Accurate Multipole Analysis for Leaky Microcavities in Two-dimensional Photonic Crystals

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***Abstract*—A multipole method is presented to analyze leaky microcavities in finite two-dimensional photonic crystals. The eigenfrequency of a leaky mode is solved from the condition that the eigenvalue with the smallest magnitude (instead of the determinant) of the coefficient matrix is zero. Accurate solutions are obtained with a relatively small truncation order in the associated cylindrical wave expansions.**

***Index Terms*—Optical cavities, photonic crystals, numerical methods, multipole method.**

I. Introduction

Due to the existence of bandgaps, photonic crystals (PhCs) are ideal material for developing microcavities with small mode volumes and high quality factors. Many different types of microcavities are needed in applications such as filters, lasers and nonlinear optical devices. In an ideal microcavity created by local defects in an otherwise perfectly periodic and infinite PhC, the cavity mode decays exponentially away from the defects and its eigenfrequency is real. In practice, the structure surrounding a microcavity cannot be an infinite and perfectly periodic, because it is necessary to couple light into and out of the microcavity. When the surrounding structure contains waveguides or unbounded homogeneous media, the microcavity becomes leaky and the eigenfrequencies of the cavity modes are complex.

To analyze microcavities in PhCs, both time and frequency domain numerical methods have been used [1]–[5]. The finite-difference time-domain (FDTD) [1] method requires small grid size to resolve material interfaces, and long simulation time to settle on the cavity modes. On the other hand, frequency domain methods, such as the finite element method [2], give rise to eigenvalue problems of large matrices which are difficult to solve. Furthermore, for leaky microcavities, the cavity modes exhibit outgoing wave behavior in nearby waveguides or homogeneous media. Therefore, techniques such as the perfectly matched layer are needed to truncate the surrounding structures.

The multipole method is a classical semi-analytic method for analyzing scattering problems associated with canonical structures such as circular cylinders and spheres, using cylindrical or spherical wave expansions [6]. The method has also been applied to compute waveguide modes. In particular, the multipole method can be used to obtain accurate solutions for guided and leaky modes in some PhC fibers [7]. In this Letter, we apply the multipole method to analyze microcavities surrounded by finite two-dimensional (2D) PhCs. Our study is restricted to 2D structures consisting of finite number of parallel and infinitely long circular cylinders embedded in a homogeneous medium. Similar to the multipole method for waveguide modes, we can solve the eigenfrequency of a cavity mode from the condition that a matrix A is singular. However, when the matrix is large, it is difficult to find the eigenfrequency from $\det(A) = 0$. We use the condition $\lambda_1(A) = 0$, where λ_1 is the eigenvalue of A with the smallest magnitude. Accurate solutions are obtained for a number of leaky microcavities in 2D PhCs composed of dielectric rods or air-holes on square or triangular lattices.

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II. The multipole method

For 2D structures which are invariant in the z direction and for waves in the E polarization, the z component of the electric field satisfies the Helmholtz equation

$$\partial_x^2 u + \partial_y^2 u + k_0^2 n^2 u = 0, \tag{1}$$

where $n = n(\mathbf{r})$ is the refractive index function, $\mathbf{r} = (x, y)$, $k_0 = \omega/c$ is the free space wavenumber, ω is the angular frequency (the assumed time dependence is $e^{-i\omega t}$), and c is the speed of light in vacuum. We are concerned with microcavities in a finite 2D PhC, where the bulk PhC consists of circular cylinders arranged as a square or triangular lattice in a homogeneous medium with refractive index n_0. Two simple examples are shown in Fig. 1. For each case, a

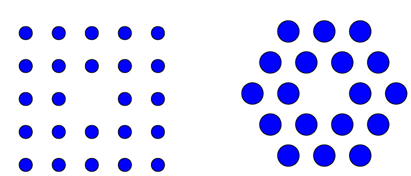

Fig. 1. Examples of leaky cavities where a missing rod is surrounded by two rings of rods in a square or triangular lattice.

microcavity corresponds to a missing cylinder at the center and it is surrounded by two rings of cylinders. Since the PhC surrounding the microcavity is finite, light cannot be fully confined, therefore Eq. (1) does not have non-zero solutions that decay to zero at infinity for any real frequency. For such a microcavity, we look for leaky modes which are non-zero solutions of Eq. (1) satisfying an outgoing radiation condition at infinity. Clearly, a leaky mode can only exist for a complex frequency, the imaginary part of which gives the damping rate of the field amplitude. Since we assumed that the time dependence is $e^{-i\omega t}$, the complex eigenfrequency of a leaky mode must have a negative imaginary part.

To use the multipole method, we choose the xy coordinate system such that the center of the microcavity is the origin and expand the cavity mode outside all cylinders as

$$u(\mathbf{r}) = \sum_{l=1}^{N} \sum_{m=-\infty}^{\infty} b_{lm} H_m^{(1)}(k_0 n_0 r_l) \exp(im\theta_l), \qquad (2)$$

where N is the number of cylinders, n_0 is the refractive index of the homogeneous medium outside the cylinders, $\mathbf{p}_l$ is the coordinates for the center of the lth cylinder, (r_l, θ_l) are the polar coordinates of $\mathbf{r} - \mathbf{p}_l$, that is $r_l = |\mathbf{r} - \mathbf{p}_l|$ and θ_l is the polar angle of $\mathbf{r} - \mathbf{p}_l$. Notice that u given in (2) satisfies the outgoing radiation condition automatically. The multipole method gives rise to a homogeneous linear system for all these coefficients b_{lm}. If the lth cylinder has a radius R_l and a refractive index n_l, the system can be written as

$$\begin{bmatrix} I & -S_1T_{12} & -S_1T_{13} & \cdots \\ -S_2T_{21} & I & -S_2T_{23} & \cdots \\ -S_3T_{31} & -S_3T_{32} & I & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \\ \vdots \end{bmatrix} = \mathbf{0} \qquad (3)$$

where $\mathbf{b}_l$ is the infinite column vector of b_{lm} for all m, I is the identity matrix, S_l is a given infinite diagonal matrix and T_{lj} is a given infinite matrix. The (m,q) entry of T_{lj} is $(T_{lj})_{mq} = H_{m-q}^{(1)}(k_0 n_0 r_l^j) \exp[i(q-m)\theta_l^j]$, where (r_l^j, θ_l^j) are the polar coordinates of $\mathbf{p}_j - \mathbf{p}_l$. For the E polarization, the (m,m) entry of S_l is

$$(S_l)_{mm} = \frac{n_l J_m(\xi) J_m'(\eta) - n_0 J_m(\eta) J_m'(\xi)}{-n_l H_m^{(1)}(\xi) J_m'(\eta) + n_0 J_m(\eta) {H_m^{(1)}}'(\xi)},$$

where $\xi = k_0 n_0 R_l$ and $\eta = k_0 n_l R_l$. For the H polarization, n_0 and n_l should be switched in the above formula for $(S_l)_{mm}$. In practice, we truncate m to $-m_* \le m \le m_*$ for a positive integer m_*, then $\mathbf{b}_l$ becomes a vector of length $M = 2m_*+1$, T_{lj} and S_l become $M \times M$ matrices. Therefore, Eq. (3) is approximated by

$$A(\omega)\,\vec{\mathbf{b}} = \mathbf{0}, \qquad (4)$$

where $\vec{\mathbf{b}}$ is a column vector with blocks $\mathbf{b}_1$, $\mathbf{b}_2$, ..., $\mathbf{b}_N$, and $A = A(\omega)$ is an $(MN) \times (MN)$ matrix. Since k_0 is involved in S_l and T_{lj}, the matrix A depends on the frequency ω.

A cavity mode corresponds to a non-zero solution of the homogeneous linear system (3) or (4) approximately. Therefore, we can find the eigenfrequency from the condition that the matrix A is singular. The standard approach is to solve ω from $\det(A) = 0$. However, the determinant of a matrix is not a good indicator for its singularity when the size of the matrix is large. If an iterative method, such as the secant method, is used to solve the eigenfrequency from $\det(A) = 0$, it is difficult to find initial guesses that lead to a convergent result. Our approach is to solve ω from

$$\lambda_1(A) = 0, \qquad (5)$$

where λ_1 is the the eigenvalue of A with the smallest magnitude. We use the secant method to solve ω from (5). Numerical examples indicate that convergent results can easily be obtained even using initial guesses that are not close to the exact eigenfrequency. The advantage of $\lambda_1(A)$ will be illustrated by an example in Section III.

III. Numerical examples

In this section, we illustrate our method by a few numerical examples. The first example was previously analyzed by a number of authors [1]–[5]. A microcavity is created in a $P \times P$ square lattice of circular rods by removing the rod at the center, where P is an odd integer. The radius and the refractive index of the rods are $R = 0.2a$ (a is the lattice constant) and $n = 3.4$, respectively. The medium surrounding the cylinders is air. The case for $P = 5$ is shown in Fig. 1 (left). Our results are listed in Table I below. From its complex frequency, the quality

TABLE I
EIGENFREQUENCIES AND QUALITY FACTORS OF LEAKY CAVITY MODES IN A FINITE SQUARE LATTICE OF DIELECTRIC RODS.

Lattice size	Normalized frequency $\omega a/(2\pi c)$	Q factor
3×3	0.37941433-0.01019708826i	18.60405
5×5	0.37843574-0.00106497948i	177.6728
7×7	0.37808105-0.00013372758i	1413.624
9×9	0.37802694-0.00001838746i	10279.48

factor of a leaky cavity mode is calculated by the formula $Q = |0.5\mathrm{Re}(\omega)/\mathrm{Im}(\omega)|$. The results in Table I are obtained using $m_* = 4$, and they have been validated by additional calculations using larger values of m_*. In fact, full double precision results (accurate to about 15 digits) can be obtained with $m_* \ge 8$. The results for $m_* > 8$ are identical to those for $m_* = 8$ in a double precision environment. The first four digits of the Q values in Table I agree with the frequency domain finite element results by Rodríguez-Esquerre *et al.* [2]. For $P = 5$, 7 and 9, they obtained $Q = 178$, 1414 and 10276, respectively. For $P = 5$, the same result ($Q = 178$) was also obtained by Obayya [3] using a finite element method with a complex time marching technique. On the other hand, it seems that the available time-domain results can only agree with these frequency-domain results for the first two digits. For example, the time domain results are $Q = 180$ in [2] and $Q = 184$ in [4] for $P = 5$, and $Q = 1423$ in [2] and $Q = 1450$ in [5] for $P = 7$.

Next, we consider microcavities in finite PhCs composed of dielectric rods in a triangular lattice, where the refractive index and the radius of the rods are $n = 3$ and $R = 0.378a$ (a is the lattice constant), respectively, and the medium surrounding the rods is air. A simple microcavity corresponds to a missing rod surrounded by a few rings of rods in a triangular lattice. The case where the microcavity is surrounded by two rings of rods is shown in Fig. 1 (right). In Table II, we show the results obtained using $m_* = 8$. This example is more difficult than the first one, since the radius of the rods is larger, and more terms are needed in the cylindrical wave expansions. Nevertheless, we are able to obtain results with full double precision using $m_* = 16$. This example was previously analyzed by Rodríguez-Esquerre *et al.* [2] using

TABLE II
EIGENFREQUENCIES AND QUALITY FACTORS FOR LEAKY CAVITY MODES IN A FINITE TRIANGULAR LATTICE OF DIELECTRIC RODS.

No. of rings	Normalized frequency $\omega a/(2\pi c)$	Q factor
1	0.46657438 - 0.0045872082i	50.85603
2	0.46704334 - 0.0020896908i	111.7494
3	0.46759852 - 0.0001811422i	1290.695
4	0.46781022 - 0.0001328438i	1760.753
5	0.46788203 - 0.0000144513i	16188.19

a finite element method. For the microcavity with four rings, the frequency-domain and time-domain finite element results given in [2] are $Q = 1745$ and $Q = 1754$, respectively. Once the eigenfrequency is calculated, we can find the eigenfunction. Since $A(\omega)$ is singular, the vector $\vec{\mathbf{b}}$ is the eigenvector corresponding to the zero eigenvalue of matrix $A(\omega)$.

For this example (cavity with three rings) and $m_* = 8$, we show the real and imaginary parts of $\det(A)$ and $\lambda_1(A)$ in Fig. 2, where the horizontal axis is the real frequency.

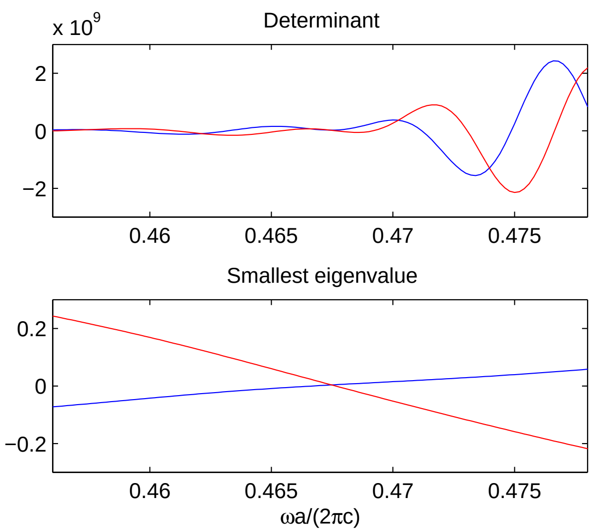

Fig. 2. The determinant and the smallest eigenvalue (in magnitude) of the matrix $A(\omega)$ as functions of a real frequency, for cavity with three rings and $m_* = 8$.

Although the true eigenfrequency is complex, its imaginary part is very small. From the curves for $\lambda_1(A)$, we can easily see that an eigenfrequency exists near $\omega a/(2\pi c) = 0.468$. The curves for $\det(A)$ are oscillatory in the frequency interval shown in Fig. 2, therefore, if $\det(A) = 0$ is used, iterative root-finding methods may not converge unless the initial guesses are very close to the true solution.

Finally, we follow [5] and consider a leaky microcavity consisting of three rings of circular air-holes (radius $R = 0.45a$) surrounded by a dielectric medium with refractive index $n_0 = \sqrt{11.4}$. For the H polarization, the microcavity has four leaky modes including a pair of doubly-degenerated ones. This example is more difficult than the previous one, since the radius is larger and the expansion (2) is given in the high index medium. Our results are given in Table III. The quadrupoles are doubly-degenerated, since two eigenvalues of the matrix A are exactly zero when ω is the given eigenfrequency. The quadrupoles, the monopole and the hexapole are obtained with

TABLE III
EIGENFREQUENCIES AND QUALITY FACTORS OF LEAKY CAVITY MODES IN A 3-RING TRIANGULAR LATTICE OF AIR-HOLES.

Modes	Normalized frequency $\omega a/(2\pi c)$	Q factor
Monopole	0.41940227 - 0.0002397509i	874.6626
Quadrupoles	0.39514759 - 0.0001009359i	1957.418
Hexapole	0.45555802 - 0.0000695536i	3274.868

$m_* = 15$, 16 and 17, respectively. These results are validated by additional calculations with even larger values of m_*. This example has been previously analyzed by Pinto *et al.* [5] using a finite volume time domain method. The Q values given in [5] are 779, 1660 and 3223, respectively.

While the examples above involve either a missing rod or a filled air-hole at the center, the multipole method is applicable to more general structures where the cylinders can be arbitrarily located and can have different radii and different refractive indices. Since the eigenfrequency of a leaky mode is solved from Eq. (5), we need $O(M^3N^3)$ operations to calculate the smallest eigenvalue in each iteration, where N is the number of cylinders and $M = 2m_* + 1$ is the number of cylindrical waves for each cylinder. For the cavity with five rings of dielectric rods in a triangular lattice and $m_* = 8$, i.e., the last row of Table II, we have $N = 90$ and $MN = 1530$. On a personal computer with a 2.33GHz CPU and using MATLAB, it takes about 4 s to generate the matrix A and 12 s to find its eigenvalues. Since the number of iterations in the secant method is typically less than 10, the total required time is less than 3 minutes.

IV. CONCLUSION

In this Letter, we use the multipole method to analyze microcavities in finite 2D PhCs composed of infinitely long and parallel circular cylinders. The eigenfrequency of a leaky cavity mode is determined from the condition that the smallest eigenvalue (in magnitude) of the coefficient matrix is zero. Accurate results are obtained with a relatively small m_*, where m_* is the truncation order of the cylindrical wave expansions. Full precision results can also be obtained using a larger m_*.

REFERENCES

[1] R. R. Villeneuve, S. H. Fan, and J. D. Joannopoulos, “Microcavities in photonic crystals: Mode symmetry, tunability, and coupling efficiency,” *Phys. Rev. B*, vol. 54, pp. 7837-7842, 1996.

[2] V. F. Rodríguez-Esquerre, M. Koshiba, and H. E. Hernández-Figueroa, “Finite-element analysis of photonic crystal cavities: Time and frequency domains,” *J. Lightw. Technol.*, vol. 23, pp. 1514-1521, 2005.

[3] S. S. A. Obayya, “Finite element time domain solution of resonant modes in photonic bandgap cavities,” *Opt. Quant. Electron.*, vol. 37, no. 9, pp. 865-873, July 2005.

[4] D. Pinto and S. S. A. Obayya, “Improved complex-envelope alternating-direction-implicit finite-difference-time-domain method for photonic-bandgap cavities,” *J. Lightw. Technol.*, vol. 25, no. 1, pp. 440-447, Jan. 2007.

[5] D. Pinto, S. S. A. Obayya, “2D Analysis of multimode photonic crystal resonant cavities with the finite volume time domain method,” *Opt. Quant. Electron.*, vol. 40, no. 11-12, pp. 875-890, Sep. 2008.

[6] G. Tayeb and D. Maystre, “Rigorous theoretical study of finite-size two-dimensional photonic crystals doped by microcavities,” *J. Opt. Soc. Am. A*, vol. 14, pp. 3323-3332, 1997.

[7] T. P. White, B. T. Kuhlmey, R. C. McPhedran, D. Maystre, G. Renversez, C. M. de Sterke, and L. C. Botten, “Multipole method for microstructured optical fibers. I. Formulation,” *J. Opt. Soc. Am. B*, vol. 19, pp. 2322-2330, 2002.