Calculation, normalization, and perturbation of quasinormal modes in coupled cavity-waveguide systems

Philip Trøst Kristensen,[1,2,*] Jakob Rosenkrantz de Lasson,[1] and Niels Gregersen[1]

[1]*DTU Fotonik, Technical University of Denmark, Lyngby DK-2800, Denmark*

[2]*Institut für Physik, Humboldt Universität zu Berlin, Berlin D-12489, Germany*

**Corresponding author: philip.kristensen@physik.hu-berlin.de*

Received August 1, 2014; revised September 25, 2014; accepted September 26, 2014; posted October 7, 2014 (Doc. ID 220143); published November 3, 2014

We show how one can use a nonlocal boundary condition, which is compatible with standard frequency domain methods, for numerical calculation of quasinormal modes in optical cavities coupled to waveguides. In addition, we extend the definition of the quasinormal mode norm by use of the theory of divergent series to provide a framework for modeling of optical phenomena in such coupled cavity-waveguide systems. As example applications, we calculate the Purcell factor and study perturbative changes in the complex resonance frequency of a photonic crystal cavity coupled to a defect waveguide.

OCIS codes: (000.3860) Mathematical methods in physics; (050.1755) Computational electromagnetic methods; (050.5298) Photonic crystals; (140.3945) Microcavities; (140.4780) Optical resonators.

http://dx.doi.org/10.1364/OL.39.006359

Quasinormal modes (QNMs) [1–3] provide a natural framework for modeling light propagation and light-matter interaction in resonant electromagnetic material systems, such as optical cavities [4–10] and plasmonic nanoparticles [11–15]. The QNMs of localized electromagnetic resonators in an otherwise homogeneous medium may be calculated as eigenmodes of the source-free Maxwell equations augmented with the Silver-Müller radiation condition [3]. The radiation condition admits only fields that propagate away from the resonator at large distances. This, in turn, leads to a discrete spectrum of complex resonance frequencies $\tilde{\omega}_\mu = \omega_\mu - \mathrm{i}\gamma_\mu$ from which the Q value may be calculated directly as $Q = \omega_\mu/2\gamma_\mu$ [16]. In numerical calculations, the radiation condition is often modeled using perfectly matched layers (PMLs) [17] in either frequency- or time-domain calculations, but alternatives are also available; for example, in the form of integral equations [8,12].

In many technologically relevant applications, light coupling to and from the cavity is controlled by waveguides, such as fibers or line defects in photonic crystal (PC) [18] circuits. In such coupled cavity-waveguide systems, the coupling to the waveguides represents by far the largest decay channel for light in the cavity; indeed, any decay through other channels than the waveguide often represents unwanted and detrimental losses and is typically minimized through careful engineering. Calculation of QNMs in these coupled systems is nontrivial because of the need for a suitable radiation condition. In particular, the Silver-Müller radiation condition applies only to problems with a homogeneous background material, and if the waveguides have discrete translational symmetry—as in PCs, for example—one cannot use PMLs to avoid reflections from the calculation domain boundary. Instead, one can formulate a suitable radiation condition by appealing to the known Bloch form of the solutions in the periodic waveguide, as was done in [7] using a Dirichlet to Neumann map technique [19] and in [10] using the Fourier modal method (FMM) [20,21]. In this Letter, we present an alternative formulation of the radiation condition in terms of a nonlocal boundary condition, which can be used with standard frequency domain methods to calculate QNMs in coupled cavity-waveguide systems. Figure 1 shows the QNM of a side-coupled cavity in a PC with lattice constant a made from high-index ($\epsilon_{\mathrm{cyl}} = 8.9$) cylinders of radius $r = 0.2a$ in air. This QNM—which is identical to the QNM that was calculated with the FMM in [10]—was calculated using the finite element method (FEM) with the nonlocal boundary condition that we present below.

The leaky nature of the QNMs leads to an exponential divergence at large distances, which means that they

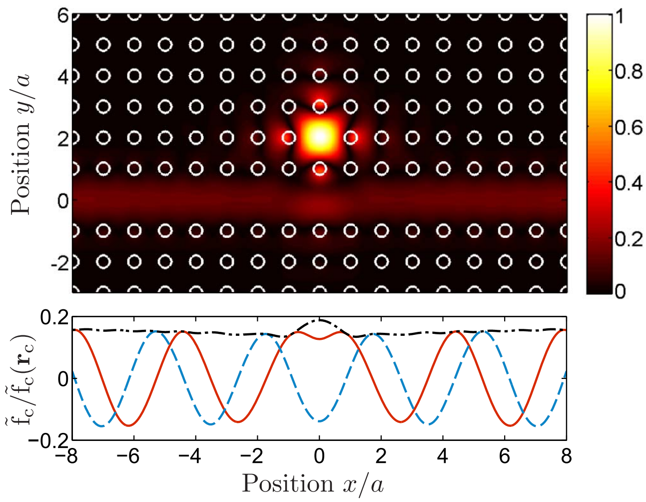

Fig. 1. Top: absolute value of the QNM $|\tilde{f}_c(\mathbf{r})|$ in a cavity side-coupled to an infinite waveguide in a PC with lattice constant a. The QNM has a complex resonance frequency of $\tilde{\omega}_c a/2\pi c = 0.39687 - 0.00136\mathrm{i}$ corresponding to $Q = 146$. Bottom: real part (red full), imaginary part (blue dashed), and absolute value (black dashed–dotted) of the QNM along the line $y = 0$ in the center of the waveguide. In both panels, the QNM is scaled to unity at $\mathbf{r} = \mathbf{r}_c$ in the center of the cavity.

cannot be normalized in the same way as the so-called normal modes calculated using Dirichlet (or periodic) boundary conditions. Instead, the QNMs may be normalized by an alternative prescription that explicitly compensates for the divergence. Such a normalization was first derived for spherically symmetric material systems in [4–6], and was adopted for general leaky optical cavities in [8] to define a generalized effective mode volume with applications, for example, in Purcell factor [22] calculations. Sauvan *et al.* [11] later derived an alternative formulation of the norm in an elegant and transparent way. When the Silver-Müller radiation condition applies, the two formulations can be shown to be identical [14]. Whereas the norm in [4–6] relies explicitly on the Silver-Müller condition, the formulation in [11] does not, but it does rely on the use of PMLs to regularize the normalization integral by a complex coordinate transform. For QNMs leaking through PC waveguides, therefore, one cannot directly use either formulation. As a remedy, we show in this Letter how one can use the theory of divergent series [23] to regularize the integral, and we use the normalization in examples of Purcell factor calculations and perturbation theory for the PC cavity-waveguide system in Fig. 1.

We consider systems of cavities coupled to waveguides that are defined in general by a periodic relative permittivity distribution $\epsilon_r(\mathbf{r})$ for which $\epsilon_r(\mathbf{r}+\mathbf{R}) = \epsilon_r(\mathbf{r})$, where $\mathbf{R}$ is a lattice vector in the direction of the waveguide. In addition, we limit the analysis to nonmagnetic, isotropic, and dispersionless materials, and to cavities coupled to waveguides with a single band of defect waveguide modes in the frequency range of interest. We focus on electric field QNMs defined as solutions to the wave equation

$$\nabla\times\nabla\times\tilde{\mathbf{f}}_\mu(\mathbf{r}) - \left(\frac{\tilde{\omega}_\mu}{\mathrm{c}}\right)^2\epsilon_r(\mathbf{r})\tilde{\mathbf{f}}_\mu(\mathbf{r}) = 0, \qquad (1)$$

where c is the speed of light, subject to a suitable radiation condition describing the light-propagation through the waveguide away from the cavity. In the periodic waveguides, Bloch–Floquet theory [18] ensures that the solutions to the wave equation may be written as

$$\mathbf{f}_\mathbf{k}(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\mathbf{u}_\mathbf{k}(\mathbf{r}), \qquad (2)$$

in which $\mathbf{k}$ is the wave vector and $\mathbf{u}_\mathbf{k}(\mathbf{r}+\mathbf{R}) = \mathbf{u}_\mathbf{k}(\mathbf{r})$. At sufficient distances from the cavity, the leaky cavity mode may be written in the form of a single Bloch mode as in Eq. (2) but with a complex wave vector $\tilde{\mathbf{k}}_\mu$ corresponding to the resonance frequency $\tilde{\omega}_\mu$ and pointing in the direction of the waveguide away from the cavity. We assume the calculation domain boundary ∂V to be a plane perpendicular to the waveguide direction (a line in two dimensions) with outward pointing unit vector $\mathbf{n}$. In this case, Eq. (2) can be used to define the waveguide radiation condition as a nonlocal boundary condition of the form

$$\tilde{\mathbf{f}}_{\tilde{\mathbf{k}}}(\mathbf{r})\big|_{\mathbf{r}\in\partial V} = \mathrm{e}^{\mathrm{i}\tilde{\mathbf{k}}\cdot\mathbf{n}a}\tilde{\mathbf{f}}_{\tilde{\mathbf{k}}}(\mathbf{r}-\mathbf{n}a). \qquad (3)$$

This nonlocal boundary condition is similar to the one introduced in [24], but the application is different in that there is no incoming field; the QNMs are defined as the solutions to the wave equation with no sources. Using Eq. (3), one can calculate the QNMs of coupled cavity-waveguide systems to high precision using standard frequency domain methods. In practice, the implementation includes a few subtleties and associated sources of error that we discuss below.

For most problems of practical interest, the dispersion of the waveguide modes has no closed form expression, and this complicates the use of Eq. (3) in QNM calculations for which the complex resonance frequency is the eigenvalue of interest. In practice, therefore, we calculate the complex wave vector $\tilde{\mathbf{k}}_\mu$ using a Taylor expansion approximation of the dispersion along the real frequency axis, which may then be readily extended to the complex frequency plane by analytic continuation. As with other frequency domain calculations of QNMs, the radiation condition results in a nonlinear problem because it depends on the complex resonance frequency. Therefore, one must calculate the QNMs by an iterative procedure in which a fixed frequency $\tilde{\omega}_{\mathrm{guess}}$ is used to set up the equation system that is then subsequently solved to find the frequency closest to $\tilde{\omega}_{\mathrm{guess}}$. The iteration continues until the difference $\delta\tilde{\omega}$ is less than some prescribed tolerance $\delta\tilde{\omega}_{\max}$. Finally, an important source of error in the calculations is linked to the size of the calculation domain and can be easily described in the language of the FMM. The FMM approach is based on an expansion using the full set of Bloch modes in the system—with either propagating, growing, or decaying characteristics. In the waveguides, the field is described by several decaying Bloch modes as well as a single growing Bloch mode [10], and Eq. (3) thus requires all purely decaying Bloch mode components of the QNM to be negligibly small at the calculation domain boundary. In practice, this leads to larger calculation domains, which is the price to pay for the relatively simple boundary condition in Eq. (3) when comparing to [7] and [10].

The procedure outlined above was applied to calculate the QNM in Fig. 1, which we denote by $\mu = \mathrm{c}$ and which has only an out-of-plane component, $\tilde{\mathbf{f}}_\mathrm{c}(\mathbf{r}) = \tilde{\mathrm{f}}_\mathrm{c}(\mathbf{r})\mathbf{e}_z$. The QNM has a complex resonance frequency of $\tilde{\omega}_\mathrm{c}a/2\pi\mathrm{c} = 0.39687 - 0.00136\mathrm{i}$, corresponding to $Q = 146$. From analytic continuation of the dispersion we find that the complex wave vector in the direction of the waveguide is $\tilde{k}_\mathrm{c}a/2\pi = 0.2837 - 0.0026\mathrm{i}$. The calculations were performed using FEM (Comsol Multiphysics 4.3a), and an absolute tolerance of $\delta\tilde{\omega}_{\max}a/\mathrm{c} = 10^{-5}$. As for discretization, the number of elements was kept sufficiently high so as not to influence the results to the quoted number of digits. The analytic continuation of the dispersion curve into the complex frequency plane was based on a fourth-order polynomial fit to the real dispersion data around the point $\omega_\mathrm{R}a/2\pi\mathrm{c} = 0.395$. Comparing to the corresponding fifth-order expansion reveals a difference $\delta ka/2\pi < 10^{-6}$ over an interval $|\omega - \omega_\mathrm{R}|a/2\pi\mathrm{c} < 0.01$. This interval is more than an order of magnitude larger than the imaginary part of the calculated resonance frequency, wherefore we expect the error in the complex dispersion to be negligible. Figure 2 illustrates the convergence of the QNM resonance frequency as the calculation domain size L_x is increased. Specifically, it shows the error $\delta\tilde{\omega}_L = |\tilde{\omega}(L_x) - \tilde{\omega}(L_{\max})|$ when comparing to a fixed domain size $L_{\max} = 18a$ as well as the error

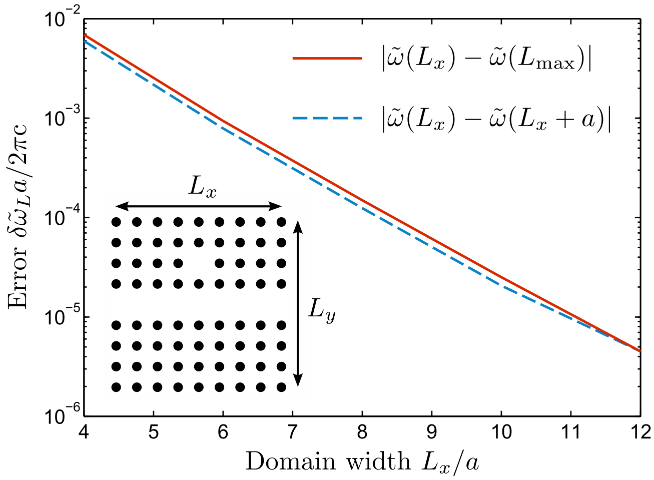

Fig. 2. Change in resonance frequency with increasing calculation domain width L_x as defined in the inset. The red solid curve shows the difference to a reference calculation with fixed domain size $L_{\max} = 18a$, and the blue dashed curve shows the difference between results using successively larger domain sizes.

$\delta\tilde{\omega}_L = |\tilde{\omega}(L_x) - \tilde{\omega}(L_x + a)|$ when comparing the results obtained using successively larger domain sizes. The error in the resonance frequency decreases exponentially with the domain size, consistent with the behavior of the nonpropagating Bloch mode components of the QNM. In all cases, we used a fixed calculation domain height of $L_y = 18a$. Because of the PC bandgap in the y direction, this was found to be large enough to not influence the results to the quoted number of digits.

Having calculated the QNM, we next turn to the question of normalization. Following [11], we start by writing the norm of the QNM $\tilde{\mathbf{f}}_\mu$ as

$$\langle\langle\tilde{\mathbf{f}}_\mu|\tilde{\mathbf{f}}_\mu\rangle\rangle = \frac{1}{2}\int_V \epsilon_\mathrm{r}(\mathbf{r})\tilde{\mathbf{f}}_\mu(\mathbf{r})\cdot\tilde{\mathbf{f}}_\mu(\mathbf{r}) + \left(\frac{\mathrm{c}}{\tilde{\omega}_\mu}\right)^2(\nabla\times\tilde{\mathbf{f}}_\mu(\mathbf{r}))\cdot(\nabla\times\tilde{\mathbf{f}}_\mu(\mathbf{r}))\,\mathrm{d}\mathbf{r}, \quad (4)$$

where the integral is formally over the entire volume of space (area in two dimensions), and we have used the source-free Maxwell curl equation to express the integrand in terms of $\tilde{\mathbf{f}}_\mu(\mathbf{r})$ only. For homogeneous surroundings, the integral in Eq. (4) can be regularized by a complex coordinate transform [11]. When the QNM leaks through a periodic waveguide this is not possible, and we must devise a means of regularization that is compatible with the Bloch form of the integrand. To this end, we split the integration into different parts; one part corresponding to the cavity, and one part for each waveguide. For the cavity part, the integrand is well-behaved, and the integral can easily be evaluated. For each semi-infinite waveguide the procedure is identical, and we limit the discussion to a single generic example waveguide. Without loss of generality, we may take this waveguide to point in the x direction. The partition of the integral along the waveguide is denoted x_0 and is chosen sufficiently large that for $x > x_0$ the QNM in the waveguide is well described by Eq. (2). With this assumption, we write the integral over the waveguide as

$$I_\mathrm{wg} = I_a(x_0)\sum_{m=0}^{\infty}\mathrm{e}^{2\mathrm{i}\tilde{k}_\mu ma}, \quad (5)$$

where

$$I_a(x_0) = \frac{1}{2}\int_\perp\int_{x_0}^{x_0+a}\epsilon_\mathrm{r}(\mathbf{r})\tilde{\mathbf{f}}_\mu(\mathbf{r})\cdot\tilde{\mathbf{f}}_\mu(\mathbf{r}) + \left(\frac{\mathrm{c}}{\tilde{\omega}_\mu}\right)^2(\nabla\times\tilde{\mathbf{f}}_\mu(\mathbf{r}))\cdot(\nabla\times\tilde{\mathbf{f}}_\mu(\mathbf{r}))\,\mathrm{d}x\mathrm{d}\mathbf{r}_\perp, \quad (6)$$

in which $\perp$ denotes the dimension(s) perpendicular to the x axis (area in three dimensions and line in two dimensions). The sum in Eq. (5) is a geometric series of the form $\sum_m b^m$, which is known to be divergent for $|b| \geq 1$. This will be the case for any application of Eq. (5), because the leaky nature of the QNMs means that $\mathrm{Im}\{\tilde{k}_\mu\} < 0$. Although the series is formally divergent, it is possible to assign a finite value to the right-hand side of Eq. (5) using Borel summation (for $\mathrm{Re}\{b\} < 1$) or Lindelöf or Mittag-Leffler summation (for $b \in \mathbb{C}\backslash[1,\infty]$) [23], in which case the sum evaluates to the same expression as in the case of $|b| < 1$:

$$I_\mathrm{wg} = \frac{I_a}{1 - \mathrm{e}^{2\mathrm{i}\tilde{k}_\mu a}}. \quad (7)$$

In effect, this procedure regularizes the integral in a way similar to what is possible with a complex coordinate transform in homogeneous media.

For the QNM in Fig. 1, we used a calculation domain size of $L_x = 18a$ and a partition between the cavity and the waveguide at $x_0 = 8a$ to find that $\langle\langle\tilde{\mathbf{f}}_\mathrm{c}|\tilde{\mathbf{f}}_\mathrm{c}\rangle\rangle/\tilde{\mathrm{f}}_\mathrm{c}^2(\mathbf{r}_\mathrm{c})a^2 = 1.441 - 0.055\mathrm{i}$. In scaling the QNM to unity in the cavity center $\mathbf{r}_\mathrm{c}$ with refractive index $n_\mathrm{c} = 1$, the norm equals the generalized effective mode volume (area in this case) that was defined in [8]. The corresponding (real) effective mode area is $A_\mathrm{eff}/a^2 = 1.443$. For out-of-plane polarization, the two-dimensional Purcell formula is

$$F_\mathrm{P} = \frac{1}{\pi^2}\left(\frac{\lambda_\mathrm{c}}{n_\mathrm{c}}\right)^2\frac{Q}{A_\mathrm{eff}}, \quad (8)$$

where $\lambda_\mathrm{c} = 2\pi\mathrm{c}/\omega_\mathrm{c}$. Inserting, we find $F_\mathrm{P} = 65$.

Last, as an additional example, we use the norm in Eqs. (4) and (5) to study the influence of small material changes. Using perturbation theory, the first-order change in the resonance frequency due to a small change in the permittivity distribution is given as

$$\Delta\tilde{\omega}_\mathrm{c}^{(1)} = -\frac{\tilde{\omega}_\mathrm{c}}{2\langle\langle\tilde{\mathbf{f}}_\mathrm{c}|\tilde{\mathbf{f}}_\mathrm{c}\rangle\rangle}\int_V\Delta\epsilon_\mathrm{r}(\mathbf{r})\tilde{\mathbf{f}}_\mathrm{c}(\mathbf{r})\cdot\tilde{\mathbf{f}}_\mathrm{c}(\mathbf{r})\mathrm{d}\mathbf{r}, \quad (9)$$

where $\Delta\epsilon(\mathbf{r})$ is the position dependent change in permittivity. Equation (9) is identical to the result for QNMs leaking to homogeneous media [4]; it may be derived, for example, using the Hellmann–Feynman theorem [25] in an operator formulation of Maxwell's equations similar to [26] but with a non-Hermitian approach using the QNM norm in Eq. (4). We consider perturbations to the material system in which an additional low-permittivity cylinder is inserted in the center of the cavity. As shown

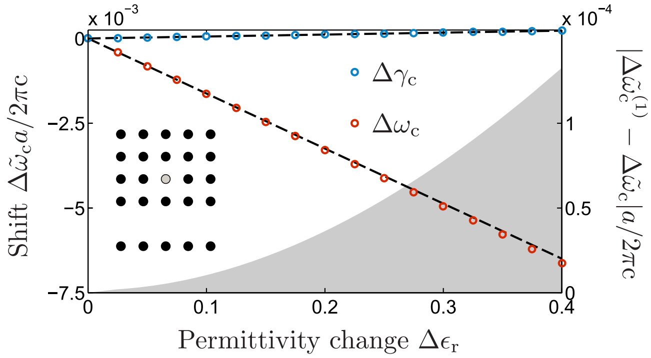

Fig. 3. Perturbative change in the resonance frequency $\Delta\tilde{\omega}_c = \Delta\omega_c - i\Delta\gamma_c$ as a function of permittivity change $\Delta\epsilon_r$ of a cylinder in the center of the cavity as indicated in the inset. Red and blue circles (left axis) show changes in resonance frequency and decay rate, respectively, using full numerical calculations, and dashed black lines show the first-order perturbation result of Eq. (9). Gray shading (right axis) shows the error in the perturbation.

in Fig. 3, the perturbation result of Eq. (9) agrees well with full numerical FEM calculations even for relatively large shifts of several linewidths.

In summary, we have described an approach for numerical calculation of QNMs in cavities coupled to waveguides. The approach relies on a nonlocal boundary condition to correctly model the radiation condition for light leaking through the waveguide. In addition, we have shown how to normalize these QNMs by use of the theory of divergent series. We expect this normalization to be useful for modeling coupled cavity-waveguide systems in terms of QNMs in ways similar to what has been done for cavities in homogeneous media [1–6,8,11,13–15]. As example applications, we have used the normalization to calculate the Purcell factor and for perturbation theory calculations to illustrate how it leads to the correct first-order prediction of the resonance shift.

This work was supported by the Carlsberg Foundation and the Danish Council for Independent Research (FTP 10-093651).

References

1. E. S. C. Ching, P. T. Leung, A. Maassen van den Brink, W. M. Suen, S. S. Tong, and K. Young, Rev. Mod. Phys. **70**, 1545 (1998).
2. E. S. C. Ching, P. T. Leung, and K. Young, *Optical Processes in Microcavities—The Role of Quasinormal Modes*, R. K. Chang and A. J. Campillo, eds. (World Scientific, 1996).
3. P. T. Kristensen and S. Hughes, ACS Photon. **1**, 2 (2014).
4. H. M. Lai, P. T. Leung, K. Young, P. W. Barber, and S. C. Hill, Phys. Rev. A **41**, 5187 (1990).
5. P. T. Leung and K. M. Pang, J. Opt. Soc. Am. B **13**, 805 (1996).
6. K. M. Lee, P. T. Leung, and K. M. Pang, J. Opt. Soc. Am. B **16**, 1409 (1999).
7. S. Li and Y. Y. Lu, J. Opt. Soc. Am. B **26**, 2427 (2009).
8. P. T. Kristensen, C. Van Vlack, and S. Hughes, Opt. Lett. **37**, 1649 (2012).
9. B. Maes, J. Petráček, S. Burger, P. Kwiecien, J. Luksch, and I. Richter, Opt. Express **21**, 6794 (2013).
10. J. R. de Lasson, P. T. Kristensen, J. Mørk, and N. Gregersen, J. Opt. Soc. A **31**, 2142 (2014).
11. C. Sauvan, J. P. Hugonin, I. S. Maksymov, and P. Lalanne, Phys. Rev. Lett. **110**, 237401 (2013).
12. J. R. de Lasson, J. Mørk, and P. T. Kristensen, J. Opt. Soc. B **30**, 1996 (2013).
13. Q. Bai, M. Perrin, C. Sauvan, J. P. Hugonin, and P. Lalanne, Opt. Express **21**, 27371 (2013).
14. R.-C. Ge, P. T. Kristensen, J. F. Young, and S. Hughes, "Quasinormal mode approach to modelling light-emission and propagation in nanoplasmonics," arXiv:1312.2939 [quant-ph] (2013).
15. R.-C. Ge and S. Hughes, Opt. Lett. **39**, 4235 (2014).
16. P. Lalanne, C. Sauvan, and J. P. Hugonin, Laser Photon. Rev. **2**, 514 (2008).
17. J.-P. Berenger, J. Comput. Phys. **114**, 185 (1994).
18. J. D. Joannopoulos, S. G. Johnson, J. N. Winn, and R. D. Meade, *Photonic Crystals—Molding the Flow of Light*, 2nd ed. (Princeton University, 2008).
19. Z. Hu and Y. Y. Lu, Opt. Express **16**, 17383 (2008).
20. E. Noponen and J. Turunen, J. Opt. Soc. Am. A **11**, 2494 (1994).
21. G. Lecamp, J. P. Hugonin, and P. Lalanne, Opt. Express **15**, 11042 (2007).
22. E. M. Purcell, Phys. Rev. **69**, 681, 1946.
23. G. H. Hardy, *Divergent Series* (Oxford at the Clarendon Press, 1949).
24. Z. Hu and Y. Y. Lu, J. Opt. Soc. Am. B **29**, 1356 (2012).
25. R. E. Allen and M. Menon, Phys. Rev. B **33**, 5611 (1986).
26. B. A. Daniel, D. N. Maywar, and G. P. Agrawal, J. Opt. Soc. Am. B **28**, 2207 (2011).