A new computing approach to problem of vibrational electromagnetic modes in one-dimensional photonic crystals with defects

Yury K Timoshenko, Sergey Yu Savchenko, and Yuri V Smirnov
Voronezh State University, Universitetskaya pl., 1, Voronezh, 394006, Russia
E-mail: yutim@phys.vsu.ru

Abstract. In this paper we describe new algorithm of calculating total density of electromagnetic states in one-dimensional photonic dielectric crystals. Our algorithm do not use unitary transformations and have low computational complexity. We are implemented it on Fortran in sequential and parallel variants.

1. Introduction

The position of the stop zones in the photon zone structure provides important information for both fundamental science and applied disciplines related to photonics [1, 2]. One of the ways to obtain data on stop zones is a computer simulation of the total density of electromagnetic states (TDES) in a photonic crystal. The standard approach to calculating TDES is connected with calculating the dispersion curves $\omega_n(k), \forall k \in BZ$, where $\omega$ is frequency of stationary oscillatory/vibrational mode, $k$ is the wave vector, $BZ$ is Brillouin's first band, $n$ is band number. To calculate $\omega_n(k)$, the plane-wave method (PWM) is often used. This method has many variants. One of the latest presented in [3] takes polariton effects into account. However, in most works that use PWM, mathematical models of photonic crystals with a frequency-independent dielectric constant [1, 2] are considered. This allows, within the framework of the PWM, to reduce the problem of determining $\omega_n(k)$ from the Helmholtz wave equation to the solution of the generalized algebraic eigenvalue problem for complex Hermitian matrices of large dimension using unitary transformations.

It should be noted that the use of unitary transformations to solve the algebraic eigenvalue problem for various reasons is not always convenient and other numerical approaches are used to calculate the distribution of eigenvalues and individual eigenvalues. In [4], for instance, they suggest three alternative methods for calculating total density of polar nanocrystals’ electronic states. One of these methods was also considered in [5]. Applying this method to calculating TDES in a photonic crystal even within very simple scalar-vector PWM variants while using sequential algorithms is very machine time-consuming. The reason is that PWM presupposes algebraic problems of calculating eigenvalues with dense matrices whereas mathematical models used in [4, 5] lead to sparse matrices which allow to use effective algorithms for matrix operations [6].

However, when using parallel algorithms, one should expect acceleration of the calculation of TDES by methods that do not use unitary transformations to calculate eigenvalues. In this work,
an attempt is made to evaluate this acceleration. In addition, one of the ways to improve our parallel algorithm to further increase the efficiency of calculations is described, while remaining within reasonable limits on the accuracy of calculation of the PPES histogram. It is noteworthy that the proposed computational techniques are applicable to photonic crystals with “defects”, which increases the range of applied problems solved by our programs.

2. Models and methods

We used PWM in scalar-vector approximation. For example, this approach presupposes finding electric-field intensity from a system of algebraic equations (2), p. 16:

$$- \sum_{G'} \alpha(G - G')(k + G') \times ((k + G') \times E_{kn}(G')) = \frac{\omega_n^2(k)}{c^2} E_{kn}(G),$$

(1)

where $G$ is the reciprocal lattice vector, $c$ is the speed of light, $E_{kn}(G)$ is Fourier-transformation coefficient:

$$E_{kn}(r) = \sum_{G} E_{kn}(G) e^{i(k + G) \cdot r},$$

(2)

and $\alpha(G)$ has the form:

$$\alpha(G) = \frac{1}{V} \int_V \frac{1}{\varepsilon(r)} e^{-iG \cdot r} d\mathbf{r},$$

(3)

Here $V$ is the volume of photonic crystal’s elementary lattice cell, $\varepsilon(r)$ is dielectric permeability constant. Since $\varepsilon(r)$ is a real function, Fourier coefficients must satisfy the equality $\alpha(-G) = \alpha^*(G)$.

For simplicity, we considered a one-dimensional model of a $Si/a - SiO_2$ dielectric photonic crystal. An elementary cell of an ideal photonic crystal consists of two layers ($Si$ and $a - SiO_2$) with thicknesses $a_1 = 2290$ Å, $a_2 = 6580$ Å and dielectric permeability constant $\varepsilon_1 = 11.6964$, $\varepsilon_2 = 2.25$ respectively. The period of a photonic crystal is $a = a_1 + a_2$. The adaptation of the MPV for a one-dimensional photonic crystal is elementary. Let the axis OX be perpendicular to the layers of a photonic crystal. Then

$$\varepsilon(x) = \begin{cases} \varepsilon_1, & x \in [0, a_1], \\ \varepsilon_2, & x \in [a_1, a] \end{cases}$$

(4)

It is easy to show that the equation (1) in the one-dimensional case takes the form:

$$\sum_{G'} \alpha(G - G')(k + G')^2 E_{kn}(G') = \frac{\omega_n^2(k)}{c^2} E_{kn}(G).$$

(5)

The integral (3) by taking (4) written as:

$$\alpha(G) = \begin{cases} \frac{1}{a} \left( \frac{a_1}{\varepsilon_1} + \frac{a - a_1}{\varepsilon_2} \right), & \text{if } G = 0; \\ \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 \varepsilon_2} \cdot \frac{1 - e^{-ia_1G}}{aG}, & \text{if } G \neq 0. \end{cases}$$

(6)

In fact, the system of equations (5) is a generalized algebraic eigenvalue and eigenvector problem of the form

$$||\alpha||B(k)||E(k)||_n = \frac{\omega_n^2(k)}{c^2} ||E(k)||_n,$$

(7)
where $\|\alpha\|$ is a complex Hermitian matrix, $\|B(k)\|$ is a real positive definite diagonal matrix, $\|E(k)\|_n$ is an eigenvector which corresponds with $n$th eigenvalue $\omega^2_n(k)/c^2$. Further, the generalized eigenvalue problem (7) by standard methods of computing linear algebra is solved with application, as a rule, of unitary transformations for each value of wave vector (number) of $k$. The obtained eigenvalues, in particular, are used to construct photon dispersion curves and calculate the TDES, for example, by the tetrahedron method.

As it has been mentioned above, in papers [4,5] suggest calculation approaches without using unitary transformations. To construct histograms of TDES of nanocrystals consisting of the “whole ions”, the author of these papers use a well-known theorem ([6], p. 204) which can formulate as follows.

**Theorem.** Let $\|H\|$ be a real symmetric matrix. For an arbitrary scalar quantity $\lambda$ we make the matrix $\|H\| - \lambda\|I\|$ and then perform a triangular factorization of the form:

$$\|H\| - \lambda\|I\| = \|U\|^T \|D\| \|U\|,$$  \hspace{1cm} (8)

where $\|I\|$ is unit matrix, $\|U\|$ is upper triangular with unit diagonal, $\|D\|$ is diagonal matrix. Then, the number of eigenvalues less than $\lambda$ is equal to the number of negative elements of the diagonal matrix $\|D\|$.

If we change $\lambda$ with a given step, then performing triangular factorization and calculating the number of negative elements of the diagonal matrix $\|D\|$, then we can easily calculate the histogram of the total density of states. It should be noted that nanocrystals contain a fixed number of atoms or ions, hence, the equation (8) does not show the dependence on the wave vector of matrix $\|H\|$ and therefore eigenvalues and eigenvectors. In the case of an ideal photonic crystal, we deal with translational invariance which, in theory, brings about a wave
vector (number) $k \in BZ$ and the necessity of calculations for all its actual values. To avoid this necessity, this work suggests using supercell approximation. A supercell comprises several elementary cells of an ideal crystal. The Brillouin’s zone for a supercell is much smaller than an ordinary Brillouin’s zone. What does this give us? Let us take a detailed look at the band structure of an ideal photonic crystal $Si/a-SiO_2$, obtained with the help of the standard PWM as well as supercell approximation. In this approximation, the integration in (3) leads to the formulas:

$$\omega(G) = \begin{cases} \frac{c^2}{a} \left( \frac{L_{1SC}^SC}{\varepsilon_{1SC}^SC} + S_0 \right), & \text{if } G = 0; \\ \frac{i c^2}{a G} \left( \frac{\exp(-i G L_{1SC}^SC)}{\varepsilon_{1SC}^SC} - 1 \right) + S_1, & \text{if } G \neq 0. \end{cases}$$

(9)

where

$$S_0 = \sum_{m=2}^{n^{SC}} \frac{L_m^{SC} - L_{m-1}^{SC}}{\varepsilon_m^{SC}},$$

(10)

$$S_1 = \sum_{m=2}^{n^{SC}} \frac{\exp(-i G L_m^{SC}) - \exp(-i G L_{m-1}^{SC})}{\varepsilon_m^{SC}}.$$  

(11)

Here $n^{SC}$ is the number of layers in the supercell, $L_m^{SC}$ is the right border coordinate of the $m$th layer, and $\varepsilon_m^{SC}$ is dielectric permeability of the $m$th layer. Numerical values of the parameters $a_1 = 2290 \, \text{Å}, a_2 = 6580 \, \text{Å}, \varepsilon_1 = 11.6964, \varepsilon_2 = 2.25$ were the same as in the work [7]. A basis set of 2403 plane waves was used. The results of the calculations are given in figure 1. In supercell approximation, the band is divided into sub-bands whose number equals the quantity of elementary cells contained in the supercell. These sub-bands do not intersect and have very slight curvature. We are primarily interested in positions of the stopband edges (rather than the ordinary problem:)

$$\|Q(k_0)\| \|Y(k_0)\| = \|Y(k_0)\| \|\Lambda(k_0)\|,$$

(12)

where

$$\|Q(k_0)\| = \|B(k_0)\|^{\frac{1}{2}} \|\omega\| \|B(k_0)\|^{\frac{1}{2}};$$

(13)

$$\|Y(k_0)\| = \|B(k_0)\|^{\frac{1}{2}} \|E(k_0)\|;$$

(14)

$$\|\Lambda(k_0)\| = \begin{pmatrix} \lambda_1(k_0) & 0 & \ldots & 0 \\ 0 & \lambda_2(k_0) & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \lambda_n(k_0) \end{pmatrix}.$$  

(15)

Here $n$ is the number of basis plane waves, $\lambda_i(k_0) = \omega_i^2(k_0)/c^2$. All matrices in (12)–(15) definitely have the $n \times n$ dimensions; $\|Q(k)\|$ is a complex Hermitian matrix; the $i_{th}$ column in the matrix $\|Y(k_0)\|$ is an eigen vector which corresponds the eigenvalue $\lambda_i(k_0)$. Instead of the
Code 1. The sub-programme for calculating diagonal elements of matrix $\parallel D \parallel$ in the expansion $\parallel A - \lambda I \parallel = \parallel L \parallel \parallel D \parallel \parallel L \parallel^T$.

```fortran
1 subroutine ldlt_m(n,A)
2 implicit none
3 integer (4) n,i,j,k
4 real (8) A(n,n), multiplier
5 do k=1 ,n -1
6   do i=k+1 ,n
7     multiplier = A(i,k)/A(k,k)
8     do j=1 ,n
9       A(i,j)=A(i,j)- multiplier*A(k, j)
10     enddo
11   enddo
12 enddo
13 end
```

The algebraic problem of calculating eigenvalues (12), it is more convenient to solve an equivalent problem for a block matrix:

$$\parallel A(k_0) \parallel = \left[ \begin{array}{cc} \text{Re} \parallel Q(k_0) \parallel & -\text{Im} \parallel Q(k_0) \parallel \\ \text{Im} \parallel Q(k_0) \parallel & \text{Re} \parallel Q(k_0) \parallel \end{array} \right].$$

It is obvious that $\parallel A(k_0) \parallel$ is a symmetric real matrix. It has duplicated dimensions, i.e. $2n \times 2n$, and its eigenvalues are confluent: $\lambda_1(k_0), \lambda_1(k_0), \lambda_2(k_0), \lambda_2(k_0), \ldots, \lambda_n(k_0), \lambda_n(k_0)$, where $\lambda_i(k_0)$ is and $i_{th}$ eigenvalue of the complex Hermitian matrix $\parallel Q(k_0) \parallel$. Now we can apply theorem 2 to matrix $\parallel A(k_0) \parallel$. To do so, we have to accomplish a triangular factorization of this matrix

$$\parallel A(k_0) \parallel - \lambda \parallel I \parallel = \parallel L(k_0) \parallel \parallel D(k_0) \parallel \parallel L(k_0) \parallel^T,$$

which will enable us to construct the TDES histogram changing $\lambda$ with the chosen step. To perform the triangular factorization such as (17), effective algorithms have been developed and computer codes have been written. Some of these algorithms and codes are contained in linear algebra routine libraries. We could have used one of those sub-programmes (functions) but we did it in a different way. The reason is that to construct the histogram, we only need diagonal elements of the matrix $\parallel D(k_0) \parallel$, and the matrix $\parallel L(k_0) \parallel$ is not used for such calculations.

Incidentally, machine time is consumed to calculate the matrix $\parallel L(k_0) \parallel$. Hence, we modified the triangular factorization algorithm eliminating redundant operations. The basis was a simple algorithm implemented in [8] Mathematica. As a result, we worked out a compact code (see Code 1). The sub-programme ldlt_m in FORTRAN-90 calculates diagonal elements of the matrix $\parallel D \parallel$ with the formula (16). The input parameter, the array $A(n, n)$, is to contain the matrix $\parallel A - \lambda I \parallel$ elements; after accomplishing the sub-programme the diagonal elements of the array $A(n, n)$ contain diagonal elements of the matrix $\parallel D \parallel$.

3. Computer Modelling

The calculated histogram TDES can be viewed on figure 2. The basis set comprised 2403 plane waves. As on figure 1, shading shows areas of permitted zones of an ideal crystal calculated using a traditional method. To calculate the TDES histogram we developed a parallel
programme using medium functions MPI. It should be noted that in our algorithm there are no data dependencies, i.e. every further iteration only depends on the starting data and does not depend on the Code 1. results of the previous one. This enabled us to implement an effective parallelization scheme for distributed-memory systems which allows to minimize the data exchange between parallel processes. To determine the amount of calculations performed by each process, a map of filling processes with tasks was implemented and this allowed to simplify the distribution of tasks. The map represents an array of dimension $N_P$, where $N_P$ is the number of processes in the calculations. Filling takes place in a cycle from $start_m$ to $end_m$. 

Figure 2. TDES histogram calculated by the suggested calculation method.

Figure 3. Computation speedup in accordance with increasing number of processes.
where $start_m$ and $end_m$ define the boundaries of the calculated area. At each step, there is an increase in the value in the corresponding cell of the array and a shift of the pointer to the element of the array corresponding to the process; when reaching the border of the array, the pointer moves to the first element. Upon completion of filling, we get an array of dimension $N_P$, in each cell of which is stored the number of steps that the process with the number $N$ should execute, where $N = 1, \ldots, N_P$. The zero process, which is not involved in the calculations, is used to send the values of this array to other processes. Processes that perform calculations, take the passed values, perform the calculation, and send the iteration number and its result to the zero process. The zero process, in turn, consistently collects the results from each iteration, providing low overheads for data waiting. Further, figure 3 shows the graph which represents computation speedup in accordance with increasing number of processes.

4. Conclusions

In this paper, we propose a computational technique for calculating the histograms of TDES of photonic crystals that does not use unitary (or orthogonal) transformations. The parallel code we created is quite efficient (see figure 2). However, the speed of the code performance when using 4 processes at most is not high enough and it cannot compete with numerical methods based upon using unitary (or orthogonal) transformations. Nevertheless, the situation may change both when using more powerful multiprocessor devices, and by improving the mathematical model. So, it is possible, while staying within the limits of reasonable calculation accuracy, to apply an approach leading to the appearance of a significant number of zero elements in the matrix $||A(k_0)||$. The use of algorithms for matrix operations with sparse matrices will undoubtedly contribute to a decrease in computer time, as in the case of calculating histograms of the total density of electronic states of polar nanocrystals [4,5].

References

[1] Qihuang Gong and Xiaoyong Hu 2013 Photonic Crystals: Principles and Applications (Singapore: Pan Stanford Publishing)

[2] Sakoda K 2004 Optical Properties of Photonic Crystals (Berlin–Heidelberg–New York: Springer)

[3] Guevara-Cabrera E, Palomino-Ovando M A, Flores-Desirena B and Gaspar-Armenta J A 2016 Physica B 484 53–59

[4] Timoshenko Yu K 2014 Journal of Physics: Conference Series 490 012173 URL http://dx.doi.org/10.1088/1742-6596/490/1/012173

[5] Timoshenko Yu K 2014 Supercomputing Technologies in Science, Education and Industry. Almanac vol 6 (Moscow State University, Moscow) pp 183–192

[6] Pissanetzky S 1984 Sparse Matrix Technology (London: Academic Press Inc.)

[7] Timoshenko Yu K, Shumina V A, Smirnov Yu V and Kazarina O V 2008 Proc. of SPIE (Nanophotonic Materials V : Conference of SPIE Symposium on NanoScience + Engineering, 10–14 August 2008, San Diego, USA) 7030 703018–1 – 703018–6

[8] Trahan J, Kaw A and Martin K 2006 Computational time for finding the inverse of a matrix: Lu decomposition vs. naive gaussian elimination, University of South Florida, URL http://mathforcollege.com/nm/simulations/nbm/04ale/nbm_sle_sim_ludecomp.pdf