Jahn-Teller effect in two-dimensional photonic crystals

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We study double degenerate defect states in the band gap of the two-dimensional photonic crystal which can be split by the Jahn-Teller distortion of the lattice. We present a group theoretical analysis of the splitting effect. The effect is supported by supercell plane wave model and by the finite difference time domain technique. We suggest ways for using the effect in photonic switching devices and in waveguides.

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Photonic crystals are of importance for numerous applications involving light modulation.1 Interest in the construction of active tunable photonic elements has led to the idea of introducing interactions into an photonic crystal. Following the analogy with the solids, interaction effects in the photonic crystals may be realized in two ways. The first is the Coulombic interaction, which in the case of the photonic crystal implies a nonlinear optical behavior.2 Another possible interaction is photon-phonon interaction, which should appear in a photonic crystal subjected to mechanical vibrations.3 It has been reported4 that tuning the driving frequency of vibrations to the frequency of interband transition leads to a coupling of the optical modes.

In this paper we show that the Jahn-Teller effect is possible as a prototype of photon-phonon interactions in photonic crystals. The splitting of the degenerate state by some interaction is photon-phonon interaction, which should be condensed, the resulting splitting of the degenerate state leads to a coupling of the optical modes.

In this paper we show that the Jahn-Teller effect is possible as a prototype of photon-phonon interactions in photonic crystals. The splitting of the degenerate state by some interaction is photon-phonon interaction, which should be condensed, the resulting splitting of the degenerate state leads to a coupling of the optical modes. The method we use is time dependent perturbation theory for non-Hermitian perturbations of the type described by Hamiltonian (1)

\[ \mathcal{H} = \mathcal{H}_0 + V = \begin{pmatrix} 0 & i \nabla \times \frac{\delta \epsilon}{\epsilon(r)} \\ -i \nabla \times \frac{1}{\epsilon(r)} & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ i \nabla \times \frac{\delta \epsilon}{\epsilon(r)} & 0 \end{pmatrix}, \]

where \( \delta \epsilon = (\delta \epsilon / \partial r)[0] \mathbf{R}(t) \) (the index 0 shows that the derivative is taken at zeroth displacement). In the frame of time dependent perturbation theory for non-Hermitian perturbations, we are interested in finding a solution of the Schrödinger equation as an extension over unperturbed states \( \Psi_i^{(0)} \) describing the degenerate state with the frequency \( \omega_0 \), \( \Psi_i = \sum a_i(t) \Psi_i^{(0)} \), where \( a_i(t) \) are time-dependent coefficients. We arrive at

\[ \frac{\partial a_i(t)}{\partial t} = -i \sum_{j} a_i(t) V_{ij} e^{i \omega t}, \]

where \( V_i = \langle \Psi_i^{(0)} | \mathcal{V} | \Psi_j^{(0)} \rangle = -\omega_0 \int (\partial \epsilon / \partial r) \mathbf{H}_i^{(0)} \cdot \mathbf{H}_j^{(0)} dr \). Since all \( \Psi_i^{(0)} \) wave functions represent just the same energy state, the resonance condition will be in the case when the driven frequency \( \omega = 0 \). This corresponds to a frozen vibronic mode. But this effect will be realized if and only if the matrix elements \( V_{ij} \) are not equal to zero.

To be more specific, we consider two-dimensional square photonic lattice of the dielectric rods in vacuum doped by the defect rod. The point group symmetry of the square lattice is \( C_4v \). If the defect rod is localized in the site of the lattice then by symmetry it may be described both by one-dimensional \( (A_{1g}, B_{1g}) \) and two-dimensional \( (E) \) irreducible representations of the group \( C_4v \). One-dimensional irreducible representations result in a nondegenerate photon state. The two-dimensional representation results in a doubly degenerate state represented by the two 1 \( \times \) 2 column basis vectors having the shape of the \( p_x \) and \( p_y \) orbitals.5,7 That is the state to be under our consideration.

All vibrations of the lattice can be presented in terms of the normal coordinates as a sum of the normal irreducible vibrations \( \alpha \). The vibronic perturbation can then be extended over normal vibrations \( \delta \epsilon(r) = \sum \alpha R_\alpha (\partial \epsilon / \partial \mathbf{r})[0] \). Each normal vibration \( \alpha \) is determined by the symmetrized displacements \( R_\alpha \) and so-called deformation potential \( \partial \epsilon / \partial \mathbf{r} \). By symmetrized displacements we mean collective (concerted) nuclear displacements which, under the symmetry operations of the molecular point group, transform according to one of its irreducible representations. For the defect crystal in ques-
tion, by molecular we mean a cell composed of the dielectric rods nearest to the defect. In this case, there are allowed $2A_1$, $B_1$, $2B_2$, and $2E$ normal irreducible vibrations of the lattice. The $A_1$ normal vibration is a totally symmetrical one, while the $B_1$ and $B_2$ modes are antisymmetrical normal vibrations described by the one-dimensional irreducible representations. The $E$ modes of the normal vibrations are characterized by the two dimensional irreducible representation with the $1 \times 2$ basis vector.

As follows from the Jahn-Teller theorem, to split the doubly degenerate $E$ photonic state the matrix element of the corresponding vibronic mode $\alpha$, $V_{ij}^\alpha = -\omega_0 \delta \langle \mathbf{H}^{(0)} \mathbf{E} \rangle \mathbf{r} \cdot V(r, \mathbf{R}_0) \mathbf{H}^{(0)} \mathbf{E} \mathbf{r} \rangle dr \neq 0$. Here $V(r, \mathbf{R}_0) = (1/e) \mathbf{R}_0 \cdot (\partial \delta / \partial \mathbf{r})$ is a perturbation potential caused by the corresponding normal vibrations $\alpha$ and described by the symmetry of the normal displacements. From the symmetry analysis, this matrix element is nonzero if and only if $E \times E = \alpha$. Since $E^2 = A_1 + A_2 + B_1 + B_2$, only the perturbations with the symmetry of the $A_1$, $B_1$, and $B_2$ vibrations can shift the degeneracy of the $E$ defect state.

In the case of the total symmetrical vibration $A_1$, $V_{yy}^{A_1} = V_{yy}^{A_1}$ and $V_{xy}^{A_1} = 0$. Solving Eq. (2) with these matrix elements, we find that the interaction of the photonic $E$ state with the $A_1$ vibration results in an equal shift of the doubly degenerate state without lifting the degeneracy. The situation is different in the case of the antisymmetrical $B_{1,2}$ modes. For the $B_1$ mode, $V_{xx}^{B_1} = -V_{yy}^{B_1}$ and $V_{xy}^{B_1} = 0$. As a result, the degeneracy of the $E$-photonic mode is removed, resulting in two levels $\omega_1^{B_1} = \omega_0 \pm V_{xx}^{B_1}$. For the $B_2$ mode, $V_{xx}^{B_2} = V_{yy}^{B_2} = 0$ and $V_{xy}^{B_2} = V_{xy}^{B_2}$. This results in the two split levels $\omega_1^{B_2} = \omega_0 \pm V_{xy}^{B_2}$.

From this analysis we note the following. First, because of the linear dependence of the perturbative potential on the amplitude of vibration $(V_{ij}^\alpha - \mathbf{R}_0)$, the splitting of the doubly degenerate level should show a linear scaling with the magnitude of the distortion of the lattice through a scaling coefficient called the constant of vibronic coupling or vibronic constant. Second, vibronic constants corresponding to different vibronic modes $\alpha$ are determined by different matrix elements $V_{ij}^\alpha$. These are the diagonal matrix element $V_{ij}^{B_1}$ for the $B_1$ mode and the non-diagonal matrix element $V_{ij}^{B_2}$ for the $B_2$ mode. It is natural to expect that the relative magnitudes of the shift of the defect mode will be greater in the case of the coupling defect state with the $B_1$ mode than with the $B_2$ mode.

Now, in order to provide numerical support for this Jahn-Teller effect, we present supercell plane wave and finite difference time domain (FDTD) calculations of the two-dimensional defect crystal. As a model crystal we consider a square photonic crystal of the dielectric rods, embedded in the air, with the lattice constant $a$, the radius of the rods $r = 0.2a$, and the dielectric constant $\varepsilon_r = 11.9$. Here, only modes with odd (TM-like) symmetry are considered, since that is the symmetry of the bands exhibiting a gap for the square lattice. We study the defect state created by the defect rod with the radius $r_d = 0.3a$ and the same dielectric constant $\varepsilon_d = 11.9$ as the other rods. That is, we are interested in the doubly degenerate defect state which in this case lies inside the first band gap. To simplify the analysis of the effect studied, we take the amplitudes of the rod displacements $|\mathbf{R}_d|$ as nonzero for only the nearest neighbors of the defect rod. We consider distortions of the lattice in the limits $\Delta r = 0 - 0.3a$, keeping in mind that only small distortions ($\Delta r \ll a$) allow for the applicability of the linear approximation of the vibronic potential [Eq. (1)].

The supercell plane wave calculations of the defect state have been performed with the number of plane waves $N = 1225$ by the usual technique. We worked with supercells including eight and 16 rods to test our data. For the frequencies inside the first band gap, the data showed a good convergence and a relative error less than 1%. A small dispersion (less than 0.05%) of the impurity band provides evidence of the small overlap between defect modes in the neighboring cells.

In Figs. 1 and 2 we present the supercell plane-wave calculations of the static Jahn-Teller splitting effect by the $B_{1,2}$ vibronic modes. Figure 1 shows the plane wave spectrum of the defect crystal for the magnitude of the distortion $\Delta r = 0.1a$. The dotted line shows the defect level in the unperturbed system. Figure 2 presents the distribution of the electric field for both split states, in the cases of coupling with the $B_1$ mode [(a) and (b)] and $B_2$ mode [(c) and (d)].

To get the defect spectrum using the FDTD technique, we have followed the approach developed in Ref. 9. Our computational domain contained $7 \times 7$ unit cells, with the defect localized at the center. Each unit cell was divided into 20 $\times$ 20 discretization grid cells. The computational domain was surrounded by perfect matched layers, with the thickness corresponding to ten layers of the discretization grid. The total number of the time steps was 80,000 with each time step $\Delta t = \Delta x/(2c)$. The analysis of the convergency of our data, performed with two times finer discretization grid cells, showed that the error in our calculations is less than 1%.

The FDTD calculations of the defect level splitting due to static Jahn-Teller distortion are shown in Fig. 3. We present the Fourier transform of the transmission spectral intensity of the Jahn-Teller splitting of the defect state by means of the $B_1$ and $B_2$ vibronic modes for the magnitude of the distortion $\Delta r = 0.1a$. The defect level of the unperturbed system $(\Delta r = 0)$ is shown by the dotted line. The corresponding distributions of the electric field for the two split modes are the same as that presented from the supercell plane wave calculation (Fig. 2) and are not repeated here. Since the intensities of the electric field have the highly symmetrical shape of the $p_x$ and $p_y$ orbitals (Fig. 2), centered on the defect, the Fourier amplitude of the defect spectrum depends on the point where the output data is collected. For the $B_1$ mode, if we collect the data on the $x$ axis, only the $p_x$ state is manifested in the Fourier spectrum (Fig. 3, dashed line). If we collect the data on the $y$ axis, only the $p_y$ state is noted (Fig. 3, dashed-dotted line). If the collecting point is selected on the line $x = y$, both $p_x$ and $p_y$ states are seen in the defect spectrum. In this case the Fourier spectrum overlaps completely with both peaks.

In the case of the $B_2$ mode, the field distributions of the
electric fields are directed along \( x = y \) and \( x = -y \) lines [Figs. 2(c) and 2(d)]. So, if we are watching the defect spectrum on the line \( x = y \) we can see only the state with the field distribution directed along \( x = y \) line (Fig. 3, dashed line). If we collect the data on the \( x = -y \) line, we can see only the state directed along \( x = -y \) line (Fig. 3, dashed-dotted line). Finally, if we collect the data at any other point (e.g., on the line \( x = 0 \)) we can see both of these states. We conclude that it is possible to manipulate the symmetry of the split photonic states of the defect level by choosing (a) the proper distortion of the nearest neighbors (\( B_1 \) or \( B_2 \) modes) and (b) the proper points for collecting data.

Figure 4(a) shows the dependence of the frequency splitting of the defect state on the relative amplitude of the distortion for the \( B_1 \) and \( B_2 \) modes. Here we present the data obtained by the supercell plane wave technique (dashed lines) and by the FDTD calculations (solid line). First, we note that the data calculated by both techniques are in rea-

**FIG. 1.** The supercell plane wave spectrum of the defect photonic crystal coupled with the \( B_1 \) (solid line) and \( B_2 \) (dashed line) vibronic modes for the magnitude of the rod displacement \( \Delta r = 0.1a \). Dotted line shows the doubly degenerate defect level in the unperturbed system.

**FIG. 2.** The distribution of the electric field intensity for two split defect states: in the cases of coupling with the \( B_1 \) mode [(a) and (b)] and the \( B_2 \) mode [(c) and (d)]. The Jahn-Teller cell with the corresponding displacements of the nearest neighbors to the central defect is shown.
sonable agreement. Second, the tangent of the slope angle gives the vibronic constant. We note that the relative slope of the curve for the $B_1$ mode is two and half times greater than for the $B_2$ mode. This supports our expectation that the diagonal matrix element $V_{xx}^{B_1}$, which determines the splitting by the $B_1$ mode, should be larger than the nondiagonal matrix element $V_{xy}^{B_2}$, determining split by the $B_2$ mode. Third, the magnitude of the splitting of the defect level shows a fairly linear scaling with the amplitude of the distortion for both the perturbations. This is an obvious consequence of the linear approximation of the vibronic potential, valid for small distortions of the lattice. It is worth mentioning that, in spite of the fact that a coupling of the defect state with the $E$ vibronic mode is forbidden by symmetry in the first approximation of the perturbation theory, it does exist in the second approximation when the second order vibronic terms $V^{(2)} \sim (\partial^2/\partial r^2)/(1/\epsilon)R^2$ are included. In this case, the splitting of the defect level is proportional to the square of the amplitude of the distortion. The dependence of the defect level frequency splitting on the square of the relative amplitude of the distortion for the $E$ vibronic mode is shown in Fig. 4(b). We note that the splitting appears only for a relatively large lattice distortion ($0.1a < \Delta r < a$), and shows a linear scaling with the square of the distortion. The disagreement between the plane wave and FDTD calculations noticeable in Fig. 4(b) is a consequence of the poor convergency of the FDTD technique for the $E$ mode.

In this paper we showed that coming from Jahn-Teller theorem, the lattice vibration with the symmetry of $B_1$ and $B_2$ modes should result in splitting the degeneracy of the $E$ mode.

FIG. 3. FDTD calculations of the defect photonic crystal coupled with the $B_1$ and $B_2$ vibronic modes for the magnitude of the rod displacement $\Delta r = 0.1a$. Fourier spectrum of the defect states coupled with the $B_1$ ($B_2$) mode, shown by dashed and dashed-dotted lines, correspond to the data collecting points on the $x$ axis (the line $x = y$) and $y$ axis (the line $x = -y$), respectively.

FIG. 4. Dependence of the frequency splitting of the double degenerate defect state on the relative amplitude of the distortion for the case of coupling the defect state with the $B_{1,2}$ (a) and E (b) vibronic modes. The data obtained from the supercell plane wave and FDTD calculations are shown by dashed and solid lines, respectively.
photon state. The symmetry of the split photon defect mode is shown to be driven by the symmetry of the lattice distortion or the corresponding vibronic mode. The splitting has a linear scaling with lattice distortion, being characterized by the vibronic constants. Now we can answer a question: what is the stable configuration for the cell in the presence of the Jahn-Teller effect? To answer this question the energy as a function of the rod displacement in the Jahn-Teller cell \( \omega(\mathbf{R}) \), that is an adiabatic potential, must be determined. For the degenerate \( E \) photon state interacting linearly with the \( B_1 \) and \( B_2 \) vibronic modes, the adiabatic potential can be found as a solution of the secular equation

\[
\begin{vmatrix}
\omega_0 + v_0(R_{B_1}^2 + R_{B_2}^2) - v_{B_1}R_{B_1} - \omega(\mathbf{R}) \\
v_{B_2}R_{B_2}
\end{vmatrix} = 0.
\]

Here, we took into account the symmetry of the \( B_1 \) and \( B_2 \) modes discussed above. The first order vibronic constants

\[
v_{B_1} = \langle p_i | \frac{\partial V^{B_1}(r)}{\partial r} | p_i \rangle
\]

and

\[
v_{B_2} = \langle p_i | \frac{\partial V^{B_2}(r)}{\partial r} | p_i \rangle,
\]

as well as the second order vibronic constant

\[
v_0 = \langle p_i | \frac{\partial^2 V(r)}{\partial r^2} | p_i \rangle
\]

can be evaluated from Fig. 4 as a tangent of the slope of the corresponding curve for the \( B_1 \) and \( B_2 \) and \( E \) modes. In Fig. 5(a) we present the solution of Eq. (3) for \( \omega(\mathbf{R}) - \omega_0 \) constructed in the space of the \( \Delta r^{B_1} = R_{B_1} \) coordinates. The coordinates of the two minima give the stable configuration of the system when both of the modes are excited, while the depth of the walls determine the so-called Jahn-Teller stabilization energy. In the case of the photonic crystal, in the system we can excite only one type of vibronic mode. The adiabatic potentials for the \( E \) degenerate photon state interacting either with the \( B_1 \) or \( B_2 \) vibronic modes are shown in Fig. 5(b) by the solid and dashed lines, respectively. The points of minima of the curves \( \Delta r^{B_1,2} = \pm 2v_{B_1,2}/v_0 \) determine the stable displacement of the Jahn-Teller cell. The Jahn-Teller stabilization energy, equal to \( \omega_{JT}^{B_1,2} = -v_{B_1,2}/4v_0 \), defines the gained energy because of the Jahn-Teller effect.

From Fig. 5 we conclude that the adiabatic potential has a characteristic shape for the Jahn-Teller effect, when for the most symmetric configuration of the cell at the point \( \Delta r = 0 \), two branches of the adiabatic potential coincide resulting in a degenerate photon state. The Jahn-Teller theorem states that at the point of degeneracy the adiabatic potential has no minimum, and hence at this point the system is unstable. The system goes to the minimum of the adiabatic potential, situated at the points \( \Delta r = \pm \Delta r_0^{B_1,2} \), being chara-
terized by a lower energy and lower symmetry. It is worth mentioning that, when calculating the adiabatic potential, we took into account only the linear terms for the interaction of the photon state with the $B_{1,2}$ vibronic modes. However, for the large magnitude of distortion, the second order terms should be included. But, as follows from our plane-wave and FDTD analysis (Fig. 4), the second order terms are small, and the second order corrections to the adiabatic potential are less than 10%.

Now we can argue that, if the proper $\alpha$ vibronic mode is excited in the photonic crystal then it may be condensed. The condition to observe the effect is that $\hbar \omega^\alpha_{JT} > K$, where $K$ is the kinetic energy of the vibrations determined by the amplitude of the vibrations and the mass of the rods. This requires that the velocity of the vibrations should satisfy inequality $v^2 < 2\hbar \omega^\alpha_{JT}/m$ (where $v$ is the velocity of the vibrations and $m$ is the mass of the rods). In the case of a photonic crystal with a nanometer scale of the lattice, this gives that the vibronic mode can be frozen if $v < 10^4$ m/s and the frequency of the vibration $f < 10^6$(1/s). In reconfigurable artificial crystals, these experimental parameters may be tuned to satisfy the above inequality.

In conclusion, we briefly describe possible applications of the Jahn-Teller distortion. Light incident on a photonic crystal with a square lattice and subject to the $B_1$ or $B_2$ vibrations will interact with all the appropriate defect states whose field distributions are nonorthogonal to the propagation direction of the light in the lattice. The straightforward way to implement the effect is to construct a photonic crystal on the piezoelectric substrate, giving a needed distortion of the lattice near the defect. This distortion could, for example, be used for the optical switch, or at the corners of sharp bends in optical waveguides to improve guiding efficiency. More sophisticated designs can include the coupling of elastic and electromagnetic waves in a lattice periodic in both dielectric and acoustic constants.

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