Strongly Localized State of a Photon at the Intersection of the Phase Slips in 2D Photonic Crystal with Low Contrast of Dielectric Constant

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Two-dimensional photonic crystal with a rectangular symmetry and low contrast (< 1) of the dielectric constant is considered. We demonstrate that, despite the absence of a bandgap, strong localization of a photon can be achieved for certain “magic” geometries of a unit cell by introducing two π/2 phase slips along the major axes. Long-living photon mode is bound to the intersection of the phase slips. We calculate analytically the lifetime of this mode for the simplest geometry: a square lattice of cylinders of a radius, r. We find the magic radius, r_c, of a cylinder to be 43.10% of the lattice constant. For this value of r, the quality factor of the bound mode exceeds 10^6. Small (~1%) deviation of r from r_c results in a drastic damping of the bound mode.

Introduction.—The field of photonic bandgap materials was pioneered by two papers [1,2]. In Ref. [1] the idea of bandgap-induced inhibition of spontaneous emission, which limits the performance of light-emitting devices, was put forward. In Ref. [2] the observation was made that a photonic bandgap facilitates strong Anderson localization of light, which otherwise is hard to achieve [3]. Both papers addressed the issue of defect-induced localized photonic modes. However, the defects considered in Refs. [1] and [2] were of a different nature. In [2] the defects were point-like scatterers, i.e. local perturbations of the spatially periodic dielectric constant. In contrast, a defect discussed in [1] represented a periodicity interruption or, in other words, a phase slip [4,5]. While both types of defects cause the formation of the in-gap states, there is a fundamental difference between them. A point-like defect does not lift the long-range order of the underlying crystal. On the contrary, in the presence of a phase-slip, the distance between two lattice sites located to the left and to the right from the phase slip is non-integer (in the units of the lattice constant).

Lately, the properties of defects in photonic bandgap structures (phase-slip-like [6] and more complex defects, specifically designed for certain manipulations of the light flow [7]) have become a branch of research of their own [8].

Theoretical studies of photonic bandgap materials are almost exclusively focused on structures with a high contrast of the dielectric constant which is sufficient for the formation of either 2D or 3D bandgap, i.e. the region of frequencies where the propagation of light is completely forbidden. For low contrast, periodicity manifests itself in the formation of narrow stop bands only along certain directions close to the Bragg condition. The overall density of photonic states is weakly perturbed by such a periodicity. This rules out the possibility of defect-induced localized modes. Although, strictly speaking, this statement is correct, we demonstrate in the present paper that strongly localized photon modes are possible in photonic crystals with contrast of dielectric constant < 1. By “strongly localized” modes we mean the modes with decay time much longer than the inverse frequency, or, in other words, with high quality factor, Q. In fact, we will demonstrate below that, when the contrast of the dielectric constant is low, the proper choice of the geometry and parameters of the 2D unit cell, combined with proper periodicity interruptions, allows to achieve a Q-factor of the localized mode as high as Q ~ 10^6.

Qualitative Consideration.—In the absence of photonic gap, it can be concluded on general grounds that formation of a defect-induced localized mode is impossible, since its frequency would be degenerate with the continuum of the extended Bloch waves. There is, however, an exception. Consider a 2D photonic crystal in which dielectric constant \( \epsilon(x,y) \) is separable, \( \epsilon(x,y) = \epsilon_0 + \epsilon_1(x) + \epsilon_2(y) \), where \( \epsilon_1 \) and \( \epsilon_2 \) are weak periodic modulations with periods a and b, respectively. Thus, for the light wave propagating strictly along the x-direction the position of a narrow stop band in the dispersion law is determined by the Bragg condition \( \epsilon_0^{1/2} \omega_x = \pi c/a \). Analogously, for the light wave along the y-direction, the Bragg condition reads \( \epsilon_0^{1/2} \omega_y = \pi c/b \). Assume now, that the phase slips along both directions, x and y, are introduced into the photonic crystal. This situation is illustrated in Fig. 1. Note, that, even in the presence of the phase slips, \( \epsilon(x,y) \) remains separable. On the other hand, it is known that, much like a point defect, a phase slip in one dimension causes a localized photonic state that decays exponentially away from the phase slip [4]. Then, in the presence of two phase slips, a truly localized photonic mode bound to the intersection of the phase slips, x = y = 0, exists. The frequency of this mode is close to \( \omega_0 \approx (\omega_x^2 + \omega_y^2)^{1/2} \). We would like to emphasize that existence of a 2D localized mode, degenerate with continuum, is unique for the case of the phase slips, since this mode is effectively decoupled from the continuum. On the other hand, even for separable \( \epsilon(x,y) \), a point defect of arbitrary strength is unable to localize a photon when the gap is absent. This is because, in the presence of a defect, the separability is lifted.

Naturally, any violation of separability of \( \epsilon(x,y) \) would result in the leakage of a mode bound to the intersection of the phase slips. It is also obvious that separability is lacking for any realistic geometry of photonic crystal (like the one illustrated in Fig. 1). Our prime observation is that, for certain “magic” geometries of the unit cell, the leakage...
can be suppressed even without separability. Then the lifetime of the mode remains much larger than $\omega_0^{-1}$.

We start with the remark that, unlike the case of a random disorder, the decay of the localized mode is, to the first approximation, determined by a single Fourier component of $\epsilon(x, y)$. Our main idea is that this component can be eliminated by a proper arrangement of a unit cell. As the simplest example, consider a rectangular lattice of cylinders of radius $r$ (Fig. 1a). In this case, the Fourier component, responsible for the leakage, is proportional to

$$J_1 \left(2\pi \sqrt{(r/a)^2 + (r/b)^2}\right),$$

where $J_1$ is the Bessel function of the first order. Correspondingly, the magic value of $r$, for which the leakage is suppressed, is determined by a first zero of $J_1(u)$, i.e. $u = u_0 \approx 3.830$. This yields for the magic radius, $r_c$, the value $r_c = 0.610ab/\sqrt{a^2 + b^2}$. In particular, for a square lattice, $a = b$, we obtain $r_c = 0.4310a$.

Away from the magic radius, the quality factor falls off as $(r - r_c)^{-2}$,

$$Q^{-1} = \frac{\text{Im} \omega}{\omega} = C \left(\frac{\delta \epsilon}{\epsilon_0}\right) \left(\frac{r - r_c}{a}\right)^2,$$

where $\delta \epsilon$ is the difference between dielectric constants of the cylinder and the background. For the coefficient $C$ in the most interesting case of $\pi/2$ phase slips we obtain below

$$C = \left(\frac{2^{11/2}}{15}\right) \frac{u_0 J_0^2(u_0)}{J_1(2^{-1/2}u_0)} \approx 4.3,$$

where $J_0$ is the Bessel function of a zero order. In the limit $r \to r_c$ the growth of $Q$ saturates due to the higher-order processes illustrated in Fig. 2. These processes involve, strictly speaking, all the Fourier components with non-zero $n$ and $m$; these components are proportional to $J_1 \left(2\pi \sqrt{(nr/a)^2 + (mr/b)^2}\right)$. Our important observation is that the leakage can be further suppressed by fine tuning of $r$ around $r_c$. This is due to the compensation of different contributions – phenomenon analogous to the Fano resonance [9]. The final expression for the quality factor, which incorporates the higher-order processes, has the form

$$Q^{-1} = C \left(\frac{\delta \epsilon}{\epsilon_0}\right) \left[\left(\frac{r - r_c}{a} - \frac{\delta \epsilon}{\epsilon_0} \kappa_1\right)^2 + \left(\frac{\delta \epsilon}{\epsilon_0}\right)^2 \kappa_2^2\right],$$

where dimensionless factors $\kappa_1$ and $\kappa_2$ involve the following lattice sums

$$\kappa_2 = \left(\frac{3^{1/2}}{2\pi^4}\right) \frac{a^4}{u_0 J_0(u_0)} \sum_{n,m > 0} F_{n,m}^2 + F_{n+1,m+1}^2 + 2F_{n,m+1}^2 \frac{n(n+1) + m(m+1)}{n(n+1) + m(m+1)},$$

$$\kappa_1 = \left(\frac{3}{2}\right)^{3/2} \kappa_2 + \frac{a^4}{2\pi^4 u_0 J_0(u_0)} \sum_{n,m > 0} \frac{F_{n,m} F_{n+1,m+1}}{n(n+1) + m(m+1)}.$$

The elements $F_{n,m}$ are related to the Fourier components of $\epsilon(x, y)$ as follows

$$F_{n,m} = \frac{\pi u_0}{2^{1/2}(n^2 + m^2)^{1/2}a^2} J_1 \left(2^{-1/2}(n^2 + m^2)^{1/2}u_0\right).$$

The sum in Eq. (4) reflects the processes $2 - 2_1$ in Fig. 2, while the sum in Eq. (5) originates from the process $2 - 2_2$. First term in Eq. (3) describes the Fano resonance. It suggests that the leakage can be reduced, if $r$ slightly exceeds $r_c$ by $(\delta \epsilon/\epsilon_0) \kappa_1 a$. Then the maximal possible value of the quality factor is given by

$$Q_m = \frac{1}{C \kappa_2^2 \left(\frac{\epsilon_0}{\delta \epsilon}\right)^3},$$

Formula (7) is our main quantitative result. In general, it could be expected that parameters $\kappa_1$ and $\kappa_2$ are $\sim 1$. Remarkably, their values turn out to be very small, $\kappa_1 \approx 5 \cdot 10^{-3}$ and $\kappa_2 \approx 0.8 \cdot 10^{-3}$. Thus, even for $\delta \epsilon = \epsilon_0$, we get a very high quality factor, $Q_m \approx 0.4 \cdot 10^9$. Achieving this value, however, requires a high precision in the choice of $r$. For example, without fine tuning (i.e. for $r = r_c$), Eq. (3) suggests that the quality factor drops from $Q_m$ to $Q_m \approx 0.03 Q_m$. 

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Derivation of Eqs. (6), (7).—For simplicity we consider the case of TM polarization with electric field, $\mathcal{E}(x, y)$, along the $z$–axis. Since the derivation is based on the perturbation theory, it is convenient to cast the wave equation for $\mathcal{E}(x, y)$ into Schrödinger-like form

$$
\left(\frac{\partial^2}{\partial x^2} + U_1(x)\right)\mathcal{E} + \left(\frac{\partial^2}{\partial y^2} + U_2(y)\right)\mathcal{E} + \nu_{\text{pert}}^{(ps)}(x, y)\mathcal{E} = -\lambda\mathcal{E},
$$

where $\lambda = \frac{\omega^2}{c^2} \epsilon_0$ stands for the “energy”, while the “potentials” $U_1(x)$, $U_2(y)$, and $\nu_{\text{pert}}^{(ps)}(x, y)$ are defined as

$$
U_1(x) = \sum_n U_{n,0}(x + d_x \text{sign}(x)), \quad U_2(y) = \sum_m U_{0,m}(y + d_y \text{sign}(y)),
$$

$$
U_{\nu_{\text{pert}}}^{(ps)}(x, y) = \sum_{n,m>0} U_{n,m}(x + d_x \text{sign}(x), y + d_y \text{sign}(y)).
$$

The arguments in r.h.s. of Eqs. (6), (7) reflect the periodicity interruptions by $2d_x$ and $2d_y$, shown in Fig. 1(a), while the functions $U_{n,m}(x, y)$ are the components of the Fourier expansion of periodic $\epsilon(x, y)$ in the absence of the phase slips

$$
\omega^2 \epsilon(x, y) = \sum_{n,m \geq 0} U_{n,m}(x, y) = \left(\frac{\delta \epsilon}{\epsilon_0}\right) \sum_{n,m \geq 0} \left(F_{n,m} e^{i(n x + m y)} + h.c.\right),
$$

where $g_x = \pi/a$ and $g_y = \pi/b$. In these notations, the known solution for the localized mode induced by a one-dimensional phase slip takes the form

$$
E_0^{(x)}(x) = (2\gamma_x)^{1/2} \cos(g_x x) \exp(-\gamma_x |x|), \quad E_0^{(y)}(y) = (2\gamma_y)^{1/2} \cos(g_y y) \exp(-\gamma_y |y|),
$$

where the decrements $\gamma_x$, $\gamma_y$ are given by

$$
\gamma_x = \left(\frac{\delta \epsilon}{\epsilon_0}\right) \frac{F_{1,0}}{2g_x} \sin\left(\frac{2\pi d_x}{a}\right), \quad \gamma_y = \left(\frac{\delta \epsilon}{\epsilon_0}\right) \frac{F_{0,1}}{2g_y} \sin\left(\frac{2\pi d_y}{b}\right).
$$

Therefore, the zero-order solution of Eq. (3) corresponding to $U_{\nu_{\text{pert}}}^{(ps)} = 0$ is $\mathcal{E}_{0}(x, y) = E_0^{(x)}(x)E_0^{(y)}(y)$ with the “energy”

$$
\lambda_0 = g_x^2 + g_y^2 + \delta \epsilon \left[|F_{1,0}| \cos\left(\frac{2\pi d_x}{a}\right) + |F_{0,1}| \cos\left(\frac{2\pi d_y}{b}\right)\right].
$$

The contour of equal intensity for $\mathcal{E}(x, y)$ is shown schematically in Fig. 1b.

Calculation of leakage of the localized mode $\mathcal{E}_0(x, y)$ requires taking into account the phase-slip-induced perturbation, $U_{\nu_{\text{pert}}}^{(ps)}(x, y)$, up to the second order. We will restrict further consideration to the most interesting case of $\pi/2$ phase slip, i.e. $d_x = a/4$, $d_y = b/4$. For this purpose we will need, in addition to $\mathcal{E}_0(x, y)$, the zero-order solutions of Eq. (3), corresponding to the continuous spectrum of propagating modes. These solutions $\mathcal{E}_0^{\mu,\nu}(x, y) = E_{\mu,\nu}^{(x)}(x)E_{0,\nu}^{(y)}(y)$ can be easily found in a similar way as $\mathcal{E}_0(x, y)$

$$
E_{\mu,\nu}^{(x)}(x) = \frac{1}{\sqrt{(1 + \tilde{p}^2)}} \left\{e^{-ig_{\mu,\nu} x} \sin(px) - e^{ig_{\mu,\nu} x} \left[\tilde{p} \cos(px) + i\mu(1 + \tilde{p}^2)^{1/2} \sin(px)\right]\right\},
$$

where $\tilde{p} = 2 \rho g_x \epsilon_0 / (\delta \epsilon |F_{1,0}|)$, and the index $\mu \pm 1$ enumerates the upper and the lower branches of a one-dimensional spectrum in the $x$–direction; these branches are separated by a narrow Bragg gap $\delta \epsilon |F_{1,0}|$ (see Fig. 2). The “energies” corresponding to $\mathcal{E}_0^{\mu,\nu}(x, y)$ are given by

$$
\lambda_{\mu,\nu}^{(0)} = g_x^2 + g_y^2 + \delta \epsilon \left[\mu |F_{1,0}| (1 + \tilde{p}^2)^{1/2} + \nu |F_{0,1}| (1 + \tilde{q}^2)^{1/2}\right].
$$

The form of the wave equation (3) allows to write down automatically the expression for the first and second-order corrections, $\lambda_0^{(1)}$, $\lambda_0^{(2)}$, to the “energy” $\lambda_0$, Eq. (14).
\[ \lambda_0^{(1)} = \langle \mathcal{E}_0 | U_{\text{pert}}^{(ps)} | \mathcal{E}_0 \rangle, \quad \lambda_0^{(2)} = \sum_{\mu, p, \nu, q} \frac{|\langle \mathcal{E}_0 | \hat{T}_{1,2} | \mathcal{E}_{p, q, \nu}^{(ps)} \rangle|^2}{\lambda_0 - \lambda_{p, q}^{\mu, \nu}}, \]  
(17)

Obviously, \( \lambda_0^{(1)} \) does not cause any leakage, and, moreover, \( \lambda_0^{(1)} = 0 \) due to symmetry of the geometry under consideration. First non-vanishing contribution to \( \text{Im} \lambda \), which describes the leakage, as follows from the golden rule,

\[ \text{Im} \lambda = \text{Im} \lambda_0^{(2)} = \pi \sum_{\mu, p, \nu, q} |\langle \mathcal{E}_0 | \hat{T}_{1,2} | \mathcal{E}_{p, q, \nu}^{(ps)} \rangle|^2 \delta (\lambda_0 - \lambda_{p, q}^{\mu, \nu}), \]  
(18)

emerges if the lowest order expression for the operator \( \hat{T}_{1,2} \)

\[ \hat{T}_{1,2}^{(0)} = U_{1, 2}^{(ps)}(x, y) + U_{2, 1}^{(ps)}(x, y) \]  
(19)

is substituted into Eq. \((18)\). Evaluation of \( \text{Im} \lambda \) leads to Eq. \((1)\) for the quality factor, \( Q = 2\lambda / \text{Im} \lambda = \omega / \text{Im} \omega \). Since for magic configuration this term is zero, the operator \( \hat{T}_{1,2} \) should be taken with higher accuracy. Namely, higher order processes, illustrated in Fig. 2, amount to the following modification of the operator \( \hat{T}_{1,2} \)

\[ \hat{T}_{1,2} = T_{1,2}^{(0)} + \sum_{m, n > 0} \sum_{m_1, n_1 > 0} \sum_{p, q} U_{m, n}^{(ps)} \mathcal{E}_{x, p, p}^{(ps)} \mathcal{E}_{y, q, q}^{(ps)} \frac{U_{m_1, n_1}^{(ps)}}{\lambda_0 - \lambda_{p, q}^{\mu, \nu}} (1 - \delta_{m_1, 1} \delta_{n_1, 1}, \delta_{m_1, 1} \delta_{n_1, 1}), \]  
(20)

where \( \mathcal{E}_{x, p, p} = \exp(ipx + ipy) \), \( \lambda_{p, q} = p_x^2 + p_y^2 \) stand for “nonresonant” solutions of Eq. \((8)\) with \( |p| > 2\pi / a \). For these solutions, periodic modulation can be neglected. Matrix elements of \( U_{m, n}^{(ps)} \) between \( \mathcal{E}_0(x, y) \) and plane waves, required for evaluation of Eq. \((18)\), can be calculated analytically. The form of these matrix elements suggests that the main contribution to \( \text{Im} \lambda \) comes from the small angular regions \( \delta \epsilon / \epsilon_0 \) in Fig. 2 (of the order of the Bragg gap) around the Bragg directions. After that, the summation in Eq. \((18)\) with the use of the \( \delta \)-function, reduces to the integrals

\[ I_n = \int_0^\infty du (1 + u)^{-(2n + 5)/2} = \frac{4}{(2n + 1)(2n + 3)} \]  
(21)

with \( n = 1, 2, \) and \( 3 \). Now, as summation over all moments in Eqs. \((18)\), \((20)\) is performed analytically, we arrive at Eq. \((8)\).

**Conclusion.**- First photonic-crystal based lasers were reported in Refs. \([11,12]\). In Ref. \([11]\) a two-dimensional photonic crystal was fabricated within the active region of the InGaAsP multiple quantum well structure using the etching procedure. The contrast of the dielectric constants between the semiconductor and etched air-holes was high (\( \approx 10 : 1 \)). This contrast was sufficient for opening of the two-dimensional bandgap. Then a defect, which was essentially a missing air-hole \([11]\), gave rise to the in-gap mode localized within approximately two periods of the host hexagonal crystal. It was demonstrated in Ref. \([11]\) that above the threshold the laser emission is dominated by this defect mode.

A low-contrast photonic crystal with array of holes etched in the SiO\(_2\) substrate (\( \epsilon = 1.46 \)) of a solid organic gain film (\( \epsilon = 1.7 \)) was reported in Ref. \([12]\). Without photonic gap, the authors did not attempt to create a localized mode, although in the later work \([13]\) a square symmetry of the lattice pattern was employed.

In the present paper we have demonstrated that a localized photon mode is possible in a 2D photonic crystal with a low contrast of the dielectric constant. In a sense, the absence of photonic gap can be compensated by a high-precision tailoring of the unit cell parameters. There is another example, when an accurate choice of point-defect parameters gives rise to a long lifetime. It pertains to the crystals with a high contrast of the dielectric constant \([14,15]\). Namely, in a finite thickness 2D photonic crystal with a complete gap for in-plane light propagation, the leakage of the in-gap mode in the \( z \)-direction can be strongly suppressed for a certain radius of a cylinder constituting a defect \([16]\).

A natural extension of the present study is to explore a possibility to guide light from one location to another using an array of phase slips in low-contrast magic crystals. It would be appealing if such crystals offered an alternative to the conventional bandgap materials \([8]\) in terms of manipulating the light flow.

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FIG. 1. (a) Schematic illustration of two intersecting phase slips in a 2D photonic crystal with rectangular symmetry. (b) The contour of equal intensity for the mode localized at the intersection.
FIG. 2. $k$-plane for a photonic crystal with low contrast of dielectric constant. Solid line is a contour of constant $|k| = \varepsilon_0^{1/2} \omega/c$. Stop bands near the Bragg conditions are indicated with long-dashed lines. Thick solid lines: (1) - second-order process responsible for the decay of the bound mode; (2) - fourth-order process responsible for the decay of the bound mode. Virtual transition 2 is followed by one of the virtual transitions $2_1$ or $2_2$ shown with dashed lines.