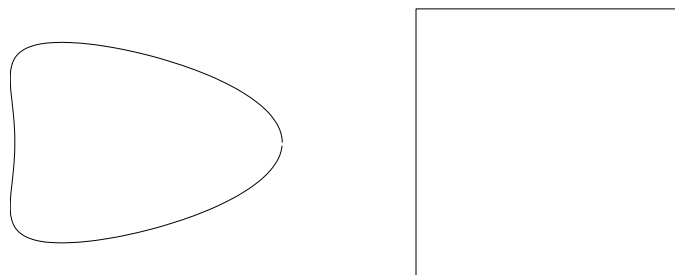


Fig. 7. Non-circular shapes for which analytical methods can not be derived. On the left a non-convex boundary and on the right a square with corners.

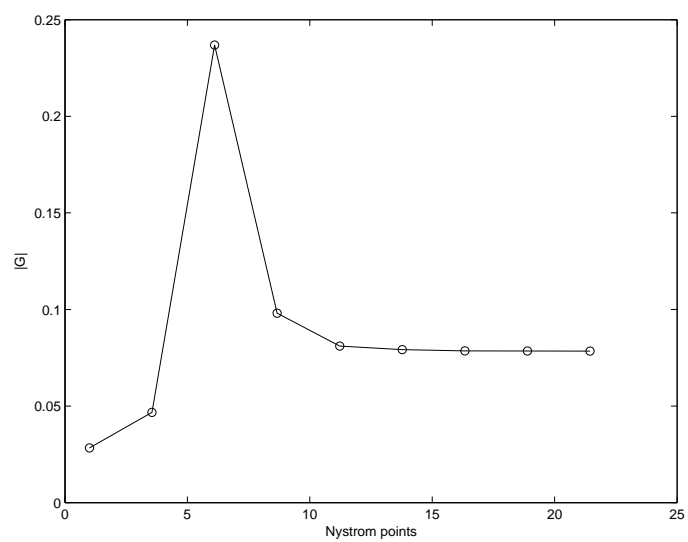


Fig. 8. Convergence test. The absolute value of the Green's function against Nyström points, at the point  $(-5,5)$ , for a finite-size photonic crystal consisting of 33 non-convex shape cylinders. Here  $\lambda = 3d$ , using the integral equation method.