

Photospin-Orbit Coupling in Photonic Structures

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We show that the inclusion of nonlocality in the constitutive relations in photonic structures has important repercussions in their eigenmode configuration and distribution. In the case of optical activity, the primary manifestation of nonlocality, these features are traced to a photospin-orbit interaction analogous to the electron spin-orbit interaction in asymmetric semiconducting compounds; its impact can be assimilated to that of a magnetic field whose magnitude and direction follow that of the photon quasimomentum, with implications in photospin transport and photospintronics.

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Photonic crystals are media in which the dielectric permittivity is spatially modulated with a period in the range of optical wavelengths. The electromagnetic (EM) mode density distribution and configuration that such dielectrics can sustain is then shaped [1] through the interplay of Bragg and Mie resonances in photonic bands separated by forbidden propagation gaps, analogous to the ones obtained for the electronic band states in crystalline semiconducting compounds. As in the latter case, their characteristics and degeneracies reflect the symmetries of the point symmetry group of the underlying photonic lattice and its constituents.

The current derivations of the EM eigenmode configuration in photonic crystals have been conducted [1] on the basis of the constitutive relation $\mathbf{D} = \epsilon_0 \epsilon \mathbf{E}$ between the electric displacement \mathbf{D} and the electric field \mathbf{E} and similarly for the relation $\mathbf{B} = \mu_0 \mu \mathbf{H}$ between the magnetic induction \mathbf{B} and magnetic field \mathbf{H} , all taken together with the corresponding field continuity conditions across interfaces of discontinuity of the dielectric permittivity ϵ and the magnetic permeability μ . These relations imply locality in the field-matter interaction, concomitant with the assumption that the electric dipole coupling is the prevailing one at the microscopic molecular level.

However, the neglect of nonlocality suppresses important features of the field-matter interaction, such as optical activity and spatial dispersion [2]. Such nonlocal effects might seem to only weakly affect the magnitude of the dielectric coefficient. However, their real impact is on transverse features of the EM propagation modes [3], such as gyrotropy, polarization state, and phase, allowing for outstanding discrimination from the background.

In this Letter, we address the impact of nonlocality in photonic crystals formed by optically active constituents. To fix the ideas, such structures can in their simplest form be obtained by three-dimensional arrays of optically active spheres, two-dimensional ones of optically active rods, or one-dimensional gratings of optically active layers. To the extent that the EM polarization states can be interpreted as

photon spin states, we show that the breakdown of space inversion symmetry and the presence of rotatory power (gyrotropy), both inherent to optical activity [2,4], endow the EM mode structure and configuration with distinctly new features analogous to those imparted by the spin-orbit coupling [5,6] on electronic band states in noncentrosymmetric semiconducting compounds like GaAs or InSb.

The starting point in the analysis is the phenomenological constitutive relations for optically active media [4],

$$\mathbf{D} = \epsilon_0(\epsilon \mathbf{E} + \alpha \nabla \times \mathbf{E}), \quad (1a)$$

$$\mathbf{B} = \mu_0(\mu \mathbf{H} + \beta \nabla \times \mathbf{H}), \quad (1b)$$

in which the nonlocal character is reflected by the presence of the spatial derivative (rotation), being a consequence of the EM induction. At the molecular level, these relations are justified by their quantum-mechanical expressions [4] for α and β , as derived by a perturbative approach with the presence of, for example, a magnetic dipole coupling term in the EM field-matter interaction. This is performed along the same line of approach used to derive the expression for the electric dipole susceptibility $\chi = \epsilon - 1$ in the local (electric dipolar) approximation.

These constitutive relations are bound to some important selection and sum rules; in particular, α and β , which in the general case are third rank tensors, vanish in centrosymmetric media and hence prohibit optical activity in media belonging to point symmetry groups possessing inversion symmetry. In isotropic media after isotropic averaging [4], ϵ and μ behave as scalars and α and β as pseudoscalars with $\alpha = \beta$, which we for simplicity assume in the following without loss of generality.

The quantum-mechanical expression for $\alpha = \beta$ for the case of magnetic dipole coupling [4] in isotropic media of molecular number density N is

$$\alpha = \frac{2N}{3\epsilon_0 \hbar} \sum_n \frac{R_{0n}}{\omega_{n0}^2 - \omega^2}, \quad (2)$$

where $R_{0n} \equiv \text{Im}[\langle 0 | \hat{\boldsymbol{\mu}} | n \rangle \cdot \langle n | \hat{\mathbf{m}} | 0 \rangle] = (e^2/2m_e) \text{Im}[\langle 0 | \hat{\mathbf{r}} | n \rangle \cdot$

$\langle n|\hat{\mathbf{L}}|0\rangle$ is the gyrotropic strength, $\hat{\boldsymbol{\mu}} = -e\hat{\mathbf{r}}$ and $\hat{\mathbf{m}} = -(e/2m_e)\hat{\mathbf{r}} \times \hat{\mathbf{p}} \equiv -(e/2m_e)\hat{\mathbf{L}}$ are, respectively, the electric and magnetic dipole operators with $\hat{\mathbf{p}} = -i\hbar\nabla$ being the linear momentum operator, and $|0\rangle$ and $|n\rangle$ the electronic ground and excited states, respectively, with corresponding transition frequency ω_{n0} . The coefficients R_{0n} satisfy [4] the Rosenfeld sum rule $\sum_n R_{0n} = 0$, being the analogue of the Thomas-Reiche-Kuhn electric dipole oscillator strength sum rule $\sum_n f_{0n} = 1$ related to the electric dipole susceptibility χ .

From Eqs. (1) and (2), it is clear that α measures the photoinduced modification of the orbital (angular) momentum; through EM induction, this sets up a time varying magnetic (electric) field which induces the additional electric (magnetic) moment related to the optical activity in Eq. (1). This is analogous to the electronic spin-orbit coupling energy in semiconducting compounds, being also a (nonlocal) manifestation of the EM induction

$$H_{so} = \frac{e\hbar}{4m_e^2 c^2} (\mathbf{E}_e \times \hat{\mathbf{p}}) \cdot \hat{\boldsymbol{\sigma}}, \quad (3)$$

where $\hat{\boldsymbol{\sigma}}$ is the electronic spin operator and $\mathbf{E}_e = \nabla V$, with V being the effective central field potential as experienced by an electron in the periodic crystalline lattice. In drawing this analogy and setting up correspondences between photonic and electronic processes, it is important to keep in sight that we argue on the polarization in one case and on the potential energy in the other.

By taking the electric field of the form $\mathbf{E}(\mathbf{r}, t) = \text{Re}[\mathbf{E}_\omega \exp(-i\omega t)]$ and similarly for all other fields in Maxwell's equations $\nabla \times \mathbf{E} = -\partial \mathbf{B}/\partial t$ and $\nabla \times \mathbf{H} = \partial \mathbf{D}/\partial t$, one by inserting the constitutive relations (1) gets

$$\nabla \times \begin{pmatrix} \mathbf{E}_\omega \\ \mathbf{H}_\omega \end{pmatrix} = \mathbf{K} \begin{pmatrix} \mathbf{E}_\omega \\ \mathbf{H}_\omega \end{pmatrix}, \quad (4)$$

where

$$\mathbf{K} = \frac{1}{(1 - \alpha\beta\omega^2/c^2)} \begin{pmatrix} \varepsilon\beta\omega^2/c^2 & i\mu_0\mu\omega \\ -i\varepsilon_0\varepsilon\omega & \mu\alpha\omega^2/c^2 \end{pmatrix}.$$

From Eq. (4), one then obtains the propagation equation

$$\nabla \times \nabla \times \begin{pmatrix} \mathbf{E}_\omega \\ \mathbf{H}_\omega \end{pmatrix} - (\nabla \mathbf{K}) \times \begin{pmatrix} \mathbf{E}_\omega \\ \mathbf{H}_\omega \end{pmatrix} - \mathbf{K}^2 \begin{pmatrix} \mathbf{E}_\omega \\ \mathbf{H}_\omega \end{pmatrix} = \mathbf{0}, \quad (5)$$

subject to the transversality conditions $\nabla \cdot \mathbf{D} = 0$ and $\nabla \cdot \mathbf{B} = 0$. With the coefficients $\varepsilon(\mathbf{r})$, $\mu(\mathbf{r})$, $\alpha(\mathbf{r})$, and $\beta(\mathbf{r})$ being spatially periodic functions over the photonic crystal lattice, this differential matrix equation provides the eigenmodes and eigenfrequencies of the electromagnetic field. The solutions to Eq. (5) can be obtained either by a plane wave expansion, which however has slow convergence, or by the Korringa-Kohn-Rostoker Green's function perturbation

technique, using an expansion in spherical harmonics with much faster convergence [1].

For the latter case, one can perform a Bohren transformation [7] in Eq. (4), with

$$\begin{pmatrix} \mathbf{E}_\omega \\ \mathbf{B}_\omega \end{pmatrix} = \mathbf{A} \begin{pmatrix} \mathbf{Q}_+ \\ \mathbf{Q}_- \end{pmatrix} \equiv \mathbf{A}\mathbf{Q},$$

to diagonalize \mathbf{K} or $\mathbf{\Lambda} = \mathbf{A}^{-1}\mathbf{K}\mathbf{A}$ with

$$\mathbf{\Lambda} = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} 1 & a_+ \\ a_- & 1 \end{pmatrix},$$

where λ_\pm and a_\pm are easily derived from Eq. (4) and explicated in Ref. [7]. Equation (4) is then recast as

$$\mathbf{A}^{-1}\nabla \times (\mathbf{A}\mathbf{Q}) = \mathbf{\Lambda}\mathbf{Q}, \quad (6)$$

while the propagation Eq. (5) transforms to

$$\nabla \times \nabla \times \mathbf{Q} + [\nabla \times (\mathbf{A}^{-1}\nabla \mathbf{A} \times \mathbf{Q}) + \mathbf{\Lambda}\mathbf{A}^{-1}\nabla \mathbf{A} \times \mathbf{Q} - \nabla \mathbf{\Lambda} \times \mathbf{Q}] - \mathbf{\Lambda}^2 \mathbf{Q} = \mathbf{0}. \quad (7)$$

For homogeneous and isotropic optically active media, \mathbf{Q}_\pm for plane waves correspond to the left/right circularly polarized (LCP/RCP) eigenmodes or the ‘‘photospin up/down states,’’ respectively. One can actually recast the terms inside the brackets in Eq. (7) in a form reminiscent of Eq. (5) by inserting the expansion [8] $\mathbf{R} = \rho_0 \mathbf{I} + \boldsymbol{\rho} \cdot \boldsymbol{\sigma}$ for any 2×2 matrix \mathbf{R} , where \mathbf{I} and $\boldsymbol{\sigma}$ are the unity matrix and the Pauli matrix vector $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$, respectively.

Eqs. (4)–(7) are invariant under time reversal, reflecting reciprocity [2], as the common ones for optically inactive photonic crystals [1] to which they reduce when $\alpha = \beta = 0$. However, in contrast to the optically inactive case, the optically active photonic crystals lack invariance under space inversion. We will now analyze some of the implications from these on the EM propagation modes, their eigenfrequencies and eigenstates. We may proceed to simplify Eqs. (5) and (7) by neglecting the magnetization [3], with $\mathbf{B} = \mu_0 \mathbf{H}$. For this case Eq. (5) reduces to

$$\nabla \times \nabla \times \mathbf{E}_\omega - (\omega/c)^2 (\varepsilon \mathbf{E}_\omega + \alpha \nabla \times \mathbf{E}_\omega) = \mathbf{0}.$$

The periodicity of $\varepsilon(\mathbf{r})$ and $\alpha(\mathbf{r})$ over the lattice of the photonic crystal is expressed by the translational symmetries $\varepsilon(\mathbf{r} + \mathbf{a}_i) = \varepsilon(\mathbf{r})$ and $\alpha(\mathbf{r} + \mathbf{a}_i) = \alpha(\mathbf{r})$, where \mathbf{a}_i , $i = 1, 2, 3$, are the elementary lattice vectors of the photonic crystal. We can accordingly express the electric permittivity and gyration coefficient in terms of their Fourier series $\varepsilon(\mathbf{r}) = \sum_{\mathbf{Q}} \tilde{\varepsilon}(\mathbf{Q}) \exp(i\mathbf{Q} \cdot \mathbf{r})$ and $\alpha(\mathbf{r}) = \sum_{\mathbf{Q}} \tilde{\alpha}(\mathbf{Q}) \exp(i\mathbf{Q} \cdot \mathbf{r})$ over the reciprocal lattice space $\mathbf{Q} = \sum_i l_i \mathbf{b}_i$ spanned by the reciprocal lattice vectors \mathbf{b}_i such that $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$, and similar for the field $\mathbf{E}_\omega(\mathbf{r}) = \sum_{\mathbf{Q}} \mathbf{E}_{n\mathbf{k}}(\mathbf{Q}) \exp[i(\mathbf{k} + \mathbf{Q}) \cdot \mathbf{r}]$. This gives the eigenmode equation

$$\sum_{\mathbf{Q}'} (\mathbf{k} + \mathbf{Q}') \times [(\mathbf{k} + \mathbf{Q}') \times \mathbf{E}_{n\mathbf{k}}(\mathbf{Q}')] + i \frac{\omega_{n\mathbf{k}}^2}{c^2} \sum_{\mathbf{Q}'} \tilde{\alpha}(\mathbf{Q} - \mathbf{Q}') (\mathbf{k} + \mathbf{Q}') \times \mathbf{E}_{n\mathbf{k}}(\mathbf{Q}') + \frac{\omega_{n\mathbf{k}}^2}{c^2} \sum_{\mathbf{Q}'} \tilde{\varepsilon}(\mathbf{Q} - \mathbf{Q}') \mathbf{E}_{n\mathbf{k}}(\mathbf{Q}') = \mathbf{0}. \quad (8)$$

As pointed out in connection with Eqs. (1) and (2), α is a measure of the coupling of the photospin state with the opticalrotatory power, and its impact on the photonic band states is analogous to the spin-orbit coupling [5,6] in the case of electronic band states in centrosymmetric compounds like GaAs or InSb. This correspondence in physical origins also reverberates in the impact on the corresponding eigenvalues and eigenmodes. As in the case of the electron spin-orbit coupling in asymmetric compounds [6], the modifications that the optical activity terms impart on the eigenmodes of the photonic crystal can be assessed by applying a perturbative approach. With the optical activity term taken as the perturbation, the primary effect of the breakdown of the space inversion term is the lifting of the two-fold degeneracy of the mode eigenstates of the underlying photonic structure if optical activity was absent, this degeneracy lifting results in different eigenfunctions for the left and right circular polarization modes or photospin states.

The mode degeneracies in the underlying optically inactive photonic structure are higher than two-fold and reflect the space group symmetry of the photonic crystal lattice; they are to a certain extent lifted in the presence of optical gyrotropy. This additional degeneracy lifting, besides the previous two-fold one, can be assessed by diagonalizing the optical activity perturbation within each degenerate manifold; this procedure exactly parallels the one used in evaluating the degeneracy splittings of the energy band states in asymmetric semiconducting compounds and the analysis of Refs. [5,6] can be transposed to the present case as such.

We highlight this point for the case of an optically active one-dimensional stratified grating with the dielectric permittivity and gyration coefficient being periodic functions along the z -axis, with $\varepsilon(z+a) = \varepsilon(z)$ and $\alpha(z+a) = \alpha(z)$. In their Fourier expansions $\varepsilon(z) = \sum_n \tilde{\varepsilon}_n \exp(inKz)$ and $\alpha(z) = \sum_n \tilde{\alpha}_n \exp(inKz)$, where $K = 2\pi/a$ is the magnitude of the reciprocal grating vector, we limit the discussion to the dominant lowest order terms $n = 0, \pm 1$, adequately describing sinusoidally modulated photonic crystals. The previously outlined diagonalization procedure shows that the eigenmodes are circularly polarized plane waves [8], and it is hence convenient to take the electric field as $\mathbf{E}(\mathbf{r}, t) = \text{Re}[\mathbf{e}_+ E_+(z, t) + \mathbf{e}_- E_-(z, t)]$, in which $\mathbf{e}_\pm = (\mathbf{e}_x \pm i\mathbf{e}_y)/\sqrt{2}$ are the LCP/RCP basis vectors. The envelopes $E_\pm(z, t)$ are expressed in terms of their Fourier expansions as

$$E_\pm(z, t) = \sum_{m=-\infty}^{\infty} \tilde{E}_m^\pm \exp[i(k_\pm + mK)z - i\omega_\pm t],$$

where \tilde{E}_m^\pm is the Fourier coefficients of the circularly polarized eigenmodes, to get the infinite chain of eigenmode equations

$$q_m^\pm \tilde{E}_{m-1}^\pm + d_m^\pm \tilde{E}_m^\pm + r_m^\pm \tilde{E}_{m+1}^\pm = 0, \quad (9)$$

for $m = 0, \pm 1, \pm 2, \dots$, in which the coefficients are

$$\begin{aligned} q_m^\pm &= (\omega_\pm/c)^2 [\tilde{\varepsilon}_{+1} \pm \tilde{\alpha}_{+1}(k_\pm + (m-1)K)], \\ d_m^\pm &= (\omega_\pm/c)^2 [\tilde{\varepsilon}_0 \pm \tilde{\alpha}_0(k_\pm + mK)] - (k_\pm + mK)^2, \\ r_m^\pm &= (\omega_\pm/c)^2 [\tilde{\varepsilon}_{-1} \pm \tilde{\alpha}_{-1}(k_\pm + (m+1)K)]. \end{aligned}$$

We may cut off the expansion at $m = \pm M$ to yield a system of $2M + 1$ terms for each circular polarization state. The requirement on the corresponding system determinant of Eq. (9) to yield zero then gives the dispersion relations $\omega_\pm(k_\pm)$, which are obtained analytically as polynomial equations in ω_\pm and k_\pm . In Fig. 1, we map these dispersion relations for a photonic crystal, possessing material parameters corresponding to those of optically active quartz, together with the dispersion for an optically inactive grating with otherwise same parameters, the later

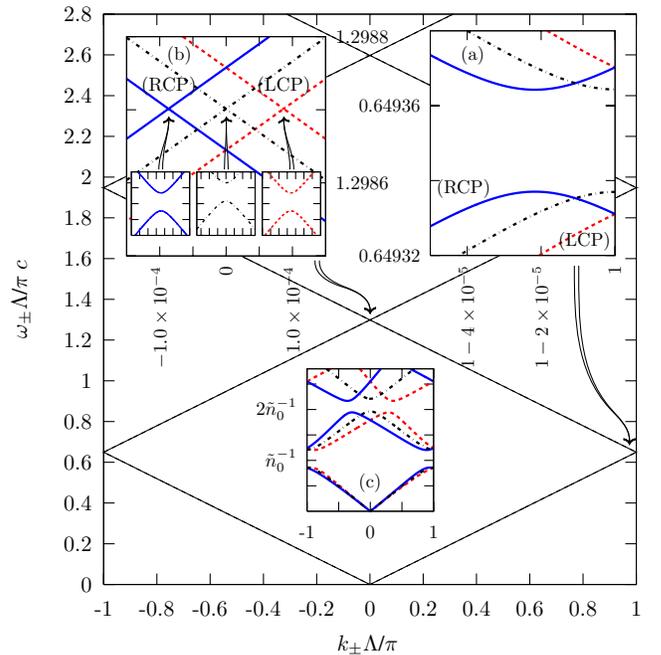


FIG. 1 (color online). The dispersion relations $\omega_-(k_-)$ of right (blue/solid line) and $\omega_+(k_+)$ of left (red/dashed line) circularly polarized modes propagating in an infinite periodic and optically active medium. The limiting band diagram in the absence of rotatory power is shown as dot-dashed curved lines. The insets show enlargements of the (a) first- and (b) second-order band gaps, in which the wave vector splitting of the circular polarization states is manifested as an asymmetry in the band diagram. Parameter values were taken as those for crystalline quartz of trigonal point symmetry group 32, which at a vacuum wavelength of 633 nm possesses a refractive index of $\tilde{n}_0 \equiv \tilde{\varepsilon}_0^{1/2} = 1.54$ and a rotatory power of 19.0 deg/mm, or $\tilde{\alpha}_0 K = 2.1 \times 10^{-4}$, with a spatial bottom-to-peak index modulation of 2.7×10^{-5} ($\tilde{\varepsilon}_{\pm 1} = 1.0 \times 10^{-4}$) and $\tilde{\alpha}_{\pm 1} = \tilde{\alpha}_0/10$. The grating period was chosen as $\Lambda = 206$ nm, corresponding to a first-order Bragg resonance at 633 nm vacuum wavelength. The wave vector splitting of the second-order bandgap is $k_+ - k_- = 1.7 \times 10^{-4} \pi/\Lambda = 26 \text{ cm}^{-1}$. For visual clarity, inset (c) shows the corresponding band diagram with parameters $\tilde{\varepsilon}_{\pm 1}$ and $\tilde{\alpha}_0$ greatly exaggerated.

possessing two-fold degeneracy. The splitting of the two-fold degeneracy in the presence of optical activity is evident as is also its vanishing at $k = 0$. Even more striking is the introduced asymmetry in the photonic band shape and the shift of the photonic band gap from the Brillouin zone border resulting from band anticrossing, as in detail illustrated in the right inset of Fig. 1, which shows the first-order band gap in the positive direction of wave propagation. The opposite horizontal shift of the dispersion relations of opposite circular polarization states increases with the value of the wave vector, as evident from Eq. (8) and explicitly demonstrated in the left inset of Fig. 1, showing the second-order band gap. This endows these gratings with functionalities such as photospin splitting and filtering. Referring for instance to inset (a) of Fig. 1 and the axis convention therein, for a linearly polarized beam of frequency close to the edge of the band gap, the RCP component will be totally transmitted while the LCP component is totally reflected. This configuration reverses by reversing the beam propagation.

The photospin-orbit splitting of the eigenmodes in photonic crystals with optical activity present is analogous to an effective Zeeman-like splitting [9] by a magnetic field whose magnitude and direction follow those of the wave vector. As can be inferred from Eq. (9) in the first Brillouin zone, the displacement $\mathbf{D}_\omega = \varepsilon_0(\varepsilon\mathbf{E}_\omega + i\alpha\mathbf{k} \times \mathbf{E}_\omega)$ has the same functional form as the displacement [3] $\mathbf{D}_\omega = \varepsilon_0(\varepsilon\mathbf{E}_\omega + i\gamma\mathbf{B}_e \times \mathbf{E}_\omega)$ in the presence of a static magnetic field \mathbf{B}_e applied in the direction of the wave vector and of magnitude $B_e = \alpha k/\gamma$, with γ being the Faraday rotation coefficient of the material. However, in contrast to the true Faraday effect in the presence of an external magnetic field, which is nonreciprocal, the present one is reciprocal as the equivalent magnetic field \mathbf{B}_e reverses direction with the wave vector and clearly vanishes with $\mathbf{k} \rightarrow \mathbf{0}$, leading to a zero photospin splitting at the center of the Brillouin zone; this is consistent with the Onsager reciprocity relations.

This exactly parallels the situation encountered in asymmetric semiconducting compounds with spin-orbit interaction included. Its effect on the electron spin dynamics there is equivalent [10] to a Zeeman-like splitting by an effective magnetic field whose magnitude and direction depend on the electron band \mathbf{k} -vector; in particular, it also for this case reverts with the later and vanishes at the center of the Brillouin zone. This plays a key role in electron spin orientation dynamics, transport and filtering, in particular, such as in the D'Yakonov-Perel and Rashba [10] mechanisms in spintronics, and the same considerations can be transposed to photospin orientation and transport in photonic structures as well, with certain provisions for the

different statistics for photons (bosons) and electrons (fermions).

In conclusion, we have in this Letter derived the eigenmode equations in photonic crystals formed with optically active constituents and shown that the combined effect of space inversion symmetry breakdown and gyrotropy there has the same impact on the eigenmode structure and configuration as in the spin-orbit coupling in electronic band states in asymmetric semiconducting compounds, allowing us to draw certain parallels between electron spin and photospin transport in such periodic structures.

Photonic crystals with optically active components embedded in an optically inactive dielectric can be made with quartz as the optically active component in the form of spheres, cylindrical rods or plane layers in three-dimensional, two-dimensional, or one-dimensional arrays; the embedding medium can be amorphous glass, a transparent polymeric solid or liquid matrix; self-organized arrays of such objects can now be envisaged. An even more interesting case is that of chiral molecular complexes, spheres or rods or layers arrayed in a throughout dielectric solid or liquid. The latter case clearly is of relevance in different situations in biophotonics where the polarization state evolution and photospin transport in ordered molecular complexes can play an important role.

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