

Eigenvalue Spectrum Estimation and Photonic Crystals

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Abstract. We have developed an algorithm for the estimation of eigenvalue spectra and have applied it to the determination of the density of states in a photonic crystal, which requires the repeated solution of a generalized eigenvalue problem. We demonstrate that the algorithm offers significant advantages in time, memory, and ease of parallelization over conventional subspace iteration algorithms. In particular it is possible to obtain more than two orders of magnitude speedup in time over subspace methods for modestly sized matrices. For larger matrices the savings are even greater, whilst retaining accurate resolution of features of the eigenspectrum.

1 Introduction

Eigenvalue problems have wide applications in mathematical physics and numerical analysis. The method described in this paper is based on those described by [6, ch. 3] and [12], which estimate the spectrum of a matrix A by calculating a distribution from values of moments derived from matrix-vector products (or solves) starting from a number of randomly chosen initial vectors. The method remains applicable when the size of the matrix is large and this is the only operation that can be performed economically.

In this paper we discuss an application of the algorithm to the problem of determining the density of states in a Photonic Band Gap (PBG) system. PBG materials are periodic dielectric crystals that exhibit a “photonic band gap” similar to the electronic band gap present in semiconductors. Photons in the frequency range of the band gap are completely excluded so that atoms within such materials are unable to spontaneously absorb and re-emit light in this region. They have applications for optical processing, optical computing, and highly efficient narrow band (tunable) lasers [15]. An illustration is in Fig. 1

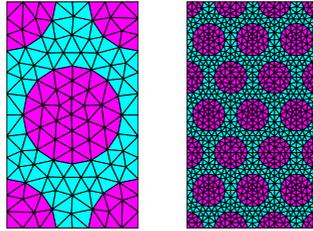


Fig. 1. Hexagonal arrangement of air rods in a dielectric medium with $\epsilon = 12.25$ [3]. The rods are 260nm in diameter and the filling fraction is 50%. Finite Element mesh is shown (with 100 independent nodes): (left) unit cell for calculation, (right) the mesh is periodic- one repeat shown in all directions

It has been shown elsewhere that the problem of characterizing the band gap can be represented as a generalized eigenvalue problem [3,2,4,1],

$$\nabla \times \frac{1}{\epsilon} \nabla \times H = \lambda H \tag{1}$$

$$\nabla \cdot H = 0, \tag{2}$$

where H is the magnetic field, ϵ is the position dependent dielectric constant, and λ are the permitted eigenmodes of propagation in the device. If the rods are considered to be infinitely long then we may reduce this to two independent Helmholtz eigenvalue problems and discretise using the finite element method giving a generalized eigenvalue problem,

$$A(k)x = \lambda Bx. \tag{3}$$

In (3), $A(k)$ is an Hermitian matrix dependent on the Bloch quasi momentum vector,

$$k \in \mathbb{R}^2, \|k\|_\infty \leq \pi. \tag{4}$$

To characterise the PBG device it is necessary to solve (3) repeatedly over values of k chosen in the region of \mathbb{R}^2 to obtain the density of states, which is a union of the resulting eigenvalues.

This problem may be solved accurately using a Krylov subspace iterative method [8], [11]. However practical characterisation and optimisation of a PBG device [5] requires only an approximate estimate of the eigenvalue distribution, since we need to determine (i) whether there are eigenvalues in a given range, and (ii) how large the gap is between consecutive groups of eigenvalues. It may also not be known in advance how many eigenvalues must be found to locate the band gaps, only that for a finite element calculation with a given mesh, roughly the first third of the eigenvalues of the full system matrix should be regarded as representing accurate eigenmodes [11].

Our algorithm overcomes both of these problems. We introduce it in the next section, and then describe how it may be applied to a test problem. Finally we demonstrate that it is straightforward to parallelise, and does not require the expensive communication steps of Krylov subspace methods [9]

2 Method

We extend the previous work in this area [6],[12] and discuss the generalised $N \times N$ eigenvalue problem

$$Ax = \lambda Bx \tag{5}$$

where A is Hermitian and B is symmetric positive definite. We further assume that the matrices are scaled such that $\lambda \in (-1, 1)$. The method constructs a sequence of vectors $b_k, k = 0, \dots, m$. The starting vector, b_0 , has elements chosen from a normal distribution with mean zero and variance 1 and is scaled to unit length. The remaining values are generated from the Chebyshev recurrence formulae:

$$b_1 = L^{-1}A(L^{-1})^T b_0 \tag{6}$$

$$b_k = 2L^{-1}A(L^{-1})^T b_{k-1} - b_{k-2}, k = 2, \dots, m. \tag{7}$$

where $B = L^T L$. From the vectors $b_k, k = 0, \dots, m$, we can define $2m + 1$ real valued moments, μ_j :

$$\mu_{2j} = 2b_j^* b_j - b_0^* b_0 \tag{8}$$

$$\mu_{2j+1} = 2b_j^* b_{j+1} - b_0^* b_1 \tag{9}$$

The vectors b_j satisfy

$$b_j = T_j(L^{-1}A(L^{-1})^T)b_0, \tag{10}$$

where $T_j(t)$ is a Chebyshev polynomial of the first kind.

The size of the problem that is feasible in this instance is determined by the ability to calculate the Cholesky decomposition of B . If the Cholesky decomposition is not economic to compute, it may nevertheless be possible to solve $Bz = w$ by an iterative method such as preconditioned conjugate gradient. A recurrence formula similar to (9) can be constructed to produce the vectors b_j and the moments.

Fundamental to our method is the spectral theory of linear self-adjoint operators in Hilbert Spaces [14] that enables us to represent the moments as a Riemann-Stieltjes integral and so the data represent integrals over the eigen-spectrum of the generalised eigenvalue problem:

$$\mu_j = \int_{-1}^1 T_j(x) d\sigma(x), \tag{11}$$

where $\sigma(x)$ is the function defined by

$$\sigma(x) = \sum_{i=1}^N |\beta_i|^2 H(x - \lambda_i) \tag{12}$$

with H being the Heaviside step function, λ_l the eigenvalues and

$$\beta_l = z_l^* b_0. \tag{13}$$

z_l is the eigenvector corresponding to λ_l . Hence the derivative $d\sigma(x)$ can be expressed as a sum of delta functions and the purpose of the subsequent analysis is to recover $d\sigma(x)$, which gives the distribution of the eigenvalues.

By the change of variables $x = \cos(\theta)$ and $\rho(\theta) = 1 - \sigma(\cos \theta)$ in (11), we can show that

$$\mu_j = \int_0^\pi \cos(j\theta) d\rho(\theta). \tag{14}$$

We identify μ_j as cosine coefficients of $d\rho(\theta)$ and the reconstruction by Fourier analysis gives [6],

$$d\rho(\theta) \sim \frac{1}{\pi} + \frac{2}{\pi} \sum_{j=1}^{2m} \mu_j \cos(j\theta). \tag{15}$$

For efficiency a fast Fourier transform may be used. However the series in (15) does not converge pointwise and ‘‘ringing’’ is observed in reconstructions based on (15). The ringing can be reduced significantly by smoothing [7, p. 65] giving a smoothed reconstruction:

$$d\rho(\theta) \sim \frac{1}{\pi} + \frac{2}{\pi} \sum_{j=1}^{2m} \tau_j \mu_j \cos(j\theta) \tag{16}$$

where

$$\tau_j = \frac{2m}{j\pi} \sin\left(\frac{j\pi}{2m}\right). \tag{17}$$

An alternative method of reconstructing the spectrum is to use the Maximum Entropy method directly on (11). In this case we compute a distribution with the largest entropy subject to the constraint (11). Details of the method are found in [10],[5] [12]. The the approximate density has the form

$$d\sigma(t) \sim x_m(t) = \exp\left(\sum_{j=0}^{2m} c_j T_j(t)\right), \tag{18}$$

where the coefficients $c_j, j = 0, \dots, 2m$ can be obtained by minimising the function

$$\Phi(c_0, \dots, c_{2m}) = \int_{-1}^1 \exp\left(\sum_{j=0}^{2m} c_j T_j(t)\right) dt - \sum_{j=0}^{2m} \mu_j c_j. \tag{19}$$

Quasi-newton methods are used for the reconstruction. This method can obtain very smooth and accurate reconstructions with significantly fewer moments than in the Fourier methods. There are drawbacks: the worst of these is the high condition number of the Hessian matrix associated with (19).

It is desirable to repeat the process for several (n_{seed}) starting vectors, b_0 and perform the analysis using the averaged moments $\bar{\mu}_j$. As is the case in Krylov

subspace methods [11] we choose $(n_{seed} - 1)$ orthogonal starting vectors and the final vector at random. This reduces the chance of missing an eigenvalue, which can occur if the starting vector is almost orthogonal to any of the eigenvectors.

2.1 Algorithm

The pseudo-code algorithm is as follows

1. compute iterates using (7);
2. compute moments using (9) and average over different starting seeds;
3. compute smoothing coefficients using (17);
4. reconstruct spectrum using (16) or maximum entropy(19).

2.2 Application to Photonic Crystal Analysis

We set up the generalised eigenvalue problem from the finite element problem (3) and use n_k k -vectors chosen as in (4). This leads to a sequence of generalised eigenvalue problems. The density of states is then the solution for λ of the eigenvalue problem:

$$\begin{pmatrix} A(k^{(1)}) & 0 & 0 & 0 \\ 0 & A(k^{(2)}) & \ddots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & A(k^{(n_k)}) \end{pmatrix} x = \lambda \begin{pmatrix} B & 0 & 0 & 0 \\ 0 & B & \ddots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & B \end{pmatrix} x \tag{20}$$

Clearly if this is tackled using a method which scales less favourably than $O(N)$ in the matrix size, N , it is much better to solve n_k separate smaller eigenproblems. For our algorithm it is straightforward to exploit the block structure in (20) and determine the vectors in (7) independently for each k , and then average the resulting moments, so that the Fourier (or Maximum Entropy) analysis of the moments immediately recovers the density of states.

3 Results

3.1 Ordinary Eigenvalue Problem

We firstly demonstrate that the method can perform extremely accurate eigenvalue spectrum estimation using relatively few iterates on a large matrix. We show results in Figure 2 for a 7000×7000 dense matrix, A , which has been given a predefined eigenspectrum. In this case we set B to be the identity matrix and solve a regular eigenvalue problem. The method resolves not only the general structure of the distribution, but also shows that there is a single eigenvalue at zero. This reconstruction is extremely accurate considering that it required *in total* only 250 matrix vector products to obtain information about the whole spectrum. An iterative method would require at least this many iterates to locate only the first few eigenvalues of a dense matrix [11].

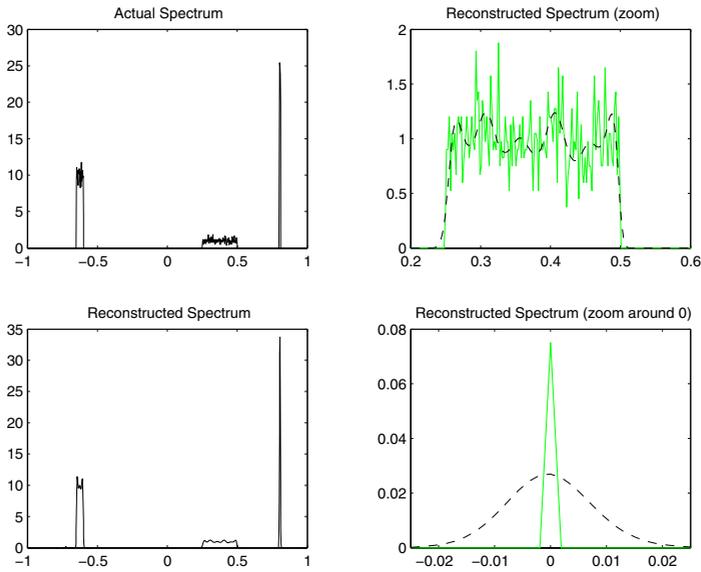


Fig. 2. Eigenvalue distribution of a 7000 square matrix reconstructed using the Maximum Entropy method with 50 iterates and 5 seed vectors. (Right) light line is actual spectrum, dashed is reconstruction

3.2 Generalised Eigenvalue Problem

We have set up and solved the eigenvalue problem in (20) for the photonic crystal in Figure 1 using 100 randomly chosen k -vectors to estimate the density of states. Two approaches may be adopted:

1. Solve 100 independent generalised eigenvalue problems of size 100. A Krylov subspace algorithm [11] was applied to the system to determine the true spectrum for comparison.
2. Solve a single 10 000 square generalised eigenvalue problem, but exploiting the block structure in (20) for any matrix-vector solves. The algorithm we describe was applied in this case.

We resolve the key features of the density of states shown in figure 3 which is in excellent agreement with those given in [15]. The eigenspectrum reconstructed using our estimation method matches precisely the form and position of the true band gaps. Furthermore our estimate was obtained nearly two orders of magnitude more quickly than the true solution, taking minutes rather than hours on a desktop machine! The results in figure 2 indicate that using the Maximum Entropy method to reconstruct the spectrum would reduce the total number of matrix-vector solves by a further factor of five.

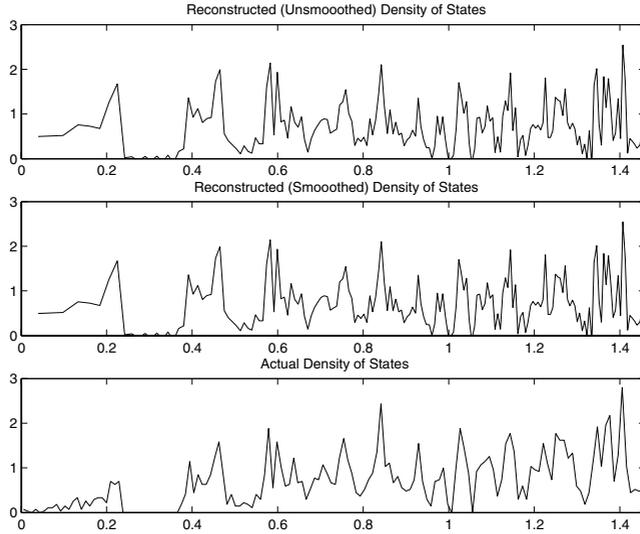


Fig. 3. Density of States for TE polarisation of a photonic crystal consisting of air rods ($\epsilon = 1$) in a dielectric substrate ($\epsilon = 12.25$). The Fourier reconstructed spectra used 256 matrix-vector solves and 5 starting seeds

3.3 Parallelism

The algorithm 2.1 proceeds in parallel in three ways for our application:

- It is possible to parallelise over the different k -vector samples in (3). This is also possible when a subspace iteration method is used. The efficiency of this ‘natural’ parallelism should not be dismissed, so long as the matrix and associated vectors can fit into the memory available on one processor. Our method, however, is considerably more memory efficient, since it is only necessary to store 2 vectors of length N to complete the iterations in (7). Subspace iteration methods require $\sim p$ full vectors where p is the number of eigenvalues required. For a sparse matrix it is this storage which can rapidly outweigh that required for the matrix and hence make it necessary to use multiple processors.
- In contrast to subspace iteration methods [11] a second level of parallelism is possible, since we can start the method with multiple random seeds in parallel on multiple processors. The resulting moments are averaged using a single global reduce step. We have implemented this in MPI, and find that it scales nearly linearly with the number of processors- this method too is ‘naturally’ parallel.
- If the matrix and two vectors of length N are too large to fit into memory on a single processor, then it is necessary to perform the steps in (7,9) in

parallel. We have implemented and described elsewhere an efficient parallel preconditioned conjugate gradient method for this, which scales linearly up to 16 nodes on a commodity cluster of Pentiums running Red Hat Linux 6.2, and also on a cluster of 21164 Compaq Alphas running Windows NT 4.0 [13].

4 Discussion and Conclusions

We have derived and implemented a new algorithm for estimating the eigenvalue spectrum of a generalised eigenvalue problem and have applied it to the calculation of the density of states of a photonic crystal. Our examples were a single large dense matrix and a sequence of small sparse generalised eigenvalue problems (equivalent to a single large block sparse problem). In each case we have demonstrated that a remarkably accurate estimation is possible using relatively few matrix-vector products offering significant advantages in time, memory, and ease of parallelisation over subspace iteration methods in the case when only information about the overall eigenspectrum is required.

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