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Analysis of the Optical Properties of a Helicoidal Liquid Crystal in a General Coupled Mode Formalism

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The optical properties of a chiral liquid crystal (CiLC) are analyzed in terms of the rotation of the principal axes (RP) together with the one-dimensional periodicity (DP) along the helicoidal axis. Within a general coupled mode formalism, the helicoidal nature of a CiLC is represented by both RP and DP. The formalism developed here is a powerful tool for calculating the optical properties of a CiLC for oblique incidence. Our numerical calculations show an exact agreement with the previous analytic results.

Keywords: chiral liquid crystals; cholesteric liquid crystals; helical structure; coupled mode

INTRODUCTION

Chiral liquid crystals (CiLCs), such as cholesteric liquid crystals (ChLCs) and smectic C* liquid crystals, exhibit several unique and interesting optical properties. The previously reported analytic results

for the normal incidence of light onto a ChLC^[1-3] show that the optical properties result from the propagation differences between two optical normal modes of a CiLC which has one-dimensional (1-D) periodic structure^[4]. In the previous approach, the optical normal modes of a CiLC were obtained by finding the non-trivial solutions of the Maxwell equations coupled with the dielectric tensor which represents the helicoidal structure. For oblique incidence, the calculations become very complicated.

In our case, the CiLC, especially ChLC, is treated as a nematic LC (NLC) which experiences the rotation of the principal axes (RP) and exhibits the 1-D periodicity (DP). The optical normal modes of a NLC is easily calculated. With the calculated normal modes of a NLC, the effect of both RP and DP are then taken into account within a general coupled mode formalism. Numerical calculations calculated in our formalism agree well with the previous analytic results.

THE ROTATION OF THE PRINCIPAL AXES

Based on the above description, we adopt the formalsim of the wave mechanics^[5] instead of the macroscopic dielectric tensor. An optical normal mode is defined as a polarization state which preserves the initial polarization state in the course of translation but having only phase change. This definition requires the optical normal modes to be the eigenstates of the wave-number operator (**K**) which is the generator of translation^[5]. Therefore, a diagonal matrix representation of **K** can be described in terms of the normal modes. For example, a NLC has two optical normal modes. These normal modes, denoted by $|\xi\rangle$ and $|\eta\rangle$, are two linearly polarized states with polarization parallel to the principal axes of NLC, having the wave-numbers of β e and β 0 respectively. The wave-number operator describing the light propagation through NLC (**K**_n) is given as

$$\mathbf{K}_{\mathbf{n}} = \beta_{\mathbf{e}} |\xi\rangle\langle\xi| - \beta_{\mathbf{o}} |\eta\rangle\langle\eta|. \tag{1}$$

For convenience, the minus sign is adopted for $|\eta\rangle$.

Now, we consider the case where one of the characteristic parameters varies. For example, a helicoidal structure, associated with the NLC director, forms along a certain axis such that the value of $2\pi/\text{pitch}$ has a finite value of q. If the change is physically meaningful, one can construct an operator which represents such change. In our case, the operator will transform an arbitrary optical mode of NLC into the corresponding mode of a helicoidal LC. Let us denote this operator by a finite chirality operator. By the same argument as that for a finite translation operator^[5], one can derive the expression for a finite chirality operator; $\exp[-i\mathbf{Q}q]$ where the nature of the helicoidal structure is contained in the generator of the chirality \mathbf{Q} . We take the viewpoint of the Heisenberg picture, and then the change in the physical system is attributed to the change in the operator. Hence, one can find the optical normal modes by observing the change in the wave-number operator, \mathbf{K}_H as follows.

$$\mathbf{K}_{\mathbf{H}} = \exp[-\mathrm{i}\mathbf{Q}\mathbf{q}]^{\dagger} \,\mathbf{K}_{\mathbf{n}} \,\exp[-\mathrm{i}\mathbf{Q}\mathbf{q}] \tag{2}$$

Note that when there exist more than one physical property, each property can be reflected by the respective term in the generator. In our case, one is associated with RP and the other is associated with DP. Accordingly, \mathbf{Q} has the following form; $\mathbf{Q} = \mathbf{Q}_R + \mathbf{Q}_D$ where \mathbf{Q}_R represents RP and \mathbf{Q}_D represents DP. Keeping \mathbf{Q}_R only in \mathbf{Q} , the effect of RP on the optical normal modes will be considered.

We now derive a definite form of the operator $\mathbf{Q_R}$. There is no formal way of deriving the generator. Thus, we construct the structure of $\mathbf{Q_R}$ under the assumption that within a small region Δz , an infinitesimal chirality (dq) appears which tends to rotate two principal axes of NLC (ξ -axis and η -axis) by an angle of $d\phi = dq \cdot \Delta z$. The difference between the wave-numbers of the two principal axes would be much smaller than the average value ($|\beta e|$ - $|\beta o|$ << $|\xi e|$ + $|\beta o|$). Under these circumstances, the rotation of the principal axes does not affect

the propagation of the individual states, $|\xi\rangle$ and $|\eta\rangle$. However, it redistributes the two states in the following manner

$$\begin{split} 1 - iQ_R dq \sim & \big[- \sin(d\phi) \big| \eta \big\rangle + \cos(d\phi) \big| \xi \big\rangle \, \big] \big\langle \xi \big| \\ + & \big[\sin(d\phi) \big| \xi \big\rangle + \cos(d\phi) \big| \eta \big\rangle \, \big] \big\langle \eta \big| \,. \end{split} \tag{3}$$

Let us consider the redistribution of the states in detail. By the rotation of $d\phi$, the projection of $|\xi\rangle$ exists in the η -axis and vice versa. Such component does not appear in the case of NLC. Hence, some fraction of one state experiences the transition to the other state. This transition is physically equivalent to the situation where it occurs between two isotropic materials. Therefore, no phase evolution is involved. For proceeding calculations, it is convenient to introduce another form of the finite chirality operator; $\exp[-i(\mathbf{Q}_R/\Delta z)(q\Delta z)] = \exp[-i\mathbf{\Phi}_R\phi]$. Mathematically, two forms are exactly equivalent but the latter has the form of the rotation operator. Note that the generator of rotation (Φ_{R}) has the dimension of the angular momentum, and \mathbf{Q}_R and Φ_R have only the off-diagonal terms in the matrix representation. Therefore, as a result of the transition, the angular momentum is transferred. The transferred angular momentum (a) is the difference in the angular momentum between $|\xi\rangle$ and $|\eta\rangle$, which is written as $a=[\Delta z](\beta e+\beta o)^{-1}$. With the help of these arguments, the complete form of Q_R can be written as

$$\mathbf{Q}_{\mathbf{R}} = (\beta_{\mathbf{e}} + \beta_{\mathbf{o}})^{-1} [|\eta\rangle\langle\xi| + |\xi\rangle\langle\eta|]. \tag{4}$$

Here, there exists a close analogy of our formalism to a well-known spin 1/2 system which can described in terms of the eigenstates of S_z in Ref. [5]. The two eigenstates of S_z , up and down, correspond to $|\xi\rangle$ and $|\eta\rangle$ of NLC. Then, the NLC wave-number operator (K_n) , having the diagonal-matrix representation, corresponds to S_z , and Q_R corresponds to S_x . In Ref. [5], the close analogy between the spin 1/2 system and the polarization state of light waves was discussed. Hence, the operator (C) which corresponds to S_y has circularly-polarized

states as the eigenstates. With this analogy kept in mind, let us evaluate K_H using Eq. (2) with the Baker-Hausdorff lemma

$$\mathbf{K}_{\mathbf{H}} = \exp[-\mathrm{i}\mathbf{Q}_{\mathbf{R}}\mathbf{q}]^{\dagger} \mathbf{K}_{\mathbf{n}} \exp[-\mathrm{i}\mathbf{Q}_{\mathbf{R}}\mathbf{q}]$$

$$= \mathbf{K}_{\mathbf{n}} + \mathrm{i}\mathbf{q} \left[\mathbf{Q}_{\mathbf{R}}, \mathbf{K}_{\mathbf{n}}\right] + (\mathrm{i}\mathbf{q})^{2}/2! \left[\mathbf{Q}_{\mathbf{R}}, \left[\mathbf{Q}_{\mathbf{R}}, \mathbf{K}_{\mathbf{n}}\right]\right] + \cdots. \quad (5)$$

In Eq. (5), the term of the *n*th-order in q represents *n*th-order photon transition. Note that $\{S_x, S_y, S_z\}$ satisfy the fundamental commutation relation of angular momentum^[5]. Therefore, the first-order transition term, $iq[Q_R, K_N]$, corresponds to C. This principle can be also applied to the higher-order term.

For the normal incidence of light onto a ChLC, keeping only the terms up to the first-order transition, the optical properties can be easily calculated. The obtained numerical results agree with the analytic results. We used the values of 1.7 and 1.5 as the refractive indices, pertinent to $|\xi\rangle$ and $|\eta\rangle$, respectively.

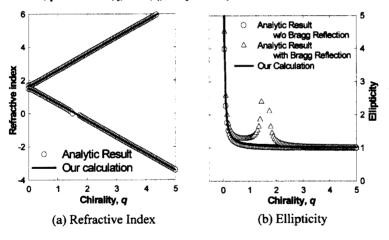


Figure 1 Comparison between numerical calculations and analytic results

Figure 1 shows the refractive index and the ellipticity as a function of

the scaled q by (ω/c) where ω and c are the angular frequency and light velocity, respectively. In fact, a selective Bragg reflection takes place as the pitch (or q) approaches the wavelength. However, our calculations do not predict the Bragg reflection because the effect of DP is ignored in our case. Outside the Bragg regime, excellent agreements are made. This tells us that the propagation difference between the optical normal modes is mainly originated from the effect of RP. Especially, as we predicted, the optical normal modes become circularly polarized states when the chirality q becomes large. Thus, our analysis based on the analogy to the spin 1/2 system is legitimate.

ONE-DIMENSIONAL PERIODICITY

Now, we examine the effect of the 1-D periodicity in a ChLC which is assumed to behave as a homogeneous medium having the dispersion relation obtained in the previous section. Let us consider that there appears a 1-DP which has the wave-vector of q and the weak periodic perturbation of $\Delta = (\beta_e - \beta_o)/2$. Assume that the ChLC under consideration is right-handed, and then the upper-branch of Figure 1-(a) (L⁺) has the opposite handedness to that of ChLC and the lower-branch (R⁺) has the same handedness.

It is well known that a weak periodic potential has its major influence near the Bragg plane^[6] (n-pitch = λ_0 with the average refractive index n and the wavelength in the vacuum λ_0). If we consider only the forward-propagating waves (L^+ , R^+), there are no two branches which are within the order Δ of each other. However, if we include the dispersion relation of the backward-propagating waves (L^- , R^-), the mirror image of Figure 1-(a) to the q-axis, we find that near the Bragg plane, the two branches of R^+ and R^- are within the order Δ of each other. Outside this regime, all the branches are far from each other compared to Δ . This means that the effect of the 1-DP comes from the resonant coupling between R^+ and R^- . This is coincident with the fact that a linearly-polarized state observed in the Bragg regime shows a

completely different dynamics from that of a linearly-polarized state in the Maugin regime^[7]. The linearly-polarized state in the Bragg regime is the standing wave because this results from the coupling between a forward-propagating wave (R⁺) and a backward-propagating wave (R⁻).

In our case, the branches with the photonic band-gap can be otained in the exactly same manner as those with the energy band-gap for a crystalline solid[6].

$$E = \left(\frac{\mathbf{R}^{+} + \mathbf{R}^{-}}{2}\right) \pm \left[\left(\frac{\mathbf{R}^{+} - \mathbf{R}^{-}}{2}\right)^{2} + \Delta^{2}\right]^{1/2}$$
 (6)

Figure 2 shows that our numerical calculations, where the 1-DP was included, are in excellent agreement with the analytic results in the entire region.

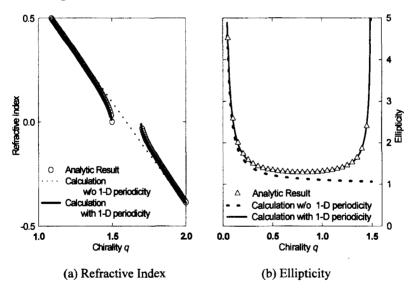


Figure 2 Numerical calculations with 1-D periodicity considered

CONLCUSION

Within a general coupled mode formalism, we calculated the optical properties of a CiLC. It was found that the propagation difference between the optical normal modes is mainly originated from the effect of the rotation of the principal axes and the 1-D periodicity plays a major role on the resonant coupling of the contra-directionally propagating normal modes. Our formalism may provide a powerful tool for calculating the optical properties of a CiLC case for oblique incidence. With the higher-order photon transitions, the modified dispersion relation and the resonant couplings, the formalism developed here is expected to study more complex phenomena.

Acknowledgments

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