Lagrangian approach to light propagation in liquid crystals

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A Lagrangian and Hamiltonian formulation of light propagation in layered nematic liquid crystals is presented in the general case of a plane wave for any incidence angle and polarization. The resulting Lagrange or Hamilton equations reproduce both Maxwell's equations and the torque equations governing the molecular director equilibrium under light action. The theory includes nonlinear optical effects due to molecular reorientation. The exact formulation is then reduced to a simpler one using the generalized geometric-optics approximation. The corresponding approximate expression for the optical torque is also derived.

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I. INTRODUCTION

Light propagation in birefringent inhomogeneous media is a difficult problem even in the case of plane incident wave and layered media. Berreman proposed to use a 4×4 matrix formalism equivalent to Maxwell's equations [1]. Oldano showed that the Berreman 4×4 matrix equation can be reduced to a simpler 2×2 matrix equation using the generalized geometric-optics approximation (GGOA) [2]. Berreman's equation has a form similar to Schrödinger's equation, so that one can use well known tools of quantum mechanics such as, for instance, perturbative approaches or eigenmode expansions.

In the case of light propagation in liquid crystalline media, the problem may become nonlinear, due to the torque exerted by the optical beam on the molecules of the medium. A Lagrangian or Hamiltonian formulation is then recommended, because nonlinearities can be handled in a natural way, and the powerful tools of analytic mechanics can be used to find conserved quantities, to formulate adiabatic theorems, and so on. This approach was proved to be possible in the case of normal incidence and in the GGOA [3]. In this paper we show that reduction to a Lagrangian problem is also possible in the case of oblique incidence, both for the exact Maxwell and torque equations and those obtained in the GGOA.

II. THE EXACT EQUATIONS

Let us consider a monochromatic plane wave propagating in a transparent anisotropic optical medium, stratified along the z direction. The electric and magnetic field components of the wave all share a common phase factor $\exp(-i\omega t + ik_x x + ik_y y)$, describing the time and transverse space dependence. Henceforth this phase factor will be omitted, so that all the fields are taken to depend on the z coordinate only. Maxwell's equations can then be cast in the form of the Euler-Lagrange equations (with $q'^i \equiv dq^i/dz$)

$$\frac{d}{dz}\frac{\partial L^o}{\partial q'^i} - \frac{\partial L^o}{\partial q^i} = 0 \qquad (i = 1, \ldots, 4), \tag{1}$$

where the four generalized coordinates q are related to the real part of the field components of the wave by

$$q \equiv \{q^i\} = \frac{1}{\sqrt{8\pi k_0}} \mathrm{Re}(E_x, E_y, H_y, -H_x) \tag{2}$$

and $L^o(q, q', z)$ is the optical Lagrangian, given by

$$L^o(q, q', z) = \frac{1}{2k_0} q'^T \tilde{G} \tilde{S}^{-1}(z) \tilde{G} q' - \frac{k_0}{2} q^T \tilde{S}(z) q, \tag{3}$$

where $\tilde{G}$ is the matrix

$$\tilde{G} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{4}$$

and $\tilde{S}$ is a symmetric 4×4 matrix characterizing the medium. In the case of transparent, nonmagnetic, birefringent media the matrix $\tilde{S}$ is given by

$$\tilde{S}(z) = \begin{pmatrix} \tilde{\varepsilon}_{xx} - \beta_y^2 & \tilde{\varepsilon}_{xy} + \beta_x\beta_y & -\beta_x \frac{\varepsilon_{xz}}{\varepsilon_{zz}} & -\beta_y \frac{\varepsilon_{xz}}{\varepsilon_{zz}} \\ \tilde{\varepsilon}_{xy} + \beta_x\beta_y & \tilde{\varepsilon}_{yy} - \beta_x^2 & -\beta_x \frac{\varepsilon_{yz}}{\varepsilon_{zz}} & -\beta_y \frac{\varepsilon_{yz}}{\varepsilon_{zz}} \\ -\beta_x \frac{\varepsilon_{xz}}{\varepsilon_{zz}} & -\beta_x \frac{\varepsilon_{yz}}{\varepsilon_{zz}} & 1 - \frac{\beta_x^2}{\varepsilon_{zz}} & -\frac{\beta_x\beta_y}{\varepsilon_{zz}} \\ -\beta_y \frac{\varepsilon_{xz}}{\varepsilon_{zz}} & -\beta_y \frac{\varepsilon_{yz}}{\varepsilon_{zz}} & -\frac{\beta_x\beta_y}{\varepsilon_{zz}} & 1 - \frac{\beta_y^2}{\varepsilon_{zz}} \end{pmatrix}, \tag{5}$$

where

$$\begin{aligned} \tilde{\varepsilon}_{xx} &= \varepsilon_{xx} - \frac{\varepsilon_{xz}^2}{\varepsilon_{zz}}, \\ \tilde{\varepsilon}_{xy} &= \varepsilon_{xy} - \frac{\varepsilon_{xz}\varepsilon_{yz}}{\varepsilon_{zz}}, \\ \tilde{\varepsilon}_{yy} &= \varepsilon_{yy} - \frac{\varepsilon_{yz}^2}{\varepsilon_{zz}}. \end{aligned} \tag{6}$$

In Eq. (5), β_x and β_y are the wave vector transverse components in units of $k_0 = \omega/c$. The ε's are the components of the dielectric tensor, that for uniaxial media is related to the local direction $\boldsymbol{n}$ of the optical axis by

$$\varepsilon(z) = \begin{pmatrix} \varepsilon_o + \varepsilon_a n_x^2 & \varepsilon_a n_x n_y & \varepsilon_a n_x n_z \\ \varepsilon_a n_x n_y & \varepsilon_o + \varepsilon_a n_y^2 & \varepsilon_a n_y n_z \\ \varepsilon_a n_x n_z & \varepsilon_a n_y n_z & \varepsilon_o + \varepsilon_a n_z^2 \end{pmatrix}, \tag{7}$$

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where $\varepsilon_a = \varepsilon_e - \varepsilon_o$ is the dielectric anisotropy, and $\varepsilon_o = n_o^2$, $\varepsilon_e = n_e^2$, where n_o and n_e are the ordinary and extraordinary indices, respectively.

Once the Euler-Lagrange Eqs. (1) are solved, the electric and magnetic fields of the optical wave in the medium can be completely evaluated because the imaginary parts of the field components along x and y are related to the conjugate momenta

$$p \equiv \partial L^o/\partial q' = \frac{1}{k_0}\tilde{G}\tilde{S}^{-1}\tilde{G}q' \tag{8}$$

according to

$$p \equiv \{p_i\} = -\frac{1}{\sqrt{8\pi k_0}}\mathrm{Im}(H_y, -H_x, E_x, E_y), \tag{9}$$

and the z components are given by

$$\begin{aligned} H_z &= \beta_x E_y - \beta_y E_x, \\ E_z &= -\frac{1}{\varepsilon_{zz}}(\varepsilon_{xz}E_x + \varepsilon_{yz}E_y - \beta_y H_x + \beta_x H_y). \end{aligned} \tag{10}$$

The equivalence between Eqs. (1) and Maxwell's equations is best made by observing that Hamilton's equations derived from the Hamiltonian

$$H^o(p,q,z) = \frac{k_0}{2}\left[p^T\tilde{G}\tilde{S}(z)\tilde{G}p + q^T\tilde{S}(z)q\right] \tag{11}$$

associated to L^o reduce to Berreman's equation

$$\frac{d\Psi}{dz} = ik_0\tilde{B}(z)\Psi, \tag{12}$$

where Berreman's wave function Ψ and matrix $\tilde{B}$ are related to our generalized coordinates and momenta and matrix $\tilde{S}$ by

$$\Psi = \sqrt{8\pi k_0}\,\tilde{G}_1(q - i\tilde{G}p), \tag{13}$$

$$\tilde{B} = \tilde{G}_1^{-1}\tilde{G}\tilde{S}\tilde{G}_1, \tag{14}$$

with matrix $\tilde{G}_1$ given by

$$\tilde{G}_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{15}$$

Both $\tilde{G}$ matrices are idempotent: $\tilde{G}^2 = \tilde{G}_1^2 = 1$.

When the medium is a liquid crystal, the direction $\boldsymbol{n}$ of the local optical axis is along the molecular director and may be different from point to point in the sample. In the plane-wave approximation we assume $\boldsymbol{n} = \boldsymbol{n}(z)$ only. Moreover, $\boldsymbol{n}$ can be changed by the optical field itself, because of the optical reorientation. The whole process becomes nonlinear and Maxwell's equations must be solved together with the torque equations governing the optical reorientation in the material. Now, both Maxwell's and torque equations can be obtained, in the plane-wave approximation, from the total Lagrangian L given by the sum of the optical Lagrangian L^o given above and of the Frank elastic free energy L^e of the liquid crystal [4]:

$$L = L^e + L^o. \tag{16}$$

This important result is based on the fact that after insertion of Eqs. (7) into Eq. (5) and Eq. (3), the optical part L^o of the Lagrangian becomes no longer explicitly dependent on z, but we have instead

$$L^o = L^o(q, q', \boldsymbol{n}) \tag{17}$$

and that we have also

$$\begin{aligned} \boldsymbol{h}^o \equiv -\frac{\partial L^o}{\partial \boldsymbol{n}} = \frac{\partial H^o}{\partial \boldsymbol{n}} &= \frac{k_0}{2}\left(p^T\tilde{G}\frac{\partial\tilde{S}}{\partial\boldsymbol{n}}\tilde{G}p + q^T\frac{\partial\tilde{S}}{\partial\boldsymbol{n}}q\right) \\ &= \frac{\varepsilon_a}{8\pi}\mathrm{Re}[(\boldsymbol{n}\cdot\boldsymbol{E}^*)\boldsymbol{E}], \end{aligned} \tag{18}$$

where $\boldsymbol{E} = (E_x, E_y, E_z)$ is the optical electric field. Using the last equation, we see that the Euler-Lagrange equations for the total Lagrangian L given by Eq. (16) reduce, on one side, to the Euler-Lagrange equations of L^o, which are equivalent to Maxwell's equations, and, on the other side, to the torque equations

$$\boldsymbol{n} \times (\boldsymbol{h}^e + \boldsymbol{h}^o) = \boldsymbol{0}, \tag{19}$$

where $\boldsymbol{h}^e \equiv (d/dz)(\partial L^e/\partial\boldsymbol{n}') - \partial L^e/\partial\boldsymbol{n}$ is the elastic molecular field derived from L^e.

Equations (19) apply to steady state only and, together with Maxwell's equations, yield the distribution of the optical and director fields $\boldsymbol{n}(z), \boldsymbol{E}(z), \boldsymbol{H}(z)$ in the medium. In nonstationary states a viscous torque $\boldsymbol{\tau}^v$ must be added on the left side of Eq. (19), depending on $\boldsymbol{n}$ and its time derivative $\dot{\boldsymbol{n}} = \partial\boldsymbol{n}/\partial t$. In the simplest cases the viscous torque is given by $\boldsymbol{\tau}^v = -\gamma(\boldsymbol{n}\times\dot{\boldsymbol{n}})$, where γ is a viscosity coefficient.

A. Conservation laws

The Lagrangian (or Hamiltonian) formulation permits us to obtain conservation laws from Noëther's theorems.

The total Lagrangian L does not depend on the z coordinate explicitly; therefore the total Hamiltonian H is constant along the z axis. In the case of normal incidence, H is equal to the sum of the elastic free energy and electromagnetic energy density and therefore this conservation law reduces to the conservation of the total energy density along the medium [3].

The total Hamiltonian H is invariant under the canonical transformation

$$\begin{aligned} q &\to q\ \cos\gamma - \tilde{G}p\ \sin\gamma\ , \\ p &\to p\ \cos\gamma + \tilde{G}q\ \sin\gamma\ , \end{aligned} \tag{20}$$

with arbitrary parameter γ, which implies the conservation law

$$S_z = \frac{ck_0}{2}(p^T\tilde{G}p + q^T\tilde{G}q) = \text{const.} \tag{21}$$

(The generating function of this transformation is $F(q,\bar{q}) = \frac{1}{2\,\sin\gamma}[(q\tilde{G}q + \bar{q}\tilde{G}\bar{q})\cos\gamma - \bar{q}\tilde{G}q]$, where $\bar{q},\bar{p}$ are the new coordinates and momenta.) From Eqs. (2) and (9) we see that the conserved quantity S_z is the Poynting vector z component of the optical wave.

Finally the total Lagrangian L is invariant under rotation of the laboratory frame around the z axis. As is well known, this rotational symmetry leads to the conservation of the z component of the total angular momentum of the whole system (radiation field plus medium). This conservation law can be written out in the divergence form

$$\operatorname{div}(\boldsymbol{l}_z^{mec} + \boldsymbol{l}_z^{int} + \boldsymbol{l}_z^{orb}) = 0, \tag{22}$$

where $\boldsymbol{l}_z^{mec}$ is the flux of z component of the mechanical angular momentum carried on by the elastic forces inside the liquid crystal. The only component of $\boldsymbol{l}_z^{mec}$ entering Eq. (22) is the z component, given by

$$l_{zz}^{mec} = -[k_{22} + (k_{33} - k_{22})n_z^2](\boldsymbol{n} \times \boldsymbol{n}')_z. \tag{23}$$

$\boldsymbol{l}_z^{int}$ and $\boldsymbol{l}_z^{orb}$ are the fluxes of z component of the intrinsic and orbital parts of the angular momentum carried on by the radiation field, given by ($\boldsymbol{z}$ is the unit vector along the positive z axis)

$$\begin{aligned} \boldsymbol{l}_z^{int} &= \frac{1}{8\pi k_0}\operatorname{Im}[\boldsymbol{H}^* \times (\boldsymbol{z} \times \boldsymbol{E})], \\ \boldsymbol{l}_z^{orb} &= [(\boldsymbol{r} \times \boldsymbol{k}) \cdot \boldsymbol{z}]\frac{\boldsymbol{S}}{\omega}, \end{aligned} \tag{24}$$

where $\boldsymbol{k} = (k_x, k_y, 0)$ and $\boldsymbol{S} = c/8\pi\,\operatorname{Re}(\boldsymbol{E}^* \times \boldsymbol{H})$ is the average Poynting vector of the optical wave.

The divergence of the flux of angular momentum z component must be equal to minus the z component of the torque acting on the unit volume. Equation (22) is therefore equivalent to the z component of the torque balance Eq. (19), as can be checked also by direct calculation. In the case of normal incidence, where the orbital part of the radiation angular momentum vanishes, the angular momentum conservation law assumes the simpler form

$$l_{zz}^{mec} + l_{zz}^{int} = \text{const.} \tag{25}$$

We notice moreover that the component l_{zz}^{int} of the flux $\boldsymbol{l}_z^{int}$ is related to our generalized coordinates and momenta by the simple relationship

$$l_{zz}^{int} = p^T\tilde{L}q, \tag{26}$$

where $\tilde{L}$ is the skewsymmetric matrix

$$\tilde{L} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}. \tag{27}$$

Definitions (24) of the orbital and intrinsic angular momentum of the light were already reported by Santamato and co-workers using a different approach [5]. In particular, from the definition of the orbital angular momentum of light, the picture emerges that inside a birefringent medium photons carry angular momentum $\boldsymbol{r} \times \hbar\boldsymbol{k}$, and hence linear momentum $\hbar\boldsymbol{k}$ along the $\boldsymbol{k}$ direction, but they move along the ray direction, i.e., the direction of the energy flux $\boldsymbol{S}$ [5].

B. Boundary conditions

In order to have a well defined mathematical problem, the Euler-Lagrange Eqs. (1) for the optical field must be supplemented with appropriate boundary conditions. (For the reorientational part, the boundary conditions are provided by the anchoring conditions of the liquid crystal molecular director at the sample walls, and will not be discussed here.) To be specific, we assume that the medium is enclosed between two external homogeneous isotropic media having refractive indices n_1 and n_2 and located at planes $z = 0$ and $z = L$, respectively. Without loss of generality we may take the x,z plane as the incidence plane so that $\beta_y = 0$ and $\beta_x = \beta = n_1\ \sin\alpha$, α being the incidence angle in the first medium. The matrix $\tilde{S}(z)$ assumes then the simpler form

$$\tilde{S}(z) = \begin{pmatrix} \tilde{\varepsilon}_{xx} & \tilde{\varepsilon}_{xy} & -\beta\frac{\varepsilon_{xz}}{\varepsilon_{zz}} & 0 \\ \tilde{\varepsilon}_{xy} & \tilde{\varepsilon}_{yy} - \beta^2 & -\beta\frac{\varepsilon_{yz}}{\varepsilon_{zz}} & 0 \\ -\beta\frac{\varepsilon_{xz}}{\varepsilon_{zz}} & -\beta\frac{\varepsilon_{yz}}{\varepsilon_{zz}} & 1 - \frac{\beta^2}{\varepsilon_{zz}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{28}$$

$$(0 \le z \le L).$$

Maxwell's equations in the external media lead to the following relationships for the optical field components of the incident, reflected, and transmitted waves:

$$\begin{array}{llll} q_4^i = \gamma_y q_2^i, & q_3^i = \gamma_x q_1^i, & p_2^i = \gamma_y p_4^i, & p_1^i = \gamma_x p_3^i, \\ q_4^\gamma = -\gamma_y q_2^\gamma, & q_3^\gamma = -\gamma_x q_1^\gamma, & p_2^\gamma = -\gamma_y p_4^\gamma, & p_1^\gamma = -\gamma_x p_3^\gamma, \\ q_4^t = \gamma_y' q_2^t, & q_3^t = \gamma_x' q_1^t, & p_2^t = \gamma_y' p_4^t, & p_1^t = \gamma_x' p_3^t, \end{array} \tag{29}$$

where

$$\begin{aligned} \gamma_x &= n_1/\ \cos\alpha, & \gamma_y &= n_1\ \cos\alpha, \\ \gamma_x' &= n_2/\ \cos\alpha', & \gamma_y' &= n_2\ \cos\alpha', \end{aligned} \tag{30}$$

and α' is related to the incidence angle α by Snell's relation $n_2\ \sin\alpha' = n_1\ \sin\alpha$. In Eqs. (29) the superscripts i, r, t refer to the incident, reflected, and transmitted wave, respectively, and the field components of all waves are related to their respective p,q by Eqs. (2) and (9). The optical field in the first medium is the sum of the incident and reflected fields, so that at $z = 0$ we have

$$q_i(0) = q_i^i + q_i^r, \quad p_i(0) = p_i^i + p_i^r$$

$$(i = 1, \ldots, 4)\ . \tag{31}$$

In the last medium there is only the transmitted wave, so that at $z = L$ we have

$$q_i(L) = q_i^t, \quad p_i(L) = p_i^t \qquad (i = 1, \ldots, 4) \; . \qquad (32)$$

Combining Eqs. (29), (31), and (32), we obtain the following homogeneous linear boundary conditions at $z = L$:

$$\begin{aligned} p_2(L) - \gamma_y' p_4(L) &= 0, \\ p_1(L) - \gamma_x' p_3(L) &= 0, \\ q_4(L) - \gamma_y' q_2(L) &= 0, \\ q_3(L) - \gamma_x' q_1(L) &= 0, \end{aligned} \qquad (33)$$

and the following inhomogeneous linear boundary conditions at $z = 0$:

$$\begin{aligned} p_2(0) + \gamma_y p_4(0) &= 2\gamma_y p_4^i, \\ p_1(0) + \gamma_x p_3(0) &= 2\gamma_x p_3^i, \\ q_4(0) + \gamma_y q_2(0) &= 2\gamma_y q_2^i, \\ q_3(0) + \gamma_x q_1(0) &= 2\gamma_x q_1^i. \end{aligned} \qquad (34)$$

Once the field of the incident wave is given at $z = 0$, the quantities p^i, q^i are fixed and Eqs. (34) and (35) provide the set of boundary conditions required to solve Eqs. (1). Once the solution $q_i(z), p_i(z)$ $(i = 1, \ldots, 4)$ is found, the transmitted fields at $z = L$ are obtained directly from the values of p and q at $z = L$, and the reflected fields are obtained by Eqs. (31).

The same formalism can be used also to find the possible guided modes of the system. In this case there is no incident wave and all p^i, q^i are zero. The boundary conditions are then homogeneous at both boundaries and the scale of the optical field remains undetermined.

III. THE GEOMETRIC-OPTICS APPROXIMATION

Our Lagrangian approach provides an appropriate framework in which to find the expression of the equations governing the light propagation and the molecular reorientation in the GGOA, which is adequate in most practical situations, where the length scale over which the molecular orientation changes appreciably is much longer than the optical wavelength. As we shall see in the following sections, the equations for the optical field may be reduced in the GGOA to a set of equations for the light polarization state only, where the intensity S_z of the incident wave enters the torque equations as a parameter. We get therefore a drastic reduction of the electromagnetic degrees of freedom from four (the real parts of the fields E_x, E_y, H_x, H_y) to only one (the angle ψ yielding the orientation of the light polarization ellipse). Our equations for the light polarization evolution are equivalent to those found by Oldano and Allia *et al.* [2,6], while our expressions for the optical torque on the liquid crystal were not deduced before and represent a not trivial extension of those found by Santamato *et al.* for the case of normal incidence [3].

A. The light equations

Following Refs. [2,6], we first solve the eigenvalue problem

$$\tilde{G}\tilde{S}\tilde{M} = \tilde{M}\tilde{\Lambda}, \qquad (35)$$

where $\tilde{M}$ is a 4×4 matrix whose columns are the eigenvector of $\tilde{G}\tilde{S}$ and $\tilde{\Lambda}$ is the diagonal matrix formed by the corresponding eigenvalues. The eigenvector normalization is chosen so that

$$\tilde{M}^T\tilde{G}\tilde{M} = \tilde{N}, \qquad (36)$$

where $\tilde{N}$ =diag(1,1,-1,-1). The eigenvalues of $\tilde{G}\tilde{S}$ are the same as the eigenvalues of Berreman's matrix $\tilde{B}$, because $\tilde{G}\tilde{S}$ and $\tilde{B}$ are related by the similarity transformation (14). Therefore the eigenvalues are the z components of the wave vectors (in units of k_0) of the extraordinary (e) and ordinary (o) waves propagating in the forward (+) and backward (−) directions. We assume the eigenvectors are ordered so that $\tilde{\Lambda} = \mathrm{diag}(\lambda_e^+, \lambda_o^+, \lambda_e^-, \lambda_o^-)$.

We then consider the coordinate transformation

$$\bar{q} = \tilde{M}^{-1}q, \qquad (37)$$

where $\bar{q}$ are the new coordinates. In the new coordinates the optical Lagrangian becomes

$$L^o = \frac{1}{2k_0}(\bar{q}' + \tilde{V}\bar{q})^T\tilde{N}\tilde{\Lambda}^{-1}(\bar{q}' + \tilde{V}\bar{q}) - \frac{k_0}{2}\bar{q}^T\tilde{N}\tilde{\Lambda}\bar{q}, \quad (38)$$

where

$$\tilde{V} = \tilde{M}^{-1}\tilde{M}' = \tilde{\boldsymbol{B}} \cdot \boldsymbol{n}', \qquad (39)$$

and $\tilde{\boldsymbol{B}} = \tilde{M}^{-1}\partial\tilde{M}/\partial\boldsymbol{n}$. Equation (21) becomes

$$S_z = \frac{ck_0}{2}\left(\bar{p}^T\tilde{N}\bar{p} + \bar{q}^T\tilde{N}\bar{q}\right) = \text{const}, \qquad (40)$$

where

$$\bar{p} = \frac{1}{k_0}\tilde{N}\tilde{\Lambda}^{-1}(\bar{q}' + \tilde{V}\bar{q}) = \tilde{M}^T p \qquad (41)$$

are the new momenta. We notice that, when expressed in the new coordinates and momenta, S_z becomes an algebraic sum of squares, where positive terms correspond to waves propagating in the forward direction, while negative terms correspond to waves propagating in the backward direction.

The GGOA approximation is made simply by retaining only the first two coordinates $\bar{q}_1$ and $\bar{q}_2$ and momenta $\bar{p}_1$ and $\bar{p}_2$ that are associated to the waves propagating in the forward direction, and the upper left 2×2 blocks $\tilde{V}_{11}, \tilde{N}_{11}, \tilde{\Lambda}_{11}$ of matrices $\tilde{V}, \tilde{N}, \tilde{\Lambda}$, appearing in Eqs. (38)

and (40) [2,6]. This leads to the GGOA total Lagrangian

$$L^{\rm GGOA} = \frac{1}{2k_0}\left[\frac{(\bar{q}_1' + v\bar{q}_2)^2}{\lambda_e} + \frac{(\bar{q}_2' - v\bar{q}_1)^2}{\lambda_o}\right] - \frac{k_0}{2}\left(\lambda_e \bar{q}_1^2 + \lambda_o \bar{q}_2^2\right), \quad (42)$$

where $\lambda_e \equiv \lambda_e^+$, $\lambda_o \equiv \lambda_o^+$, and $v = v_{12} = -v_{21}$, where v_{ij} are the elements of the matrix $\tilde{V}$ defined by Eq. (39). It is also useful to introduce the vector $\boldsymbol{b} = \boldsymbol{b}_{12} = -\boldsymbol{b}_{21}$, $\boldsymbol{b}_{ij}$ being the elements of the matrix vector $\tilde{\boldsymbol{B}}$, so that $v = \boldsymbol{b}\cdot\boldsymbol{n}'$. In the GGOA, the Poynting vector conservation law is given by

$$S_z^{\rm GGOA} = \frac{ck_0}{2}\left[\bar{p}_1^2 + \bar{p}_2^2 + \bar{q}_1^2 + \bar{q}_2^2\right] = \text{const.} \quad (43)$$

The Hamiltonian associated with $L^{\rm GGOA}$ is

$$H^{\rm GGOA} = \frac{k_0}{2}[\lambda_e(\bar{p}_1^2 + \bar{q}_1^2) + \lambda_o(\bar{p}_2^2 + \bar{q}_2^2)] - v(\bar{p}_1\bar{q}_2 - \bar{p}_2\bar{q}_1). \quad (44)$$

Introducing the Jones vector $\bar{J} = (\bar{J}_1, \bar{J}_2)$, with components $\bar{J}_1 = \sqrt{8\pi k_0}(\bar{q}_1 - i\bar{p}_1)$ and $\bar{J}_2 = \sqrt{8\pi k_0}(\bar{q}_2 - i\bar{p}_2)$, one can easily check that Hamilton's equations associated to $H^{\rm GGOA}$ may be written as

$$\bar{J}' = \tilde{\bar{Q}}\bar{J}, \quad (45)$$

where

$$\tilde{\bar{Q}} = ik_0\tilde{\Lambda}_{11} - \tilde{V}_{11} = \begin{pmatrix} ik_0\lambda_e & -v \\ v & ik_0\lambda_o \end{pmatrix}. \quad (46)$$

These equations are the same as reported in Refs. [2,6] and describe the evolution of the light polarization in the medium in the local frame formed by the principal axes of the matrix $\tilde{G}\tilde{S}$. Equations (45) have the first integral $|\bar{J}_1|^2 + |\bar{J}_2|^2 = 16\pi(S_z/c)$ corresponding to the conservation of the power flux along the z axis. Therefore, introducing the local Stokes unit vector $\bar{\boldsymbol{s}} = (\bar{s}_1, \bar{s}_2, \bar{s}_3) = (|\bar{J}_1|^2 - |\bar{J}_2|^2, 2\mathrm{Re}(\bar{J}_1\bar{J}_2^*), 2\mathrm{Im}(\bar{J}_1\bar{J}_2^*))/(|\bar{J}_1|^2 + |\bar{J}_2|^2)$, Eqs. (45) may be written out in the precession form

$$\bar{\boldsymbol{s}}' = \bar{\boldsymbol{\Omega}} \times \bar{\boldsymbol{s}}, \quad (47)$$

where $\bar{\boldsymbol{\Omega}} = (k_0\Delta\lambda, 0, 2v)$ and $\Delta\lambda = \lambda_e - \lambda_o$.

Jones's vector $\bar{J}$ and Stokes's vector $\bar{s}$ refer to the polarization state in the locally rotated frame. The passage from the fixed laboratory frame to the local one is defined by Eqs. (37) and (41). From these equations we obtain

$$J = \tilde{M}_{11}\bar{J}, \quad (48)$$

where $J = (E_x, E_y)$ is Jones's vector in the fixed frame and $\tilde{M}_{11}$ is the 2×2 upper-left block of $\tilde{M}$. Since we assumed $\bar{q}_3 = \bar{q}_4 = \bar{p}_3 = \bar{p}_4 = 0$, we have the following useful relation connecting the components of the magnetic and electric field of the optical wave in the GGOA:

$$\begin{pmatrix} H_y \\ -H_x \end{pmatrix} = \tilde{M}_{21}(\tilde{M}_{11})^{-1}\begin{pmatrix} E_x \\ E_y \end{pmatrix}. \quad (49)$$

These relations permit us to evaluate the optical electric and magnetic field transverse components, once the Jones vector $\bar{\boldsymbol{J}}$ (or Stokes vector $\bar{\boldsymbol{s}}$) in the local frame is known. The longitudinal field components are then given by Eqs. (10).

B. The reduced Lagrangian

Since S_z =const, Eqs. (47) describe only the evolution of the light "polarization" state in the medium. We may, in fact, further reduce the degrees of freedom from two to only one, inserting back into the Lagrangian the conservation law (43) as a constraint, and using as new coordinate the angle $\psi = \frac{1}{2}\arctan(\bar{s}_2/\bar{s}_1)$, formed by the major axis of the light polarization ellipse with the x axis of the local frame. This approach has the further advantage that the incident wave power flux S_z enters the final equations as an external parameter. The new Lagrangian is

$$L^{\rm GGOA}(\psi, \psi') = -\frac{S_z}{ck_0}\left(k_0\bar{\lambda} + \sqrt{(\psi' - v)^2 + \frac{1}{4}k_0^2\Delta\lambda^2\cos^2 2\psi}\right), \quad (50)$$

where $\bar{\lambda} = (\lambda_e + \lambda_o)/2$.

The Hamiltonian corresponding to the Lagrangian (50) is

$$H^{\rm GGOA} = \frac{S_z}{c}\left[\bar{\lambda} + \frac{\Delta\lambda}{2}\cos 2\psi\sqrt{1 - \left(\frac{ck_0}{S_z}\right)^2 p_\psi^2}\right] + vp_\psi, \quad (51)$$

where p_ψ is the momentum conjugate to ψ. It is worth noting that the momentum p_ψ conjugate to the ellipse angle ψ has a simple physical meaning. We have, in fact,

$$p_\psi = \frac{S_z}{\omega}\bar{s}_3, \quad (52)$$

where $\bar{s}_3$ is the ellipticity of the light polarization in the local frame and ω the optical frequency. We may then consider p_ψ as the negative of the z component of the intrinsic angular momentum carried on by the light along the laboratory z axis. A similar result was previously reported for the case of normal incidence [3].

The Euler-Lagrange equations resulting from the reduced Lagrangian (50) are equivalent to Eqs. (45) and (47). The Lagrangian $L^{\rm GGOA}$, as given in Eq. (50), is fully determined once the eigenvalues λ_e and λ_o for the extraordinary and ordinary waves in the forward direction as well as the quantity v are given. Taking the x, z plane as the incidence plane, these quantities have been calculated elsewhere [6] and are reported here:

$$\lambda_e = -m_t \cos\phi + \sqrt{\varepsilon_t - (1-\mu)\beta^2 \frac{\varepsilon_t \varepsilon_f}{\varepsilon_o^2}},$$
$$\lambda_o = \sqrt{\varepsilon_o - \beta^2},$$
$$v = b_\phi \phi' + b_\theta \theta', \tag{53}$$
$$b_\theta = \frac{1}{2} c_e c_o \beta \frac{\sin\phi}{\sin^2\theta}\left(1 + \frac{\lambda_e}{\lambda_o}\right),$$
$$b_\phi = -\frac{1}{2} c_e c_o \left[\lambda_e + \lambda_o - \beta \cot\theta \cos\phi \left(1 + \frac{\lambda_e}{\lambda_o}\right)\right],$$

where

$$c_e = \left[\lambda_e \left(1 - \frac{\beta^2 \cos^2\phi}{\varepsilon_o}\right) - \beta \cos\phi \cot\theta \times \left(1 - \frac{\beta^2}{\varepsilon_o} + \frac{\lambda_e^2}{\varepsilon_o}\right) + \beta^2 \cot^2\theta \frac{\lambda_e}{\varepsilon_o}\right]^{-\frac{1}{2}},$$
$$c_o = \left[\lambda_o \cos^2\phi + \frac{\varepsilon_o}{\lambda_o} \sin^2\phi - 2\beta \cos\phi \cot\theta + \frac{\beta^2 \cot^2\theta}{\lambda_o}\right]^{-\frac{1}{2}},$$
$$\varepsilon_t = \frac{\varepsilon_o}{1 - \mu \sin^2\theta}, \tag{54}$$
$$\varepsilon_f = \varepsilon_o \sin^2\phi + \varepsilon_t \cos^2\phi,$$
$$m_t = \beta \frac{\mu \sin\theta \cos\theta}{1 - \mu \sin^2\theta},$$
$$\beta = \frac{k_x}{k_o} = n_1 \sin\alpha.$$

In these equations θ and ϕ are the polar angles of the molecular director $\boldsymbol{n}$, α is the beam incidence angle, and $\mu = 1 - \varepsilon_o/\varepsilon_e$, ε_e and ε_o being the principal values of the material dielectric tensor at the optical frequency. We notice that, unlike the exact optical Lagrangian L^o, the GGOA Lagrangian $L^{\rm GGOA}$ depends, through v, on the derivatives θ' and ϕ' of the director polar angles. [A lower order approximation, called the geometric-optics approximation (GOA), is often used in which the quantity v containing the spatial derivatives of the molecular director is neglected. To neglect v is, however, impossible for particular directions of the optical axis, where v may become infinite.]

C. The boundary conditions in the GGOA

The boundary conditions are fixed by the anchoring conditions of the molecular director at the walls and by the intensity, polarization, and incidence angle of the incoming optical wave. It should be stressed, however, that the GGOA is no longer applicable at boundaries, where the refractive index is discontinuous. The relevant boundary conditions can be obtained eliminating the magnetic field components from Eqs. (34) and Eqs. (49), evaluated at $z = 0$. Thus we find the following relationship between the Jones vector $\boldsymbol{J}(0)$ at $z = 0$ and the Jones vector J^i of the incident wave (the latter taken in the reference frame having the z axis along the beam propagation direction):

$$J(0) = \tilde{Z}(0) J^i, \tag{55}$$

where $\tilde{Z}(0)$ is the 2×2 matrix given by

$$\tilde{Z}(0) = 2n_1 \left[\tilde{M}_{21}(0)(\tilde{M}_{11})^{-1}(0) + \begin{pmatrix} \gamma_x & 0 \\ 0 & \gamma_y \end{pmatrix}\right]^{-1} \times \begin{pmatrix} 1 & 0 \\ 0 & \cos\alpha \end{pmatrix}. \tag{56}$$

Relation (55) permits us to evaluate the Jones vector at the input plane $z = 0$ from the Jones vector of the incident wave. The Jones vector $\bar{J}$ in the local frame is then obtained from Eq. (48) at $z = 0$.

D. The optical torque in the GGOA

The more direct way to evaluate the optical torque is by expressing Eq. (18) in terms of the local frame coordinates and momenta $\bar{p}, \bar{q}$. We thus obtain

$$\boldsymbol{h}^o = \frac{k_0}{2}(\bar{p}^T \tilde{N} \tilde{\boldsymbol{A}} \tilde{N} \bar{p} + \bar{q}^T \tilde{\boldsymbol{A}} \bar{q}), \tag{57}$$

where we introduced the 4×4 matrix vector

$$\tilde{\boldsymbol{A}} = \tilde{M}^T \frac{\partial \tilde{S}}{\partial \boldsymbol{n}} \tilde{M}. \tag{58}$$

Derivation of Eq. (35) with respect to $\boldsymbol{n}$ yields

$$\tilde{\boldsymbol{A}} = \tilde{N}\left(\frac{\partial \tilde{\Lambda}}{\partial \boldsymbol{n}} + \tilde{\boldsymbol{B}}\tilde{\Lambda} - \tilde{\Lambda}\tilde{\boldsymbol{B}}\right). \tag{59}$$

The GGOA expression of $\boldsymbol{h}^o$ is then obtained by retaining only the terms containing $\bar{p}_i, \bar{q}_i$ with $i = 1, 2$ in Eq. (57). Using as before Jones's vector and Stokes's parameters, we get

$$\boldsymbol{h}^{\rm GGOA} = \frac{1}{16\pi} \bar{J}^\dagger \tilde{\boldsymbol{A}}_{11} \bar{J}, \tag{60}$$

where $\tilde{\boldsymbol{A}}_{11}$ denotes the upper left 2×2 block of $\tilde{\boldsymbol{A}}$. Using Stokes's parameters, Eq. (60) can be rewritten as

$$\boldsymbol{h}^{\rm GGOA} = \frac{S_z}{2c}\left[\frac{\partial \lambda_e}{\partial \boldsymbol{n}}(1 + \bar{s}_1) - 2\Delta\lambda \boldsymbol{b} \bar{s}_2\right]. \tag{61}$$

If one starts directly from the GGOA Lagrangian (42) or (50) a slightly different expression is found for $\boldsymbol{h}^{\rm GGOA}$:

$$\boldsymbol{h}^{\rm GGOA} \equiv \frac{d}{dz}\left(\frac{\partial L^{\rm GGOA}}{\partial \boldsymbol{n}'}\right) - \frac{\partial L^{\rm GGOA}}{\partial \boldsymbol{n}} = (61) + \boldsymbol{h}^{extra}, \tag{62}$$

where the components of the extra term are

$$h_i^{extra} = \left(\frac{S_z}{ck_0}\right)\left[\sum_{j=1}^{3}\left(\frac{\partial b_j}{\partial n_i} - \frac{\partial b_i}{\partial n_j}\right) n_j'\right] \bar{s}_3 \tag{63}$$
$$(i = 1, 2, 3).$$

This extra term in the optical contribution to the torque is very small, because it is proportional to $\boldsymbol{n}'/k_0$, but it is needed in order to preserve the Lagrangian character of the theory in passing to the GGOA. We may consider it as a small contribution from higher order terms in the GGOA.

Using the relations (53), we may express $\boldsymbol{h}^{\mathrm{GGOA}}$ as a function of the director polar angles θ and ϕ. In the special cases of normal incidence and elliptical polarization and of oblique incidence and p polarization, $\boldsymbol{h}^{\mathrm{GGOA}}$ reduces to the expressions which have already appeared in the literature [3,7].

IV. FINAL COMMENTS

We have shown how the equation governing the motion of the molecular director and the change of the light polarization in the medium can be derived by a unique Lagrangian even in the GGOA, for any incidence angle and polarization. The Euler-Lagrange equation obtained by $L(\psi,\psi';\boldsymbol{n},\boldsymbol{n}') = L^e + L^{\mathrm{GGOA}}$, with L^{GGOA} given by Eq. (50) may also be used for numerical integration in the GGOA. Problems may arise, however, in the numerical integration of the light polarization Eqs. (47) [or Eqs. (45)] in the local frame, because, for particular directions of the optical axis $\boldsymbol{n}$, the quantity v appearing in these equations may become undetermined and even infinite. We can see this by evaluating the components v_{ij} of the matrix $\tilde{V}$, defined by Eq. (39), from Eq. (59). After scalar multiplication of Eq. (59) by $\boldsymbol{n}'$, we get a matrix equation that can be solved explicitly with respect to v_{ij}, yielding

$$v_{ij} = \frac{f_{ij}}{\lambda_j - \lambda_i} \quad (i \neq j),$$
$$v_{ii} = 0, \quad (i,j = 1,\cdots,4)\ , \tag{64}$$

where f_{ij} $(i,j = 1,\ldots,4)$ are the elements of the matrix

$$\tilde{F} = \tilde{N}\tilde{\boldsymbol{A}}\cdot\boldsymbol{n}' = \tilde{N}\tilde{M}^T\tilde{S}'\tilde{M} \tag{65}$$

and $\tilde{S}' = d\tilde{S}/dz$. We see therefore that $v \equiv v_{12}$ is undetermined when the eigenvalues λ_1 and λ_2 become degenerate. This happens, indeed, when the direction $\boldsymbol{n}$ of the local optical axis is parallel to the wave vector, i.e., when $n_x = \beta/n_o, n_y = 0, n_z = \lambda_o/n_o$. For direction of the optical axis close to the degeneration direction, v may be very large, contrarily to what is supposed in the GGOA. It is evident that the origin of this problem is not physical, because the spatial distribution of the refractive index in the medium is really smooth, but it is due to the fact that the local frame where Eqs. (45) and (47) are evaluated is ill defined in the degenerate eigenvalue case. We expect therefore that any singularity could be removed simply by solving the equations governing the evolution of the light polarization in the fixed laboratory frame, rather than in the local frame. Thus using transformations (48) to return back to the fixed frame Jones vector $J = (E_x, E_y)$, Eq. (45) is changed to

$$J' = \tilde{Q}J, \tag{66}$$

where

$$\tilde{Q} = \tilde{M}_{11}[ik_0\tilde{\Lambda}_{11} - \tilde{V}_{11} + (\tilde{M}_{11})^{-1}\tilde{M}'_{11}](\tilde{M}_{11})^{-1}. \tag{67}$$

The divergency occurring in $\tilde{V}_{11}$ is then cancelled out, because from $\tilde{M}' = \tilde{M}\tilde{V}$ it follows that

$$\tilde{M}'_{11} = \tilde{M}_{11}\tilde{V}_{11} + \tilde{M}_{12}\tilde{V}_{21}, \tag{68}$$

and hence we may rewrite $\tilde{Q}$ as

$$\tilde{Q} = ik_0\tilde{M}_{11}\tilde{\Lambda}_{11}(\tilde{M}_{11})^{-1} + \tilde{M}_{12}\tilde{V}_{21}(\tilde{M}_{11})^{-1}. \tag{69}$$

Since the eigenvectors in the forward direction are positive, while the eigenvectors in the backward direction are negative, the elements of the 2×2 matrix $\tilde{V}_{21}$ in Eq. (69) are always well determined by Eq. (64).

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