Electrical tuning of photonic crystals infilled with liquid crystals

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Abstract

In this paper we perform a complete study of electrical tuning in liquid crystal-infilled two-dimensional (2D) photonic crystals (PCs). The nematic liquid crystal (NLC) is characterized by a full range of bulk and surface elastic parameters. An essentially DC tuning field is applied in the axial direction. By minimizing the total (elastic plus electromagnetic) free energy, the configuration of the NLC directors, as a function of radial distance, is obtained. Three possible configurations are considered: escaped radial, planar radial, and axial. It is found that, in general, the escaped radial configuration is the preferred one. However, for sufficiently large applied fields, a phase transition occurs to the axial configuration. For example, in the case of the NLC 5CB, this transition is realized at about 14 V/\mu m provided that the cylinder radius is greater than about 50 nm. The configuration of the NLC directors determines the dielectric tensor as function of radial distance and this, in turn, leads to the eigenvalue equation for the PC. We present two such equations: one exact and the other approximate. The exact eigenvalue equation is based on the full anisotropy of the dielectric tensor and does not result in the usual separation of normal modes in a 2D PC. The approximate eigenvalue equation is derived from the average (over the cylinder cross-section) dielectric tensor and leads to modes that are polarized in the directions either parallel (\textit{E}-mode) or perpendicular (\textit{H}-mode) to the cylinders. Our calculations of the photonic band structure, by both methods, show that the approximate calculation works very well for the 5CB NLC cylinders in a silicon oxide (silica) host. This allows us to introduce the terminology quasi-\textit{E} and quasi-\textit{H} polarizations. We show how the partial photonic band gap in the [100] direction for these polarizations can be tuned and even completely closed. This behavior could be applied to the design of versatile, tunable polarization filters.

1. Introduction

This paper deals with two kinds of crystals, neither of which is a crystal in the usual sense. One of these is photonic crystal (PC) – by now a household term among condensed-matter scientists. The basic optical properties of these man-made, periodic structures, as well as numerous applications, are covered by several books [1]. The other type of nonconventional crystal is a liquid crystal, characterized by some particular microscopic regularity; liquid crystals occupy an intermediate position between ordinary crystals and amorphous materials [2]. For many decades, liquid crystals are a much favored optoelectronic substance on account of easy tunability of their properties with pressure, temperature, electric fields, and magnetic fields. This suggests a marriage of convenience with PCs, whose most prominent feature is the photonic band gap (PBG). Indeed, in 1999 Bush and John proposed that, by infilling a PC with a liquid crystal, an applied electric field would tune the PBG [3]. Enthusiastic response led to rapid growth, reported in a recent review [4] and a specialized conference [5]. We proceed to describe some of the advances in liquid crystal-infilled, two-dimensional (2D) and three-dimensional (3D) PCs and a few applications of related structures. Most of this work was done on nematic liquid crystals (NLCs) which, on account of their rodlike molecules, have the simplest macroscopic properties.

The first tuning experiment was performed by Leonard et al. [6], who infiltrated the NLC \textit{E7} into the air pores of a 2D macroporous silicon PC. Strong, polarization-sensitive tuning of the band edges was attained as the sample...
was heated from the nematic phase, beyond the phase transition, to the isotropic phase. The results were interpreted in terms of the escaped radial (ER) configuration of NLC directors. While this work concerned continuous tuning, in Ref. [7] the shifts in band structure and transmission were contrasted in the nematic and isotropic phases, assuming that the NLC 5CB occupies the space between a 2D lattice of metallic plasma bars. The axial (AX) NLC configuration was arbitrarily assumed. Takeda and Yoshino [8] came to the theoretical conclusion that a NLC-infilled 2D PC does not support independent $E$- and $H$-modes – as is the rule for isotropic ingredient materials. As a result, an incident wave polarized perpendicular to the cylinders gives rise to transmission with parallel polarization, as well as perpendicular one. It is assumed that the NLC directors have a fixed direction within all the cylinders and that this direction can be altered by the application of an electric field [8].

A promising application of these ideas is the recent advent of NLC-infilled PC fibers. Proposed by Larsen et al. [12], the authors demonstrated thermo-optic tuning and switching that utilized shifts of the photonic bands with temperature. Electrical tuning of similar fibers was accomplished by Du et al. [13], who observed variations in the light output of the fiber with transversely applied voltage, as well as the switching function. All optical modulation [14] and continuous electrically controlled tunability [15] were also demonstrated.

As for 3D PCs infilled with NLCs, ever since the original idea of Busch and John [3], there was a strong preference for synthetic opal structures. The first such experimental work was done by Yoshino et al. [16], who showed that the optical stop band in the transmission spectrum shifts drastically by the infiltration of liquid crystals. Subsequent work, also on silica opal, demonstrated tuning of the optical response by an external electric field [17]. Mertens et al. [18] studied both normal and inverted colloidal crystals infilled with the E7 NLC. They found that the Bragg reflection peak in the (111) direction can be temperature-tuned. Interestingly, in Ref. [19] it was shown that, in specially prepared synthetic opals, the nematic directors can self-align in a unique, well-defined direction. Also, Escuti et al. [20] reported on the fabrication and electro-optic measurements of fcc lattices in holographic polymer-dispersed NLCs.

Several NLC-infilled defect structures were also tuned. In Ref. [21] it was demonstrated that a NLC defect layer within a 1D PC gives rise to a transmission peak whose spectral position could be tuned by an external voltage. Schuller et al. [22] fabricated a planar microcavity in a 2D PC of air holes, thus producing a linear waveguide.

In an experiment similar to that of Leonard et al. [6], with the E7 NLC having been injected into the holes, the transmission peak was tuned by sweeping the temperature from 20 °C up to 72 °C (beyond the nematic–isotropic phase transition at 60 °C). Takeda and Yoshino [23] studied theoretically a NLC polymer film forming a defect layer within a 2D PC. It was found that the transmission peaks depend on the direction of the NLC director – assumed to be constant, as in ref.[8]. The same authors also designed a Y-shaped wave guide in a 2D PC, with the three arms of the Y having different radii [24]. The path taken by the light could then be controlled by an applied field – although not assumed explicitly.

It is noteworthy that an electrically tunable laser has been devised; it is based on infiltrating a NLC into the void cylinders of a 2D PC with a defect cavity (produced by replacing one of the cylinders by a narrower one) [25]. Application of a voltage realigns the NLC molecules, changing the effective index and laser cavity’s optical length, thus blue-shifting the lasing wavelength (≈1.6 μm).

After this survey of advances in tuning of PCs by means of infiltration of NLCs, it is evident that deeper understanding and future applications much depend on in-depth studies of the configuration of the NLC within a PC of interest. That is, what is the precise direction of the NLC director $\hat{n}(r)$ at every point within the infiltrated voids? How does this direction depend on an applied electric field or on the temperature? Is it possible to have a change of the type of configuration, that is, a phase transition even below the usual nematic phase–isotropic phase transition point? The only way to answer these questions is to minimize the free energy of the system. In a 3D PC the infiltrated voids have very complicated geometrical forms; for example, a general solution for the much-favored synthetic opals is a formidable problem[3,17,19]. On the other hand, 2D PCs – given their simple, cylindrical voids – are a manageable task.

In the next section we establish the basic formulas for the free energy of an isolated NLC cylinder subject to an external, axial DC electric field. In doing so we take fully into account the bulk and surface interactions of the NLC molecules. The free energy is minimized in Section 3, considering three possible configurations: ER, the planar radial (PR), and the AX. The direction of the director $\hat{n}(r)$ is calculated as function of the radial distance in the cylinder and of the magnitude of the applied field. For sufficiently large values of this field a phase transition occurs, as shown in Section 4, from the ER to the AX configuration. In Section 5 the dielectric tensor for the NLC cylinder – which is both inhomogeneous and anisotropic – is used to derive the eigenvalue equation for the magnetic field in the NLC-infilled PC. This equation separates into the usual, independent $E$- and $H$-polarization modes only for applied electric fields above the critical value – when the NLC configuration is axial. Nevertheless, we also show that such two independent modes follow from an approximate treatment (Section 6) that averages the dielectric tensor over the cross-section of a cylinder. Rather surprisingly, graphical
comparison of the PBSs obtained from the approximate and exact theories yield a very good fit (Section 7). From this fact we conclude that, while for sub-critical electric fields, strictly speaking, there is no separation into $E$- and $H$-modes, such a classification is a very reasonable approximation – at least for the materials considered in this paper ($5CB$ NLC in silicon oxide (silica) PC). Finally, the conclusions are given in Section 8; substantial tuning of the photonic bands and band gaps, as well as polarization effects, can be accomplished by means of the external electric field.

2. Model and basic equations for nematic liquid crystal cylinder

In this section, instead of considering the photonic crystal (PC) as a whole, we concentrate on a single, circular and infinitely long, cylinder of LC that is contained within an isotropic dielectric material. In what follows we comment on the assumptions and approximations involved in our calculation.

We assume homeotropic anchoring of the nematic liquid crystal (NLC) molecules at the cylinder walls. This means that the easy direction for the molecular orientation is the direction perpendicular to the wall at every point. According to Burylov [26], “in essentially every experiment to date the anchoring is of homeotropic type”. This, however, does not mean that the directors are perpendicular to the walls; the actual inclination also depends on elastic forces due to neighboring molecules, on external fields, and on the strength of anchoring. This leaves us with three possible structures [26], namely the PP, the PR, and the ER. In the first two structures all the directors of the LC lie in the plane perpendicular to the cylinder. In case of the ER structure the directors form a certain angle with the normal to the wall; the angle gradually increases as the cylinder axis is approached and, on the axis itself, the directors are parallel to it.

The macroscopic description of the Van der Waals forces between the NLC molecules is given in terms of the following formula [26] for the elastic contribution to the free energy density:

$$\mathcal{F}_e = (1/2) \int_V dV [K_{11}(\nabla \cdot \mathbf{n})^2 + K_{22}(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_{33}(\mathbf{n} \times \nabla \times \mathbf{n})^2 - K_{24} \cdot [\nabla \cdot (\mathbf{n} \nabla \cdot \mathbf{n} + \mathbf{n} \nabla \times \mathbf{n})]] + (1/2) \int W_0 \cos^2 \theta(r) dS$$

Here the unit vector $\mathbf{n}$ is the director, the elastic moduli $K_{11}, K_{22},$ and $K_{33}$ describe, respectively, transverse bending (splay), torsion (twist), and longitudinal bending (bend) deformations. $K_{24}$ is called the surface elastic constant because it is the coefficient of a divergence term which can be transformed to a surface integral by using Green’s theorem. The last term provides the interaction between the NLC and the confining surface. There $\theta(r)$ is the angle between $\mathbf{n}$ and the axial direction evaluated at the surface of the cylinder, and $W_0$ denotes the strength of interaction, in units of energy per area, between a nematic molecule and the surface.

We assume that the wave field $\mathbf{E}$ is much weaker than the applied field $\mathbf{E}_0$; $| \mathbf{E} | \ll | \mathbf{E}_0 |$, so that the dielectric tensor of the LC will not depend on the wave field. Thus our study of the optical response of the LC-infilled PC is linear. Additionally, we assume that the external field $\mathbf{E}_0$ is larger than the critical (Freedericksz) field, below of which no reorientation of the nematic LC molecules occurs. Finally, we neglect absorption in both the LC and the dielectric host.

The free energy of the LC cylinder has, in addition to the above elastic part, also an electromagnetic part due to the applied electrostatic field. As we have already discussed, the first contribution is given by Eq. (1). The electromagnetic free energy density, taking $\mathbf{E}_0$ along the $z$-axis is, in MKS units

$$\mathcal{F}_{em} = -(1/2) \int_V dV [\mathbf{D} \cdot (\mathbf{E}_0 + \mathbf{E}) + \mathbf{B} \cdot \mathbf{H}] dV$$

$$\simeq -(1/2) \int_V \varepsilon_0(r) E_0^2 dV$$

where we have used the fact that $| \mathbf{E} | \ll | \mathbf{E}_0 |$.

Now we must express the element of the dielectric tensor $\varepsilon_{ij}(r)$ in terms of the ordinary and extraordinary dielectric constants of the NLC, $(\varepsilon_o = n_o^2)$ and $(\varepsilon_e = n_e^2)$, respectively. At a point where the director forms an angle with the $z$-axis, the dielectric tensor in the proper coordinate system of the NLC has the uniaxial form. This must be transformed into the “laboratory” coordinate system $x,y,z$, resulting in the following expression for the dielectric tensor elements:

$$\varepsilon_{ij} = \varepsilon_o \delta_{ij} + \varepsilon_e n_i n_j$$

(3)

$$n_x = \sin \theta(r) \cos \phi$$

(4)

$$n_y = \sin \theta(r) \sin \phi$$

(5)

$$n_z = \cos \theta(r)$$

(6)

The angle $\phi$ is measured with respect to the (arbitrarily oriented) $x$-axis. For infinite circular cylinders the symmetry implies that $\theta = |\mathbf{n} \cdot \hat{z}|$ only depends on the radial distance $r$. Since $\mathbf{n}$ is a position dependent vector, Eqs. (3)-(6) show explicitly that we have inhomogeneity, as well as anisotropy. Using Eqs. (1) and (2), the total free energy becomes

$$\mathcal{F} = \mathcal{F}_e + \mathcal{F}_{em} = (1/2) \int_V dV [K_{11}(\nabla \cdot \mathbf{n})^2 + K_{22}(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_{33}(\mathbf{n} \times \nabla \times \mathbf{n})^2 - K_{24} \cdot [\nabla \cdot (\mathbf{n} \nabla \cdot \mathbf{n} + \mathbf{n} \nabla \times \mathbf{n})]] + (1/2) \int W_0 \cos^2 \theta(r) dS - (1/2)\mathbf{E}_0^2 \int_V \varepsilon(r) dV$$

(7)

We conclude this section with an important note: While Eqs. (3)-(6) are valid for any frequency, the static limiting values $\varepsilon_o(\omega \to 0)$ and $\varepsilon_e(\omega \to 0)$ must be used for the tuning with the essentially DC applied field $\mathbf{E}_0$, while
the high-frequency (optical) values $\epsilon_n(\omega \to \infty)$ and $\epsilon_s(\omega \to \infty)$ apply to the infrared EM fields in the PC. Hence, the static (optical) values are used in Sections 2–4 (5–7).

3. Nematic configurations

The free energy of the LC is obtained by integrating Eq. (7) over the cylindrical volume. Then, expressing $\nabla \cdot \mathbf{n}$ and $\nabla \times \mathbf{n}$ in cylindrical coordinates we obtain the free energy per unit length. The calculation is done for the ER configuration which covers the PR and the AX configurations as special cases. Taking $L$ as the cylinder length and normalizing the radial distance $r$ with the cylinder radius $R(r)/R = x$ we obtain

$$\mathcal{F}/L \equiv F_{\text{ER}} = \int_0^1 \mathrm{d}x f_b(\theta, \mathrm{d}\theta/\mathrm{d}x) + f_s[\theta(1)]$$

(8)

where the bulk $f_b$ and surface $f_s$ expressions are defined as

$$f_b(\theta, \mathrm{d}\theta/\mathrm{d}x) = \pi K_{11} x \left[ \left( \frac{\mathrm{d}\theta}{\mathrm{d}x} \right)^2 \left( \cos^2 \theta + \eta \sin^2 \theta \right) + \frac{\sin \theta}{x^2} \right]$$

$$-q \left( \cos^2 \theta + \epsilon_n \right)$$

(9)

$$f_s(\theta) = \pi K_{33}/K_{11}$$

(10)

Here

$$\eta \equiv K_{33}/K_{11}$$

$$\sigma \equiv RW_0/K_{11} + K_{24}/K_{11} - 1$$

(11)

(12)

and $q$ is the important parameter defined as

$$q \equiv \epsilon_n E_0^2 R^2 / K_{11}$$

(13)

The $q$-parameter represents the ratio of the electric and elastic energies; for $q \ll 1$ the influence of the applied field is weak, while, for $q \gg 1$ the field essentially overcomes the Van der Waals forces between the molecules. Note that the effectiveness of the field $E_0$ is greatly augmented for large radii $R$ of the tubes.

The dependence of the director inclination $\theta(r)$ on the radial distance, for the ER configuration (our general case), is obtained by minimization of the free energy $F_{\text{ER}}$. With this purpose in mind, in Eq. (8) we consider $\theta$ and $\mathrm{d}\theta/\mathrm{d}x$ in $f_b(\theta, \mathrm{d}\theta/\mathrm{d}x)$ as two independent variables. Then the variation of $F_{\text{ER}}$ is

$$\delta F_{\text{ER}} = \int_0^1 \mathrm{d}x \left[ \frac{\mathrm{d}f_s[\theta(1)]}{\mathrm{d}\theta} \delta \theta + \frac{\mathrm{d}f_b(\theta, \mathrm{d}\theta/\mathrm{d}x)}{\mathrm{d}\theta} \frac{\mathrm{d}\theta}{\mathrm{d}x} \delta \frac{\mathrm{d}\theta}{\mathrm{d}x} \right]$$

$$+ \frac{\mathrm{d}f_s[\theta(1)]}{\mathrm{d}\theta} \delta \theta(1)$$

(14)

Notice that even though $f_s$ in Eq. (10) is not a function of $x$, it is nevertheless a function of $\theta(1)$. Then, as usual in variational calculus [27], we exchange the order of the variation and the derivative: $\delta (\mathrm{d}\theta/\mathrm{d}x) = \delta \theta/\mathrm{d}x$ and use the identity

$$\frac{\mathrm{d}}{\mathrm{d}x} \left( \frac{\mathrm{d}\theta}{\mathrm{d}x} \right) = \frac{\mathrm{d}}{\mathrm{d}x} \delta \theta$$

(15)

to rewrite Eq. (14) as

$$\delta F_{\text{ER}} = \int_0^1 \mathrm{d}x \left[ \frac{\mathrm{d}f_s[\theta(1)]}{\mathrm{d}\theta} \delta \theta + \frac{\mathrm{d}f_b(\theta, \mathrm{d}\theta/\mathrm{d}x)}{\mathrm{d}\theta} \frac{\mathrm{d}\theta}{\mathrm{d}x} \delta \frac{\mathrm{d}\theta}{\mathrm{d}x} \right]$$

$$+ \left[ \frac{\mathrm{d}f_s[\theta(1)]}{\mathrm{d}\theta} \delta \theta(1) \right]$$

(16)

Here we have used the fact that $\theta(0) = 0$ in the ER configuration, implying that $\delta \theta(0) = 0$. To find the extrema we set the condition $\delta F_{\text{ER}} = 0$ which can be fulfilled by satisfying simultaneously the conditions:

$$\frac{\mathrm{d}f_b(\theta, \mathrm{d}\theta/\mathrm{d}x)}{\mathrm{d}\theta} = \frac{\mathrm{d}}{\mathrm{d}x} \left( \frac{\mathrm{d}f_b(\theta, \mathrm{d}\theta/\mathrm{d}x)}{\mathrm{d}\theta} \right)$$

$$= 0$$

(17)

$$\frac{\mathrm{d}f_s[\theta(1)]}{\mathrm{d}\theta} = \frac{\mathrm{d}}{\mathrm{d}x} \left( \frac{\mathrm{d}f_s[\theta(1)]}{\mathrm{d}\theta} \right)$$

$$= 0$$

(18)

Eq. (17) describes the nematic’s bulk and is the well-known Euler–Lagrange equation which assumes the explicit form

$$\frac{\mathrm{d}^2 \theta}{\mathrm{d}x^2} + \eta \sin^2 \theta = \frac{\mathrm{d}\theta}{\mathrm{d}x} \frac{\mathrm{d}^2 \theta}{\mathrm{d}x^2}$$

$$+ \frac{1}{2} \sin 2\theta - \frac{q^2}{2} \sin 2\theta = 0$$

(19)

Eq. (18) leads to the “arbitrary anchoring” boundary condition at the surface

$$\frac{\mathrm{d}\theta}{\mathrm{d}x} \bigg|_{x=1} = \frac{\sigma \sin \theta \cos \theta}{\cos^2 \theta + \eta \sin^2 \theta} \bigg|_{x=1}$$

(20)

In the above procedure we have just performed a free-endpoint variation [27] for which $\theta$ is subjected to a finite force $\delta \theta/\delta \theta$ at the cylinder border. To check that Eq. (20) is indeed consistent with the hard-anchoring boundary condition $\theta(1) = \pi/2$, valid for a very large surface force, let us divide Eq. (20) by $\sigma$ and take the limit when $W_0 \to \infty$. Then according to Eq. (12) $\sigma \to \infty$ and we obtain that

$$\sin \theta(1) \cos \theta(1) = 0$$

(21)

This equation has the solutions $\theta(1) = 0$ and $\theta(1) = \pi/2$. The former condition is associated with the AX configuration that we will discuss below, and the second one is what we were looking for.

Notice that Eq. (19) has two simple exact solutions, namely, $\theta(1) = \pi/2$ and $\theta(1) = 0$. The first possibility corresponds to the PP or PR configurations, the second one to the AX structure. A third solution is the ER configuration which depends on the radius and fields through the parameter $q$, Eq. (13), and should be obtained by solving Eq. (19) subject to the condition Eq. (20). To discern which of these configurations the nematic actually adopts, we
should calculate their corresponding total energies from Eqs. (8)–(10) to choose the one with smallest value. We shall discuss this below.

Numerical solutions of Eq. (19) subjected to the conditions given by Eq. (20) and \( \theta(0) = 0 \) were calculated by using the shooting method [28] for different values of \( q \) and are shown in Figs. 1–4. We performed the calculations for the NLC 5CB at \( T_{IN} = T = 10 \, ^\circ \text{C} \) where \( T_{IN} = 35 \, ^\circ \text{C} \) is the clearing temperature at which 5CB suffers the transition from nematic to isotropic phase. The other parameters [29] are \( \eta = 1.316, K_{11} = 1.2 \times 10^{-11} \, \text{N}, W_0/K_{11} = 40 \, \mu \text{m}^{-1}, \) \( K_{24}/K_{11} = 1, \epsilon_a = 7 \) and \( \epsilon_s = 11.5 \). In Figs. 1–4 the angle \( \theta \), between the nematic director and the cylinder axis is plotted versus the radial distance. In all these figures the various curves are characterized by the field parameter \( q \), defined in Eq. (13). The uppermost curve corresponds to \( q = 0 \) and describes the ER configuration in the absence of an applied field. The value of \( q \) increases from top to bottom, the last curve – a straight line coinciding with the \( q \)-axis – corresponding to the critical value of \( q \), at which the phase transition \( \text{ER} \rightarrow \text{AR} \) occurs. The specific values of \( q \) for each curve are given in the figure captions.

These figures clearly show that, for any value of the field parameter \( q \), the directors are constrained to the axial direction on the cylinder axis and to some angle \( 0 < \theta < \pi/2 \) at the wall. Notice how the value of \( \theta \) at the cylinder wall \( x = 1 \) diminishes with increasing field, which implies that for general anchoring the field has stronger effect on the configuration than it has in the strong anchoring limit. Moreover, for a given finite value of \( \sigma > 1 \), we can find numerically a value of \( q \) for which \( \theta(x) = 0 \) at every point; that is, a phase transition occurs from the ER to the AX configuration. This is indicated by the largest value of \( q \) in Figs. 1–4, that corresponds to \( \theta(x) = 0 \). In the next section we explore the phase transition in detail.

Fig. 1. Inclination of the NLC director \( \theta \) versus the dimensionless radial distance \( x = r/R \) for the nematic 5CB with \( \eta = 1.316 \) and \( \sigma = 1.25 \) (\( R = 31.25 \, \text{nm} \)). The field parameter takes the values (from above to below) \( q = 0, 0.25, 0.5, 0.75, 1.045, 1.049 \). For the last value of \( q \), \( \theta(x) = 0 \).

Fig. 2. As in Fig. 1 for \( \sigma = 2 \) (\( R = 50 \, \text{nm} \)) and \( q = 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 11, 13, 15, 17, 19, 19.2 \).

Fig. 3. As in Fig. 1 for \( \sigma = 4 \) (\( R = 0.1 \, \mu \text{m} \)) and \( q = 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 11, 13, 15, 17, 19, 19.2 \).

4. Phase transition from escaped radial to the axial configuration

We can obtain the free energy density for the PR configuration from Eq. (8) by setting \( \theta = \pi/2 \); this leads to

\[
F_{PR} = \pi K_{11} [\ln(R/\rho) + 1 - K_{24}/K_{11} - q\epsilon_a/2\epsilon_s] \tag{22}
\]

where \( \rho \) is the radius of the dislination core which should be of the order of the molecular size. The energy for the AX configuration is obtained by setting \( \theta = 0 \) and is given by

\[
F_{AX} = \pi K_{11} [-(\epsilon_a + \epsilon_s)q/2\epsilon_a + RW_0/K_{11}] \tag{23}
\]

The PR configuration becomes energetically more favorable than the ER if \( F_{PR} < F_{ER} \). Thus the boundary between both configurations in the parameter space is described by the equation
\[
\ln(R/\rho) + 1 - K_{24}/K_{11} - E_0^2R^2/2K_{11}\epsilon_0 - F_{ER}(\eta, RW_0/K_{11}) + K_{24}/K_{11} - 1, \epsilon_2E_0^2R^2/K_{11})/\pi K_{11} = 0
\] (24)

Similarly, the AX configuration becomes energetically more favorable than the ER if \( F_{AX} < F_{ER} \) that is, the boundary between these configurations is defined by

\[
- (\epsilon_4 + \epsilon_6)E_0^2R^2/2K_{11} + RW_0/K_{11} - F_{ER}(\eta, RW_0/K_{11}) + K_{24}/K_{11} - 1, \epsilon_2E_0^2R^2/K_{11})/\pi K_{11} = 0
\] (25)

Using the numerical solutions for \( \theta(x) \), shown for several of values of \( \sigma \) in Figs. 1–4, and those of \( d\theta(x)/dx \), we calculate numerically \( F_{ER}(\eta, \sigma, q) \) as given by Eq. (8) and insert it in the last two equations. We find no realistic solutions for Eq. (24). This is essentially due to the fact that the parameter \( \rho \) has to be taken of the order of the molecular size \( \rho \approx 2 \text{ nm} \) so that \( \ln \rho \) is very large unless \( R \ll 10 \text{ nm} \). In contrast, we do find a solution for Eq. (25) that we plot in Fig. 5 for an AC electric field of 1 Khz. In the context of the photonic crystal, this can be considered a DC field.

Note that, for this particular NLC, \( K_{24} = K_{11} \) and thus \( \sigma = (W_0/K_{11})R \). The variation of the parameter \( \sigma \) in Figs. 1–4 then corresponds simply to variation of the cylinder radius \( R \).

From Fig. 5 we can see that for large values of \( R \), the necessary field \( E_0 \) to cause the phase transition seems to tend to a constant value. It can be shown analytically that the solution of Eq. (19) has this behavior, by calculating its asymptotic form for large values of \( q \).

As is well known, the effect of the external field on the nematic is usually opposed to the that of elastic forces, particularly at frontiers of the nematic where the molecules anchor to the walls. This competition is stronger for intense fields since in the regions which lie “far” from the border (bulk), the nematic director is practically aligned with the field, whereas within a layer of nematic in contact with the solid walls, the orientation of \( \mathbf{n} \) displays strong spatial gradients, so as to satisfy the boundary conditions. These two regions with different behaviors can be described simultaneously by using the boundary layer technique [30] for which the solution in the bulk is denoted by \( \theta_b(x) \) and the solution within the layer is represented by \( \theta_l(x) \). The solutions for both regions are coupled or matched asymptotically to give rise to a continuous solution \( \theta_{adj}(x) \), valid for the entire domain and is given by

\[
\theta_{adj}(x) = \theta_b(x) + \theta_l(x) - \theta_{match}(x)
\] (26)

Here \( \theta_{match} \) must be determined so that the solution in the boundary layer \( \theta_l(x) \) and the solution in the bulk \( \theta_b(x) \) are joined asymptotically. In other words, \( \theta_{match} \) is defined as the solution within the region where \( \theta_l(x) \) and \( \theta_b(x) \) overlap each other, that amounts mathematically to write [30]

\[
\theta_{match}(x) = \lim_{k \to \infty} \theta_l(x) = \lim_{x \to \gamma} \theta_b(x)
\] (27)

where \( \gamma \) represents the region in which \( \theta_b \) cannot satisfy at least one of the boundary conditions (in our case at the border of the cylinder) and \( h \) is related with the thickness of the boundary layer.

To apply this formalism, we note first, that, for large \( q \), Eq. (19) reduces to \( q^2 \sin 2\theta = 0 \) which means that the AX solution \( \theta_b(x) = 0 \) (bulk), which does not satisfy the boundary condition given by Eq. (20), is reached apparently for the whole domain \( 0 \leq x \leq 1 \). To get around this problem, \( \theta_b(x) \) should be no longer valid for a narrow region near \( x = 1 \). Thus, there must exist a region (not a point) near the boundary \( x = 1 \) (that we call the boundary layer) where the solution varies on a rapid spatial scale so as to both satisfy the boundary condition given by Eq. (20) and tend to the bulk solution \( \theta_b \) outside of this thin layer. To find this boundary layer solution \( \theta_l(x) \) we need to express Eq. (19) in terms of a rapid scale variable \( \ln x' \equiv \sqrt{q} \ln x \) or \( x' \equiv x^{1/2} \), which is selected in such a way...
that the highest order derivative of $\theta$ is to be proportional to the last term, (field term) of this equation. This derivative term will allow $\theta$ to vary adequately near the boundary. In this way, even for large values of $q$ we keep the highest derivative by using this fast variable, which allows to write $x d\theta/dx = \sqrt{x^2 d\theta/dx}$, leading to

$$q\sqrt{\cos^2 \theta + \eta \sin^2 \theta} \frac{d}{dx} \left[ x \frac{d\theta}{dx} \sqrt{\cos^2 \theta + \eta \sin^2 \theta} \right] - \frac{1}{2} \sin 2\theta - \frac{q^2 x^2 / \sqrt{\eta}}{2} \sin 2\theta = 0$$

Taking the limit of large $q$ this equation turns out to be Eq. (19) for a vanishing $q$ value. Similarly, using the fact that $d\theta/dx|_{x=1} = \sqrt{\eta} d\theta/dx|_{x=1}$, Eq. (20) remains the same after replacing $\sigma$ by $\sigma = \sigma/\sqrt{\eta}$. Thus, the boundary layer solution $\theta_l$ for large $q$ can be obtained by replacing $x$ and $\sigma$ by $x/\sqrt{\eta}$ and $\sigma/\sqrt{\eta}$, respectively, in the solution $\theta = \theta(x)$ in the absence of external fields ($q = 0$). This solution of Eq. (19), without the last term has been found by Crawford et al. [29] in the inverse form $x = x(\theta)$, as follows:

$$x = \sqrt{\frac{\sigma + 1}{\sigma - 1}} \frac{\Delta - 1}{\Delta + 1} \exp \left[ \sqrt{\eta - 1} \arctan \left( \frac{\sqrt{\eta - 1} (\Delta - \sigma)}{\Delta \sigma + \eta - 1} \right) \right],$$

for $q = 0$ (29)

This is the solution of Eq. (19) when there is no applied field ($q = 0$). Here $\Delta = 1 + \eta \tan^2 \theta$.

As we showed above, for $q \rightarrow \infty$ the bulk solution is $\theta_b = 0$ and it can be proved consistently that $\lim_{\sqrt{\eta} \rightarrow \infty} \theta_l = \theta(x/\sqrt{\eta}, \sigma/\sqrt{\eta}, \eta) \rightarrow 0$ so that $\theta_{\text{match}}$ vanishes and as a consequence $\theta_{\text{adj}}$ from Eq. (26) reduces to $\theta_l$ which yields

$$\theta_{\text{adj}} = \theta(x/\sqrt{\eta}, \sigma/\sqrt{\eta}, \eta)$$

At this point, it is convenient to recall that the ER solution $\theta \neq 0$, given by Eq. (29), valid in the absence of a field, is only possible for $\sigma > 1$. Otherwise, the anchoring at the cylinder wall is no longer possible [26] and the system acquires the AX solution ($\theta = 0$). In fact, if we take the limit $\sigma \rightarrow 1$ in Eq. (29), $x$ will remain finite only if $\Delta \rightarrow 1$, implying $\theta \rightarrow 0$. According to Eq. (30), rescaling of $\sigma$ to the variable $\sigma' = \sigma/\sqrt{\eta}$ implies that the threshold value for the realization the ER–AX phase transition is translated by the influence of the field from $\sigma = 1$ to $\sigma/\sqrt{\eta} = 1$. Hence, using Eqs. (12) and (13), we find the expression for the threshold or critical field $E_\theta = E_c$

$$E_c = \frac{W_0}{\sqrt{\epsilon_a K_{11}}}$$

Using numerical values for the 5CB nematic we get $E_c = 13.45$ V/μm. Actually, because in the particular case of the NLC 5CB, $K_{24} = K_{11}$, Eq. (31) is independent of $R$. Because, according to Eq. (13), $\sqrt{q} \propto R$, our asymptotic calculation should not work well for small values of $R$ as is apparent from Fig. 5.

Also, Eq. (19) admits the AX solution for all $q$

$$\theta_q(x) = 0$$

However, as we have noted in the discussion of Eq. (25), the AX configuration is not favorable energetically for subcritical fields, while for a field larger than the value given by Eq. (31), it is the only solution.

Once $\theta(x)$ is calculated numerically, the Eq. (3) completely determine the dielectric tensor at every point of the LC cylinders and for all values of the field. Now one can proceed to the calculation of the PB structure, with allowance for the inhomogeneity and anisotropy of the LC cylinders, as done by Hornreich et al. [31] for cholesteric blue phases.

5. Photonic crystal composed of nematic liquid crystal cylinders

Sections 2–4 were devoted to the dielectric response of a single NLC cylinder subject to an axial DC electric field $E_0 \hat{z}$, neglecting the contribution of the AC wave field in our linear approximation. The conditions at the cylinder surface were specified in terms of the parameters $W_0$ and $K_{24}$, encapsulated in the important quantity $\sigma$, Eq. (12). We expect $\sigma$ to be practically independent of the thickness of the cylinder wall, and this thickness has not been taken into account explicitly. Summarizing our results up to this point, the NLC cylinder is characterized by the dielectric tensor $\varepsilon_{ij}$, Eq. (3),

$$\varepsilon = \begin{bmatrix} \epsilon_a + \epsilon_a \sin^2 \theta \cos^2 \phi & \epsilon_a \sin^2 \theta \sin \phi \cos \phi & \epsilon_a \sin \theta \cos \theta \cos \phi \\ \epsilon_a \sin^2 \theta \sin \phi \cos \phi & \epsilon_a + \epsilon_a \sin^2 \theta \sin^2 \phi & \epsilon_a \sin \theta \cos \theta \sin \phi \\ \epsilon_a \sin \theta \cos \theta \cos \phi & \epsilon_a \sin \theta \cos \theta \sin \phi & \epsilon_a + \epsilon_a \cos^2 \theta \end{bmatrix}$$

in the laboratory frame of reference. Here $\theta(r) = \angle(n, \hat{z})$ is the angle formed by the director $\mathbf{n}$ with respect to the cylinder axis and $\phi$ is the angle between the projection of $\mathbf{n}$ onto the $xy$ plane and an arbitrarily oriented $x$-axis. The angle depends on the radial distance $r$, is however independent of $z$ for our infinitely long cylinders. This angle $\theta(r)$ is found from the solution of the differential Eq. (19) subject to the boundary condition Eq. (20). Examples of the solution, for four values of the
parameter $\sigma$ (corresponding to progressively increasing cylinder radii $R$) are shown in Figs. 1–4. For applied fields $E_0$ that are greater than the critical field $E_{cr}$, as given by Eq. (25) or (31) and Fig. 5, all the directors assume the axial direction ($\mathbf{n} = \mathbf{z}$), that is, $\theta(r) = 0$ for all $r$. Then Eq. (34) reduces to
\begin{equation}
\tilde{\varepsilon}_{aK} = \begin{bmatrix}
\varepsilon_0 & 0 & 0 \\
0 & \varepsilon_0 & 0 \\
0 & 0 & \varepsilon_{a}
\end{bmatrix}
\end{equation}
(35)
as it should, recalling that the anisotropy is defined as the difference between the extraordinary and ordinary dielectric constants, $\varepsilon_a = \varepsilon_e - \varepsilon_o$.

Now we turn to a PC of NLC cylinders. We are assuming that the applied electric field $E_0\hat{z}$ has the same value at every point $r$ within the PC. Given this and the molecular origin of the director orientation, we can safely assume that the configuration $\theta(r)$ at any given cylinder is not affected by neighboring cylinders. That is, we take Eq. (34) to represent the dielectric tensor within all the cylinders of the PC ($r \leq R$). The space between the cylinders is filled by a uniform and isotropic dielectric having the dielectric constant $\varepsilon_b$. In what follows we will need the inverse dielectric tensor or dyadic $\eta(r)$ that satisfies the definition
\begin{equation}
\eta(r) \cdot \tilde{e}(r) = \mathbf{I} \quad \text{for all } r
\end{equation}
(36)
$I = \hat{x}x + \hat{y}y + \hat{z}z$ being the unit dyadic. By inverting the matrices (34) and (35) we find that
\begin{equation}
\eta(r) = \frac{1}{\varepsilon_e} \mathbf{I}, \quad \text{outside of cylinders}
\end{equation}
(37)
Clearly, the problem at hand is anisotropic, as well as inhomogeneous.

Every element of $\eta(r)$ is periodic in the $xy$ plane, permitting its expansion in a 2D Fourier series
\begin{equation}
\eta(r) = \sum_G \tilde{\eta}(G)e^{iGr}
\end{equation}
(38)
where $G = Gx \hat{x} + Gy \hat{y}$ are the 2D reciprocal lattice vectors. The Fourier coefficients $\tilde{\eta}(G)$ are obtained as
\begin{equation}
\tilde{\eta}(G) = \frac{1}{A_c} \int_{A_c} dV \eta(r)e^{-iGr}
\end{equation}
(39)
$A_c$ being the area of the unit cell. For $G = 0$, this is just the average of $\eta(r)$ over the unit cell. When integrating over de angle $\phi$, for $G = 0$ the off-diagonal elements of $\eta(r)$ give vanishing contribution, while the diagonal elements lead to integrals over the radius of the form $\int_0^1 dx \sin^2 \theta(x)$. Because $\int dV e^{-iGr} = 0$ for any $G \neq 0$, in this case Eq. (39) takes the form
\begin{equation}
\tilde{\eta}(G) = \frac{1}{A_c} \int_0^R rdr \int_0^{2\pi} d\phi \tilde{\eta}(r, \phi) - \frac{1}{\varepsilon_b} \mathbf{I} e^{-iGr} G_\alpha \cos \phi + G_\beta \sin \phi
\end{equation}
(40)
This dyadic is not diagonal, and its elements must be calculated numerically. Considering Eq. (37), $\tilde{\eta}(G)$ is symmetric, namely $\tilde{\eta}_{\alpha\beta}(G) = \tilde{\eta}_{\beta\alpha}(G)$.

Now we turn to Maxwell’s Equations for the PC. For harmonic waves of circular frequency $\omega$, Faraday’s Law is $\nabla \times \mathbf{E} = io\mathbf{B}(r)$. (41)
For our periodic medium both $\mathbf{E}(r)$ and $\mathbf{B}(r)$ must be Bloch waves
\begin{equation}
\mathbf{E}(r) = \sum_G \mathbf{E}_G(e^{i(k + G)r})
\end{equation}
(42)
\begin{equation}
\mathbf{B}(r) = \sum_G \mathbf{B}_G(e^{i(k + G)r})
\end{equation}
(43)
Here $k$ is the Bloch wave vector and $\mathbf{E}_G(k)$ and $\mathbf{B}_G(k)$ are the Fourier coefficients, respectively, of the amplitudes of $\mathbf{E}(r)$ and $\mathbf{B}(r)$. Substituting Eqs. (42) and (43) in Eq. (41), we can conclude that
\begin{equation}
(k + G) \times \mathbf{E}_G = \omega \mathbf{B}_G
\end{equation}
(44)
Therefore, for every partial plane wave in Eqs. (42) and (43), the magnetic induction amplitudes $\mathbf{B}_G(k)$ are perpendicular to the electric field amplitudes $\mathbf{E}_G(k)$ and to the wave vector $(k + G)$. Hence, $\mathbf{B}_G(k)$ is represented as having two independent components that are perpendicular to $(k + G)$. It is convenient to choose one of these components to be parallel to the cylinders, the other component then lying in the plane of periodicity. Then
\begin{equation}
\mathbf{B}_G(k) = \sum_{j=1}^{2} \tilde{B}_{kj}(G) \hat{c}_{kj}(G)
\end{equation}
(45)
\begin{equation}
\hat{c}_{k2}(G) = \hat{z}, \quad \hat{c}_{k1}(G) = \hat{z} \times \frac{k + G}{|k + G|}
\end{equation}
(46)
the unit vectors $(k + G)/|k + G|$, $\hat{c}_{k1}(G)$ and $\hat{c}_{k2}(G)$ form a right-handed triad of unit vectors, see Fig. 6. Note that, unlike $\mathbf{B}_G(k)$, the electric field $\mathbf{E}_G(k)$ has in general a longitudinal component parallel to $(k + G)$.

Because we are considering non-magnetic materials and there are no currents, the Ampère–Maxwell Law reads
\[ \nabla \times \mathbf{B}(\mathbf{r}) = -i(\alpha/c^2)\hat{e}(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r}) \]  

Multiplying this equation by \( \tilde{\eta}(\mathbf{r}) \), as given by Eq. (37), and using Eq. (36), we can eliminate \( \mathbf{E}(\mathbf{r}) \) from Eqs. (41) and (47). This yields the wave equation for \( \mathbf{B}(\mathbf{r}) \),

\[ \nabla \times [\nabla \times \mathbf{B}(\mathbf{r})] = k_0^2\mathbf{B}(\mathbf{r}) \]  

where \( k_0 = \omega/c \) is the vacuum wavevector. We transform this equation to inverse space by substituting Eq. (38) for \( \tilde{\eta}(\mathbf{r}) \) and Eqs. (43) and (45) for \( \mathbf{B}(\mathbf{r}) \). Standard algebra leads to

\[
\sum_{G} \sum_{j=1}^2 \sum_{\beta=1}^3 \eta_{\beta\beta}(\mathbf{G} - \mathbf{G'}) \hat{e}_\beta \cdot \hat{e}_\beta \\
\sum_{G} \sum_{j=1}^2 [\tilde{\xi}_{k_1}(\mathbf{G}) \cdot (\mathbf{k} + \mathbf{G})] \cdot \tilde{\eta}(\mathbf{G} - \mathbf{G'}) \cdot [(\mathbf{k} + \mathbf{G'})] \\
\times \sum_{G} \sum_{j=1}^2 \tilde{\xi}_{k_2}(\mathbf{G'}) B_{0\lambda}(\mathbf{G'}) + k_0^2 B_{0\lambda}(\mathbf{G}) = 0, \quad \lambda = 1, 2
\]

In order to simplify this equation, we note that, using Eq. (46)

\[
(\mathbf{k} + \mathbf{G}) \times (\tilde{\xi}_{k_1}(\mathbf{G})) = |\mathbf{k} + \mathbf{G}| \tilde{\xi}_{k_2}(\mathbf{G})
\]

\[
(\mathbf{k} + \mathbf{G}) \times (\tilde{\xi}_{k_2}(\mathbf{G})) = -|\mathbf{k} + \mathbf{G}| \tilde{\xi}_{k_1}(\mathbf{G})
\]

In addition, we may express the dyadic \( \tilde{\eta}(\mathbf{G}) \) as

\[
\tilde{\eta}(\mathbf{G}) = \sum_{\alpha, \beta=1}^3 \eta_{\alpha\beta}(\mathbf{G}) \hat{e}_\alpha \hat{e}_\beta
\]

in a coordinate system convenient for the PC. Naturally, we select \( \hat{e}_3 = \hat{z} \), see Fig. 6. Then Eq. (49) may be conveniently rewritten as

\[
\sum_{G} \sum_{j=1}^2 [\tilde{\xi}_{k_1}(\mathbf{G}) \cdot (\mathbf{k} + \mathbf{G})] \cdot \tilde{\eta}(\mathbf{G} - \mathbf{G'}) \cdot [(\mathbf{k} + \mathbf{G'})] \\
\sum_{G} \sum_{j=1}^2 \tilde{\xi}_{k_2}(\mathbf{G'}) B_{0\lambda}(\mathbf{G'}) + k_0^2 B_{0\lambda}(\mathbf{G}) = 0, \quad \lambda = 1, 2
\]

The summation over \( \alpha \) and \( \beta \) greatly simplifies because \( \tilde{\xi}_{k_1}(\mathbf{G}) = \tilde{\xi}_{k_2}(\mathbf{G'}) = \hat{z} \). The few surviving terms lead to our final result

\[
\sum_{G} |\mathbf{k} + \mathbf{G}| |\mathbf{k} + \mathbf{G'}| \\
\times \begin{bmatrix}
M_{11}(\mathbf{k} + \mathbf{G}, \mathbf{k} + \mathbf{G'}) & M_{12}(\mathbf{k} + \mathbf{G}, \mathbf{k} + \mathbf{G'}) \\
M_{21}(\mathbf{k} + \mathbf{G}, \mathbf{k} + \mathbf{G'}) & M_{22}(\mathbf{k} + \mathbf{G}, \mathbf{k} + \mathbf{G'})
\end{bmatrix} \\
\times \begin{bmatrix}
B_{k_1}(\mathbf{G'}) \\
B_{k_2}(\mathbf{G'})
\end{bmatrix}
= k_0^2 \begin{bmatrix}
B_{k_1}(\mathbf{G}) \\
B_{k_2}(\mathbf{G})
\end{bmatrix}
\]

where \( M_{ij} \) and \( B_{ij} \) are the components of the magnetic field and the magnetic induction, respectively.

\[
M_{11}(\mathbf{k} + \mathbf{G}, \mathbf{k} + \mathbf{G'}) = \eta_{xz}(\mathbf{G} - \mathbf{G'}) \sin \psi - \eta_{yz}(\mathbf{G} - \mathbf{G'}) \cos \psi
\]

\[
M_{12}(\mathbf{k} + \mathbf{G}, \mathbf{k} + \mathbf{G'}) = \eta_{xz}(\mathbf{G} - \mathbf{G'}) \cos \psi - \eta_{yz}(\mathbf{G} - \mathbf{G'}) \sin \psi
\]

Here \( \psi(\psi') \) is the angle between \( \mathbf{k} + \mathbf{G} \) and the \( x \)-axis.

Eq. (54) represents a doubly infinite number of equations; infinite, because all values of \( \mathbf{G} \) must be considered (in principle) and doubly, because for every value of \( \mathbf{G} \) there are two components of the magnetic induction – \( B_{k_1}(\mathbf{G}) \) and \( B_{k_2}(\mathbf{G}) \). However, these two components are coupled, as already noted in Ref. [8], meaning that they do not correspond to independent polarization modes related to the direction of the cylinders. In this context we recall that 2D PCs made from \textit{isotropic} materials with propagation in the plane of periodicity (\( \mathbf{k} \perp \mathbf{z} \)), support an \textit{E}-mode with \( \mathbf{E}(\mathbf{r}) \) parallel to the cylinders and an \textit{H}-mode with \( \mathbf{H}(\mathbf{r}) \) or \( \mathbf{B}(\mathbf{r}) \) along the cylinders. This separation into two polarizations is dictated by the existence of a mirror symmetry plane perpendicular to the homogeneous cylinders, such that \( \epsilon(-z) = \epsilon(z) \). On the other hand, no such plane exists for the NLC cylinders. This is so because the positive and negative \( z \)-directions are not equivalent; note that there are no NLC molecules, in our description, with \textit{downward} – pointing directors (always \( \hat{n} \cdot \hat{z} > 0 \)). This asymmetry originates in an implicit impurity at \( z = +\infty \) that attracts the molecules \textit{upward}. Eq. (54) thus describes a situation not unlike that of a 3D PC, where the components of the magnetic field are also coupled.

Now consider what happens for \textit{super-critical fields} \( E_0 > E_c \). In this axial configuration the dielectric dyadic is given by Eq. (35). Then the inverse dyadic (as also follows directly from Eq. (37) upon substituting \( \theta = 0 \)) is

\[
\tilde{\eta}_{AX} = \begin{bmatrix}
1/\epsilon_o & 0 & 0 \\
0 & 1/\epsilon_o & 0 \\
0 & 0 & 1/\epsilon_e
\end{bmatrix}
\]

independent of position, as long as \( \mathbf{r} \) is within a NLC cylinder. The Fourier transform is gotten from Eq. (40):

\[
\tilde{\eta}_{AX} = \begin{bmatrix}
\epsilon_{o}^{-1} - \epsilon_{b}^{-1} & 0 & 0 \\
0 & \epsilon_{o}^{-1} - \epsilon_{b}^{-1} & 0 \\
0 & 0 & \epsilon_{e}^{-1} - \epsilon_{b}^{-1}
\end{bmatrix} \frac{1}{\mathcal{A}} \int d\mathbf{r} e^{-i\mathbf{G} \cdot \mathbf{r}},
\]

\( \mathbf{G} \neq 0 \)
The integral over the cylinder cross-sectional area gives rise to a Bessel function, namely the well-known form factor \( F(|G| R) = J_1(|G| R) \) for circular cylinders. The matrix has the usual uniaxial structure, with

\[
\eta_{ax}^{XX}(G) = \eta_{ay}^{XX}(G) = \left( \frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) \frac{2fJ_1(GR)}{GR} = \eta_H(GR)
\]

\[
\eta_{ax}^{YY}(G) = \left( \frac{1}{\epsilon_a} - \frac{1}{\epsilon_b} \right) \frac{2fJ_1(GR)}{GR} = \eta_E(GR)
\]

(58)

\[
\eta_{ay}^{YY}(G) = 0 \quad \text{for} \quad \alpha \neq \beta, \quad G \neq 0
\]

For \( G = 0 \), the average of \( \tilde{\eta}(r) \) over the unit cell gives, simply

\[
\eta_H(0) = \frac{1}{\epsilon_a} f + \frac{1}{\epsilon_b} (1 - f), \quad f = \frac{\pi R^2}{A_c}
\]

\[
\eta_E(0) = \frac{1}{\epsilon_a} f + \frac{1}{\epsilon_b} (1 - f), \quad f = \frac{\pi R^2}{A_c}
\]

(59)

where \( f \) is the cylinder filling fraction. Eq. (55) then become

\[
M_{11}^{ax}(k + G, k + G') = \eta_H(|G - G'| R)
\]

\[
M_{12}^{ax}(k + G, k + G') = M_{21}^{ax}(k + G, k + G') = 0
\]

\[
M_{22}^{ax}(k + G, k + G') = \eta_H(|G - G'| R) \cos(k + G, k + G')
\]

(60)

The matrix in Eq. (54) then becomes diagonal, so that this equation reduces to

\[
\sum_{\alpha} \eta_{ax}(|G - G'| R)(k + G)\cdot(k + G')B_{ax1}(G') = k_a^2 B_{ax1}(G)
\]

(61)

\[
\sum_{\alpha} \eta_{ay}(|G - G'| R)(k + G)\cdot(k + G')B_{ay2}(G') = k_b^2 B_{ay2}(G)
\]

(62)

Eq. (61) involves only the field component \( B_{ax1}(G') \), but not the component \( B_{ay2}(G') \), while it is the other way round for Eq. (62). This means that, in the axial configuration, we have two independent polarizations. By Eqs. (45) and (46) \( B_{ax1}(G) \) is the component that is perpendicular to the cylinders. Then it follows from Eq. (44) that the accompanying electric field \( E_{ax1}(G) \) must be parallel to the cylinders. Hence, Eq. (61) is an eigenvalue equation for \( E \)-modes. By similar reasoning, Eq. (62) governs the \( H \)-modes, their magnetic field being parallel to the cylinders. However, when comparing with the corresponding eigenvalue equations for isotropic cylinders, a word or caution is in order: unlike the case of isotropic cylinders, in Eqs. (61) and (62) the Fourier coefficients \( \eta_{ax}^{ax}(GR) \) and \( \eta_{ax}^{ay}(GR) \) are different. From Eq. (59) we see that the only difference arises from having to use the extraordinary dielectric constant \( \epsilon_e \) of the NLC for the \( E \)-modes, while the ordinary dielectric constant \( \epsilon_o \) applies to the \( H \)-modes.

Summarizing, for supercritical fields \( E_0 > E_c(R) \), the general eigenvalue Eq. (54) – corresponding to complex polarization of the fields – decomposes into the two eigenvalue Eqs. (61) and (62) that determine, respectively, the properties of modes polarized with their electric field parallel and perpendicular to the cylinders.

6. Approximate photonic band structure

This approximate approach is based on the intuitive idea of replacing the dielectric dyadic \( \tilde{\epsilon}(r, \varphi) \), Eq. (34), by its average \( \langle \tilde{\epsilon} \rangle \) over the cross-sectional area of a NLC cylinder, namely

\[
\langle \tilde{\epsilon} \rangle = \frac{1}{\pi R^2} \int_0^R \int_0^{2\pi} \, dr \, d\varphi \langle \tilde{\epsilon}(r, \varphi) \rangle
\]

(63)

From Eq. (34) we see that the off-diagonal elements all vanish and the diagonal elements are

\[
\langle \epsilon_{ax} \rangle = \langle \epsilon_{ay} \rangle = \epsilon_o + \epsilon_a \int_0^1 \, dx \cdot x \sin^2 \theta(x) \equiv \epsilon_H(q)
\]

\[
\langle \epsilon_{az} \rangle = \epsilon_o + 2\epsilon_a \int_0^1 \, dx \cdot x \cos^2 \theta(x) \equiv \epsilon_E(q)
\]

(64)

the field parameter \( q \) being given by Eq. (13). We note that \( \epsilon_H \) and \( \epsilon_E \) are related by

\[
2\epsilon_H(q) + \epsilon_E(q) = 2\epsilon_o + \epsilon_e = \text{const}
\]

(65)

It is interesting that an intrinsically positive nematic \( \epsilon_o > \epsilon_e \) may become effectively negative, in the sense that \( \epsilon_H(q) < \epsilon_E(q) \) for a range of field strengths – and vice versa for an intrinsically negative nematic \( \epsilon_o < \epsilon_e \). It can even happen that \( \epsilon_E(q) \) and \( \epsilon_H(q) \) become equal for some value of \( q \), corresponding to isotropy in the average of the NLC cylinder.

By Eq. (64), the inverse dielectric tensor is

\[
\tilde{\eta} = \langle \tilde{\epsilon} \rangle^{-1} = \begin{bmatrix}
\frac{1}{\epsilon_H(q)} & 0 & 0 \\
0 & \frac{1}{\epsilon_H(q)} & 0 \\
0 & 0 & \frac{1}{\epsilon_E(q)}
\end{bmatrix}, \quad r < R
\]

(66)

This has the same uniaxial structure as Eq. (56), obtained for supercritical fields – which is not the case being considered at this point – however with \( \epsilon_o \) and \( \epsilon_e \) replaced, respectively, by \( \epsilon_H(q) \) and \( \epsilon_E(q) \). We can thus directly conclude that the present approximation leads to the eigenvalue Eqs. (61) and (62), however with \( \eta_{ax} \) and \( \eta_{ay} \) not given by the Eq. (58), but rather by

\[
\eta_{ax}(GR) = \begin{cases}
\frac{1}{\epsilon_o} + \frac{1}{\epsilon_e} & \text{if} \quad G = 0 \\
\frac{1}{\epsilon_o} - \frac{2fJ_1(GR)}{GR} & \text{if} \quad G \neq 0
\end{cases}
\]

(67)

\[
\eta_{ay}(GR) = \begin{cases}
\frac{1}{\epsilon_o} + \frac{1}{\epsilon_e} & \text{if} \quad G = 0 \\
\frac{1}{\epsilon_o} - \frac{2fJ_1(GR)}{GR} & \text{if} \quad G \neq 0
\end{cases}
\]

(68)

with \( \epsilon_E(q) \) and \( \epsilon_H(q) \) defined, respectively, in Eq. (64)

As we see then, the approximate calculation leads to independent \( E \)- and \( H \)-modes even for subcritical fields \( E_0 < E_c(q) \).

7. Graphical results

In Ref. [32] we have computed the components \( B_{ax}(r) \) and \( B_{ay}(r) \) of the magnetic field eigenvectors, corre-
responding to the directions perpendicular and parallel to the cylinders, respectively. It was found that $B_{\perp}(r)$ is the dominant component (with $B_{\parallel}(r) \ll B_{\perp}(r)$) in the first and third photonic bands. These two bands then can be said to have nearly-$E$ or quasi-$E$ polarization, even though, of course, we are concerned now with subcritical fields. Just the opposite occurs for the second band, which turns out to be characterized by $B_{\parallel}(r) \gg B_{\perp}(r)$; to this situation we refer as nearly-$H$ or quasi-$H$ polarization. This suggests that the usual separation into $E$- and $H$-modes might be approximately valid for NLC-infilled two-dimensional PCs – at least for the low-lying photonic bands. The approximate theory presented in the previous sections led, precisely, to independent $E$- and $H$-modes. It is then instructive to compare band structures calculated from Eqs. (61) and (62) with the substitution of Eqs. (67) and (68) with exact band structures from Eq. (54). This is done in Fig. 7 for the 5CB NLC cylinders in a silicon oxide (silica) host (square lattice), using our results for the director inclination $\theta(x)$.

About the first 6 bands are shown in Fig. 7 for $q = 20$. It is seen that, in general, the approximate bands for either the $E$- or the $H$-polarization nearly coincide with one of the exact bands. The fit is excellent for lower lying bands and it is very good even for the higher ones. This the justifies the concept of nearly-$E$ and nearly-$H$ polarizations and the use of much simpler approximate calculation in Section 6. Here is important to note that, the higher the value of $q$, the more the NLC directors align with the cylinders and the better this concept of quasi-polarization is expected to work. In fact, for $q \geq q_c$, the modes are strictly separated into the $E$- and $H$-polarizations.

Fig. 8a, shows the band structure for the case $q \geq q_c$. As a consequence of the low dielectric contrast there is no complete band gap, but there exist partial band gaps for both polarizations in the [100] direction. These partial band gaps are tuned by the external DC electric field as shown by Fig. 8b and c for the $E$- and $H$- modes, respectively. We should note that for $q = 0$, both gaps share a frequency region around \( \sim 0.32 \). When the $q$ parameter is increased, the $E$-band gap shifts downwards and the $H$-band gap shifts upwards in frequency.

Now, if unpolarized light with a normalized frequency of 0.317 is incident at the PC in the direction [100] and there is no applied field, all the light will be reflected. When $q$ is increased a little ($q = 9$), the $E$-polarized component of the light will still be reflected, while now the $H$-polarized component will be transmitted. Finally, all the light will be transmitted for any value of $q$ greater than 20. This demonstrates a significant application of NLC-infilled PCs,
namely polarizers whose optical response can be tuned or switched by means of an applied field.

8. Conclusions

In the first part of this paper we have determined the configuration of NLC molecules within an infinite circular cylinder. Namely, we calculated the angle \( \theta(r) \), formed by NLC director as function of radial distance and applied axial electric field, for a cylinder of given radius and specified elastic and surface parameters of the nematic (chosen to be 5CB). We came to the conclusion that, for a given radius, the configuration is escaped radial up to rather high fields. However, for a critical value of this DC field, a phase transition occurs to the axial configuration, with all the directors aligned with the cylinder axis. We have determined the value of this critical field as function of the cylinder radius. For radii that are not very small \( (R \geq 50 \text{ nm}) \), the critical field is \( E_c = 14 \text{ V/}\mu\text{m} \).

The NLC directors \( \vec{n}(\theta) \) lead to the dielectric tensor \( \epsilon_{ij}(r) \) of the NLC cylinder. In turn, this paved the way toward the eigenvalue equation that yields the photonic band structure. This was obtained for hollow cylinders in silica infilled with the nematic 5CB. It is important to note that, in principle, there are no independent \( E \)- and \( H \)-modes, as is the case for ordinary two-dimensional PCs with propagation in the plane of periodicity. That is, the electric and magnetic fields possess components both parallel and perpendicular to the cylinders that are coupled. This is occasioned by the special anisotropy of the nematic molecules that in our model escape upwards from the radial direction; hence there is no mirror plane parallel to the cylinders that are coupled. This work is expected to facilitate a more quantitative approach to the study of NLC-infilled PCs.

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