

A numerical approach to complex eigenvalues with moduli close to a specified value

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Abstract. In this paper, we consider computing all the complex eigenvalues with moduli close to a specified value. Such problems arise in the application of photonic crystals. For solving the problems efficiently, we extend the projection method based on the residue theorem. We also analyze the errors of the eigenvalues computed by an extended method.

1 Introduction

We consider solving the generalized eigenvalue problem

$$Ax = \lambda Bx \quad (x \neq 0), \quad (1)$$

where A and B are $n \times n$ matrices, $\lambda \in \mathbb{C}$ is an eigenvalue, and $x \in \mathbb{C}^n$ is its corresponding eigenvector. The problem arises in many applications of scientific computing, such as structural analysis and stability analysis of fluid dynamics [1]. In these problems, it is often needed to find a few eigenvalues near a specified point in the complex plane, and iterative methods [2] are available for the problem.

Here, we focus on the eigenvalue problems which arise in the application of photonic crystals. In recent years, photonic crystals [3] have attracted much attention due to their potential applications in future integrated circuits based on light, instead of electrons. In these practical problems, one has to find all the complex eigenvalues on the unit circle in the complex plane [4]. To be more precise, in numerical computations, the eigenvalues of interest will not be strictly on the unit circle. The number of the needed eigenvalues are small, though the needed eigenvalues are usually scattered, not located near one point in the complex plane. Hence, the computational task is to find all the eigenvalues with moduli close a specified value; the value is 1 in this problem.

Since the needed eigenvalues are not located near one point in the complex plane, we consider the following approach to the needed eigenvalues without using iterative methods. We first consider a domain near the unit circle. The domain is surrounded by two circles whose centers are the origin and radii are $1 \pm \varepsilon$, where ε is a small positive number. This finite and

multiply connected domain includes all the eigenvalues of interest. Thus, we can say that the computational task is to find all the eigenvalues within the domain. To compute all the eigenvalues within the domain efficiently, we focus on the projection method based on the residue theorem [6]. We consider extending the method so that we can compute all the eigenvalues within the domain without computing the other eigenvalues.

The rest of this paper is organized as follows. In section 2, we give a brief exposition of the projection method based on the residue theorem. In section 3, we extend the method to the need for the eigenvalues with moduli close to a specified value. To illustrate the availability of a new extended method, we report numerical experiments in section 4. Finally, we summarize this paper in section 5.

Throughout this paper, i denotes the imaginary unit, $\mathbf{0}$ and O denote the zero vector and the zero matrix with appropriate size in the context, and $(\cdot)^*$ denotes the conjugate transpose. A positively oriented closed Jordan curve in the complex plane is simply called a closed curve.

2 The projection method based on the residue theorem

In this section, we briefly sketch the projection method based on the residue theorem [6]. The method is recently used to find the eigenvalues within a simply connected domain of the complex plane [5, 7].

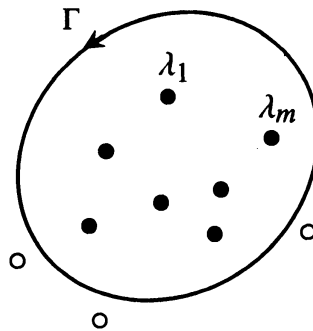


Figure 1: Distribution of eigenvalues in the complex plane. The eigenvalues within the domain enclosed by Γ are shown by $\bullet$, and the other eigenvalues are shown by $\circ$. The method can compute all the eigenvalues $\bullet$ without computing the eigenvalues $\circ$.

We assume that the matrix pencil $A - \lambda B$ is regular and A is diagonalizable [6]. However, the symmetry and singularity of the matrices A and B in (1) are not restricted. Let Γ be a closed curve and γ be a point within the domain enclosed by Γ . Let $\lambda_1, \dots, \lambda_{n'}$ be finite and distinct eigenvalues of (1). We assume that any eigenvalues do not lie on Γ . Let $\lambda_1, \dots, \lambda_m$ ($m \leq n'$) be the distinct eigenvalues within the domain. We suppose that the eigenval-

ues within the domain are of interest, see Figure 1. The needed eigenvalues can be computed in the following two steps [6]. The first step is computing complex moments which include the information of the needed eigenvalues $\lambda_1, \dots, \lambda_m$. It is important that the unneeded eigenvalues are not included in the moments. The second step is extracting the needed eigenvalues from the moments. This can be done by solving a generalized eigenvalue problem with smaller scale matrices than A and B in (1).

At the first step, let us consider computing the following complex moments for $p = 0, 1, \dots, 2m - 1$:

$$\mu_p = \frac{1}{2\pi i} \oint_{\Gamma} f(p, \gamma, z) dz, \quad (2)$$

where f is given with nonzero vectors $\mathbf{u}$ and $\mathbf{v}$ as follows:

$$f(p, \gamma, z) = (z - \gamma)^p (\mathbf{u}^* (zB - A)^{-1} \mathbf{v}). \quad (3)$$

The function f is expanded into two terms as follows [6]:

$$f(p, \gamma, z) = \sum_{k=1}^{n'} \frac{(z - \gamma)^p \nu_k}{z - \lambda_k} + g(z), \quad (4)$$

where ν_k is a scalar which we assume nonzero, and $g(z)$ is a polynomial. From (2), (4), and the residue theorem, it follows that

$$\mu_p = \sum_{k=1}^m (\lambda_k - \gamma)^p \nu_k, \quad (5)$$

where $(\lambda_k - \gamma)^p \nu_k$ is the residue of the function f at $z = \lambda_k$. From (5), the moment μ_p includes the information of the needed eigenvalues $\lambda_1, \dots, \lambda_m$.

At the second step, let us consider extracting the eigenvalues in the moments. Here, $m \times m$ matrices H_m and $H_m^<$ are given by

$$H_m = \begin{bmatrix} \mu_0 & \mu_1 & \dots & \mu_{m-1} \\ \mu_1 & \mu_2 & \dots & \mu_m \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{m-1} & \mu_m & \dots & \mu_{2m-2} \end{bmatrix}, \quad H_m^< = \begin{bmatrix} \mu_1 & \mu_2 & \dots & \mu_m \\ \mu_2 & \mu_3 & \dots & \mu_{m+1} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_m & \mu_{m+1} & \dots & \mu_{2m-1} \end{bmatrix}. \quad (6)$$

Let us consider solving the eigenvalue problem

$$H_m^< \mathbf{y} = \tilde{\lambda} H_m \mathbf{y} \quad (\mathbf{y} \neq \mathbf{0}). \quad (7)$$

In [6], it is shown that the eigenvalues of (7) are given by $\tilde{\lambda} = \lambda - \gamma$ ($\lambda \in \{\lambda_1, \dots, \lambda_m\}$). In this way, the eigenvalues of (1) within the domain, $\lambda = \tilde{\lambda} + \gamma$, can be computed by solving (7). This method can efficiently compute the needed eigenvalues λ when $m \ll n$.

3 An approach to the practical needs for eigenvalues

The previous section has given the brief summary of the method for the eigenvalues within a simply connected domain. In this section, we consider extending the method so that we can compute all the complex eigenvalues with moduli close to 1. To begin with, we give an extension of the method in section 3.1. Then, we describe the details of an extended method in section 3.2. In section 3.3, we analyze the error of the eigenvalues computed by the extended method.

3.1 Extension to a finite and multiply connected domain

To solve the eigenvalue problems which arise in the applications of photonic crystals, one has to compute the eigenvalues $\lambda_1, \dots, \lambda_m$ which are scattered near the unit circle in the complex plane, $|\lambda_i| \simeq 1$ ($i = 1, \dots, m$). To find them, it is natural in the method to specify a closed curve Γ_1 by a circle with the property that a center is the origin and a radius is $1 + \varepsilon$, where ε is a small positive number, see Figure 2. Then, the domain enclosed by Γ_1 includes both the needed eigenvalues near the unit circle and the unneeded eigenvalues within the unit circle. Let m' be the number of eigenvalues within the domain. Let us consider a moment

$$\mu_p^{(1)} = \frac{1}{2\pi i} \oint_{\Gamma_1} f(p, 0, z) dz.$$

By (2) and (5), the moment is shown by

$$\mu_p^{(1)} = \sum_{k=1}^m \lambda_k^p \nu_k + \sum_{k=m+1}^{m'} \lambda_k^p \nu_k.$$

Thus, the cluster of the needed eigenvalues can be decomposed into two terms as follows:

$$\sum_{k=1}^m \lambda_k^p \nu_k = \mu_p^{(1)} - \sum_{k=m+1}^{m'} \lambda_k^p \nu_k. \quad (8)$$

The second term in (8) includes the cluster of the unneeded eigenvalues inside the unit circle. To vanish them, we consider another moment. Let Γ_2 be a circle with the property that a center is the origin and a radius is $1 - \varepsilon$, see Figure 3. Let us consider a moment

$$\mu_p^{(2)} = \frac{1}{2\pi i} \oint_{\Gamma_2} f(p, 0, z) dz.$$

By (2) and (5), the moment is shown by

$$\mu_p^{(2)} = \sum_{k=m+1}^{m'} \lambda_k^p \nu_k. \quad (9)$$

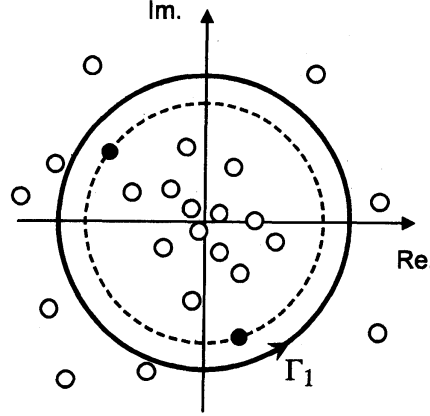


Figure 2: The eigenvalues of interest near the unit circle (dot line) are shown by $\bullet$, and the other eigenvalues are shown by $\circ$. All the needed eigenvalues $\bullet$ are included within the domain enclosed by Γ_1 .

From (8) and (9), it follows that

$$\sum_{k=1}^m \lambda_k^p \nu_k = \mu_p^{(1)} - \mu_p^{(2)}. \quad (10)$$

Let $\pm \tilde{\Gamma}_2$ be lines which connect Γ_1 to Γ_2 , as shown in Figure 3, and C be a closed curve

$$C = \Gamma_1 + \tilde{\Gamma}_2 - \Gamma_2 - \tilde{\Gamma}_2. \quad (11)$$

Then, (10) can be expressed as follows:

$$\sum_{k=1}^m \lambda_k^p \nu_k = \frac{1}{2\pi i} \oint_C f(p, 0, z) dz. \quad (12)$$

As shown in (12), the needed eigenvalues are included in the moment specified by C in (11), whereas the other eigenvalues are not included in the moment. From the above remark, let us consider using the following moments for $p = 0, 1, \dots, 2m - 1$ to give the elements of the matrices in (6):

$$\mu_p = \frac{1}{2\pi i} \oint_C f(p, 0, z) dz.$$

Then, by solving (7), we can get all the needed eigenvalues with moduli close to 1.

The above approach can be extended to general case: we can get the eigenvalues within a finite and multiply connected domain, see Figure 4. For $t = 1, \dots, d$, let Γ_t be a closed curve. We assume that any closed curves do not overlap with each other. Let D_t be a simply connected domain enclosed by Γ_t , and γ_t be a point within D_t . The outside of D_t is denoted

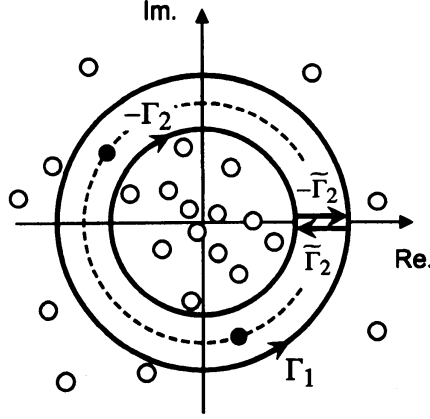


Figure 3: The needed eigenvalues shown by • can be treated as the eigenvalues within the multiply connected domain between Γ_1 and Γ_2 .

by $\overline{D}_t$. We assume that $D_2, \dots, D_d \subset D_1$ and define a finite and multiply connected domain Ω as follows:

$$\Omega = D_1 \cap \overline{D}_2 \cap \dots \cap \overline{D}_d. \quad (13)$$

The domain Ω is enclosed by a closed curve

$$C = \Gamma_1 + \sum_{t=2}^d (\tilde{\Gamma}_t - \Gamma_t - \tilde{\Gamma}_t), \quad (14)$$

where $\pm \tilde{\Gamma}_t$ are lines connecting Γ_1 to Γ_t . Let us consider a moment

$$\mu_p^{(t)} = \frac{1}{2\pi i} \oint_{\Gamma_t} f(p, \gamma_1, z) dz. \quad (15)$$

By (2) and (5), the information of all the eigenvalues within Ω are included in the following moment specified by C in (14):

$$\mu_p = \frac{1}{2\pi i} \oint_C f(p, \gamma_1, z) dz = \mu_p^{(1)} - \sum_{t=2}^d \mu_p^{(t)}, \quad (16)$$

where $\mu_p^{(t)}$ is given by (15). Note that (16) with $d = 2$ and $\gamma_1 = 0$ corresponds to (12). Let us consider using the moment in (16) to give the elements of the matrices in (6). Then, we can get all the eigenvalues within Ω in (13) by solving (7).

3.2 Algorithm

We present an algorithm for computing all the eigenvalues within a finite and multiply connected domain. We consider the case in which Γ_t ($t = 1, \dots, d$)

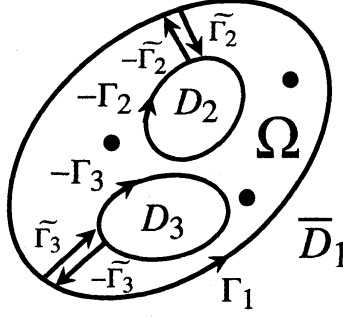


Figure 4: The eigenvalues within the multiply connected domain Ω ($d = 3$) are shown by $\bullet$.

is given by a circle with a center γ_t and a radius ρ_t . From (3) and (15),

$$\mu_p^{(t)} = \frac{1}{2\pi} \int_0^{2\pi} (\gamma_t + \rho_t e^{i\theta} - \gamma_1)^p \rho_t e^{i\theta} \left(\mathbf{u}^* ((\gamma_t + \rho_t e^{i\theta})B - A)^{-1} \mathbf{v} \right) d\theta. \quad (17)$$

Let N be a natural number, $\omega_N = \exp(2\pi i/N)$, and $z_j^{(t)} = \gamma_t + \rho_t \omega_N^j$. Then, an approximation $\tilde{\mu}_p^{(t)}$ of (17) by the N -point trapezoidal rule is given by

$$\tilde{\mu}_p^{(t)} = \frac{1}{N} \sum_{j=0}^{N-1} (z_j^{(t)} - \gamma_1)^p (z_j^{(t)} - \gamma_t) \left(\mathbf{u}^* (z_j^{(t)} B - A)^{-1} \mathbf{v} \right). \quad (18)$$

By (18), an approximation $\tilde{\mu}_p$ of (16) is given by

$$\tilde{\mu}_p = \tilde{\mu}_p^{(1)} - \sum_{t=2}^d \tilde{\mu}_p^{(t)}. \quad (19)$$

The matrices H_m and $H_m^<$ in (6) are generated by using $\tilde{\mu}_p$ in (19) instead of μ_p , and then (7) is solved. The above procedure is summarized in Algorithm 1.

3.3 Error analysis of computed eigenvalues

We analyze the error of the eigenvalues computed by Algorithm 1. Let m_t ($2 \leq t \leq d$) be the number of finite and distinct eigenvalues within D_t . Let m_1 be the number within Ω : $m_1 = m$, and m_{d+1} be the number in $\bar{D}_1$. Let $M(\ell) = \sum_{t=1}^{\ell} m_t$ ($1 \leq \ell \leq d+1$) with $M(0) = 0$. Then, $M(\ell)$ shows the number of finite and distinct eigenvalues: within Ω when $\ell = 1$; within $\Omega \cup D_2 \cup \dots \cup D_\ell$ when $2 \leq \ell \leq d$; of (1) when $\ell = d+1$. The finite and

Algorithm 1 Algorithm for all the eigenvalues within a finite and multiply connected domain

Input parameters: $m, N, d, \gamma_1, \dots, \gamma_d, \rho_1, \dots, \rho_d$.

Set nonzero vectors $\mathbf{u}, \mathbf{v} \in \mathbb{C}^n$.

for $t = 1, 2, \dots, d$ **do**

 Compute $z_j^{(t)} \leftarrow \gamma_t + \rho_t \exp(2\pi i j / N)$ ($j = 0, \dots, N-1$). $\triangleright i = \sqrt{-1}$

 Solve linear systems $(z_j^{(t)} B - A) \mathbf{q}_j = \mathbf{v}$ ($j = 0, \dots, N-1$).

 Compute $\tilde{\mu}_p^{(t)} \leftarrow \frac{1}{N} \sum_{j=0}^{N-1} (z_j^{(t)} - \gamma_1)^p (z_j^{(t)} - \gamma_t) (\mathbf{u}^* \mathbf{q}_j)$.

if $t = 1$ **then**

$\tilde{\mu}_p \leftarrow \tilde{\mu}_p^{(t)}$ ($p = 0, \dots, 2m-1$).

else

$\tilde{\mu}_p \leftarrow \tilde{\mu}_p - \tilde{\mu}_p^{(t)}$ ($p = 0, \dots, 2m-1$).

end if

end for

Set $H_m \leftarrow \begin{bmatrix} \tilde{\mu}_0 & \tilde{\mu}_1 & \dots & \tilde{\mu}_{m-1} \\ \tilde{\mu}_1 & \tilde{\mu}_2 & \dots & \tilde{\mu}_m \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{\mu}_{m-1} & \tilde{\mu}_m & \dots & \tilde{\mu}_{2m-2} \end{bmatrix}$, $H_m^< \leftarrow \begin{bmatrix} \tilde{\mu}_1 & \tilde{\mu}_2 & \dots & \tilde{\mu}_m \\ \tilde{\mu}_2 & \tilde{\mu}_3 & \dots & \tilde{\mu}_{m+1} \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{\mu}_m & \tilde{\mu}_{m+1} & \dots & \tilde{\mu}_{2m-1} \end{bmatrix}$.

Compute the eigenvalues $\tilde{\lambda}_1, \dots, \tilde{\lambda}_m$ of the pencil $H_m^< - \tilde{\lambda} H_m$.

Output the eigenvalues $\lambda_j \leftarrow \tilde{\lambda}_j + \gamma_1$ ($j = 1, \dots, m$).

distinct eigenvalues of (1) are indexed as follows:

$$\lambda_{M(\ell-1)+1}, \dots, \lambda_{M(\ell)} \begin{cases} \in \Omega & (\ell = 1), \\ \in D_\ell & (2 \leq \ell \leq d), \\ \in \overline{D}_1 & (\ell = d+1). \end{cases}$$

The eigenvalues computed by Algorithm 1 are denoted by $\tilde{\lambda}_1, \dots, \tilde{\lambda}_m$. Then, we show the errors of the computed eigenvalues as follows.

Theorem 1 *If the matrix H_m is nonsingular, then*

$$|\lambda_j - \tilde{\lambda}_j| = O(\varepsilon^N) \quad (j = 1, \dots, m),$$

$$\varepsilon = \max(\varepsilon_1, \varepsilon_2),$$

$$\varepsilon_1 = \max_{2 \leq \ell \leq d} \max_{M(\ell-1)+1 \leq k \leq M(\ell)} \left(\frac{|\lambda_k - \gamma_1|}{\rho_1}, \frac{|\lambda_k - \gamma_\ell|}{\rho_\ell}, \max_{2 \leq t \leq d, t \neq \ell} \frac{\rho_t}{|\lambda_k - \gamma_t|} \right),$$

$$\varepsilon_2 = \max_{M(d)+1 \leq k \leq M(d+1)} \max_{1 \leq t \leq d} \frac{\rho_t}{|\lambda_k - \gamma_t|}.$$

From Theorem 1, we can say that the absolute errors of the computed eigenvalues linearly decrease as N increases. The convergence ratio ε depends on the eigenvalues which are located outside Ω and are closest to Ω . If there are eigenvalues outside and very near Ω , ε becomes large. In this case, N is needed to be large to get the accurate eigenvalues.

4 Numerical experiments

In this section, we report some numerical experiments to show the availability of Algorithm 1 in section 3.2 and the validity of Theorem 1 in section 3.3. The following experiments were carried out with Matlab in double precision arithmetic.

4.1 Example 1

First, we compute all the eigenvalues on the unit circle. For this example, the order of the matrices A and B is $n = 20$, and the matrices are given by

$$A = Q^* \begin{bmatrix} 0.7D_1 & O \\ O & D_2 \\ O & 1.3D_1 \end{bmatrix} Q, \quad B = Q^*Q,$$

where $D_1 = \text{diag}(d_0, \dots, d_7)$, $d_j = \exp(2\pi i j/8)$, $D_2 = \text{diag}(1, -1, i, -i)$, and Q is a 20×20 matrix whose elements are given by random numbers. The distribution of the eigenvalues of (1) for the matrices is shown in Figure 5.

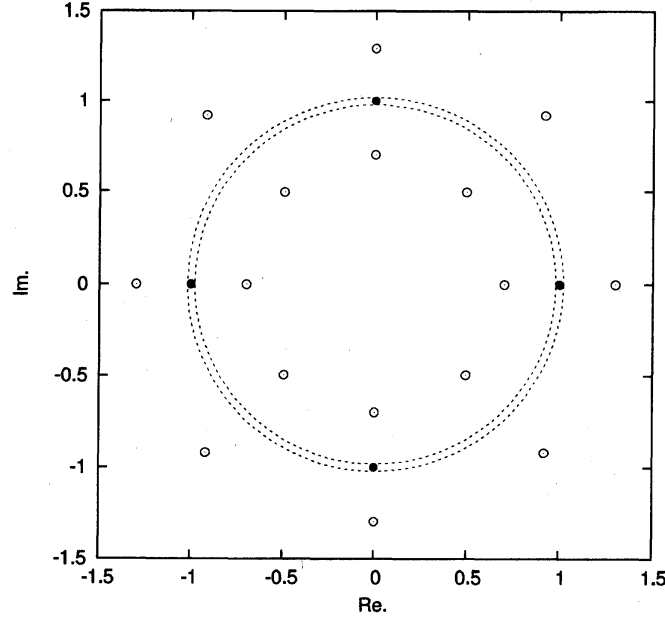


Figure 5: The eigenvalues on the unit circle are shown by $\bullet$, and the other eigenvalues are shown by $\circ$.

To find all the eigenvalues on the unit circle, $\lambda_1 = 1, \lambda_2 = -1, \lambda_3 = i, \lambda_4 = -i$, we set the parameters in Algorithm 1 as follows:

$$\begin{aligned} m &= 4, \quad N = 128, \quad d = 2, \\ \gamma_1 &= 0.00, \quad \rho_1 = 1.02, \\ \gamma_2 &= 0.00, \quad \rho_2 = 0.98. \end{aligned}$$

By using the parameters, we computed all the eigenvalues within a multiply connected domain, see Figure 5. The computed eigenvalues are

$$\begin{aligned}\lambda_1 &= 1.0000000000000035 + 0.0000000000000037i, \\ \lambda_2 &= -1.0000000000000061 - 0.0000000000000007i, \\ \lambda_3 &= -0.0000000000000003 + 1.0000000000000085i, \\ \lambda_4 &= -0.0000000000000038 - 1.0000000000000031i.\end{aligned}$$

From this result, we observe that Algorithm 1 can compute all the eigenvalues on the unit circle.

4.2 Example 2

For the second example, the order of the matrices A and B is $n = 100$, and the matrices are given by

$$A = \begin{bmatrix} \frac{99}{100} & \frac{1}{100} & & & 0 \\ & \frac{98}{100} & \ddots & & \\ & & \ddots & \ddots & \\ & & & \frac{1}{100} & \frac{1}{100} \\ 0 & & & & 0 \end{bmatrix}, \quad B = \begin{bmatrix} O & O \\ O & I_{20} \end{bmatrix},$$

where I_{20} is the 20×20 identity matrix. For the matrices, the finite eigenvalues of (1) are given by

$$\lambda_j = \frac{j-1}{100} \quad (j = 1, \dots, 20).$$

We set the parameters in Algorithm 1 as follows:

$$\begin{aligned}m &= 4, \quad d = 4, \\ \gamma_1 &= 0.040, \quad \rho_1 = 0.051, \\ \gamma_2 &= 0.021, \quad \rho_2 = 0.015, \\ \gamma_3 &= 0.058, \quad \rho_3 = 0.009, \\ \gamma_4 &= 0.080, \quad \rho_4 = 0.005.\end{aligned}$$

By the parameters, a multiply connected domain is specified, see Figure 6. We computed the eigenvalues within the domain, $\lambda_1 = 0.00$, $\lambda_2 = 0.04$, $\lambda_3 = 0.07$, $\lambda_4 = 0.09$, see Figure 6. In this case, $\lambda = 0.05$ is the eigenvalue which is located outside the domain and is closet to the domain. From Theorem 1, the convergence ratio is estimated to be $\varepsilon = |\lambda - \gamma_3|/\rho_3 \simeq 0.89$.

We show the errors of the computed eigenvalues in Figure 7. From Figure 7, we observe that the errors linearly decrease. The gradient shows the convergence ratio as $\varepsilon \simeq 10^{-0.05} \simeq 0.89$. From these results, we observe that the error analysis in Theorem 1 is valid.

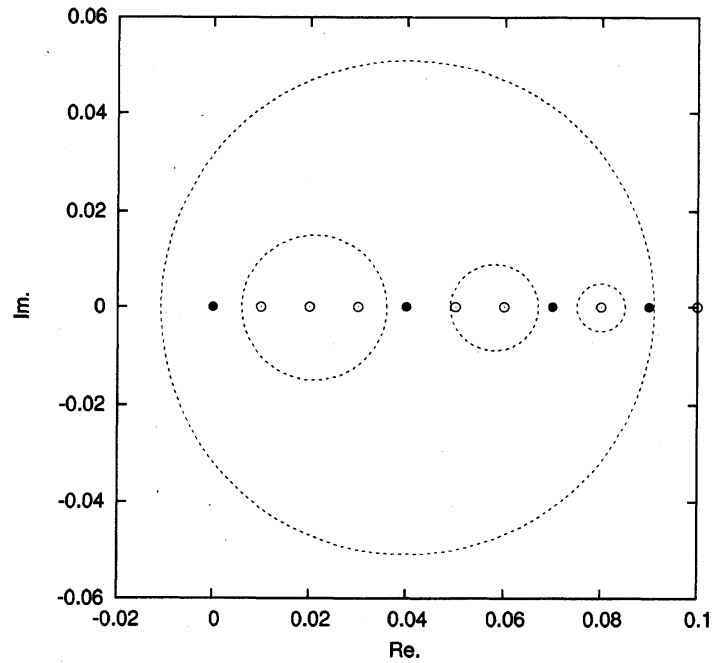


Figure 6: The eigenvalues within the multiply connected domain are shown by ●, and the other eigenvalues are shown by ○.

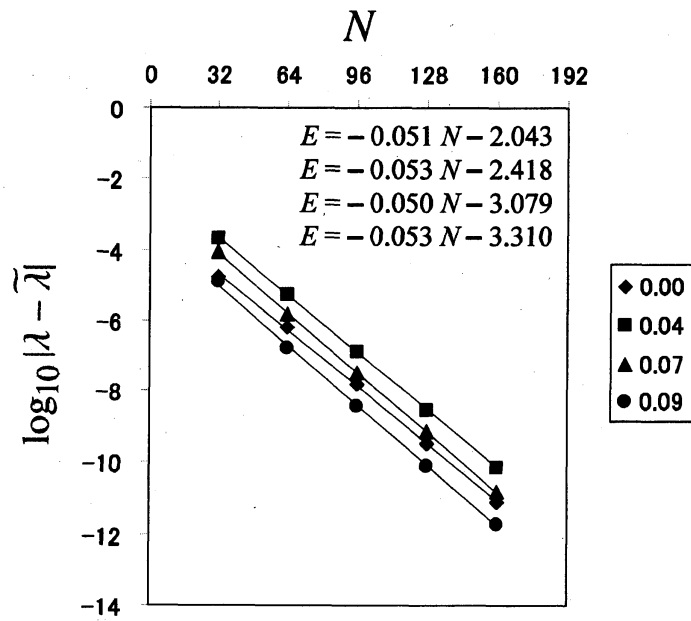


Figure 7: As N increases, the error $|\lambda - \tilde{\lambda}|$ linearly decreases, where λ is the exact eigenvalue and $\tilde{\lambda}$ is the computed eigenvalue. The gradient shows the convergence ratio as $\varepsilon \simeq 10^{-0.05} \simeq 0.89$.

5 Concluding remarks

In this paper, we have considered computing the eigenvalues whose absolute values are close to a specified value. Such problems arise in the application of photonic crystals. For solving the problems efficiently, we have extended the projection method based on the residue theorem. From our experiments, we have learned that an extended method can compute the eigenvalues within a finite and multiply connected domain. Since the needed eigenvalues in the application of photonic crystals are within a multiply connected domain, the extended method is promising for computing the needed eigenvalues. We have also analyzed the errors of the eigenvalues computed by the extended method. The analysis has been verified by numerical experiments.

Acknowledgment

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