Lower and upper bounds to photonic band gap edges

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A photonic band gap is determined by its edges, which are frequently calculated by the Rayleigh-Ritz method, producing a sequence of upper bounds. Since there are no error estimates available on these approximations, the level of accuracy of the computed band-gap edges, and thus of the extent of the band gap, remains undetermined. We adopt the method of intermediate problems to develop a procedure to calculate the lower bounds to the photonic band-gap edges. Lower bounds, supplemented with the Rayleigh-Ritz approximations, determine a band gap with arbitrary and known degree of accuracy, as well as provide error bounds on approximate calculations by other methods. Calculation of the lower bounds by the present method requires slightly more computational effort than the Rayleigh-Ritz method with a plane-wave basis. A parallel method to compute the alternative upper bounds is also developed in the process.

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I. INTRODUCTION

Mediums with periodic structures are known to block electromagnetic waves except for a discrete set of frequencies.[1,2] The allowed frequencies, as functions of the wave number, form the edges of the interior, containing the prohibited frequencies and defining the band gap. The allowed frequencies, for a wide class of realistic structures, are determined by the eigenvalues of a self-adjoint operator (Ref. 3, pp. 11–14). A widely used algorithm to determine the boundaries of the photonic band gaps is by computing the eigenvalues by the Rayleigh-Ritz (RR) method. While this method may be used with a variety of basis functions, in the case of periodic crystals plane waves are frequently used for convenience[4–8] (Also see Ref. 3, pp. 127–129). With any basis, the RR method produces a sequence of upper bounds to the exact values.

With plane wave basis, the RR method is known to suffer from a slow rate of convergence for the geometries of interest, due to the Gibbs phenomenon.[9–11] A variety of methods have been developed to determine the band gaps more efficiently, some with an overlap with the RR method and others with quite independent foundations.[9–16] To the best of our knowledge, no error estimates are available on the approximations produced by the RR method with any basis, or by these methods. The convergence and accuracy of the results are intuitively inferred on the basis of the numerical stability. For the lack of error estimates, the degree of the accuracy of the band-gap edges remains undetermined, leaving the extent of the band gap correspondingly uncertain. If a band gap determined by these methods is narrow, then even its existence remains uncertain. Existence and a knowledge of the extension of the band gaps, are critical for their exploitation to design usable devices, and for an adequate understanding of the properties of the photonic band-gap material. The availability of the upper and lower bounds to the band-gap edges would substantially improve the understanding of the extension of a band gap.

In the present paper, we develop a numerical scheme to determine converging lower bounds to the edges, based on the method of intermediate problems.[17] These approximations, together with the upper bounds, determine the extension of a band gap with certainty, as it covers at least the region between the upper bound to the lower edge and the lower bound to the upper edge. Although useful in all cases, this information is quite valuable, if a band gap is narrow, to establish its existence, and if one exists, to establish its extent, which for a narrow band gap is even more critical than for a broader one.

Supplementing the Rayleigh-Ritz approximations with lower bounds has been a topic of wide interest, particularly in calculations of the atomic binding energies for which a number of methods with differing properties have been developed.[18–22] We use the method of intermediate problems[17] for its suitability to the present problem. The computational procedure is simplified with a special choice of the basis functions, of the type first proposed by Bazley, to calculate the lower bounds to the He binding energy.[18] The resulting numerical procedure is only slightly more complex than the Rayleigh-Ritz method with a plane-wave basis.

A parallel procedure was also developed to obtain alternative upper bounds. While the lower bounds calculated by the present method provide valuable information, the parallel procedure for the upper bounds is mainly of an academic interest. The RR method, since it is based on a minimum principle, yields the optimal upper bounds, with a given basis set. Also, the methods based on the intermediate problems are computationally more complex, as are all the other methods to compute lower bounds. While the additional computational effort is justified for the calculation of the lower bounds, for the upper bounds it is not, since a better method is available.

Test calculations were carried out for a standard case consisting of cylindrical dielectric material arranged in a two-dimensional periodic structure to form a photonic crystal. The upper bounds produced by the present method are found to be higher than the Rayleigh-Ritz approximations, as expected. Both sequences of the upper bounds, and the sequence of the lower bounds, converge to each other from above and below, respectively.

II. RAYLEIGH-RITZ METHOD

In this section, we formulate the basic problem in a form suitable for the present analysis, and briefly describe the RR method for a comparison with the method to determine the lower bounds, developed here. For the materials of interest, Maxwell's equations can be reduced to (Ref. 3, pp. 8–11)

$$\nabla\times\left(\frac{1}{\varepsilon(\mathbf{r})}\nabla\times\mathbf{H}(\mathbf{r})\right)=\omega^2\mathbf{H}(\mathbf{r}), \tag{1}$$

where $\varepsilon(\mathbf{r})$ is the dielectric distribution of the material, $\mathbf{H}(\mathbf{r})$ is the magnetic field, and ω is the frequency of the propagating electromagnetic wave, in units with the speed of light in vacuum being equal to 1. By Bloch's theorem, $\mathbf{H}(\mathbf{r})$ can be expressed as $\mathbf{H}(\mathbf{r})=e^{i(\mathbf{k}\cdot\mathbf{r})}\mathbf{H}_{\mathbf{k}}(\mathbf{r})$, where it is sufficient to restrict the wave vector $\mathbf{k}$ to the irreducible Brillouin zone. Here $\mathbf{H}_{\mathbf{k}}(\mathbf{r})$ is a periodic function with period equal to that of the crystal. Substitution for $\mathbf{H}(\mathbf{r})$ in Eq. (1) yields

$$(i\mathbf{k}+\nabla)\times\left(\frac{1}{\varepsilon(\mathbf{r})}(i\mathbf{k}+\nabla)\times\mathbf{H}_k(\mathbf{r})\right)=\omega^2(\mathbf{k})\mathbf{H}_{\mathbf{k}}(\mathbf{r}). \tag{2}$$

Let $\mathcal{H}$ be the Hilbert space of the square-integrable vector functions covering the region occupied by the crystal with the scalar product $(\ ,\ )$ defined by

$$(\mathbf{u},\boldsymbol{v})=\int d\mathbf{r}\,\mathbf{u}^*(\mathbf{r})\cdot\boldsymbol{v}(\mathbf{r}),$$

where the dot denotes the usual scalar product of the vectors in the pertaining Euclidian space, and the integral is over the region covered by the material. The space $\mathcal{H}$ can be expressed as a direct sum of the copies of the space $\mathcal{H}'$, where $\mathcal{H}'$ is the Hilbert space of the square integrable, scalar functions, with the scalar product $\langle\ ,\ \rangle$ defined by

$$\langle u,v\rangle=\int d\mathbf{r}\,u^*(\mathbf{r})v(\mathbf{r}).$$

The scalar product $(\mathbf{u},\boldsymbol{v})$ is then expressed as $(\mathbf{u},\boldsymbol{v})=\Sigma_j\langle u_j,v_j\rangle$, where the index j runs over the dimension of the underlying Euclidian space, and u_j and v_j are the components of vectors $\mathbf{u}$ and $\boldsymbol{v}$, respectively. Equation (2) may be expressed as an eigenvalue equation in $\mathcal{H}$,

$$(ABA)\mathbf{H}_{\mathbf{k}}=\omega^2(\mathbf{k})\mathbf{H}_{\mathbf{k}}, \tag{3}$$

where $(A\mathbf{u})(\mathbf{r})=(i\mathbf{k}+\nabla)\times\mathbf{u}(\mathbf{r})$, and $(B\mathbf{u})(\mathbf{r})=\mathbf{u}(\mathbf{r})/\varepsilon(\mathbf{r})$. The operator (ABA) is defined on the divergence-free functions, with further restrictions imposed by the boundary conditions. For the periodic condition and various other boundary conditions of interest, (ABA) is a non-negative operator, in addition to being self-adjoint (Ref. 3, pp. 11–15, 31, and 32). Thus the determination of the frequencies of the waves propagating through a crystal is reduced to the calculation of the eigenvalues of a non-negative operator in a Hilbert space $\mathcal{H}$.

In the RR method, the eigenvector $\mathbf{H}_{\mathbf{k}}(\mathbf{r})$ is expanded as

$$\mathbf{H}_{\mathbf{k}}(\mathbf{r})=\sum_{(\mathbf{G}\lambda)}\mathbf{h}_{(\mathbf{G}\lambda)}\phi_{(\mathbf{G}\lambda)}(\mathbf{r}),$$

where $\{\phi_{(\mathbf{G}\lambda)}\}$ is a suitable basis set, $\mathbf{G}$ are the vectors describing the reciprocal lattice, λ is the index for the polarization vector $\mathbf{e}_\lambda$, and $\mathbf{h}_{(\mathbf{G}\lambda)}$ are as yet undetermined constants. The minimization principle reduces Eq. (3) to the matrix eigenvalue equation

$$\sum_{(\mathbf{G}\lambda)'}\Theta^k_{(\mathbf{G}\lambda)(\mathbf{G}\lambda)'}\mathbf{h}_{(\mathbf{G}\lambda)}=\omega_R^2(\mathbf{k})\mathbf{h}_{(\mathbf{G}\lambda)}, \tag{4}$$

where $\Theta^k_{(\mathbf{G}\lambda)(\mathbf{G}\lambda)'}=(\phi_{(\mathbf{G}\lambda)},(ABA)\phi_{(\mathbf{G}\lambda)'})$.

The set of plane waves $\{\phi_{(\mathbf{G}\lambda)}(\mathbf{r})\}=\{\mathbf{e}_\lambda e^{i(\mathbf{G}\cdot\mathbf{r})}\}=\{\mathbf{e}_\lambda\phi^0_{\mathbf{G}}(\mathbf{r})\}$, being a set of eigenvectors of a self-adjoint operator with discrete spectrum A^2 in $\mathcal{H}$, forms a basis. This property of the plane waves also simplifies the computational procedure. For this reason, they are frequently used as basis, which reduce the matrix elements to

$$\Theta^k_{(\mathbf{G}\lambda)(\mathbf{G}\lambda)'}=[(\mathbf{k}+\mathbf{G})\times\mathbf{e}_\lambda]\cdot[(\mathbf{k}+\mathbf{G}')\times\mathbf{e}_{\lambda'}]B_{\mathbf{G}\mathbf{G}'} \tag{5}$$

with $B_{\mathbf{G}\mathbf{G}'}$ being the matrix elements of B, in $\mathcal{H}'$, given by $B_{\mathbf{G}\mathbf{G}'}=\langle\phi^0_{\mathbf{G}},(1/\varepsilon)\phi^0_{\mathbf{G}'}\rangle$, i.e., the coefficients in the Fourier series expansion of $[1/\varepsilon(\mathbf{r})]$. With bases, other than the plane waves, the RR method yields a matrix with more complicated structure than given by Eq. (5).

III. LOWER BOUNDS

The present procedures to calculate the lower and upper bounds to ω^2, based on the method of intermediate problems, are described below. The exposition is focused on the lower bounds. The scheme for the upper bounds follows by obvious modifications, which are indicated.

Let $\varepsilon_{\max}$ be the maximum value of the dielectric function $\varepsilon(\mathbf{r})$, and $a_0<(1/\varepsilon_{\max})$ be a positive constant. With $a_0>(1/\varepsilon_{\min})$, where $\varepsilon_{\min}$ is the minimum value of $\varepsilon(\mathbf{r})$, the following inequalities are reversed, yielding a parallel procedure to determine the upper bounds. For the lower bounds case, the operator (ABA) can be expressed as $(ABA)=(a_0A^2+ACA)$, where $C=(B-a_0)$ defines a positive operator in $\mathcal{H}'$, as well as in $\mathcal{H}$, and hence, from the monotonicity principle (Ref. 17, Sec. 2.5, Theorem 1), $\sigma_{n0}\leqslant\omega_n^2$, where $\{\omega_n^2\}$ and $\{\sigma_{n0}\}$, for $n=0,1,2....$, are the eigenvalues of (ABA) and the base operator (a_0A^2), respectively, ordered in a nondecreasing sequence. The eigenvalues $\{\sigma_{n0}\}$ are given by $\sigma_{n0}=a_0|[(\mathbf{k}+\mathbf{G}_n)\times\mathbf{e}_\lambda]|^2$, where $[\mathbf{e}_\lambda\phi^0_{\mathbf{G}_n}(\mathbf{r})]$ and $\mathbf{G}_n$ are the corresponding eigenvector and the reciprocal-lattice vector, respectively. Let $\{(ACA)_N\}$ be a sequence of operators in $\mathcal{H}$ such that

$$0=(ACA)_0\leqslant(ACA)_N\leqslant(ACA)_{(N+1)}\leqslant(ACA)_\infty=(ACA) \tag{6}$$

for $N=1,2,...$. A sequence of the intermediate operators $(ABA)_N$ may now be defined by $(ABA)_N=[a_0A^2+(ACA)_N]$. It follows from the monotonicity principle that $\sigma_{nN}\leqslant\sigma_{n(N+1)}\leqslant\omega_n^2$, where $\{\sigma_{nN}\}$ is the nondecreasing ordered set of the eigenvalues of the operators $(ABA)_N$. Since $(\mathbf{u},ACA\mathbf{u})=(\boldsymbol{v},C\boldsymbol{v})=\Sigma_j\langle v_j,Cv_j\rangle$, where $\boldsymbol{v}=A\mathbf{u}$, it is suf-

ficient to find a sequence $\{C_N\}$, such that $0=C_0\leqslant C_N \leqslant C_{(N+1)}\leqslant C_\infty=C$, in $\mathcal{H}'$, and let $(ACA)_N=(AC_NA)$, for Eq. (6) to hold in $\mathcal{H}$.

Let Z_N be the inverse of p_NCp_N, restricted to the N-dimensional subspace $p_N\mathcal{H}'$, of $\mathcal{H}'$, where p_N is the orthoprojection defined by $p_Nu=\Sigma_{j=1}^N\psi_j\langle\psi_j,u\rangle$, with $\{\psi_j\}$ being an arbitrary orthonormal basis in $\mathcal{H}'$. The operator C_N, defined by $C_Nu=Cp_NZ_Np_NC$, satisfies the above requirement (Ref. 17, pp. 79–82). This result may also be obtained as a special case of the standard variational inequality for the positive operators [see, e.g. Ref. 22, Lemma 3(ii)],

$$\langle p_N,g,Z_Np_Ng\rangle\leqslant\langle g,C^{-1}g\rangle.$$

The inequality $C_N\leqslant C$ follows by letting $g=Cu$, for an arbitrary u in $\mathcal{H}'$, and the monotonicity, by taking $g=p_{(N+1)}Cu$, together with $p_Np_{(N+1)}=p_{(N+1)}p_N=p_N$. In detail, the operator C_N is defined by

$$C_Nu=\sum_{j,m=1}^{N}[Z_N]_{jm}C\psi_j\langle C\psi_m,u\rangle,$$

where $[Z_N]$ is the inverse of the matrix $[C_N]$, with elements $[C_N]_{jm}=\langle\psi_j,C\psi_m\rangle$. In this representation of C_N, the basis $\{\psi_j\}$ need not be orthonormal. It is sufficient that $\{\psi_j\}$ be a linearly independent basis.

Computational evaluation of $\{\sigma_{nN}\}$ is considerably simplified with the special choice[18] $\psi_m(\mathbf{r})=C^{-1}\phi^0_{\mathbf{G}_m}$. With these basis functions, the eigenvalues and the eigenvectors of $(ABA)_N$, for $n>N$, are identical to those of (a_0A^2), i.e., $\sigma_{nN}=\sigma_{n0}$, with the corresponding eigenvector $\mathbf{e}_\lambda\phi^0_{\mathbf{G}_n}(\mathbf{r})$. For $n\leqslant N$, σ_{nN} are the solutions of the matrix eigenvalue equation:

$$\sum_{(\mathbf{G_j}\lambda')}\Phi^k_{(\mathbf{G_m}\lambda)(\mathbf{G_j}\lambda')}\mathbf{h}'_{(\mathbf{G_j}\lambda')}=\sigma_{nN}(\mathbf{k})\mathbf{h}'_{(\mathbf{G}_m\lambda)}. \tag{7}$$

The matrix elements on the left side of Eq. (7) are given by

$$\Phi^k_{(\mathbf{G_m}\lambda)(\mathbf{G_j}\lambda')}=[(\mathbf{k}+\mathbf{G_m})\times\mathbf{e}_\lambda]\cdot[(\mathbf{k}+\mathbf{G_j})\times\mathbf{e}_{\lambda'}] \times\{a_0\delta_{mj}+[C_N^{-1}]^{-1}_{\mathbf{G_mG_j}}\},$$

where $[C_N^{-1}]^{-1}_{\mathbf{G_mG_j}}$ are the elements of the inverse of the matrix with elements $\langle\phi^0_{\mathbf{G_m}},C^{-1}\phi^0_{\mathbf{G_j}}\rangle$, and $\delta_{\mathbf{mj}}$ is the Kronecker delta. For $n>N$, we have that $\sigma_{nN}=\sigma_{n0}\leqslant\omega_n^2$, and, for $n\leqslant N'\leqslant N$, σ_{nN} provide nontrivial bounds to ω_n^2, i.e., $\sigma_{nN}\leqslant\omega_n^2$, as long as $\sigma_{N'N}\leqslant\sigma_{(N+1)N}$. This condition restricts the smallest value allowed for a_0.

The present method to calculate the lower bounds parallels the RR method with a plane-wave basis, quite closely, differing as follows. In the RR method, the second multiplicative factor, defining the matrix in Eq. (5), is equal to the matrix elements of $(1/\varepsilon)$, which in the method for lower bounds, is replaced by $\{a_0+[C_N^{-1}]^{-1}_{\mathbf{G_mG_j}}\}$. The elements $(a_0\delta_{\mathbf{mj}})$ define a constant, diagonal matrix, and $[C_N^{-1}]^{-1}_{\mathbf{G_mG_j}}$ are the matrix elements of the inverse of the matrix with elements $\langle\phi^0_{\mathbf{G_m}},[\varepsilon/(1-a_0\varepsilon)]\phi^0_{\mathbf{G_j}}\rangle$. The function $[\varepsilon/(1-a_0\varepsilon)]$ has properties similar to $(1/\varepsilon)$. In the limit of infinite basis set, $\{a_0+[C_N^{-1}]^{-1}_{\mathbf{G_mG_j}}\}$ reduces to a matricial representation of $(1/\varepsilon)$. Additional computational effort in calculating the lower bounds by this method arises out of the need to invert $[C_N^{-1}]$.

The method of intermediate problems may be used with basis different from the one used here. However, the present choice simplifies the computational procedure considerably.

IV. EXAMPLE

The method was applied to a standard test case, of a square lattice of cylindrical dielectric columns, with $\varepsilon=8.9$, embedded in air with $\varepsilon=1$. The lattice was assumed to be homogeneous in the Z direction, and periodic along X and Y axes, with the lattice constant equal to a, and the radius of the dielectric $\rho=0.2a$ (Ref. 3, pp. 54–57). In this structure, $\mathbf{G_m}=\mathbf{m}$, and the two polarization modes decouple into transelectric (TE) and transmagnetic (TM), enabling one to obtain the solutions separately. In case of the RR method, we have used the plane-wave basis for a comparison with the bounds calculated by the present method.

For the TE mode, only the Z component of the magnetic field is nonzero. The matrix elements $\Theta^{\mathbf{k}}_{(\mathbf{G_m}\lambda)(\mathbf{G_j}\lambda')}$ and $\Phi^{\mathbf{k}}_{(\mathbf{G_m}\lambda)(\mathbf{G_j}\lambda')}$, in this case reduce to $\Theta^{\mathrm{TE}}_{\mathbf{mj}}$ and $\Phi^{\mathrm{TE}}_{\mathbf{mj}}$, respectively, given by

$$\Theta^{\mathrm{TE}}_{\mathbf{mj}}=\varepsilon^{-1}_{\mathbf{mj}}[(\mathbf{k}+\mathbf{m})\cdot(\mathbf{k}+\mathbf{j})]$$

and

$$\Phi^{(\mathrm{TE})}_{\mathbf{mj}}=[(\mathbf{k}+\mathbf{m})\cdot(\mathbf{k}+\mathbf{j})](a_0\delta_{\mathbf{mj}}+[\xi^{-1}]_{\mathbf{mj}}), \tag{8}$$

where $\mathbf{m}$ and $\mathbf{j}$ are the integer vectors with components m_x, m_y and j_x, j_y, respectively, $\varepsilon^{-1}_{\mathbf{mj}}=\langle\phi^0_{\mathbf{m}},[1/\varepsilon]\phi^0_j\rangle$ are the Fourier coefficients of $[1/\varepsilon]$, and $[\xi^{-1}]$ is the inverse of the matrix with elements $\langle\phi^0_{\mathbf{m}},[\varepsilon/(1-a_0\varepsilon)]\phi^0_j\rangle$. The range of integers m_x, m_y, j_x, $j_y=-L$ to L, and thus the size of the basis set, is equal to $(2L+1)^2=N$.

For the TM case, both, the X and Y components of the magnetic field are nonzero. This increases the rank of the matrix in Eqs. (4), and (7) by a factor of 2. However, each mode $\mathbf{E_k}(\mathbf{r})$ of the electric field $\mathbf{E}(\mathbf{r})$, defined by $\mathbf{E}(\mathbf{r})=e^{i(\mathbf{k}\cdot\mathbf{r})}\mathbf{E_k}(\mathbf{r})$ satisfies

$$(A'BA')\mathbf{E}'_{\mathbf{k}}=\omega^2(\mathbf{k})\mathbf{E}'_{\mathbf{k}}, \tag{9}$$

where $[(A')^2\mathbf{u}](\mathbf{r})=(i\mathbf{k}+\nabla)\times(i\mathbf{k}+\nabla)\times\mathbf{u}(\mathbf{r})$, and $\mathbf{E}'_{\mathbf{k}}=A'\mathbf{E}_{\mathbf{k}}$. Equation (9) has all the properties of Eq. (3), required for the derivations based on the method of intermediate problems. Thus the above results are applicable in the present case, yielding a similar method. The matrices for this case, $\Theta^{\mathbf{k}}_{(\mathbf{G_m}\lambda)(\mathbf{G_j}\lambda')}=\Theta^{\mathrm{TM}}_{\mathbf{mj}}$ and $\Phi^{\mathbf{k}}_{(\mathbf{G_m}\lambda)(\mathbf{G_j}\lambda')}=\Phi^{\mathrm{TM}}_{\mathbf{mj}}$, are given by

$$\Theta^{\mathrm{TM}}_{\mathbf{mj}}=\varepsilon^{-1}_{\mathbf{mj}}|\mathbf{k}+\mathbf{m}||\mathbf{k}+\mathbf{j}|$$

and

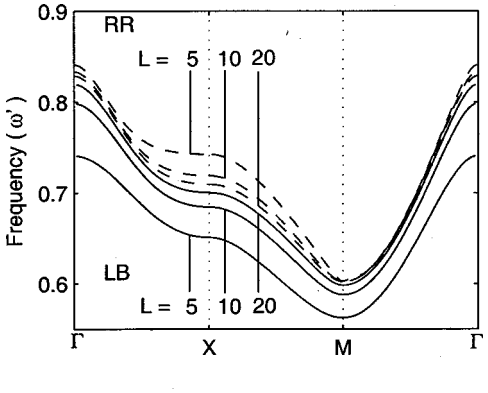

FIG. 1. Comparison of the lower bounds (LB) and the Rayleigh-Ritz (RR) upper bounds to the third lowest, normalized frequency $\omega' = \omega a/2\pi$, for the TE mode.

$$\Phi^{\mathrm{TM}}_{\mathbf{mj}} = |\mathbf{k}+\mathbf{m}||\mathbf{k}+\mathbf{j}|(a_0\delta_{\mathbf{mj}} + [\xi^{-1}]_{\mathbf{mj}}), \tag{10}$$

with the symbols as defined above.

Similarity of the present method with the RR method with a plane wave basis is transparent from the sets of Eqs. (8) and (10), which is, in replacing $\varepsilon^{-1}_{\mathbf{mj}}$ of the RR method with $(a_0\delta_{\mathbf{mj}} + [\xi^{-1}]_{\mathbf{mj}})$. Thus the two methods differ only by similar, but different, approximations of $(1/\varepsilon)$. An additional computational effort is required in the present method in obtaining $[\xi^{-1}]$.

The calculations were carried out for the lowest three frequencies in both the TE and TM modes. The behavior of the approximations was found to be similar to the cases displayed in Figs. 1, 2, and 3. Figure 1 compares the lower bounds obtained by the method of intermediate problems, and the upper bounds obtained by the RR method, with plane waves, for the third lowest frequency for the TE mode propagation for different values of L. The same comparison is made in Fig. 2 for the second lowest frequency in TM mode. In these and all the other cases studied, the sequences of the lower and upper bounds show monotonically convergent behaviors toward each other as the size of the basis set is increased. The accuracy of the lower bounds is comparable with that of the upper bounds, with a moderate size basis set. Two sets of bounds determine the accuracy of the edges and

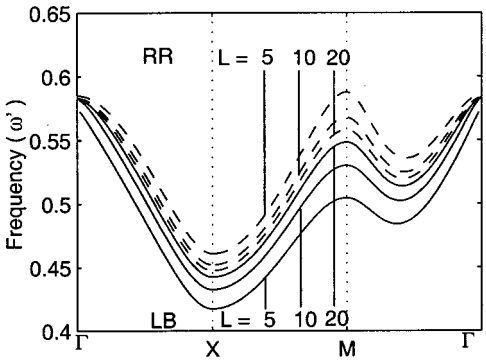

FIG. 2. Comparison of the lower bounds (LB) and the Rayleigh-Ritz (RR) upper bounds to the second lowest, normalized frequency $\omega' = \omega a/2\pi$, for the TM mode.

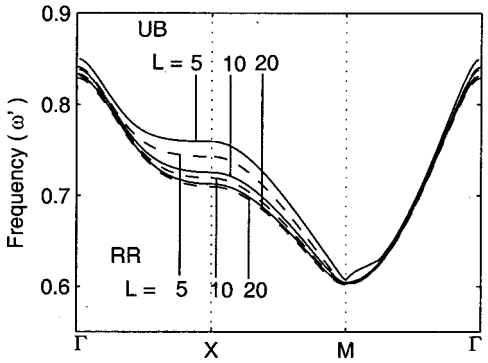

FIG. 3. Comparison of the upper bounds (UB) by the method of intermediate problems and the Rayleigh-Ritz (RR) method to the third lowest, normalized frequency $\omega' = \omega a/2\pi$, for the TE mode.

thus of the extension of the band gap, which may be exploited in designing, and in the studies of, photonic band-gap material.

Figure 3 compares the upper bounds obtained by the method of intermediate problems and by the RR method for the third lowest frequency in the TE mode, which also closely represents all the other cases. While the upper bounds obtained by the method of intermediate problems are higher than the RR values for all values of L, both sequences converge to each other as the basis size is increased. There is a modest increase in computational complexity in obtaining both bounds by the method of intermediate problems, compared to the RR method with the same size basis set.

V. CONCLUDING REMARKS

We have developed a convenient numerical scheme to calculate lower bounds to the photonic band-gap edges, which are determined by the eigenvalues of a non-negative operator. The present procedure adopts the method of intermediate problems to calculate the lower bounds to the eigenvalues of the type of operators encountered in the studies of the photonic band-gap material. The exploitation of some of the properties of this class of operators results in considerable computational simplification, by allowing the use of special basis functions to construct a sequence of operators converging from below to the exact operator. A parallel method to calculate the upper bounds is also developed in the process. Both these methods are computationally slightly more complex than the RR method, which is widely used to determine the upper bounds. In a realistic test case, the rate of convergence of the lower bounds from below is found to be comparable with that of the RR approximations from above. The upper bounds obtained by the present method are higher than the RR approximations, but converge to them, yielding almost the same values for moderate basis size. While it is interesting to note that the method of intermediate problems, although motivated by a need to determine lower bounds to the eigenvalues, may be used to calculate the upper bounds, the resulting procedure is less attractive than the RR method for the present case.

The lower bounds complement the upper bounds, com-

puted by the RR method or by the present method, to determine the accuracy of the band-gap edges and thus of the extension of the band gap for all basis sizes. The availability of the opposite bounds, or other error bounds, is desirable in all cases, to establish a confidence level in the calculated values, and to determine the extent of the band gap, irrespective of the rate of convergence of the method used. In a number of cases, the extent of the band gap determined by any of the other methods is quite narrow. In such cases, the lower and upper bounds would be useful in determining whether an exploitable band gap exists or not, with certainty, before attempts to experimentally exploit it are undertaken.

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