ACCURACY IMPROVEMENT OF THE FOURIER SERIES EXPANSION METHOD FOR FLOQUET-MODE ANALYSIS OF PHOTONIC CRYSTAL WAVEGUIDES

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Abstract—The Fourier series expansion method is a useful tool to approach the problems of discontinuities in optical waveguides, and it applies to analyze the Floquet-modes of photonic crystal waveguides. This paper shows that the Floquet-mode calculation with large truncation order is limited and explains the reason. Furthermore, two techniques of the formulation are presented to relieve this limitation. One of them is a use of the symmetric properties of the Floquet-modes, and another is a use of the Rayleigh quotients to improve accuracy of eigenvalue calculation. They are validated by numerical experiments.

1. INTRODUCTION

Photonic crystals are periodic structures that are designed to reject the propagation of electromagnetic waves at certain wavelength range. Local collapses of the periodicity provide significant advantages for field confinement, wave guiding, and directing radiation and have received attentions of researchers. Especially, defects introduced into the photonic crystals compose optical devices such as cavities, waveguides, splitter, coupler, etc. and they constitute photonic crystal circuits. The optical propagation along the photonic crystal circuits

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has been simulated using various numerical methods such as the beam propagation method [1], the finite difference time domain method [2], and the plane wave expansion method [3]. These methods require adequate treatments of terminating conditions for optical waves at the output ends of the circuits. However, the structure of photonic crystal waveguide is nonuniform along the optical propagation, and the Floquet-mode analysis is necessary to decompose the fields in input/output waveguides into the forward and the backward propagating components. The Floquet-modes are the eigenmodes of a periodic structure.

The present paper considers the Floquet-modes propagating in a photonic crystal waveguides schematically shown in Fig. 1. The photonic crystal consists of rectangular cylinders located parallel in rectangular lattice characterized by the periods d_x and d_z in the x- and z-directions, respectively. Each cylinder has common dimensions a_x and a_z along the x- and z-directions, and infinitely long in the y-direction. The waveguide is formed by a straight line defect in the photonic crystal, and the structure is uniform in the y-direction. The cylinder and the surrounding media are linear and isotropic, and the permeability of free space is assumed. The permittivity of rectangular cylinders is denoted by ε_c and that of the surrounding medium is denoted by ε_s. Throughout the paper, we consider only time-harmonic TE-polarized fields assuming a time-dependence in $e^{-i\omega t}$ and the electric field is parallel to the cylinders. Then the fields are represented by complex vectors depending only on the space variables x and z.
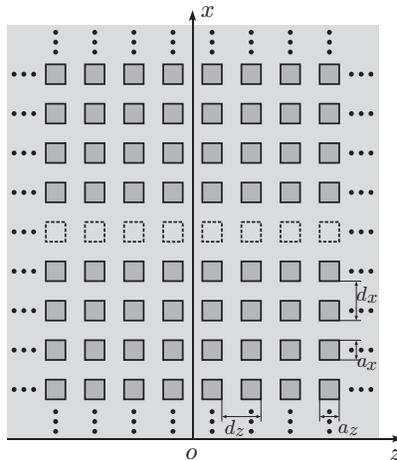

Figure 1. Two-dimensional photonic crystal waveguide formed by rectangular cylinders.

Since the structure is periodic in the z-direction, the generalized Fourier series is usually introduced to expand the electromagnetic fields [4, 5]. Maxwell's equations and the constitutive relations yield a coupled ordinary differential equation set in terms of the generalized Fourier coefficients. Then the dispersion equation for guided modes was derived based on the scattering-matrix propagation algorithm. The derived dispersion equation is written by a complex function with a complex argument and the zeros give the propagation constants of the eigen modes. Müller's method is usually used to find the zeros, but it is not so easy to give an adequate initial value to obtain a desired zero.

The present paper deals with the Fourier series expansion method to calculate the Floquet-modes propagating in the photonic crystal waveguides. The method was originally developed to analyze the discontinuities in dielectric waveguides [6–8]. Miyamoto et al. [9] proposed a formulation of grating waveguides based on the Fourier series expansion method, and the Floquet-modes were obtained by the eigenvalue calculation of the transfer matrix for one periodicity cell. Their formulation was applied to Floquet-mode analysis of photonic crystal waveguides [10, 11], and provided sufficiently accurate results in many applications. Recently, we found there is a limitation of the truncation order when increasing the accuracy. This paper presents the origin of this limitation and shows some techniques to relieve it. These techniques make us possible to obtain results that are more accurate.

2. OUTLINE OF THE FORMULATION

The aim of this section is to make clear the formulation that we used to calculate the Floquet-modes of photonic crystal waveguides. We introduce artificial boundaries at $x = 0$ and $x = w$, which are supposed to be sufficiently far from the defects (see Fig. 2(a)). The original electromagnetic fields in $0 < x < w$ are then approximated by periodic functions with the period w and expressed in the Fourier series expansion. For example, the y-component of electric field is approximately expressed as

$$E_y(x,\, z) = \sum_{n=-N}^{N} E_{y,\, n}(z)\, e^{ink_w x} \tag{1}$$

where N denotes the truncation order and $k_w = 2\pi/w$. The Fourier coefficients $\{E_{y,\, n}(z)\}_{n=-N}^{N}$ are functions of z, and the field profile can be derived by calculating the z-dependence of the coefficients. The structure under consideration is periodic in the z-direction and the
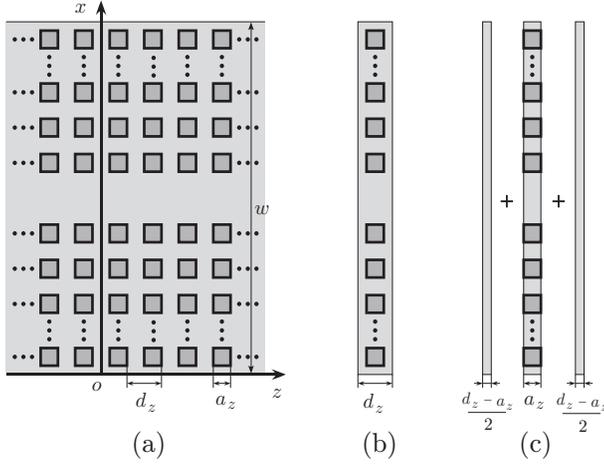
Figure 2. Analysis regions, (a) introduction of artificial boundaries
with periodicity condition, (b) periodicity cell for analysis, and (c)
segments uniform in the z-direction.

Floquet theorem asserts that the analysis region for calculating the
wave propagation can be reduced to a periodicity cell. In this paper,
the periodicity cell is taken to be the region $0 < z < d_z$ as shown in
Fig. 2(b). Furthermore, the periodicity cell is decomposed into three
segments as shown in Fig. 2(c). We denote the region $(d_z - a_z)/2 <
z < (d_z + a_z)/2$ as segment c and the regions $0 < z < (d_z - a_z)/2$ and
$(d_z + a_z)/2 < z < d_z$ as segments s. Also, the permittivity distribution
of segment c is denoted by $\varepsilon^{(c)}(x)$.

Let, for example, $\mathbf{e}_y(z)$ be the $(2N + 1) \times 1$ column matrix
generated by the Fourier coefficients of $E_y(x, z)$. Then, from Maxwell's
curl equations, the coefficients of TE-polarized fields in the segment c
are expressed as follows:

$$\begin{pmatrix} \mathbf{e}_y(z) \\ \mathbf{h}_x(z) \end{pmatrix} = \mathbf{Q}^{(c)} \begin{pmatrix} \mathbf{a}^{(c,+)}(z) \\ \mathbf{a}^{(c,-)}(z) \end{pmatrix} \tag{2}$$

with

$$\mathbf{Q}^{(c)} = \begin{pmatrix} \mathbf{P}^{(c)} & \mathbf{P}^{(c)} \\ -\frac{1}{\omega\mu_0}\mathbf{P}^{(c)}\mathbf{Z}^{(c)} & \frac{1}{\omega\mu_0}\mathbf{P}^{(c)}\mathbf{Z}^{(c)} \end{pmatrix} \tag{3}$$

$$\mathbf{P}^{(c)} = \begin{pmatrix} \mathbf{p}_1^{(c)} & \cdots & \mathbf{p}_{2N+1}^{(c)} \end{pmatrix} \tag{4}$$

$$\left(\mathbf{Z}^{(c)} \right)_{n,m} = \delta_{n,m}\gamma_n^{(c)}. \tag{5}$$

$\gamma_n^{(c)\,2}$ and $\mathbf{p}_n^{(c)}$ denote respectively the nth-eigenvalues and the associated eigenvectors of the matrix $\mathbf{C}^{(c)} = \omega^2 \mu_0 \left[\!\left[\varepsilon^{(c)}\right]\!\right] - \mathbf{X}^2$, where (n, m)-entries of the square matrices $\left[\!\left[\varepsilon^{(c)}\right]\!\right]$ and $\mathbf{X}$ are given by

$$\left(\left[\!\left[\varepsilon^{(c)}\right]\!\right]\right)_{n,\,m} = \frac{1}{w} \int_0^w \varepsilon^{(c)}(x) e^{-i(n-m)k_w x}\, dx \qquad (6)$$

$$(\mathbf{X})_{n,\,m} = \delta_{n,\,m} n k_w. \qquad (7)$$

Two column matrices $\mathbf{a}^{(c,+)}(z)$ and $\mathbf{a}^{(c,-)}(z)$ give the amplitudes of eigenmodes propagating in the $+z$- and $-z$-directions, respectively, and the relation between the modal amplitudes at $z = z'$ and $z = z''$ is given as

$$\begin{pmatrix} \mathbf{a}^{(c,+)}(z') \\ \mathbf{a}^{(c,-)}(z') \end{pmatrix} = \mathbf{U}^{(c)}(z' - z'') \begin{pmatrix} \mathbf{a}^{(c,+)}(z'') \\ \mathbf{a}^{(c,-)}(z'') \end{pmatrix} \qquad (8)$$

with

$$\mathbf{U}^{(c)}(z) = \begin{pmatrix} \mathbf{V}^{(c)}(z) & \mathbf{0} \\ \mathbf{0} & \mathbf{V}^{(c)}(-z) \end{pmatrix} \qquad (9)$$

$$\left(\mathbf{V}^{(c)}(z)\right)_{n,\,m} = \delta_{n,\,m} e^{i\gamma_n^{(c)} z} \qquad (10)$$

where z', z'' are both in the segment c. The permittivity inside the segments s is a constant value ε_s. We obtain the relations in the same form with Eqs. (2) and (8) in these segments but replace the superscript (c) by (s) to indicate the matrices defined in the segments s. The coefficient matrix $\mathbf{Q}^{(s)}$ is defined by replacing $\mathbf{P}^{(c)}$ by the identity matrix and $\mathbf{Z}^{(c)}$ by the diagonal matrix generated with $\gamma_n^{(s)} = \sqrt{\omega^2 \varepsilon_s \mu_0 - n^2 k_w{}^2}$.

The fields in segments c and s are matched at the boundaries $z = (d_z \pm a_z)/2$ by the boundary conditions, which are given by continuing the coefficients column matrices $\mathbf{e}_y(z)$ and $\mathbf{h}_x(z)$ at the boundaries. Then, the relations between the modal amplitudes $\mathbf{a}^{(s,\pm)}(0)$ and $\mathbf{a}^{(s,\pm)}(d_z)$ are derived as

$$\begin{pmatrix} \mathbf{a}^{(s,+)}(d_z) \\ \mathbf{a}^{(s,-)}(d_z) \end{pmatrix} = \mathbf{F} \begin{pmatrix} \mathbf{a}^{(s,+)}(0) \\ \mathbf{a}^{(s,-)}(0) \end{pmatrix} \qquad (11)$$

where the transfer matrix of the periodicity cell $\mathbf{F}$ is given by

$$\mathbf{F} = \mathbf{U}^{(s)}\left(\tfrac{d_z - a_z}{2}\right) \mathbf{Q}^{(s)^{-1}} \mathbf{Q}^{(c)} \mathbf{U}^{(c)}(a_z) \mathbf{Q}^{(c)^{-1}} \mathbf{Q}^{(s)} \mathbf{U}^{(s)}\left(\tfrac{d_z - a_z}{2}\right). \qquad (12)$$

Let β_n and $\mathbf{r}_n$ be, respectively, the nth-eigenvalues and the associated eigenvectors of the transfer matrix $\mathbf{F}$. Then, we define a column matrix $\mathbf{b}(z)$ by

$$\mathbf{b}(z) = \mathbf{R}^{-1} \begin{pmatrix} \mathbf{a}^{(s,+)}(z) \\ \mathbf{a}^{(s,-)}(z) \end{pmatrix} \tag{13}$$

with

$$\mathbf{R} = (\mathbf{r}_1 \quad \cdots \quad \mathbf{r}_{4N+2}). \tag{14}$$

The nth-component of $\mathbf{b}(z)$ is denoted by $b_n(z)$, and Eqs. (11) and (13) yield a relation:

$$b_n(d_z) = \beta_n b_n(0). \tag{15}$$

This means that $\{b_n(0)\}$ gives the amplitudes of the Floquet-modes propagating in the photonic crystal waveguide at $z = 0$, and the propagation constants are calculated by

$$\eta_n = -i\frac{\mathrm{Ln}(\beta_n)}{d_z}, \tag{16}$$

where Ln denotes the principal natural logarithm function. Also, the Fourier coefficients of the modal profile functions corresponding to the nth-Floquet-modes are given by

$$\begin{pmatrix} \mathbf{e}_y(0) \\ \mathbf{h}_x(0) \end{pmatrix} = \mathbf{Q}^{(s)} \mathbf{r}_n. \tag{17}$$

The propagation direction of each Floquet-mode can be judged as follows:

- if $|\beta_n| < 1$, the corresponding mode is the evanescent one propagating in the $+z$-direction.
- if $|\beta_n| > 1$, the corresponding mode is the evanescent one propagating in the $-z$-direction.
- if $|\beta_n| = 1$, the corresponding mode is the guided one. The modal power carried in the z-direction is calculated by $-\frac{w}{2}\Re(\mathbf{e}_y(0) \cdot \mathbf{h}_x(0)^*)$ where $\mathbf{e}_y(0)$ and $\mathbf{h}_x(0)$ are obtained by Eq. (17). If the modal power is positive (negative), the corresponding mode propagates in the $+z$ $(-z)$-direction.

3. LIMITATION ON NUMERICAL CALCULATION

Here, we show some results of a numerical experiment. The parameters of the photonic crystal are chosen as $\varepsilon_s = \varepsilon_0$, $\varepsilon_c = 12.25\varepsilon_0$, $d_x = d_z = 0.67\lambda_0$, and $a_x = a_z = \sqrt{0.41}d_x$. The rectangular cylinders are situated with the center at $x = (m - 1/2)\,d_x$ for positive integer m though one layer of cylinder array is removed at $x = 5.5d_x$ to form the waveguide structure, and $w = 11d_x$ is used for the periodic boundary condition. The numerical results are obtained by double precision computation, and the eigenvalues and eigenvectors of **F** are computed using the routine DEVCCG from IMSL Library, which is a commonly used routine. Figure 3 shows the normalized propagation constants of the guided Floquet-modes calculated by the present formulation as a function of the truncation order N. The photonic crystal waveguide with these parameters supports two guided modes, and Jia and Yasumoto [5] have calculated their normalized propagation constants η_n/k_d with $k_d = 2\pi/d_z$ as 0.415946 for the even-mode and 0.219867 for the odd-mode, though they did not mention the propagation direction. The obtained results converge to the values given in Ref. [5] though the value 0.415946 should be the normalized propagation constant of the even-mode propagating in the $-z$-direction. The results with $N = 68$ are ± 0.4165, ± 0.2127, and thought to be in a good agreement with the reference values.

It is worth noting that computation with truncation order $N = 50$ may be sufficiently accurate to characterize the photonic crystal devices of several wavelength dimension [10]. However, we are here interested
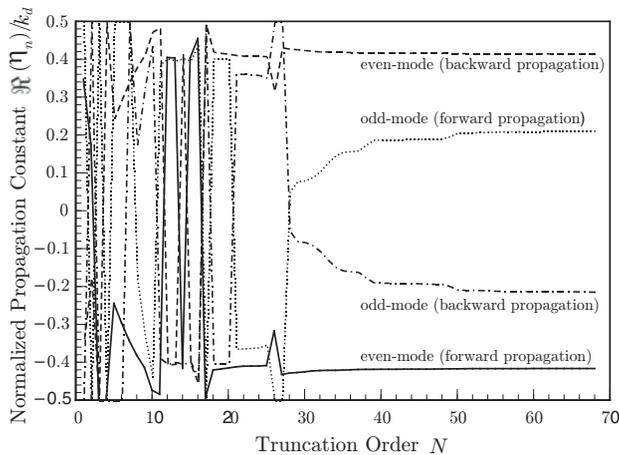

Figure 3. Convergence of the normalized propagation constants of the guided modes.
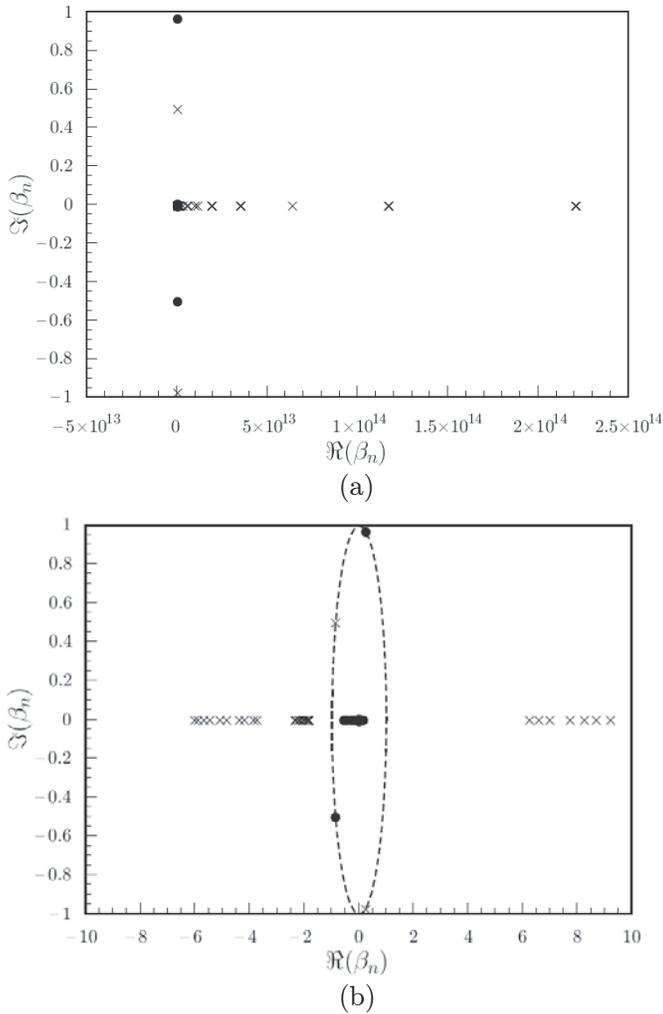
Figure 4. Distribution of the eigenvalues $\{\beta_n\}$ in the complex-plane, (a) whole view and (b) close view near the origin.

in the results that are more accurate. It is observed that the values in Fig. 3 are plotted for the truncation order $N \leq 68$ only. When N is larger than 68, we cannot find the guided modes and the number of Floquet-modes propagating in the $+z$-direction is not equal to that propagating in the $-z$-direction. This means that a precise calculation is impossible due to the limitation of truncation order. To consider the origin of difficulty, the obtained eigenvalues of the transfer matrix
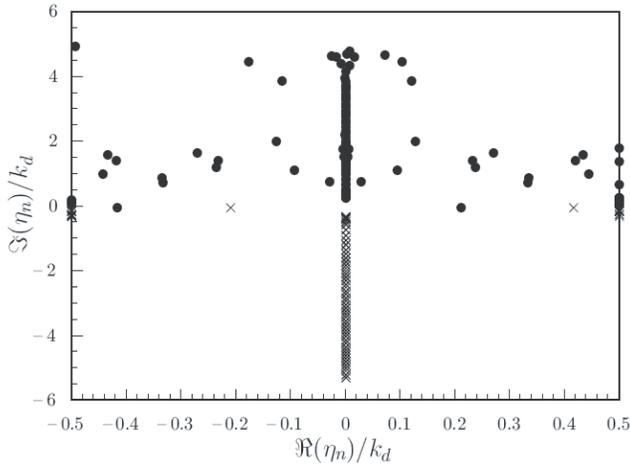
Figure 5. Distribution of the normalized propagation constants $\{\eta_n/k_d\}$ in the complex-plane.

$\mathbf{F}$ for $N = 60$ are plotted on the complex-plane in Fig. 4. The dots and the crosses denote the eigenvalues correspond to the Floquet-mode propagating in the $+z$- and the $-z$-directions, respectively. Fig. 4(b) is a close view near the origin and the dashed curve denotes a circle with a unit radius. The values on the dashed curve correspond to the guided modes, and those corresponding to the forward and the backward propagating modes are respectively distributed inside and outside the circle. A whole view is given in Fig. 4(a) and shows that the spectral radius of $\mathbf{F}$ (maximum absolute value of β_n) is about 2.2×10^{14}. This implies that the double precision computation leads to roundoff errors in the order of 10^{-2} and the obtained eigenvalues with $|\beta_n| \lesssim 10^{-2}$ may not be accurate. To show more clearly, we plot the calculated propagation constants $\{\eta_n\}$ on the complex-plane in Fig. 5. If η is a propagation constant of Floquet mode, $-\eta$ is also the propagation constant because of the structural symmetry. The distribution of $\{\eta_n\}$ should be therefore point symmetric to the origin. However, it is clearly observed in Fig. 5 that the distribution of calculated values is not point symmetric. The eigenvalues with $|\beta_n| < 10^{-2}$ correspond to the propagation constants with $\Im(\eta_n)/k_d > 0.73$ and the roundoff error is unnegligible in this region. The spectral radius of $\mathbf{F}$ becomes larger with the increase of the truncation order N, and the computation with $N > 68$ lead to significant errors for the guided modes and the evanescent modes with large $\Im(\eta_n)$.

4. NUMERICAL TECHNIQUES TO IMPROVE ACCURACY

4.1. Use of the Symmetry Properties

As mentioned in Section 3, the distribution of the propagation constants $\{\eta_n\}$ should be point symmetric to the origin due to the structural symmetry. However, it is clearly observed in Fig. 5 that the symmetry is broken by the roundoff error, which is unneglible for the propagation constants with large $\Im(\eta_n)$. This means that the calculated evanescent modes propagating in the $-z$-direction are more accurate than ones propagating in the $+z$-direction. The order of $\mathbf{F}$ is $4N + 2$, and the eigenvalues $\{\beta_n\}$ and the eigenvectors $\{\mathbf{r}_n\}$ are here supposed to be arranged in such a way that $\{\beta_n\}_{n=1}^{2N+1}$ and $\{\mathbf{r}_n\}_{n=1}^{2N+1}$ correspond to the Floquet-modes propagating in the $+z$-direction and $\{\beta_n\}_{n=2N+2}^{4N+2}$ and $\{\mathbf{r}_n\}_{n=2N+2}^{4N+2}$ correspond to ones propagating in the $-z$-direction. Also, let $\mathbf{R}_1$ and $\mathbf{R}_2$ be $(2N + 1) \times (2N + 1)$ square matrices defined by

$$\begin{pmatrix} \mathbf{R}_1 \\ \mathbf{R}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{r}_{2N+2} & \cdots & \mathbf{r}_{4N+2} \end{pmatrix}. \tag{18}$$

Then, when the error is negligible for the guided modes, more accurate results are obtained by replacing $\{\beta_n\}_{n=1}^{2N+1}$ and $\{\mathbf{r}_n\}_{n=1}^{2N+1}$ in the
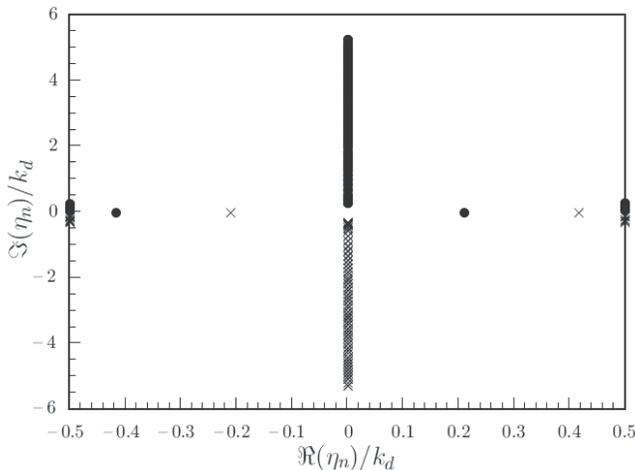

Figure 6. Distribution of the normalized propagation constants $\{\eta_n/k_d\}$ in the complex-plane.

following ways:

$$\eta_n = -\eta_{n+2N+1} \tag{19}$$

$$(\mathbf{r}_1 \quad \cdots \quad \mathbf{r}_{2N+1}) = \begin{pmatrix} \mathbf{R}_2 \\ \mathbf{R}_1 \end{pmatrix}, \tag{20}$$

where n in Eq. (19) is an integer $1 \leq n \leq 2N + 1$ and Eq. (20) is presented in [9]. Figure 6 shows the normalized propagation constants of the Floquet-modes that are computed for $N = 60$, and the constants corresponding to the Floquet-modes propagating in the $+z$-direction are obtained by Eqs. (19) and (20). As the result, if we calculate accurately the Floquet-modes corresponding to the values located in the lower half-plane, the other Floquet-modes are obtained by the symmetry property.

4.2. Use of the Rayleigh Quotients

We cannot avoid the roundoff errors in a finite precision computation, and the technique presented in the previous subsection is effective only when the error is negligible for the guided modes. Consequently, accurate computation with the truncation order $N > 68$ is still difficult. This subsection provides a technique to relieve this limitation.

As mentioned before, we use the routine DEVCCG from IMSL library to compute the eigenvalues and the associated eigenvectors of the transfer matrix $\mathbf{F}$. DEVCCG transforms a complex matrix to an upper Hessenberg matrix and use the QR algorithm to compute all of the eigenvalues and eigenvectors. Of course, the obtained eigenvalues and eigenvectors involve numerical errors, and there is a possibility that some more accurate values of eigenvalues are calculated by the Rayleigh quotients [12]. Since $\mathbf{r}_n$ denotes an obtained eigenvector of $\mathbf{F}$, the corresponding eigenvalue β_n is approximately given by

$$\beta_n = \frac{\mathbf{r}_n \cdot \mathbf{F} \mathbf{r}_n}{\mathbf{r}_n \cdot \mathbf{r}_n}. \tag{21}$$

Figure 7 shows the calculated values of normalized propagation constants $\{\eta_n/k_d\}$ for the truncation order $N = 75$. The results in Fig. 7(a) are from the eigenvalues obtained with the direct use of DEVCCG, and ones in Fig. 7(b) are from the eigenvalues obtained by Eq. (21). The spectral radius of $\mathbf{F}$ for $N = 75$ reaches to 1.5×10^{18}, and DEVCCG may yield the eigenvalues β_n with the roundoff errors in the order of 10^2. This eigenvalues $|\beta_n| < 10^2$ correspond to the normalized propagation constants with $\Im(\eta_n)/k_d > -0.73$ and, as shown in Fig. 7(a), the guided modes are no longer distinguished from
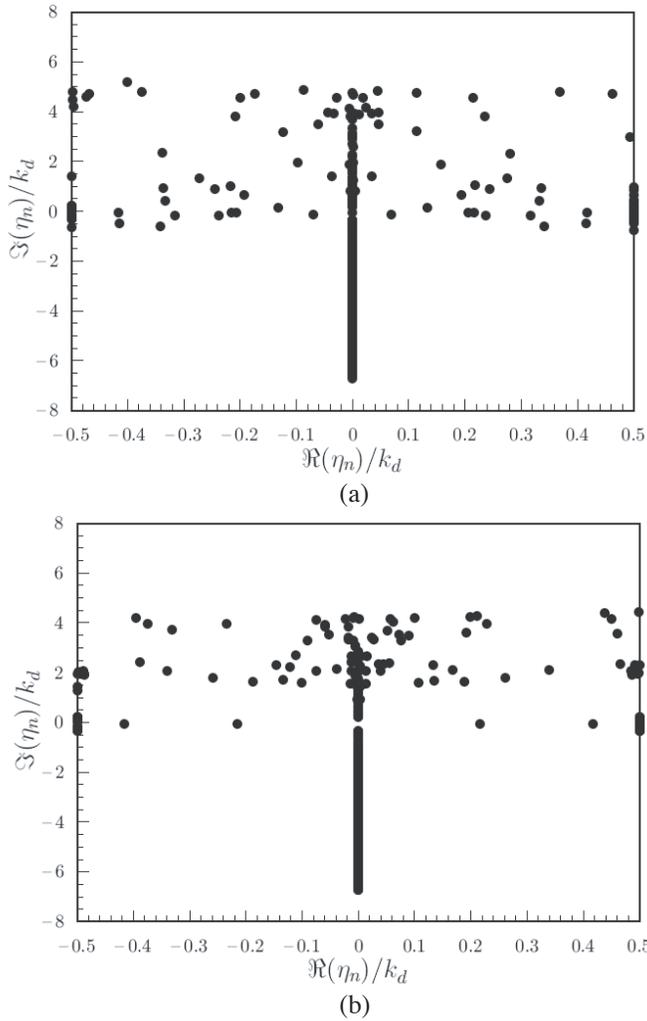
Figure 7. Distribution of the normalized propagation constants $\{\eta_n/k_d\}$ in the complex-plane. The eigenvalue computation is performed for $N = 75$ with the use of (a) the routine DEVCCG from IMSL library and (b) the Rayleigh quotients.

the evanescent ones. On the other hand, four guided modes are clearly distinguished in Fig. 7(b) though the values corresponding to the evanescent modes propagating in the $+z$-direction still have significant errors. The normalized propagation constants corresponding to the

guided modes given in Fig. 7(b) are ± 0.4162 for the even-modes and ± 0.2156 for the odd-modes, and they are surely in better agreement with the referred values than ones calculated with $N = 68$. The values located in the lower half-plane of Fig. 7(b) are sufficiently accurate, and the technique presented in the previous subsection should be available.

5. CONCLUSION

The Fourier series expansion method has been known as a powerful tool to analyze dielectric waveguide devices. We have dealt with an analysis of the Floquet-modes propagating in a photonic crystal waveguide, which are obtained from the eigenvalues of the transfer matrix for one periodicity cell. This approach provides sufficiently accurate results in many applications though this paper showed a limitation for highly accurate computation. The limitation comes from the eigenvalue calculation of the transfer matrix. Accurate computations with large truncation order should include evanescent modes with large attenuation constants, and the roundoff errors in finite precision computation limit the accuracy of calculated eigenvalues. This paper presented two techniques to relieve this limitation. When the Floquet-modes propagating in the $-z$-direction can be accurately calculated, ones propagating in the $+z$-direction, which always include larger numerical errors, can be accurately obtained with the use of the symmetry property. In addition, the Rayleigh quotients, which are calculated from the obtained eigenvectors, improve the accuracy of the eigenvalues. Unfortunately, the validities of these techniques are still limited, but they make us possible to perform analyses that are more accurate. This paper concentrates TE-polarized fields propagating in a two-dimensional photonic crystal waveguide consisting of rectangular cylinders, but the same difficulty exists in the analyses of TM-polarized fields or other photonic crystal waveguides.

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