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Creating a gap without symmetry breaking in two-dimensional photonic crystals

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Degeneracy can be broken and spectral gap (including absolute gap) can be created by adding a small fraction of metallic component at the center of each dielectric cylinder without breaking the space group symmetry in two-dimensional photonic crystals. This phenomenon can occur for both normal and accidental degeneracies and does not exist in electron systems. Physical explanations are given for both cases. This facilitates the opening of large absolute gaps. The method can be generalized to three-dimensional photonic crystals and opens a unique way to engineer photonic band gaps.

In recent years there has been a great deal of interest in fabricating photonic crystals that possess a frequency region in which electromagnetic (EM) waves cannot propagate in any direction.¹⁻⁴ This frequency region is called the photonic band gap (PBG), which is analogous to the electronic band gap due to spatial periodic electrostatic potential in natural crystals. The absence of normal modes of EM waves inside PBG can give rise to some peculiar physical phenomena,¹⁻⁴ as well as wide application in several scientific and technical areas.^{1,2}

Since all the novel properties as well as the application of photonic crystals rely on the existence of PBG, it is essential to design crystal structures with a spectrum gap as large as possible. In fact, people have been searching for materials with large PBG since the beginning of the investigation of photonic crystals. In general, there are two ways to produce large PBG material. The first is to construct artificially new structures which possess large PBG.^{1,5,6} This method is often limited in scope. The second is to draw on the experience of the band structure of electron systems in order to break the symmetry of the structure and material.⁷⁻⁹ One of the most severe limits to the formation of PBG comes from the degeneracy of photonic bands at high symmetry points in the Brillouin zone. It has recently been reported that the symmetry reduction of “atom” configuration by introducing a two-point basis set in simple two-dimensional (2D) lattices can remarkably increase the gap,⁷ similar to the 3D case for diamond structure.⁵ In addition, anisotropy in “atom” dielec-

tricity can also break the degeneracy of photonic bands to create a gap.^{8,9}

In this work, we report a unique way to produce large gaps. Here we demonstrate that the degeneracy can be broken and the gap can be created without breaking the symme-

FIG. 1. The calculated photonic band structure for a square lattice. (a) Dielectric cylinder with radius $R=0.42$ in air for P wave. (b) Coated cylinder with dielectric cylinder radius $R=0.42$ and inner metallic cylinder radius $r=0.12$. The dielectric constant for the dielectric and metallic components are taken as 11.4 and -1000 , respectively. The insets in (a) and (b) show the microstructures.

FIG. 2. The displacement field energy distribution in Wigner unit cell for A and A' points marked in Fig. 1(a). The structure and parameter are the same as in Fig. 1.

try of the structure or the isotropy of the material. This embodies the special feature of PBG, which is different from electronic systems. We'll take 2D photonic crystals as an example to describe the physical principle in the following.

Two-dimensional photonic crystals can be fabricated more easily than three-dimensional ones in the infrared (IR) or the visible to near-IR wavelength ranges,^{10–12} it can also find some important uses such as a feedback mirror in laser diodes¹³ and waveguide for light transmission.^{14,15} Perhaps for this reason, much attention has been drawn towards them. It is well known that the electromagnetic wave can be de-

composed into E polarization (S wave) and H polarization (P wave) modes for a 2D structure. An absolute band gap exists for a 2D PBG crystal only when band gaps in both polarization modes are present and they overlap each other. Thus it is our aim to search for some structures with an optimal overlapping band gap (absolute gap). It is reported that the square lattice of dielectric cylinder have gaps for S wave in the normal frequency region (in dimensionless units). But, for the P wave, there are no significant gaps in this frequency region due to either normal or accidental degeneracies. Therefore, a square lattice of dielectric cylinder in air does

Fig.3

FIG. 3. The magnetic-field energy distribution in Wigner unit cell. (a) For B point in Fig. 1(a), (b). For C point in Fig. 1(a). (c) For B' point in Fig. 1(b). (d) For C' point in Fig. 1(b). The structure and parameter are the same as in Fig. 1.

fig.4

FIG. 4. The calculated photonic band structure of a square lattice of coated cylinder in air for P wave (solid lines) and S wave (dashed lines). The radii of the dielectric cylinder and inner metallic cylinder are $R=0.42$ and $r=0.2$. The dielectric constant for the dielectric and metallic cylinder are taken as 11.4 and -1000 , respectively. An absolute gap (shaded region) appears between 0.643 and $0.683(\omega a/2\pi c)$.

not give rise to the absolute PBG's. However, in this work we find that both normal and accidental degeneracies can be broken after adding a small fraction of metallic component in the center of the dielectric cylinder without breaking the symmetry of the system. Thus, the square lattice of dielectric cylinder can exhibit photonic gap for the P wave and the absolute gap can be created by adjusting the size of the metal cylinder.

The photonic band structures for a photonic crystal can be well handled by band theoretic methods, such as the plane-wave method⁹ and the multiple-scattering method.^{16–18} Here we use the multiple-scattering method but generalize it to treat complex coated scatterers that include the metallic component. The lattice sums involved in our method are represented in terms of an absolutely converging series over the reciprocal lattice,¹⁶ and in contrast to the method used by Ewald,¹⁷ these series may be accelerated by successive integration to any order. Because there are no series expansions of the dielectric constant, the method may also be applied in cases when the dielectric constant takes on imaginary values.

We first calculate the band structure of the square lattice of the dielectric cylinder in air. For S wave, some gaps exist as reported in Ref. 2. However, there are no gaps for P wave, and hence no absolute gap. Figure 1(a) displays the band structure of P wave in square lattice with dielectric cylinders of radius $R=0.42$ and dielectric constant $\epsilon=11.4$. Here, we take the lattice constant as the length unit. It is easy to see from this figure that there exist many degeneracies at high symmetry points, which precludes the existence of photonic gaps.

The situation can be changed by introducing a metallic

component in the center of every dielectric cylinder, resulting in “coated cylinder” photonic crystals. The coated structures have the same symmetry group as the former. That is to say, adding a small fraction of metal in the center of every dielectric cylinder does not break the symmetry of the structure. However, the degeneracy marked by A and A' in Fig. 1(a) can be lifted as shown in Fig. 1(b). Figure 1(b) displays the band structure of the square lattice of coated cylinder with a dielectric cylinder of radius $R=0.42$ with an inner metallic cylinder of radius $r=0.12$. The dielectric constant of the dielectric region in this system is taken as the same as that shown in Fig. 1(a), whereas the dielectric constant of the metallic component is taken as -1000 . It has been shown in Refs. 20, 21 that this choice of the dielectric constant for the metal can produce almost the same band structures as that obtained from a realistic metal dielectric constant. Now one can raise the question of whether the metallic cylinder is the only contributing factor to the opening of gaps at A and A' points? As a control calculation, we calculate the band structure of metallic cylinders in air with various radii r and $\epsilon=-1000$. For $r<0.2$, we do not find any gap in the region $\omega a/2\pi c<2.0$.

What is the key factor that leads to the breaking of degeneracy and hence the creation of a gap when the metal cylinder is introduced? In order to clarify this issue, we calculate the field distribution at this symmetry point. The displacement field distributions in a Wigner unit cell which correspond to A and A' points in Fig. 1(a) are plotted in Fig. 2. When a metallic cylinder is inserted into the center of each cylinder, the field distribution in the unit cell will change and lead to the shift of frequencies of A and A' . According to perturbation theory,¹⁹ the frequency shift for P wave can be estimated by the following formula:

$$\left(\frac{\bar{\omega}_{nk}}{\omega_{nk}}\right)^2 - 1 = \frac{\int [\bar{\epsilon}^{-1}(r) - \epsilon^{-1}(r)] |D_{nk}(r)|^2 dr}{\int \epsilon^{-1}(r) |D_{nk}(r)|^2 dr}.$$

Here $\bar{\epsilon}(r)$ and $\bar{\omega}_{nk}$ represent the dielectric constant and eigenfrequency, respectively, corresponding to the original ϵ and ω_{nk} . The function $\bar{\epsilon}^{-1}(r) - \epsilon^{-1}(r)$ is nonzero, say, δ , only at the insertion position. $D_{nk}(r)$ describes the displacement field in unit cell. From Fig. 2, we observe that $|D_{nk}(r)|$ for A is small in the center of cylinder, but it is large for A' . The insertion of a metal cylinder in the center of every cylinder will push the eigenfrequency down for A' and the frequency of A will remain unaffected as can be estimated from the above formula. Owing to the different amount of frequency shift for A and A' , the degeneracy is lifted naturally with the insertion of a metallic cylinder. For example, when a metal cylinder with $r=0.02$ is inserted in the center of cylinder, the degeneracy of A and A' is lifted. The frequency from the band calculation for A and A' are 0.498 and 0.491, respectively. The corresponding results estimated by the above formula are 0.498 and 0.493. The excellent agreement between the estimated and calculated results confirms our understanding of the physical origin of this degeneracy breaking.

We would like to point out that the fields for the degeneracy points, A and A' in Fig. 1(a), are not related by a simple symmetry transformation. This kind of degeneracy is called accidental degeneracy. However, for some degeneracy

points such as B and B' in Fig. 1(a), their field distributions are symmetry related. Figure 3(a) describes the magnetic-field distribution of B point in Fig. 1(a). The field of B' point can be obtained by rotating 90° from the field of B point. This kind of degeneracy is called normal degeneracy. For these normal degeneracy points, the situation is not as simple as the accidental one when the metallic cylinder is inserted. When the radius of the metallic cylinder is $r < 0.11$, the frequencies of the B and B' points will shift down together with the increase of the radius of the metallic cylinder, and the degeneracy will not be broken. This is a result of normal degeneracy. However, the frequency of C point will also shift downwards but in a much slower rate when compared to the shift of B and B' . These can also be explained by the above perturbation formula combined with the displacement field distributions of corresponding points. When the radius of the metal cylinder inserted is about 0.113, B , B' , and C join altogether. If the radius of the metal cylinder inserted continues to be increased such as $r = 0.12$ [Fig. 1(b)], B' and C will possess the degeneracy properties of the original degeneracy points of B and B' , while leaving B alone will break the original degeneracy of B and B' points. The magnetic-field distribution of B' point in Fig. 1(b) is plotted in Fig. 3(c). The field of C point in Fig. 1(b) can be obtained by rotating 90° from Fig. 3(c). The feature of field distribution for the original C point which is shown in Fig. 3(b) transfers to B point as shown in Fig. 3(d). It should be pointed out that the fact that the degeneracy of B and B' is lifted at the same time when a new degeneracy at B' and C is formed is due to the nonsymmetry breaking insertion. This behavior occurs only for normal degeneracy points, not for accidental degeneracy. As will be shown later, this switching of degeneracy points can facilitate the creation of absolute gaps. Thus, both accidental and normal degeneracies can be broken and new gaps can be created by inserting a metallic component without breaking the space group symmetry of the structure.

According to the above notion, we can create an absolute gap which does not exist in square lattice of pure dielectric cylinders. Figure 4 depicts the photonic band structure for a square lattice of coated cylinder in air. The radii of the coated cylinders and metallic cylinders are 0.42 and 0.2, respectively. The dielectric constant of the dielectric cylinder is 11.4. The solid and dotted lines in Fig. 4 correspond to P and S waves, respectively. A gap for P wave around $\omega a/2\pi c = 0.65$ appears in this coated system. This gap is created by the switching of the ordering of the normal degeneracy at D and D' in Fig. 1(a), i.e., the degeneracy of 8Γ [D' in Fig. 1(a)] and 9Γ [D in Fig. 1(a)] is lifted while the new degeneracy of 7Γ and 8Γ [D' in Fig. 1(b)] is formed. An absolute PBG occurs where the 7–8 band gap for S wave and the 8–9 band gap for P wave overlap. The shaded area represents the absolute PBG.

In conclusion, we find that the degeneracy can be lifted and the gap (including the absolute gap) can be created without breaking the space group symmetry. This phenomenon can occur for both accidental and normal degeneracies and does not exist in electronic systems. For both cases the physical origin of the degeneracy breaking can be understood from the a perturbative approach together with the eigenfield analysis. The creation of gaps demonstrated here provides a unique way to search for large absolute gaps in 2D photonic crystals.

Although what we have discussed here is for the 2D square lattice, nevertheless, our physical analysis is not limited to this system. This way of creating gaps should also be valid in other microstructures in 2D and 3D photonic crystals. Thus, it opens a unique method to engineer photonic band gaps.

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¹See, for example, *Photonic Band Gaps and Localization*, edited by C. M. Soukoulis (Plenum, New York, 1993); J. Opt. Soc. Am. B **10**, 208 (1993); *Photonic Band Gap Materials*, edited by C. M. Soukoulis (Kluwer, Dordrecht, 1996).

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