Bound states in photonic crystal waveguides and waveguide bends

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We investigate the mechanism for the appearance of bound states in two-dimensional photonic crystal waveguides and contrast it with the corresponding mechanism for conventional guides. It is shown that the periodicity of the photonic crystal can give rise to frequency ranges above cutoff where no guided modes exist in the waveguides. Such mode gaps make possible the creation of bound states in constrictions and in bends. Bound states are found to correspond to analogous cavity modes and it is shown that their appearance strongly depends on the lattice geometry and cannot be described in a one-dimensional framework.
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I. INTRODUCTION

Bound states in waveguides, and especially in waveguide bends, have recently been the subject of widespread theoretical and experimental investigation. Goldstone and Jaffe proved[1] that bends, which behave like local bulges in the guide, always support bound states in constant cross-section quantum waveguides under the condition that the wave function vanishes on the boundary. Papers by Carini *et al.*[2–4] deal with calculating energies of single and multiple bound states in bent quantum waveguides and comparing them to results from microwave experiments. Much effort has also been spent on finding new and calculationally efficient approaches for determining bound-state energies in waveguide bends.[5,6] Such research was ultimately prompted by an interest in semiconductor device miniaturization. Since electronic transport properties through such quantum wires are influenced by the existence of localized states,[7,8] having a good understanding of bound states in bends is relevant to building small-scale integrated circuits.

There is also considerable current interest in designing integrated optoelectronic or all-optical circuits. A set of essential components in these circuits are electromagnetic waveguides. Traditionally, two main types of guides are used in controlling the linear propagation of electromagnetic (EM) waves: metallic guides for microwaves and dielectric guides for optical light. In two-dimensional (2D) structures, planar symmetry implies that the waveguide modes can have either TM or TE polarizations.[9] One can then reformulate the problem for metallic waveguides in terms of a single scalar field. On the boundary the field amplitude is zero for TM modes and the field derivative vanishes for TE modes. The results of Ref. 1 thus carry over to electromagnetic waves with TM polarization in 2D metallic waveguides as well: Any bulge or bend will generate a bound state. We note that in the case of a dielectric waveguide with a high dielectric contrast, the fields are similar to those of a metallic guide, so we expect that bulges and bends in these waveguides will also generate localized states in a similar manner. However, since these states can couple to free space modes, they will be decaying resonances and not bound states.

As an alternative to conventional (metallic or dielectric) components, photonic band gap (PBG) materials are well suited as building blocks of devices comprising all-optical circuits.[10–14] PBG waveguides, linear defects in PBG materials, are capable of guiding light at optical wavelengths without appreciable losses.[13] Furthermore, it has also been demonstrated that such guides can transmit EM waves efficiently through sharp corners.[14] The question of whether bound states exist in PBG waveguide bends arises naturally. In this paper, we study the conditions and the mechanism for the appearance of bound states in such guides. For simplicity, we consider only two-dimensional photonic crystals. However, the analysis presented here applies also to three-dimensional crystals. We present general arguments on PBG waveguide band structures, mode gaps, and bound states and illustrate the arguments with specific examples. We find that PBG waveguides, unlike conventional ones, can possess mode gaps. These gaps make it possible for bound states to exist in bends and in constrictions even above the cutoff frequency for guided modes. It is also shown that the appearance of bound states in bends cannot be described in a purely one-dimensional framework and that these states are closely related to cavity modes.

The outline of the paper is as follows. In Sec. II the methods of calculation are presented and in Sec. III PBG waveguides are studied. In Sec. IV, we investigate bound states in photonic crystal waveguides in both straight and bent waveguides.

II. METHODS OF CALCULATION

The dispersion relations for the PBG waveguides in this paper are calculated by solving Maxwell's equation in the frequency domain for given dielectric configurations.[15] A supercell with periodic boundary conditions is taken as the computational domain. The length of the cell corresponds to the periodicity of the dielectric in the direction of the guide, whereas the width was taken to be several (usually 12) lattice constants. The photonic crystal simulated in this way contains parallel, evenly spaced waveguides. We increased the distance between the guides by taking wider and wider unit cells until the frequencies obtained for the eigenmodes no longer depended on the cell size. In this way we ensure that the distance between the guides is sufficient so that modes localized in the guides do not appreciably couple to each other through the bulk. Therefore, we obtain the correct frequencies for the localized modes associated with an individual waveguide at each wave vector.

The bound states in various PBG waveguide configurations are studied by solving Maxwell's equations in the time domain. The computational domain used is rectangular and is bounded by a perfectly matching layer material[16] to minimize back reflections. Modes with a wide range of frequencies are excited by a dipole source with a Gaussian temporal profile. The modes that remain after transient ones decay are either bound states or slowly decaying resonances; they both show up as peaks on the time Fourier transform of the field measured inside the waveguide. The resonances can easily be distinguished from bound states by noting that bound states have an essentially infinite quality factor when a large enough supercell is used. Also, in waveguide configurations, resonances occur at frequencies corresponding to zero group velocity in the waveguide or in the frequency range corresponding to guided modes, whereas bound states exist inside the mode gaps. The frequencies of all the bound states can be identified by using a pulse short in time. Each bound state can be studied individually by using a long excitation pulse whose Fourier spectrum is peaked at the bound state frequency. The electric field configurations shown in this paper are snapshots taken after a long time once every transient mode has decayed, leaving only a single mode.

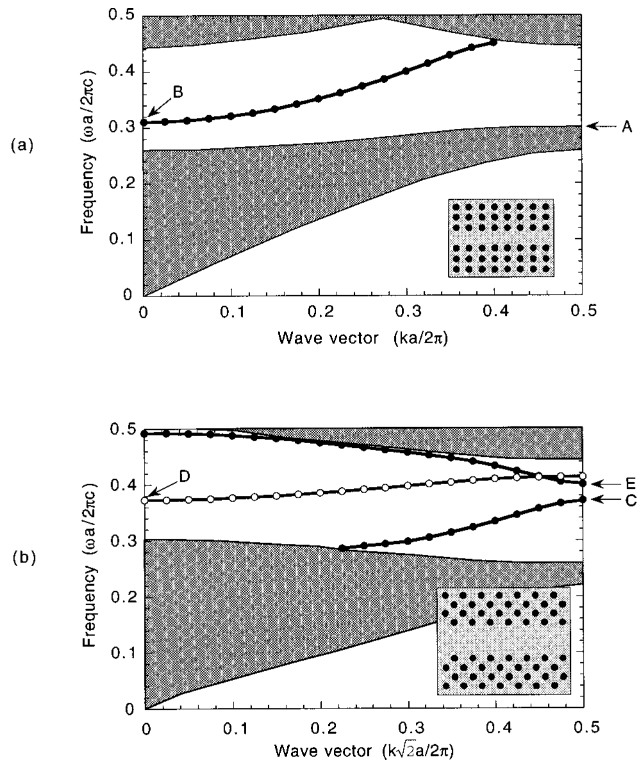

FIG. 1. Dispersion relations for the two photonic crystal waveguides. The geometry of the waveguides is shown in the insets. The gray areas are the projected band structure of the perfect crystal. The filled circles correspond to even modes and the open circles correspond to odd modes. The frequencies at the points indicated are (in units of $2\pi c/a$) $A=0.302$, $B=0.312$, $C=0.371$, $D=0.373$, and $E=0.400$.

III. GUIDED MODES IN PHOTONIC CRYSTAL WAVEGUIDES

Just as the regular arrangement of atoms in a crystal gives rise to band gaps, the periodicity of the spatial dielectric distribution in a photonic crystal may prevent electromagnetic waves of certain frequencies from propagating inside the bulk. Because of the periodicity, the modes of the electromagnetic waves in the crystal can be expanded in Bloch functions defined by their wave vectors **k**. While in the photonic band gap there are no solutions to Maxwell's equations for an infinite crystal for any real **k**, one does obtain solutions with complex **k**'s. These solutions will only become physical if the periodicity of the crystal is broken by introducing a defect.

We consider a square array of parallel, infinitely long high dielectric rods in air. The removal of a row of rods breaks the periodicity in one spatial direction. If the parameters of the crystal are such that there is a complete band gap for wave vectors perpendicular to the rods, then this defect can introduce modes that decay exponentially away from the defect but can still be described by a wave vector pointing along the missing row of rods. Such a defect acts like a waveguide: Waves of the right frequencies can propagate down the guide.[17]

For definiteness, we assume GaAs rods of circular cross section, with an index of refraction of 3.4, appropriate at optical wavelengths. From now on we restrict our analysis to TM modes. The largest TM band gaps (38%) occurs when the rods have a radius $r=0.18a$, where a is the distance between two neighboring rods.[17] The gap is centered at frequency $\omega=0.37\times 2\pi c/a$, which corresponds to the canonical free-space wavelength for light of 1.55 μm when $a=0.57$ μm.

We determine the TM band structures for two different PBG waveguides in order to illustrate their features that are different from those in conventional waveguides. The results are shown in Fig. 1. The horizontal axis is the wave vector in the direction of the guide, and we show the band structure in the reduced Brillouin zone scheme. The gray areas are the projections in the direction perpendicular to the guide of every mode in the band structure of the perfect crystal; These are extended modes in the crystal bulk. The modes inside the gap are localized to the row of missing rods.

In Fig. 1(a) we show the band structure for the guide created by removing a row of rods in the (10) direction of the crystal, as shown in the inset. We find a single guided mode inside the band gap. The electric field of the mode has even symmetry with respect to the mirror plane along the guide axis. The mode itself bears a close resemblance to the fundamental mode of a conventional dielectric waveguide: It has a sinusoidal profile inside the guide and decays exponentially outside.

In Fig. 1(b) the waveguide is made by removing three rows of rods in the (11) direction of the crystal (see the inset). There are now three guided modes inside the gap that can again be classified according to their symmetry with respect to the mirror plane along the guide axis. The first and the third modes are even, whereas the second mode is odd.

It is generally true that the number of bands inside the band gap equals the number of rows of rods removed when creating the guide. This can be understood from a simple counting of the states in the crystal. If we decrease the dielectric constant of a single rod in a perfect crystal, we pull up one defect state from the dielectric band.[17,18] If we repeat this for a whole row of rods, we pull up N localized states in an $N\times N$ crystal: one state at each k point for $\mathbf{k}$ along the guide. Analogously, when M rows of rods are removed, we pull up M guided modes at each $\mathbf{k}$ from the dielectric band. Nevertheless, at some $\mathbf{k}$'s the modes may have frequencies outside the band gap and the entire band may not be contained in the gap, as is the case, for instance, for the lowest guided mode band in Fig. 1(b).

For small k, the dispersion relations behave like conventional guided modes in a metallic waveguide with a cutoff $\omega-\omega_{\mathrm{cutoff}}\propto|\mathbf{k}|^2$. For these wave vectors, the wavelengths of the light is much larger than the variation in the dielectric function, so the light ''sees'' only an average uniform dielectric in the direction of the guide. However, close to the boundary of the Brillouin zone the bands level off. Because of the discrete translational symmetry of the crystal, the dispersion relations are repeated outside the first Brillouin zone; consequently, each band is restricted to a certain frequency range. The frequencies of the modes do not grow indefinitely with increasing $|\mathbf{k}|$, as in the case of conventional dielectric and metallic waveguides. This means that there may arise situations where a complete frequency gap will exist between the guided modes themselves. We term this frequency range a *mode gap.*

Such mode gaps do exist for the waveguide in Fig. 1(b): a small complete gap between the first and second guided mode bands, between points C and D. A larger gap for even symmetry modes can be seen between points C and E. In the case shown in Fig. 1(a), there is also a frequency range, below the cutoff, with no guided modes or extended modes, between points A and B.

In the Appendix we present a group-theoretical analysis on the origins and on the presence and absence of mode gaps in PBG waveguides. The arguments presented can facilitate the design of waveguide configurations with suitable mode gaps.

IV. BOUND STATES IN PHOTONIC CRYSTAL WAVEGUIDES

In this section we investigate how the existence of mode gaps affect the bound-state spectrum. As in conventional waveguides, one can try to create a bound states in a PBG waveguide in two different ways: by altering either the width or the curvature of the guide. First we consider what happens if only the guide width changes.

A. Bound states in straight guides

In a metallic waveguide, a wave packet trapped in a constriction has a larger transverse momentum than any guided mode, so its frequency will be higher than the cutoff frequency (if the cutoff exists). Such a state would decay into open channels in the guide. Therefore, to create a bound state in a metal guide, one has to put a bulge into the guide because bound states can exist only below the cutoff frequency for guided modes. If we view the guide with a bulge as three waveguide sections, two semi-infinite sections and one of finite length, the above requirement translates in terms of the dispersion relations for the two types of waveguide sections as follows: The existence of bound states requires the existence of guided modes for the finite guide section within the frequency range where no guided modes exist in the semi-infinite section.

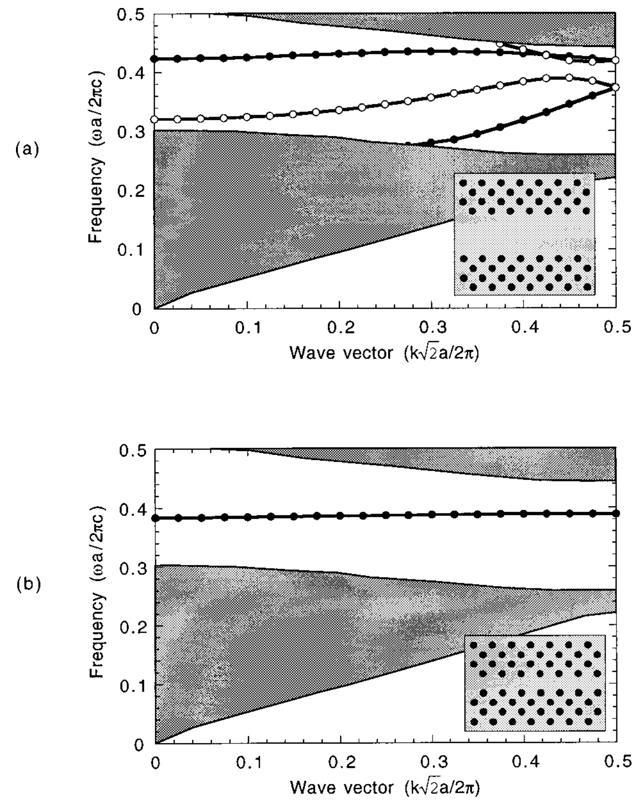

FIG. 2. Dispersion relations for the two PBG waveguides shown in the insets. The gray areas are the projected band structure of the perfect crystal. The filled circles correspond to even modes and the open circles correspond to odd modes.

As in conventional guides, it is possible to find bound states in photonic crystal waveguides with a bulge as well, except that we have the additional restriction that the state lie inside the band gap. If the bottom of the first guided mode is higher in frequency that the lowest frequency of the band gap, bound states can be created by increasing the width of the guide by, for instance, removing another row of rods in one section of the guide. However, in PBG waveguides, one also has an unconventional choice: We can look for a state in the gaps *between* the guided modes. As long as a part or all of a guided mode for the finite section falls into the mode gap, there is a possibility that bound states can exist within that frequency range. We illustrate this point in the following.

A guide with a mode gap for the rectangular array of rods can be formed by taking out four rows of rods in the (11) direction of the lattice. The band structure for the guide is shown in Fig. 2(a). We find four guided modes inside the gap. Because of the symmetry of the dielectric function of the guide, the modes can again be classified as even or odd with respect to a glide plane operation consisting of a trans-

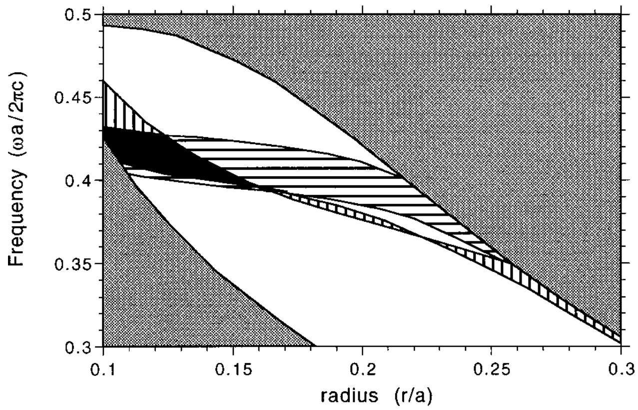

FIG. 3. Range of frequencies (black shaded area) for which bound states are allowed as a function of the radius of the rods. Horizontally hatched area, frequency range of the mode gap for the guide in Fig. 2(a); vertically hatched area, frequency range covered by the guided mode at the guide in Fig. 2(b); black shaded area, overlap of the two frequency ranges. The gray areas are the projected band structure of the perfect crystal.

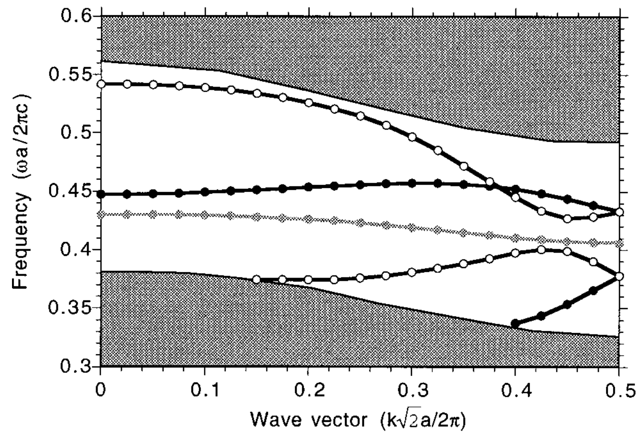

FIG. 4. Superimposed dispersion relations for the two guides in Fig. 2 when the radius of the rods is $r=0.12a$. Black line, guided modes for the wider guide, gray line, guided mode for the narrow guide. Filled circles correspond to even modes and open circles correspond to odd modes. The gray areas are the projected band structure of the perfect crystal.

lation by $a/\sqrt{2}$ parallel to the guide axis and of a reflection across the axis. the filled circles in the figure correspond to even modes and the open circles to odd modes. The upper two bands, having different symmetries, do cross. The two odd modes repel each other, creating a mode gap from $\omega=0.390\times 2\pi c/a$ to $0.417\times 2\pi c/a$.

In order to emphasize the contrast between PBG and conventional waveguides, we use a narrow constriction as the finite section to form a bound state: the guide in the (11) direction consisting of only one missing row of rods. Figure 2(b) displays the band structure of this guide. The single mode in the gap is even with respect to the mirror plane and covers a frequency range from $\omega=0.384\times 2\pi c/a$ to $0.388\times 2\pi c/a$.

For the rod radius used so far ($r=0.18a$) the mode gap and the guided mode do not overlap. However, we can tune r so that the guided mode of the narrow guide falls inside the mode gap of the wide guide. Figure 3 shows the frequency range of the mode gap (horizontal hatch) and that of the guided mode (vertical hatch) as a function of the radius of the rods. In the black shaded area the two frequency ranges overlap. The optimal radius is found to be $r=0.12a$ for the creation of bound states. Figure 4 shows the two band structures at this value of r superimposed on one another. The entire guided mode band of the guide chosen as the constriction falls inside the mode gap, thereby enabling the creation of a bound state in the constriction.

By choosing a configuration such that the constriction has length $3\sqrt{2}a$, we indeed find a bound state at $\omega=0.411\times 2\pi c/a$. The electric field of the mode is displayed in Fig. 5. We note that, in general, a dielectric defect in a metallic waveguide gives rise to a completely different field distribution for the defect mode. In that case, most of the field lies inside the high dielectric region, whereas in our case most of the field is confined to the inside of the narrow guide section. Since the mode is close in frequency to the mode gap edge, the decay constant κ is small ($\kappa\cong 0.27/a$) (Ref. 19) and the electric field decays slowly in the semi-infinite section. Nevertheless, it is a bona fide bound state whose counterpart would be impossible to obtain in conventional waveguides.

B. Bends in waveguides

Let us now turn our attention to bends in photonic crystal waveguides. Like straight waveguides with a bulge, bent waveguides can also be viewed as one finite and two semi-infinite waveguide sections of different wave vectors and dispersion relations joined together.[14] In analogy to the straight waveguide, we can create a bound state in a bend by joining three sections, the two semi-infinite sections having a mode gap and the finite section having a guided mode in that mode gap. As an example, we show a 180° bend in Fig. 6, where each of the three sections is identical to the three sections in Fig. 5. We indeed find a bound state in the waveguide bend, at $\omega=0.411\times 2\pi c/a$. Note that the localized electric field of this mode is nearly the same as that in Fig. 5.

We again emphasize that in a metallic waveguide with this bend configuration a state inside such a narrow bend section would have a higher transverse momentum than the lowest guided mode of the semi-infinite section. This state then would decay by coupling into guided modes. This does not happen in the PBG case, even though the finite section is roughly two and a half times narrower than the semi-infinite sections. The bound state also lies closer to the guided modes

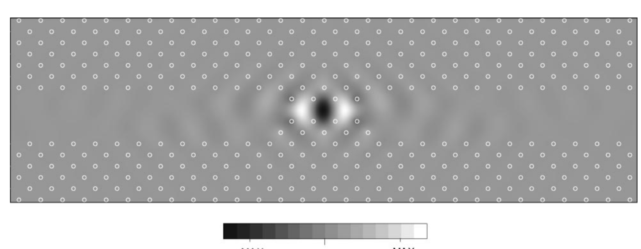

FIG. 5. Electric field for the bound state at $\omega=0.411\times 2\pi c/a$ in a constriction of length $3a$. Most of the field power is concentrated in the constriction itself. White circles indicate the dielectric rods.

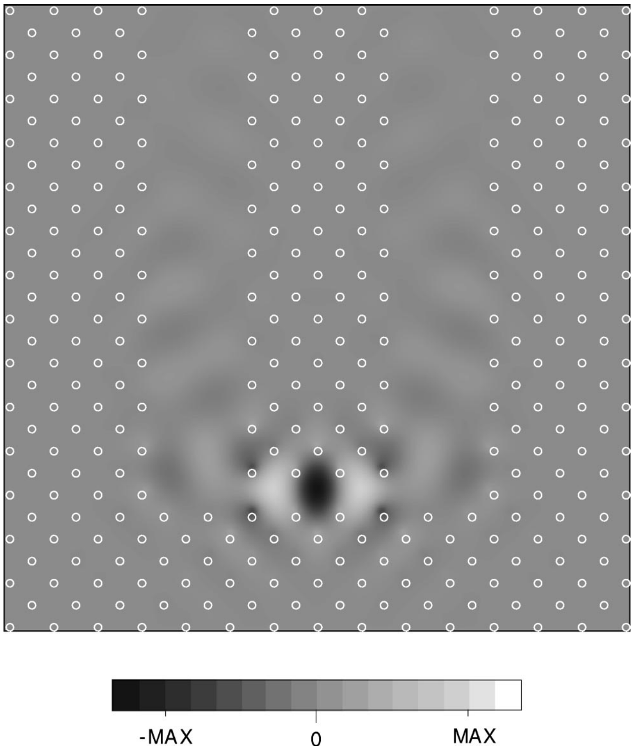

FIG. 6. Electric field for the bound state at $\omega = 0.411 \times 2\pi c/a$ in the 180° bend. White circles indicate the dielectric rods.

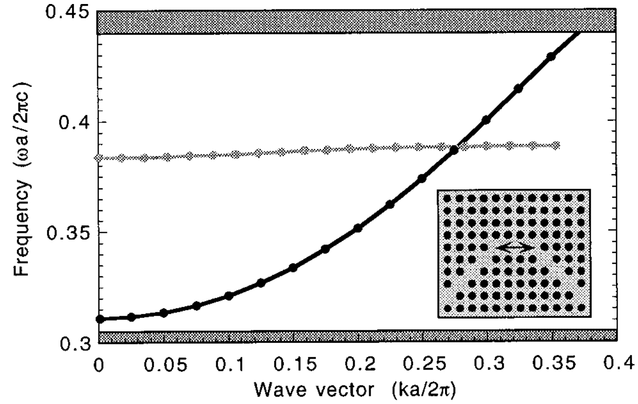

FIG. 7. Superposition of two band structures inside the photonic band gap. Black line, guided mode for the guide in the (1,0) direction with one row of rods removed; gray line, guided mode for the guide in the (1,1) direction with one row of rods removed, gray area, extended modes in the crystal.

than to the bulk modes in frequency, so the decay constant for the state is smaller in the guide that in the bulk. This implies that, from an experimental point of view, coupling into this bound state would be easier through the guide than through the bulk.

In order to investigate further the mechanism for the appearance of bound states in bends, we need a configuration that allows for a number of bound states to exist. Such a configuration preferably would consist of a finite section, whose guided mode covers most of the bulk gap, and of two semi-infinite sections, each possessing a guided mode band with a narrow bandwidth. We create one such configuration by removing one row of rods from the square array in the (10) and (11) directions, respectively. The guides and their band structures at $r = 0.18a$ are shown in Fig. 7 superimposed on one another. The dispersion relations indeed satisfy our requirements.

As the length L (indicated by the arrow in the inset) of the bend section is changed, we observe bound states of different frequencies. When $L = 3a$, we find three bound states, two even and one odd mode with respect to the mirror plane. The dielectric function and the electric field for these states is shown in the left panels of Fig. 8. We note that the highest frequency mode is above the upper cutoff frequency of the guided mode of the infinite guide section. Such a mode would not exist in analogous conventional waveguide structures, where there can only be a lower cutoff.

These bound states resemble cavity modes. Indeed, after removing the semi-infinite guide sections on both sides of the bend, we obtain similar eigenmodes at frequencies almost identical to the bound-state frequencies. These modes are shown in the right panels of Fig. 8.

We present two arguments to explain the close correspondence between bound states in PBG guides and cavity modes. In a metallic waveguide the boundary conditions for a TM bound state are $\mathbf{E} = \mathbf{0}$ at the guide boundaries. The bound-state frequencies are determined by matching the decaying solution outside the bend to the field inside the bend. By closing off the bend section, we require that the field be zero at the ends of the bend section, so the frequencies of the

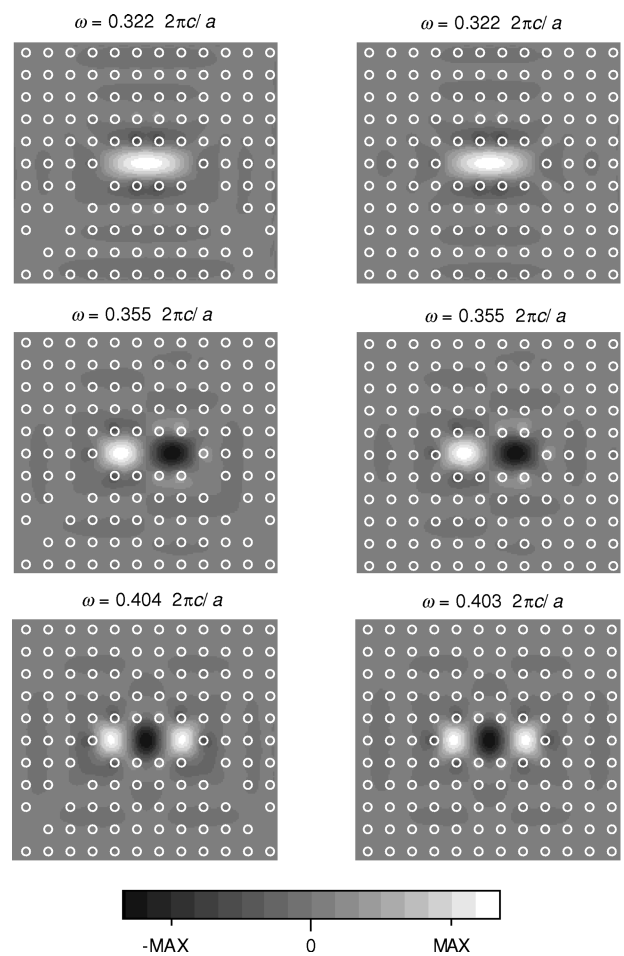

FIG. 8. Left panels, electric fields and frequencies of the three bound state inside the gap for the bend with length of the bend section $L = 3a$; right panels, electric fields and frequencies of the corresponding cavity modes.

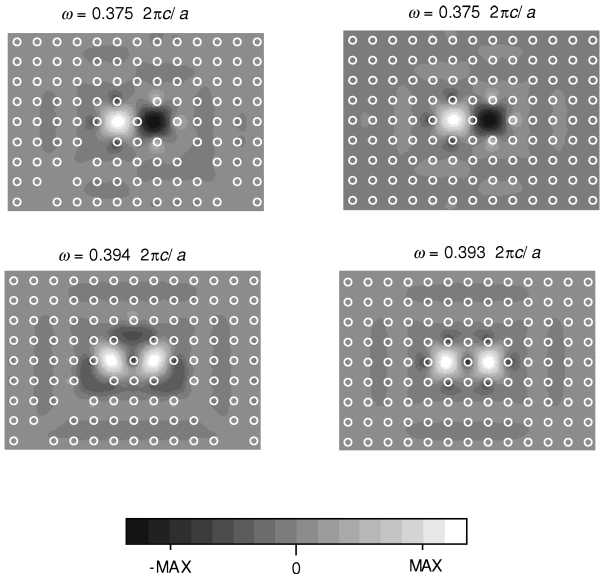

FIG. 9. Left panels, electric fields and frequencies of the two bound state inside the gap for the 90° bend; right panels, electric fields and frequencies of the corresponding cavity modes.

cavity modes may differ considerably from those of bound states. In the case of photonic crystals, zero boundary conditions are not required at the guide edges because there are exponentially decaying solutions in the crystal bulk. Thus the mode-matching requirement at the ends of the open bend (decaying field into the guide) does not differ greatly from the boundary condition for a cavity mode (decaying field into the bulk).

Another reason for the small shift in the frequencies when the waveguide is closed off is the following. To calculate the TM modes of a 2D photonic crystal structure with dielectric function $\epsilon(\mathbf{r})$, one can solve the following eigenvalue equation for the scalar electric field $E(\mathbf{r})$:

$$-\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)E(\mathbf{r})=\frac{\omega^2}{c^2}\,\epsilon(\mathbf{r})E(\mathbf{r}) \tag{1}$$

by minimizing the energy functional

$$\frac{\displaystyle\int \frac{1}{\epsilon(\mathbf{r})}\,E^*(\mathbf{r})\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)E(\mathbf{r})dr}{\displaystyle 2\int E(\mathbf{r})^2 dr}. \tag{2}$$

If the waveguides are open, the solution $E(\mathbf{r})$ is small outside the bend section since the bound states decay exponentially into the guide. Changing $\epsilon(\mathbf{r})$ in that part of the guide by closing off the bend section then causes only a small perturbation in the quantity in the numerator, so the frequencies change only minimally.

For shorter bend sections, we find the following bound states: for $L=2a$, $\omega=0.330\times 2\pi c/a$ (even) and $\omega=0.379\times 2\pi c/a$ (odd); for $L=a$, $\omega=0.344\times 2\pi c/a$ (even), all corresponding to cavity modes (the fields are not shown). In analogy, we might expect the 90° bend $(L=0)$ to have one bound state, in the bend corner, corresponding to the cavity mode for one missing rod in an otherwise perfect crystal. Yet, instead we find two bound states, neither of which is localized in the corner. One of the states is even and the other one is odd with respect to the mirror plane, as shown in the left panels of Fig. 9. Both states are localized at the two vacancy sites $\sqrt{2}a$ away from the corner.

This anomalous behavior is due to the fact that the frequency of the mode for the single rod cavity is $\omega=0.385\times 2\pi c/a$, which falls in the guided range of the semi-infinite sections of the guide. (This is reasonable because this cavity mode locally is similar to the guided mode for wavelength $\lambda=2\sqrt{2}a$ or for $k=\pi/\sqrt{2}a$.) This cavity mode couples with the guided modes and it shows up as a resonance in the bend corner.

The two bound states instead correspond to the coupled cavity modes shown in the right panels of Fig. 9. The cavity is composed of two vacancies, with their centers separated by two lattice constants. As pointed out earlier, each vacancy by itself supports a cavity mode at $\omega=0.385\times 2\pi c/a$, which would lie in the guided range of the infinite sections of the guide. However, since the vacancies are in close proximity to each other, there is a finite coupling between them, which in turn splits the other wise degenerate levels into an odd and an even bound state, with frequencies that respectively fall just below and just above the guided mode frequency range. Such unconventional bound states demonstrate that bound-state creation in PBG waveguide bends cannot always be described in a one-dimensional framework and they can strongly depend on dielectric function.

V. SUMMARY

We have shown that the periodicity of the photonic crystal waveguide gives rise to mode gaps between different guided modes. Such mode gaps make it possible to create bound states in a waveguide with a constriction and in bends. Bound states in PBG bends closely correspond to cavity modes. We have also observed that the existence of certain bound states can critically depend on the geometry of the bend in question and cannot always be predicted using arguments based on one-dimensional models.

ACKNOWLEDGMENTS

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APPENDIX

In this part of the paper we demonstrate how it is possible to give a simple explanation of the main qualitative and quantitative characteristics of the PBG waveguide dispersion relations, including the appearance of mode gaps. We show that the different types of mode gaps in band structures seen earlier arise from simple symmetries of the dielectric function. The following group-theoretical analysis allows one to design waveguides with suitable mode gaps easily.

As we have seen, photonic crystal guided mode fields resemble modes in conventional waveguides. So, in order to

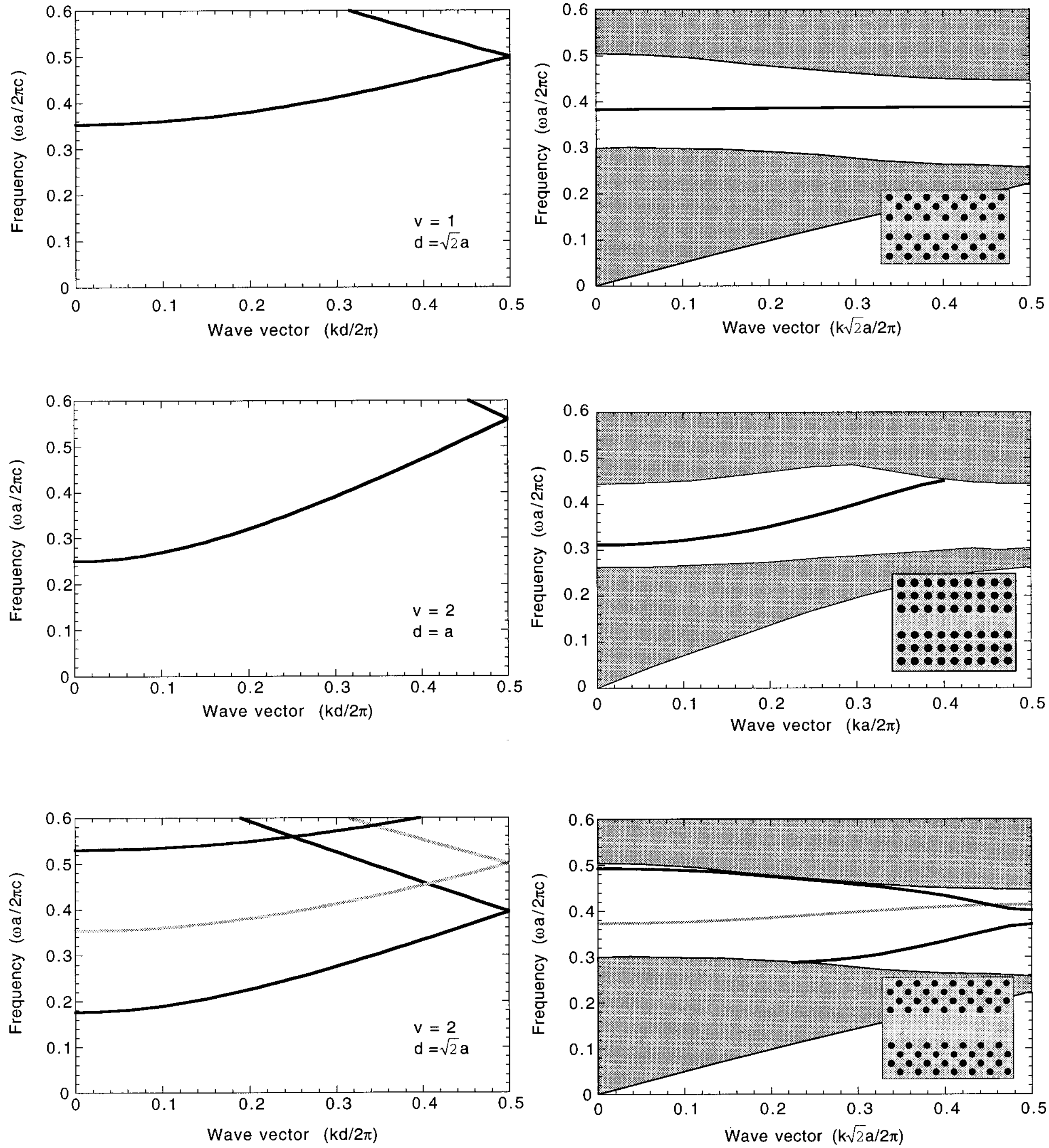

FIG. 10. Left panels, dispersion relations calculated from symmetrizing a set of basis functions for the symmetry group *G*. The periodicity *d* and the relative width v used are shown on each of the graphs. Right panels, band structures for the PBG waveguides displayed in the insets. The gray areas are the projected band structure of the perfect crystal. Black lines, even modes; gray lines, odd modes.

find the band structure for PBG guides, we start out with the exactly solvable case of TM modes in a straight hollow two-dimensional metallic waveguide. First we consider a metallic waveguide of width b, on which we have imposed an artificial periodicity *d*. For TM modes, Maxwell's equations for the electric field $\mathbf{E}=E(x,y)e^{i\omega t}$ yield

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)E(x,y)=\frac{\omega^2}{c^2}E(x,y), \qquad \text{(A1)}$$

with boundary conditions $E(x,y)=0$ at $y=\pm b/2$. Because of the periodicity in the x direction, we can classify the modes by their wave vector $\mathbf{k}=(2\pi/d)\tilde{k}\hat{x}$. One possible set of basis functions for this $\mathbf{k}$ is $\{e^{2(l+\tilde{k})\pi i x/d}\sin[m\pi(y/b+\frac{1}{2})]\}$, with $l=0,\pm1,\pm2,\ldots$ and $m=1,2,3,\ldots$. Each function in the set corresponds to an eigenvalue with $\omega=(2\pi c/d)\sqrt{(l+\tilde{k})^2+m^2/4v^2}$, where $v=b/d$ is the relative width of the waveguide.

The dispersion relations for the metallic waveguide are altered in two ways in PBG guides. First, the bands that are

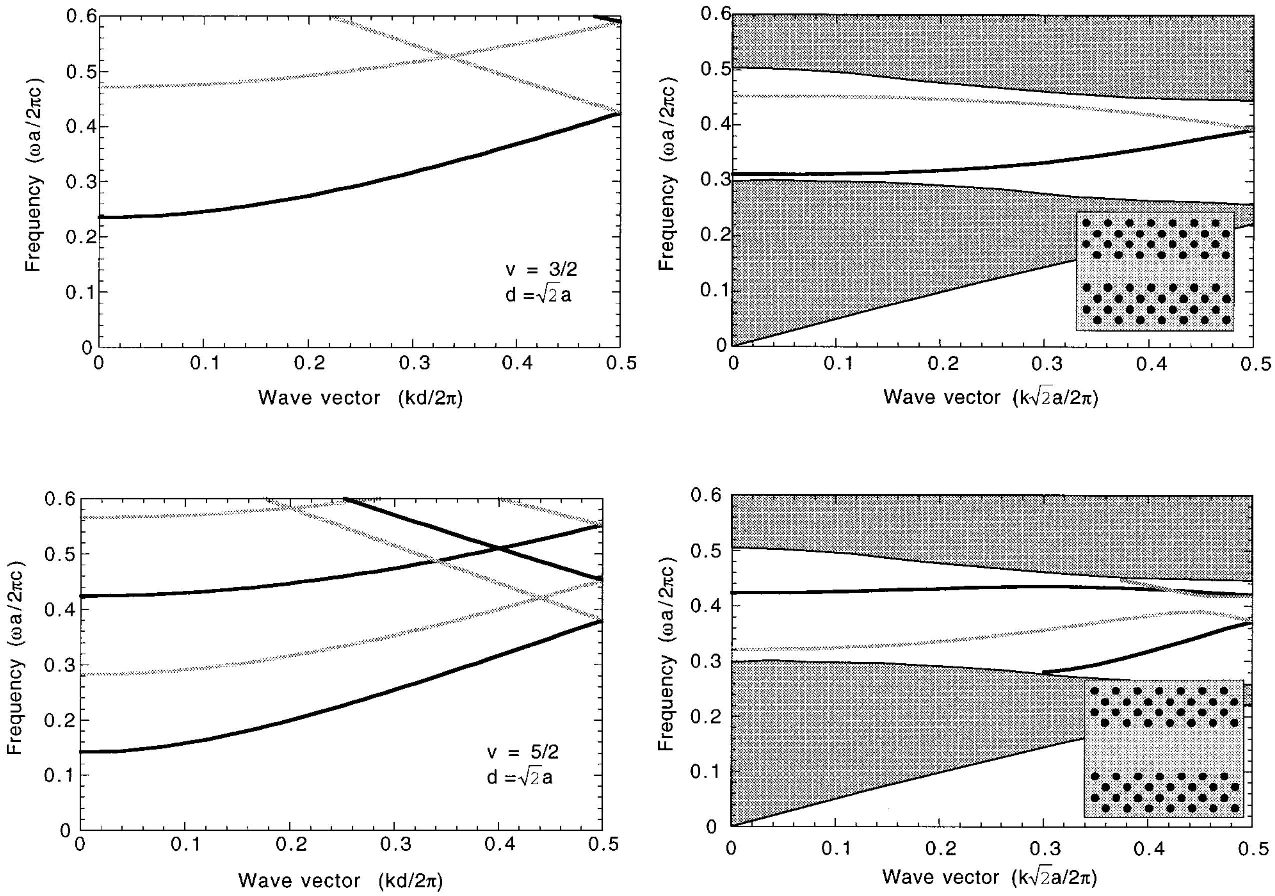

FIG. 11. Left panels, dispersion relations calculated from symmetrizing a set of basis functions for the nonsymmetry group G'. The periodicity d and the relative width v used are shown on each of the graphs. Right panels, band structures for the PBG waveguides displayed in the insets. The gray areas are the projected band structure of the perfect crystal. Black lines, even modes; gray lines, odd modes.

outside the first Brillouin zone fold back because the periodicity is no longer artificial. Second, bands crossing may repel each other when continuous translational symmetry is lost as the metallic boundaries are replaced by the PBG material. Yet discrete translational symmetry is always retained, as well as symmetry under a certain point group G, which depends on the dielectric function of the guide.

First, let us consider guides that are invariant under $G = \{E, \sigma_x, \sigma_y, I\}$. E here is the identity operator, σ_x and σ_y are reflections across the x and the y axes, respectively, and I is inversion through the origin. (Such are the guides in Fig. 1.) Since the periodicity is only in the x direction, the irreducible Brillouin zone is a line from $\Gamma(\tilde{k}=0)$ through $\Delta(0<\tilde{k}<\frac{1}{2})$ to $X(\tilde{k}=\frac{1}{2})$. For Δ, the point group is $\{E, \sigma_y\}$, so the guided modes can be divided into ones that are even or odd under σ_y. At both of the high symmetry points Γ and X the point group is just G, which has four irreducible one dimensional representations.

Keeping the symmetry under σ_x in mind, we choose the unit cell such that the centers of the rods at the guide edge are at $x=0$. In vacuum, a pair of degenerate modes at X consists of an even and an odd mode under σ_x. They always have the same symmetry under σ_y. The odd mode has a node at $x=0$, whereas the even one has a maximum there. Since in the PBG guide the even mode has a higher fill factor[20] than the odd one, it must have a lower frequency. In this way the degeneracy of the modes at X is removed and the level splitting creates mode gaps at the Brillouin zone edge.

The left panels of Fig. 10 show the band structures calculated from symmetrizing the basis function set, with the actual dispersion relations for three PBG guides to the right of each plot. The periodicity d and the relative width v used in the three calculations are indicated on the plots. The black lines denote even modes, and the gray lines denote odd ones. Having taken into account the fact that degenerate modes repel each other, a remarkable similarity can be seen between the corresponding band structures in the frequency range of the band gap.

In this work we also investigated another type of guide, shown in Fig. 3(a). This guide is invariant under a different group of symmetry operations $G = \{E, \{\sigma_x|\mathbf{f}\}, \{\sigma_y|\mathbf{f}\}, I\}$, where $\mathbf{f}$ is the fractional translation equal to $d/2\hat{x}$. Because the group is now nonsymmorphic, the point group size doubles at X and we obtain five irreducible representations. The degenerate pairs of the basis functions at X always belong to the same two-dimensional irreducible representation. This representation is compatible with the sum of an even and an odd representation along Δ. The essential degeneracy at X is due to the nonsymmorphicity of the symmetry group and is not influenced by the specific features of the dielectric function; therefore, no mode gaps open up at the Brillouin zone edge. However, because the symmetries of individual bands have also changed, some bands that were allowed to cross in the case of the symmorphic group will now repel and this effect produces new mode gaps.

We compare two PBG guide band structures with the dispersion relations calculated from symmetrizing the basis function set in Fig. 11. The two guides examined are ones created by removing two and four rows of rods in the (11) crystal direction, respectively, as shown in the insets. The periodicity d and the relative width v used are indicated on the plots. As expected, mode gaps open up solely when bands of the same symmetry repel.

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[20] The fill factor is defined as the ratio $I_{\text{high dielectric}}/I_{\text{crystal}}$, where $I_V = \int_V E(\mathbf{r}) D(\mathbf{r}) d\mathbf{r}$. A high fill factor means that a lot of field is in the high dielectric, so the frequency of the mode is low.