Computing interior eigenvalues of nonsymmetric matrices: Application to three-dimensional metamaterial composites

Takamichi Terao

Department of Mathematical and Design Engineering, Gifu University, Gifu 501-1193, Japan (Received 18 May 2010; published 6 August 2010)

We propose a numerical method to calculate interior eigenvalues and corresponding eigenvectors for nonsymmetric matrices. Based on the subspace projection technique onto expanded Ritz subspace, it becomes possible to obtain eigenvalues and eigenvectors with sufficiently high precision. This method overcomes the difficulties of the traditional nonsymmetric Lanczos algorithm, and improves the accuracy of the obtained interior eigenvalues and eigenvectors. Using this algorithm, we investigate three-dimensional metamaterial composites consisting of positive and negative refractive index materials, and it is demonstrated that the finite-difference frequency-domain algorithm is applicable to analyze these metamaterial composites.

DOI: [10.1103/PhysRevE.82.026702](http://dx.doi.org/10.1103/PhysRevE.82.026702)

PACS number(s): 02.60 .Dc, 42.70 . - a, 78.67 .Pt

I. INTRODUCTION

The photonic properties of metamaterials in which the refractive index becomes negative have attracted much attention $\lceil 1-5 \rceil$ $\lceil 1-5 \rceil$ $\lceil 1-5 \rceil$. Wave propagation in these metamaterials shows many characteristic features, and various photonic devices have been proposed such as a perfect lens $[5]$ $[5]$ $[5]$. For example, one-dimensional stacking of alternating layers of positive and negative index materials has been studied by several groups $[6-8]$ $[6-8]$ $[6-8]$. Li *et al.* have shown that a new type of photonic gap appears when the volume averaged effective refractive index equals zero in such material composites $\lceil 6 \rceil$ $\lceil 6 \rceil$ $\lceil 6 \rceil$. Analysis of the photonic properties of three-dimensional metamaterials is of great interest $[9,10]$ $[9,10]$ $[9,10]$ $[9,10]$.

In general, the analysis of electromagnetic wave propagation in the medium leads to eigenvalue problems. Most numerical methods for large-scale eigenvalue analysis such as the Lanczos and Arnordi methods are based on the technique of Krylov subspace projection $[11]$ $[11]$ $[11]$. The subspace is spanned by a series of vectors $\{x_0, Ax_0, A^2, x_0, ...\}$, where **A** is a coefficient matrix of the eigenvalue problem and x_0 is an arbitrary vector. Such numerical techniques are more adapted for eigenvalue analysis with the maximum eigenvalue because the direction of vector A^n x_0 with sufficiently large *n* comes close asymptotically to that of the eigenvector, which belongs to the maximum eigenvalue of matrix **A**. Based on Krylov subspace projection, the numerical method referred to as the nonsymmetric Lanczos (NLZ) algorithm has been also proposed to obtain interior eigenvalues $[12]$ $[12]$ $[12]$. However, this numerical approach is not applicable to nonsymmetric matrices for which the dimension is large, because the accuracy of obtained eigenvalues and corresponding eigenvectors is lost.

We propose herein a new numerical method for interior eigenvalue analysis. This method is especially suitable to large-scale eigenvalue calculations for nonsymmetric matrices, and is applicable to problems with complex, non-Hermitian matrices. This method is based on the novel subspace projection technique, and using this method we numerically study the photonic properties of electromagnetic waves in three-dimensional metamaterial composites by the finite-difference frequency-domain (FDFD) method.

In Sec. [II,](#page-0-0) we briefly describe the FDFD method. In Sec. [III,](#page-1-0) we present details of the numerical method for interior eigenvalue analysis of nonsymmetric matrices. Section [IV](#page-2-0) presents calculated results for three-dimensional metamaterial composites by this algorithm. Conclusions are given in Sec. [V.](#page-3-0)

II. FINITE-DIFFERENCE FREQUENCY-DOMAIN METHOD

In previous theoretical studies of photonic materials, calculations by the plane-wave expansion (PWE) method or the finite-difference time-domain (FDTD) method have been performed [[13,](#page-4-8)[14](#page-4-9)]. The PWE method proposed by Ho *et al.* was formulated for a system in which the relative permeability is equal to unity, and is not directly applicable to metamaterials when the permeability of the system becomes negative $\lceil 13 \rceil$ $\lceil 13 \rceil$ $\lceil 13 \rceil$. In this study, we instead employed the FDFD method, which has not been referred to in previous studies, with just a few exceptions $[15,16]$ $[15,16]$ $[15,16]$ $[15,16]$. In the FDFD method, it becomes much easier to separate the adjacent eigenfrequencies. In addition, calculated results are not negatively affected by the spectral noise that often appears in calculations using time-domain techniques $\lceil 15 \rceil$ $\lceil 15 \rceil$ $\lceil 15 \rceil$.

Another reason to adopt the FDFD method in photonic metamaterials is as follows: In the FDTD method, numerical treatment of dispersive mediums such as PLRC algorithm has been proposed $[14,17]$ $[14,17]$ $[14,17]$ $[14,17]$, but in general the function forms regarding permittivity and permeability of the system are limited. Negative refractive index materials are fabricated in experiments, and the permittivity and permeability of these materials have been shown to be dispersive, where the frequency dependence in general cannot be written using simple function forms. In the FDFD method, there is no limitation to the frequency dependence of the dispersive medium, and there is an advantage to analyzing numerically negative refractive index materials in which the frequency dependence of the refractive index obeys more general conditions.

In this section, the outline of the FDFD method is briefly described. We begin with the Maxwell equations written by

$$
\text{rot } \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \quad \text{rot } \mathbf{H} = \mathbf{j} + \frac{\partial \mathbf{D}}{\partial t}, \tag{1}
$$

where **E** and **H** denote the electric field and the magnetic field, respectively. For a given wave vector **k**, all the referred components outside the unit cell boundary can be obtained using Bloch's periodic boundary condition such as

$$
\mathbf{E}(\mathbf{r} + \mathbf{R}) = \exp(i\mathbf{k} \cdot \mathbf{R})\mathbf{E}(\mathbf{r})
$$
 (2)

and

$$
H(r + R) = exp(ik \cdot R)H(r),
$$
 (3)

where **R** is an arbitrary lattice vector in the unit cell. Thus, we can obtain the dispersion relation, which indicates the resonance frequency as a function of **k**. The system in the unit cell is divided into *Yee cells* to apply to the FDFD method [[14](#page-4-9)]. Using the substitution $\frac{\partial}{\partial t}$ → −*i*ω and the condition of the current density $\mathbf{j} = 0$, Eqs. (1) (1) (1) – (3) (3) (3) are transformed into an eigenvalue problem, which is used to compute interior eigenvalues of large and sparse non-Hermitian matrices. In this study, there are $4n³$ physically meaningful eigenfrequencies when the number of divided mesh on each side is *n*, and there are also $2n³$ nonphysical eigenvalues that are degenerated at zero. It is difficult to solve these problems numerically by existing methods, and a computational method for nonsymmetric eigenvalue problems is therefore required. In the next section, we describe the details of our numerical method that is especially suitable for this purpose.

III. LARGE-SCALE EIGENVALUE PROBLEM FOR NONSYMMETRIC MATRICES

We first explain Lanczos biorthogonalization (two-sided Lanczos recursion) procedures in the eigenvalue problem for nonsymmetric or non-Hermitian matrix **A** written by

$$
Ax = \lambda x, \tag{4}
$$

where λ and **x** are the eigenvalue and eigenvector, respec-tively [[11](#page-4-6)[,12](#page-4-7)]. We start with $v_0 = 0$, $w_0 = 0$, and $\beta_1 = 0$. Let v_1 and w_1 be arbitrary vectors that satisfy $(w_1, v_1) = 1$, and we choose the vector \mathbf{w}_1 such as $\mathbf{w}_1 = \mathbf{v}_1^*$. For $j = 1, 2, ..., m$, we use the following recursions to define Lanczos vectors \mathbf{v}_i and **w***^j* such that

$$
\hat{\mathbf{v}}_{j+1} = \mathbf{A}\mathbf{v}_j - \alpha_j \mathbf{v}_j - \beta_j \mathbf{v}_{j-1} \tag{5}
$$

$$
\hat{\mathbf{w}}_{j+1} = \mathbf{A}^* \mathbf{w}_j - \alpha_j \mathbf{w}_j - \beta_j \mathbf{w}_{j-1},
$$
\n(6)

where $\{v_i\}$, $\{w_i\}$, $\{\alpha_i\}$, and $\{\beta_i\}$ are given by

$$
\alpha_j = (\mathbf{w}_j, \mathbf{A}\mathbf{v}_j),\tag{7}
$$

$$
\beta_{j+1} = (\hat{\mathbf{w}}_{j+1}, \hat{\mathbf{v}}_{j+1})^{1/2},\tag{8}
$$

$$
\mathbf{v}_{j+1} = \hat{\mathbf{v}}_{j+1} / \beta_{j+1},\tag{9}
$$

and

$$
\mathbf{w}_{j+1} = \hat{\mathbf{w}}_{j+1} / \beta_{j+1},\tag{10}
$$

respectively [[11](#page-4-6)[,12](#page-4-7)[,18](#page-4-13)]. Here the sets of vectors V_m $\mathbf{v} = \{ \mathbf{v}_1, \dots, \mathbf{v}_m \}$ and $\mathbf{W}_m \equiv \{ \mathbf{w}_1, \dots, \mathbf{w}_m \}$ are biorthogonal to

each other such as $(\mathbf{w}_i, \mathbf{v}_j) = \delta_{i,j}$. Using the recursion relation in Eqs. ([5](#page-1-3)) and ([6](#page-1-4)), the tridiagonal matrix \mathbf{T}_m is defined by the scalars $\{\alpha_i\}$ and $\{\beta_i\}$ such as

$$
\mathbf{T}_{m} = \begin{pmatrix} \alpha_{1} & \beta_{2} & & & \\ \beta_{2} & \alpha_{2} & \beta_{3} & & \\ & & \ddots & & \\ & & & \beta_{m-1} & \alpha_{m-1} & \beta_{m} \\ & & & & \beta_{m} & \alpha_{m} \end{pmatrix}, \qquad (11)
$$

where α_i and β_i are in general complex, and the tridiagonal matrix \mathbf{T}_m is non-Hermitian. Consider the eigenvalue problem for the tridiagonal matrix \mathbf{T}_m written by

$$
\mathbf{T}_m \mathbf{y}_j = \theta_j \mathbf{y}_j \quad (1 \le j \le m), \tag{12}
$$

where θ_i and \mathbf{y}_i are the eigenvalues and eigenvectors of the matrix \mathbf{T}_m , respectively. Thus, the set of Ritz vectors \mathbf{X}_m $\equiv \{x_1, \ldots, x_m\}$, which are the approximate solutions of the right eigenvectors in Eq. (4) (4) (4) , are given by

$$
\mathbf{X}_m \equiv \mathbf{V}_m \mathbf{Y}_m,\tag{13}
$$

where $Y_m \equiv \{y_1, \ldots, y_m\}$ is the set of eigenvectors in Eq. $(12).$ $(12).$ $(12).$

To calculate the interior eigenvalues for large-scale eigenvalue problems, Cullum and Willoughby have proposed a Lanczos algorithm without reorthogonalization $\lceil 12,19 \rceil$ $\lceil 12,19 \rceil$ $\lceil 12,19 \rceil$ $\lceil 12,19 \rceil$. In their algorithm, the dimension of the tridiagonal matrix T_m is taken to be $3N \sim 5N$, and the eigenvalues are obtained by eliminating spurious solutions. For symmetrical matrices, this algorithm is very efficient and has already been applied to many problems in computational physics $\lceil 20-22 \rceil$ $\lceil 20-22 \rceil$ $\lceil 20-22 \rceil$. Elsner *et al.* have performed a comparative study of modern eigenvalue algorithms for large-scale symmetric matrices $[23]$ $[23]$ $[23]$. For non-Hermitian matrices, however, the accuracy of the eigenvalue obtained by this approach deteriorates seriously, when the dimension of the matrix is large. As a result, it becomes difficult to distinguish correct eigenvalues from spurious solutions. In past studies regarding the nonsymmetric Lanczos method, the dimensions of the matrix *N* have been small such as $N < 10^4$ [[12](#page-4-7)], and there has been no systematic way of improving the accuracy of obtained interior eigenvalues and eigenvectors for large-scale eigenvalue problems.

In many scientific computations, it is often the case that only the *right* eigenvectors (and corresponding eigenvalues) are required. In this case, you can save the computation time if you do not need to explicitly calculate "Ritz vectors" for the left eigenvectors. In the following, we describe a numerical method for obtaining eigenvalues and right eigenvectors. The extension of our method to the calculation of left eigenvectors is straightforward and presents no difficulties. We consider the subspace, which is composed of the set of Ritz vectors and is obtained by the Lanczos biorthogonalization procedures. As described above, the Ritz vectors obtained from Eq. ([13](#page-1-7)) do not give good approximations of the solutions for nonsymmetric matrices, especially for large-scale eigenvalue problems. However, each Ritz vector may have a nonzero projection over the true eigenvector, and a subspace spanned by this set of Ritz vectors is useful for obtaining correct eigenvectors. The set of m_1 Ritz vectors $\{x_i\}$ for

$$
\mathbf{A}'_{m_1} = \mathbf{X}^{\prime *}_{m_1} \mathbf{A} \mathbf{X}'_{m_1},\tag{14}
$$

where X'_{m_1} is a matrix consisting of the orthonormalized Ritz vectors \mathbf{x}'_i ($1 \le i \le m_1$) given by $\mathbf{X}'_{m_1} = {\mathbf{x}'_1, ..., \mathbf{x}'_{m_1}}$. In principle, the approximate solution of the eigenvalues near the target and the corresponding eigenvectors of matrix **A** can be obtained from Eq. (14) (14) (14) .

In many cases, however, Eq. (14) (14) (14) does not give sufficiently accurate solutions. One way to improve the accuracy of calculated results is to make the dimension of subspace for projection much larger. In the following, we expand the subspace by the following procedures: Starting with different sets of initial vectors \mathbf{v}_1 and \mathbf{w}_1 , we perform the calculations of Lanczos biorthogonalization, and calculate again the Ritz values near the target and corresponding Ritz vectors. After the repetition of these procedures, we obtain the assembly of $(m_1+m_2+\cdots+m_q)$ vectors such as $\{ \mathbf{x}_1, \ldots, \mathbf{x}_{m_1}, \mathbf{x}_{m_1+1}, \ldots, \mathbf{x}_{m_1+m_2}, \mathbf{x}_{m_1+m_2+1}, \ldots, \mathbf{x}_{m_1+m_2+\cdots+m_q} \}$ where q denotes the degree of expansion of the subspace, and m_p ($1 \leq p \leq q$) is the number of Ritz vectors obtained by the *p*-th Lanczos biorthogonalization procedure. We construct a matrix $\mathbf{X}'_{\{m_p\}}$ from the set of $\{\mathbf{x}'_i\}$, the orthonormalized vectors of $\{x_i\}$, such as

$$
\mathbf{X}'_{\{m_p\}} \equiv \{ \mathbf{x}'_1, \dots, \mathbf{x}'_{m_1}, \mathbf{x}'_{m_1+1}, \dots, \mathbf{x}'_{m_1+m_2}, \mathbf{x}'_{m_1+m_2+1},
$$

$$
\dots, \mathbf{x}'_{m_1+m_2+\dots+m_q} \}.
$$
(15)

Next, we construct the matrix \mathbf{A}'_{m} given by

$$
\mathbf{A}'_{\{m_p\}} = \mathbf{X}'^{\ast}_{\{m_p\}} \mathbf{A} \mathbf{X}'_{\{m_p\}},\tag{16}
$$

for the projection onto the expanded Ritz subspace. In the following, we call such a subspace spanned by the vectors in Eq. ([15](#page-2-2)) an *expanded Ritz subspace* (ERS). The eigenvalues can be obtained by the diagonalization of matrix A'_{m} in Eq. (16) (16) (16) such as

$$
\mathbf{A}'_{\{m_p\}}\mathbf{y}'_j = \theta'_j\mathbf{y}'_j,\tag{17}
$$

where θ'_j and \mathbf{y}'_j are the eigenvalues and eigenvectors of $\mathbf{A}'_{\{m_n\}}$, respectively.

As a next step, we group the obtained eigenvalues $\{\theta'_j\}$ of matrix $\mathbf{A}'_{\{m_p\}}$ which satisfy $|\theta'_j - \lambda'| < \varepsilon$ (ε is a small constant), where λ' is a target. Using the corresponding vectors $\{y'_j\}$ in Eq. ([17](#page-2-4)), we calculate the set of vectors $\{x'_j\}$ given by

$$
\mathbf{X}'_{\{m_p\}} \equiv \mathbf{V}_m \mathbf{Y}'_{\{m_p\}}\tag{18}
$$

where $\mathbf{X}'_{\{m_p\}}$ and $\mathbf{Y}'_{\{m_p\}}$ are the matrices written by $\mathbf{X}'_{\{m_p\}}$ $\mathbf{X}_{m_1}^{\prime}, \dots, \mathbf{X}_{m_1 + \dots + m_q}^{\prime}$ and $\mathbf{Y}_{\{m_p\}}^{\prime} \equiv \{\mathbf{y}_1^{\prime}, \dots, \mathbf{y}_{m_1 + \dots + m_q}^{\prime}\}$, respectively. For these obtained vectors \mathbf{x}'_j , we calculate the norm of residual vector δ_i given by

$$
\delta_j \equiv |\mathbf{A}\mathbf{x}_j' - \theta_j' \mathbf{x}_j'|,\tag{19}
$$

where the norm of each vector \mathbf{x}'_j is normalized, such as $|\mathbf{x}'_j| = 1$. From this set of θ'_j and \mathbf{x}'_j , we choose one for which the norm of residue δ_i becomes the smallest as an eigenvalue and an eigenvector of matrix **A**, respectively. This numerical procedure improves the accuracy of the obtained eigenvalues and eigenvectors for the nonsymmetric matrix. In Eq. (15) (15) (15) , the parameter *q* determines the expansion of subspace for convergence, where the optimal value of *q* may depend on the properties of matrix **A**. Our method provides a systematic way of improving the accuracy of interior eigenvalues and eigenvectors by means of the Lanczos algorithm without reorthogonalization for nonsymmetric matrices $[12]$ $[12]$ $[12]$.

IV. NUMERICAL RESULTS

We numerically studied the three-dimensional metamaterial composites by the FDFD method. In this study, we considered the case in which both the permittivity and permeability of the system simultaneously take negative values, and these two quantities are frequency independent. The numerical treatment of frequency-dependent negative refractive index materials will be described in the latter part of this section.

Consider a cubic cell with system size L ($0 \le x, y, z \le L$), with periodic boundary conditions being imposed in *x*, *y*, and *z* directions. We consider the system for which the relative permittivity $\varepsilon_r(\mathbf{r})$ and relative permeability $\mu_r(\mathbf{r})$ of the system are given by

$$
\varepsilon_r(\mathbf{r}) = \begin{cases} \varepsilon_r^p & (0 \le x < L/2) \\ \varepsilon_r^n & (L/2 \le x < L) \end{cases} \tag{20}
$$

and

$$
\mu_r(\mathbf{r}) = \begin{cases} \mu_r^p & (0 \le x < L/2) \\ \mu_r^n & (L/2 \le x < L) \end{cases} \tag{21}
$$

respectively.

We first calculate the eigenvalues of a matrix $[Eq. (4)]$ $[Eq. (4)]$ $[Eq. (4)]$ with smaller dimensions, to clarify the characteristics of the eigenvalue distribution in a complex plane. The dimension of the matrix is taken to be *N*= 24 576, and all eigenvalues are calculated by the QR method $[11]$ $[11]$ $[11]$. In positive refractive index material, the relative permittivity ε_r^p and the relative permeability μ_r^p are taken to be $(\varepsilon_r^p, \mu_r^p) = (1, 1)$. In negative refractive index material, we consider three different sets of relative permittivity ε_r^n and the relative permeability μ_r^n . Figures $1(a)-1(c)$ $1(a)-1(c)$ show the results of all eigenvalues with parameters $(e_r^n, \mu_r^n) = (-0.3, -0.3), (-0.8, -0.8),$ and $(-1.3,$ -1.3 -1.3), respectively. The wave vector **k** in Eqs. ([2](#page-1-8)) and (3) is taken to be $\mathbf{k} = (0, 0, 0)$. In these figures, the eigenvalues appear not only on the real axis but also all over the complex plane. This result is of interest because the refractive indices on each material $(\sqrt{\epsilon_r^p \mu_r^p})$ and $\sqrt{\epsilon_r^p \mu_r^p}$ are real and the optical attenuation effect is not considered. This is a characteristic feature in composite metamaterials with a positive and negative refractive index, and Fig. [1](#page-3-1) also suggests that it is diffi-

FIG. 1. Eigenvalue distribution with *N*= 24 576. The relative permittivity ε_r^p and the relative permeability μ_r^p in positive refractive index material are taken to be $(\varepsilon_r^p, \mu_r^p) = (1, 1)$. (a) The relative permittivity ε_r^p and the relative permeability μ_r^p in negative refractive index material are taken to be $(\varepsilon_r^n, \mu_r^n)$ = (-0.3, -0.3). (b) $(eⁿ, \muⁿ_r) = (-0.8, -0.8)$. (c) $(eⁿ, \muⁿ_r) = (-1.3, -1.3)$.

cult to numerically treat the optical properties on these composite metamaterials by the traditional FDTD method. Instead, the FDFD method described in Sec. [II](#page-0-0) will become an alternative approach to this problem.

Next, we apply the numerical method using ERS projection described in Sec. [III](#page-1-0) to the problem of metamaterial composites. We calculate the eigenvalues and eigenvectors of the matrix in Eq. (4) (4) (4) with the dimension $N=196,608$ and *N*= 279, 936, where it is impossible to calculate the eigenvalues of these matrices by traditional diagonalization techniques such as the QR method. The sets of the relative permittivity and the relative permeability are taken to be $(e_r^p, \mu_r^p) = (1, 1)$ and $(e_r^p, \mu_r^p) = (-0.3, -0.3)$, and the wave vector **k** is given by $\mathbf{k} = (k_0 \pi / L, k_0 \pi / L, k_0 \pi / L)$, where k_0 is a constant. We first calculate the eigenvalues of the system by the traditional NLZ method $\lceil 12 \rceil$ $\lceil 12 \rceil$ $\lceil 12 \rceil$. In the following calculations, the dimension of tridiagonal matrix \mathbf{T}_m is taken to be 4*N*. Calculated results of the eigenvalues θ'_j which are located adjacent to the real axis in the low-frequency regime $(0 \leq \theta'_j \leq 1)$, and their norms of residue vectors δ_j are shown in Table [I.](#page-4-14) It is clear that the calculated values of δ_i obtained by the NLZ method become larger than 10−1. Though we confirm that such an NLZ method produces accurate results when the dimension of matrix *N* is smaller than a few thousand, the results in Table [I](#page-4-14) indicate that the traditional NLZ method is impractical for a large-scale nonsymmetric eigenvalue problem.

We calculate the eigenvalues of matrix by means of the ERS projection method. Calculated eigenvalues θ'_j of the matrix $\mathbf{A}'_{\{m_p\}}$ in Eq. ([17](#page-2-4)) and the norms of the corresponding residue vector δ_i are shown in Table [I.](#page-4-14) The typical CPU time for calculating eigenvalues for *N*= 279 936 is approximately 40 h with an Itanium 1.6 GHz processor. With *q*= 1, the accuracy of the obtained eigenvalues and eigenvectors is not yet sufficient. Though it is not shown in Table [I,](#page-4-14) the calculated results produce not only the approximation of eigenvalues but also many spurious solutions, and the screening out of these spurious solutions becomes difficult when the accuracy of the obtained eigenvectors is not good enough. (In Table [I,](#page-4-14) we display, for convenience sake, the solutions only which will be clarified as genuine eigenvalues in the subsequent stage.) Compared with previous results by the NLZ method, the accuracy of the results is improved, and the eigenvalues and eigenvectors are reliable for nonsymmetric matrices with large dimension. With $q=2$, the accuracy of the eigenvalues obtained by the ERS projection method obviously improves, and we can confirm the efficiency of the subspace expansion approach in this method.

Finally, we comment on the numerical treatment of dispersive medium by the FDFD method. Instead of Eqs. (20) (20) (20) and ([21](#page-2-6)), we consider the frequency-dependent relative permittivity $\varepsilon_r^n(\omega)$ and the relative permeability $\mu_r^n(\omega)$ of the system $\lceil 3 \rceil$ $\lceil 3 \rceil$ $\lceil 3 \rceil$. We first calculate the eigenfrequencies by the ERS projection method using the parameters $\varepsilon_r^n(\omega)$ and $\mu_r^n(\omega)$ at a target frequency. We then recalculate the eigenfrequencies using the parameters with the frequency obtained in the previous stage. After repeating these procedures several times, self-consistent solutions can be found in dispersive medium. For example, four iterations are required to obtain an eigenfrequency to 5 digits in our calculations.

V. CONCLUSIONS

In conclusion, we have studied the properties of threedimensional metamaterial composites consisting of positive

\boldsymbol{N}	k_0	Method	q	θ_i'	δ_i
196608	0.2	NLZ		$(0.56688467, -0.00485904)$	2.1×10^{0}
	0.2	N _{LZ}		$(0.57192020, -0.00006070)$	4.7×10^{-1}
	0.2	N _L Z		(0.57363302, 0.00042317)	1.2×10^{-1}
	0.2	N _L Z		$(0.83231659, -0.00205953)$	6.6×10^{-1}
	0.2	N _L Z		(0.88738888, 0.00267784)	5.4×10^{0}
	0.2	ERS	1	$(0.57369594, -0.00000009)$	5.1×10^{-6}
	0.2	ERS	1	$(0.83285874, -0.00000323)$	4.6×10^{-4}
	0.2	ERS	2	$(0.57369616, -0.00000001)$	3.9×10^{-6}
	0.2	ERS	2	$(0.83285863, -0.00000001)$	2.2×10^{-6}
279936	0.1	ERS	2	$(0.36362658, -0.00000004)$	2.5×10^{-6}
	0.1	ERS	2	$(0.45072961, -0.00000024)$	3.4×10^{-5}
	0.2	ERS	2	(0.57361000, 0.00000000)	3.8×10^{-7}
	0.2	ERS	2	$(0.80838517, -0.00000004)$	1.3×10^{-5}

TABLE I. Calculated results of eigenvalues in three-dimensional metamaterial composites by the nonsymmetric Lanczos (NLZ) method and the expanded Ritz subspace (ERS) method.

and negative refractive index materials. We have studied the eigenvalue spectrum of these systems for given wave vectors **k**, and it has been clarified that characteristic absorption modes appear in the metamaterial composites. The present results demonstrate that the FDFD algorithm is suitable for analyzing the photonic properties of these metamaterial composites.

We have also proposed a numerical method for obtaining interior eigenvalues and corresponding eigenvectors for nonsymmetric matrices. Based on the subspace projection technique onto expanded Ritz subspace, it becomes possible to obtain the set of eigenvalues and eigenvectors with sufficiently high precision. Our method overcomes the difficulties of the NLZ algorithm, in which the accuracy of the obtained eigenvalue is destroyed when the dimension of the matrices becomes large. In addition, we show a systematic way of making further improvements in accuracy to obtain interior eigenvalues and eigenvectors for the Lanczos algorithm without reorthogonalization. This numerical method is applicable to not only electromagnetics but also to any large-scale eigenvalue problems, and will also shed light on different problems in the field of computational physics and engineering.

ACKNOWLEDGMENTS

The author acknowledges the Research Center for Computational Science, Okazaki, Japan, for the use of their facilities. This work was supported in part by a Grant-in-Aid from the Japan Ministry of Education, Science, Sports, and Culture for Scientific Research.

- [1] V. G. Veselago, [Sov. Phys. Usp.](http://dx.doi.org/10.1070/PU1968v010n04ABEH003699) **10**, 509 (1968).
- [2] S. A. Ramakrishna, [Rep. Prog. Phys.](http://dx.doi.org/10.1088/0034-4885/68/2/R06) 68, 449 (2005).
- 3 R. A. Shelby, D. R. Smith, and S. Schultz, [Science](http://dx.doi.org/10.1126/science.1058847) **292**, 77 $(2001).$ $(2001).$ $(2001).$
- [4] V. M. Shalaev, [Nat. Photonics](http://dx.doi.org/10.1038/nphoton.2006.49) 1, 41 (2007).
- [5] J. B. Pendry, *[Phys. Rev. Lett.](http://dx.doi.org/10.1103/PhysRevLett.85.3966)* **85**, 3966 (2000).
- 6 J. Li, L. Zhou, C. T. Chan, and P. Sheng, [Phys. Rev. Lett.](http://dx.doi.org/10.1103/PhysRevLett.90.083901) **90**, [083901](http://dx.doi.org/10.1103/PhysRevLett.90.083901) (2003).
- [7] H. Daninthe, S. Foteinopoulou, and C. M. Soukoulis, [Photon](http://dx.doi.org/10.1016/j.photonics.2006.01.001)[ics Nanostruct. Fundam. Appl.](http://dx.doi.org/10.1016/j.photonics.2006.01.001) 4, 123 (2006).
- [8] A. A. Asatryan, L. C. Botten, M. A. Byrne, V. D. Freilikher, S. A. Gredeskul, I. V. Shadrivov, R. C. McPhedran, and Y. S. Kivshar, *[Phys. Rev. Lett.](http://dx.doi.org/10.1103/PhysRevLett.99.193902)* 99, 193902 (2007).
- 9 J. Valentine, S. Zhang, T. Zentgraf, E. Ulin-Avila, D. A. Genov, G. Bartal, and X. Zhang, Nature ([London](http://dx.doi.org/10.1038/nature07247)) 455, 376 $(2008).$ $(2008).$ $(2008).$
- [10] N. Liu, H. Guo, L. Fu, S. Kaiser, H. Schweizer, and H. Gies-sen, [Nature Mater.](http://dx.doi.org/10.1038/nmat2072) 7, 31 (2008).
- [11] F. Chatelin, *Eigenvalues of Matrices* (Wiley, New York, 1993).
- [12] Large-scale Eigenvalue Problem: Proceedings of the IBM Europe Institute Workshop on Large Scale Eigenvalue Problems, edited by J. Cullum and R. A. Willoughby (North-Holland, Amsterdam, 1986).
- [13] K. M. Ho, C. T. Chan, and C. M. Soukoulis, *[Phys. Rev. Lett.](http://dx.doi.org/10.1103/PhysRevLett.65.3152)* 65[, 3152](http://dx.doi.org/10.1103/PhysRevLett.65.3152) (1990).
- [14] A. Taflove and S. C. Hagness, *Computational Electrodynamics: The Finite-Difference Time-Domain Method*, 3rd ed. (Artech House, Boston, 2005).
- 15 S. Guo, F. Wu, S. Albin, and R. Rogowski, [Opt. Express](http://dx.doi.org/10.1364/OPEX.12.001741) **12**, [1741](http://dx.doi.org/10.1364/OPEX.12.001741) (2004).
- 16 S. G. Johnson and J. D. Joannopoulos, [Opt. Express](http://dx.doi.org/10.1364/OE.8.000173) **8**, 173 $(2001).$ $(2001).$ $(2001).$
- [17] D. F. Kelley and R. J. Luebbers, [IEEE Trans. Antennas Propag.](http://dx.doi.org/10.1109/8.509882) 44[, 792](http://dx.doi.org/10.1109/8.509882) (1996).
- 18 Y. Saad, *Iterative Methods for Sparse Linear Systems*, 2nd ed. (SIAM, Philadelphia, 2003).
- 19 J. K. Cullum and R. A. Willoughby, *Lanczos Algorithms for Large Symmetric Eigenvalue Computations, Vol. 1, Theory* (Birkhauser, Boston, 1985).
- 20 Th. Koslowski and W. von Niessen, [Phys. Rev. B](http://dx.doi.org/10.1103/PhysRevB.42.10342) **42**, 10342 $(1990).$ $(1990).$ $(1990).$
- 21 M. Schreiber and H. Grussbach, [Phys. Rev. Lett.](http://dx.doi.org/10.1103/PhysRevLett.67.607) **67**, 607 $(1991).$ $(1991).$ $(1991).$
- [22] T. Terao, *[Phys. Rev. B](http://dx.doi.org/10.1103/PhysRevB.56.975)* **56**, 975 (1997).
- 23 U. Elsner, V. Mehrmann, F. Milde, R. A. Römer, and M. Schreiber, [SIAM J. Sci. Comput.](http://dx.doi.org/10.1137/S1064827598332217) **20**, 2089 (1999).