Light Propagation in Liquid Crystal Samples

Intro To LC

Liquid crystals (LC) are substances that are fluid yet have their molecules arranged with some degree of order. For instance, a nematic liquid crystal is composed of elongated molecules which align along a common headless direction, called the director, without positional order of the center of mass of the molecules. Owing to their unique electro-optical properties stemming from their anisotropic nature, these soft, reconfigurable, and birefringent materials can be found in many applications, ranging from TV displays to advanced optical instruments. Additionally, LCs have potential applications in smart reconfigurable devices and metamaterials. This project focuses on the propagation of light with LCs, a crucial aspect in both optical applications and the characterization of LC samples.

In this work, we use a continuum description of the liquid crystal that is considered a continuous material.. At every point in space r(vector), we consider a fluid element, that is a ball just large enough to contain a sufficient number of molecules for statistics, but small enough to be considered homogeneous. We are only interested in the local average direction of the molecules contained in the fluid element to obtain a unit director field n. The director n(r) is a field that can vary with space and with time, and is conveniently parameterized by the zenithal angle theta(r), and the azimuthal angle phi(r) (see figure 1). While this headless unit vector describes the average direction of molecular alignment, an order parameter S measures the degree of this alignment. S ranges from 0 to 1, with 0 signifying complete disorder and 1 corresponding to perfect nematic alignment (see figure 2).

One problem arising from the use of the continuum model is that the individual orientations and positions of the LCs can not be used. Instead, a director field is created, which consists of LC director vectors that represent the local average orientation of the liquid crystal molecules at each point in space. That is, this field holds no information regarding the location of individual LC particles, rather, it specifies the average direction in which they point. However, the continuous description allows us to write partial differential equations to describe the system over large length scales, and to coarse grain the effect of liquid crystal anisotropic molecules on electromagnetic waves.

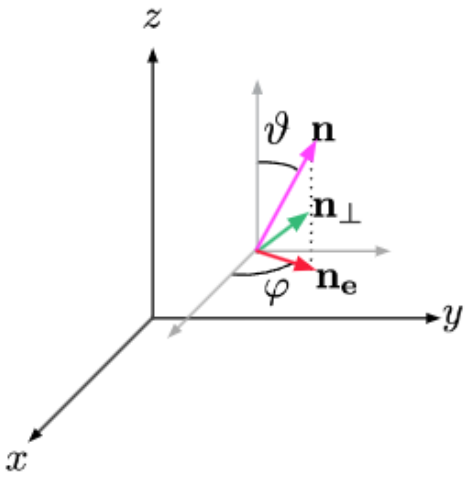

Figure 1: The two relevant angles for a director vector **n**. Phi is the polar angle and theta is the azimuthal angle.

Liquid crystals have several phases that they can naturally exist in. Two that will be discussed in this paper are the nematic (S>0) and the isotropic phase (S=0), which differ in molecular arrangement. In the nematic phase, the liquid crystals are roughly aligned along some common angle, which is effectively the local director vector. As a nematic liquid crystal is heated, molecules deviate more and more from the director. At a critical temperature of roughly 38°C for 5CB, the transition from the nematic phase to the isotropic phase occurs. In the isotropic phase, the molecules don't orient in any particular direction, therefore the director is not defined.These two phases are illustrated in figure 2.

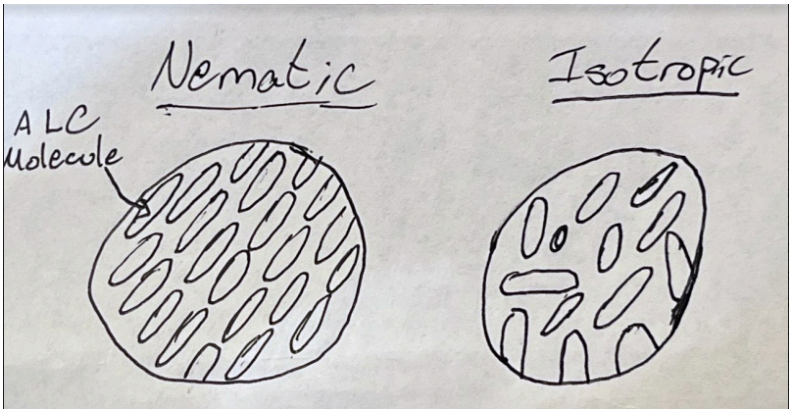

Figure 2: The left image shows a region of a liquid crystal in the nematic phase with perfect alignment S=1 and the right image shows a region in the isotropic phase S=0.

Two fundamental properties essential to understanding the optical behavior of liquid crystals are anisotropy and birefringence. Anisotropy in liquid crystals means that the material properties depend on the direction due to the nematic ordering of the molecules. Birefringence, a direct consequence of this anisotropy, means that the material has two distinct refractive indices, hence light of different polarizations will travel at different speeds through the material. Analyzing how a light beam propagates through a liquid crystal sample necessitates a thorough consideration of these optical properties.

Light Analysation

One effective method to studying materials such as LCs is polarized optical microscopy. This technique is based on LC's ability to alter polarized light passing through it. It works by placing two perpendicular linear polarizers around the sample. Any polarized light beam that propagates in the z direction can be decomposed into a beam linearly polarized along x and a beam linearly polarized along y. A linear polarizer is a filter that lets light with a specific linear polarization pass through and absorbs the orthogonal component. Typically, such as if there was an isotropic material (air or water, for example) in between the polarizers, then no light would be able to pass through the second polarizer. However, since the LC is able to alter the polarization of light, some light could get through the second polarizer. The intensity image after a LC placed between crossed-polarizers, called a cross-polarized image, therefore contains partial information about the structure of the director field in the sample, with brighter areas corresponding to regions where the director structure is such that the polarization of light was altered by the LC.

There are several methods to determine the amount of propagated light from a collimated beam through a characterized sample of LCs. The most accurate method would be to use Maxwell's equations and relationships between the magnetic and electric field to set up and solve wave equations. This can be computationally difficult and requires the use of sophisticated computer software.

A simpler way to estimate the cross polarized image would be to use the Jones Matrix Formalism, which uses vectors of complex exponentials to describe the polarization state of light. Furthermore, the Jones Matrix Formalism describes how light is altered by optical elements, so it can model the light properties of LCs.

This formalism works by representing light as a 2x1 Jones vector, which contains components denoting the electric field in the x and y direction. Indeed, Jones formalism assumes that light propagates in the z-direction and that the electric field is perpendicular to the z-direction. Optical elements, such as the polarizers, are represented with 2x2 Jones Matrices that convert the incoming light into the outgoing light. This transformation can be calculated by multiplying the Jones matrix by the Jones vector. A slab of uniform birefringent material can also be represented by a 2x2 Jones Matrix. A LC sample is birefringent but non uniform in general, as the director is allowed to vary with x, y, z. Thus, the liquid crystal sample needs to be discretized in x, y, z direction into tiny birefringent slabs, each one represented by a Jones matrice with the

local optical axis. The goal of this paper is to introduce a Python notebook capable of utilizing this formalism to create cross polarized images of LC samples.

Before using this method to approximate the polarization of the output wave, it is necessary to draw some assumptions on the sample and the light. First, Jones Calculus assumes that no light is diffracted, reflected, or absorbed within the sample. This holds true for thin samples, on the order of a few micrometers in depth, as they have shorter optical path lengths and less opportunities for the scattering of light. In other words, the variation of the optical index must be relatively small. This does not hold true for defect regions, which are local isotropic areas in which the optical index variation is large. In a practical sense, collimated light can be directed perpendicular to the sample, with its entire beam being directed perpendicular to the sample. For consistency, it is also assumed that the light propagates in the positive z-direction of the sample. For Jones Calculus to be most accurate, the variation of the optical index must be less than the thickness of the sample.

Additionally, by using collimated light, it can be assumed that the incident light is a coherent plane wave. With this assumption, complex exponentials can be used to represent the components of the light's electric field. This complex exponential holds the frequency, amplitude, and phase information for the light. Thus mathematical operations such as matrix multiplication can be used to determine how light is changing.

Program Methodology

To implement the Jones Matrix Formalism in code, the director field of the LC sample must be inputted in some manner. A COMSOL program can be used to generate a text file with all of the director field information. This file can then be parsed by Python, and stored in a Pandas dataframe, which allows for efficient processing of the data.

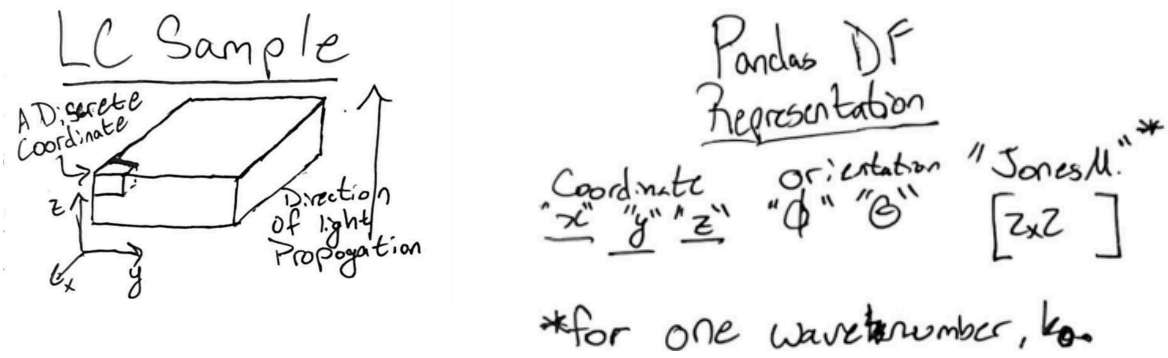

Figure 2: The initial manner of representing the LC sample after parsing from a .txt file.

The Python storage scheme for the director fields of the LC sample is depicted in Figure 2. The physical LC sample is shown on top, with one of the 3D discrete coordinates shown. Each of these discretized locations is associated with a director field orientation, which is also parsed from the input file. These variables are stored in a Pandas dataframe, which allows for easy and efficient indexing. An additional piece of information stored in the dataframe is the Jones matrix. This matrix contains a complex exponential with the light altering properties of the LC molecules, $\hat{\mathbf{J}} = \begin{pmatrix} e^{ik_0(n_e - n_\perp)dz} & 0 \\ 0 & 1 \end{pmatrix}$. Hence, the Jones matrix is dependent on the wavenumber, k_0 and the refraction indices. In addition to this, the Jones matrix must be rotated by phi, the polar angle of the LC director. This is done with a matrix rotation operation $\mathbf{J}=RJR^{-1}$, where **J** is the rotated Jones matrix, J is the original Jones matrix, and R and R^{-1} are the rotation matrix and its inverse, respectively.

Additionally, it is pertinent that each discrete location in the sample has its own Jones matrix. This can be repeated for several wavenumbers, which would result in several Jones matrices corresponding to each coordinate. To store these, the list of wavenumbers is stored as an instance in the class and the column name of each set of Jones matrices for a given wavenumber is the wavenumber itself. In this sense, a for loop can iterate over the k values and operations can

be performed quickly and independently over different wavenumbers. This will prove advantageous because in averaging the results of several wavenumbers a more accurate result is obtained.

To simplify future calculations, the Jones Matrices corresponding to a particular z-column in the LC sample can be multiplied together in the direction of light propagation to determine a matrix that effectively represents the entire column of the sample. In this spatial manner, the once 3 dimensional sample of LCs is flattened into the x, y plane, as in Figure 3, where each coordinate in this plane holds a Jones matrix depicting how polarized light will change upon propagating through that section of the sample.

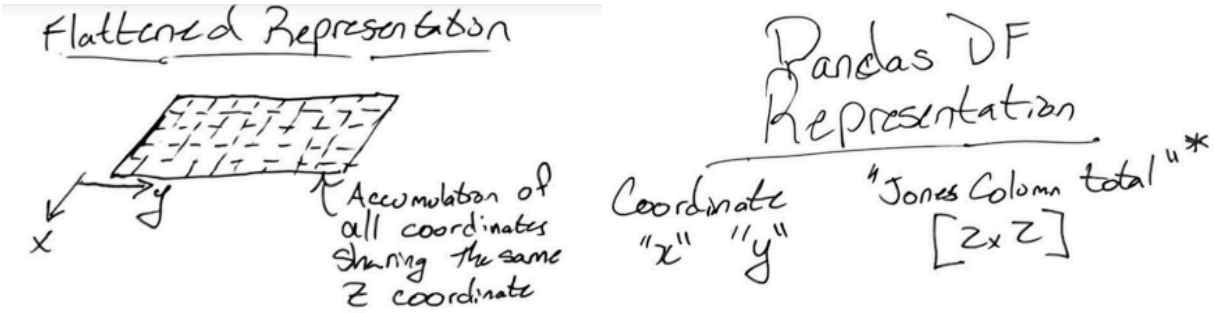

Figure 3: The flattened representation of the LC sample after computing the Jones matrices.

In other words, one can filter the original dataframe by some particular xy coordinate, and then find the total Jones matrix for light propagating through that z axis. This dataframe is costly to compute but much lighter to work with and only needs to be created once. This flattening operation is shown in Figure 4.

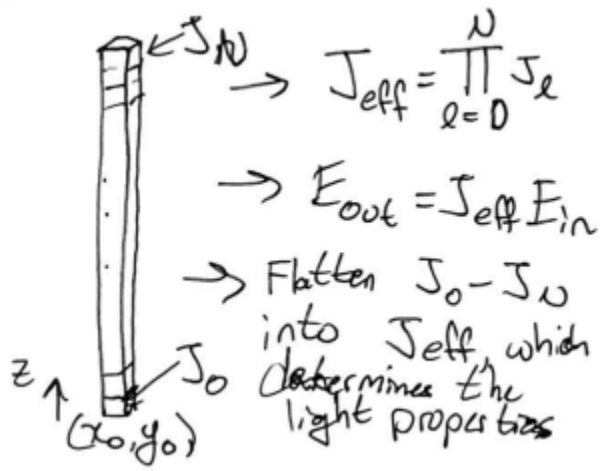

Figure 4: The effective Jones matrix is the product of all of the matrices in a ‘column’ (a particular xy coordinate).

The LCProcessor class does the flattening computation for each xy coordinate. Furthermore, the entire process can be repeated several times for various wavenumbers. Each wavenumber will have its own dataframe column in both the original and flattened dataframe. An intensity plot, showing the cross polarized image for some particular polarized input light vector, can be found for each set of Jones matrices of a wavenumber. Then these can be averaged for a more accurate cross-polarized image. Furthermore, a sequence of images for different cross polarizer angles can be generated, in turn producing a video of the light output with a rotating cross polarizer.

To find the intensity plot, linear polarized light is multiplied with the flattened Jones matrix each vertical axis of the sample. The output of this represents the light seen coming out of the sample. Then this light is multiplied with the crossed polarizers matrix, and the intensity of each point is plotted on a 2D grid. Further analysis can be performed by rotating either one or both of the cross polarizers. A video can be made of the cross polarizers rotating at a constant rate, which assists in the classification of defect structures.

A major drawback of the Jones matrix formalism is the computational bottleneck of creating the flattened dataframe, which is the largest source of delay due to the amount of matrix multiplication necessary. Other functions have been vectorized where possible, allowing them to take a vector as an input to work more efficiently. For example, when computing the Jones matrix for the original dataframe, numpy functions are used to represent all of the Jones matrices in one matrix and all of the rotation matrices in two other matrices. Thus only 2 matrix multiplication operations are required.

Results

The JonesCaclculusforLC Jupyter notebook is capable of producing vector field plots of the LC directors, generating the cross polarized image, and generating a video the cross polarized output as the LC sample is rotated. The results from experimenting with this notebook will be explored in this section.

Consider, for example, an LC sample where all LCs are oriented in the xy-plane (theta = 90°) and all oriented in the same direction in the xy-plane. It is expected that this sample will act as a linear polarizer, as the Jones matrix is consistent across the sample. We also expect that the light will propagate through the cross polarizers when the LC director is diagonal to the cross polarizers. To determine if this holds true for the Python simulation, rotation matrices are used to rotate the Jones matrix, which is effectively the same as rotating the sample on a microscope stage. In doing so, the resulting video should switch between an entirely black output as the LC director goes in phase with one of the cross polarizers, and an entirely white output when the LC is diagonal.

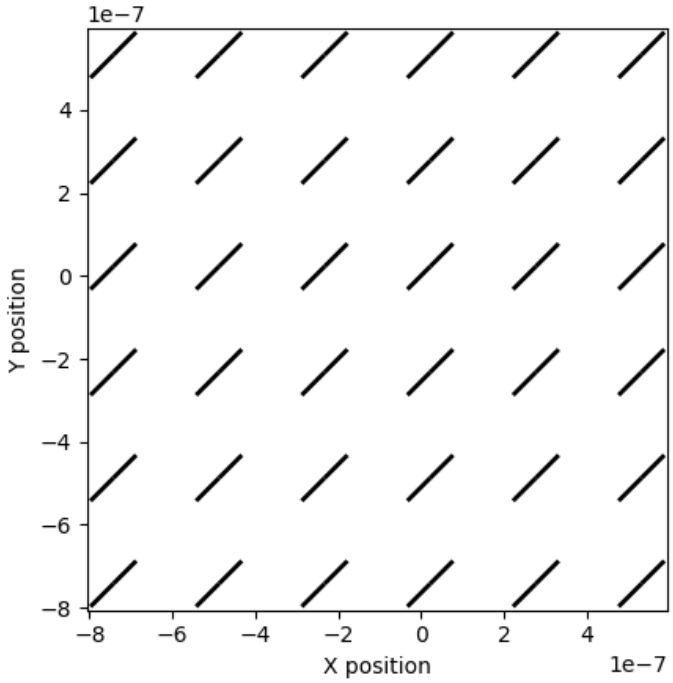

Figure 5: The sampled director field for LCs configured as a linear polarizer. This is the orientation of angle = 0.

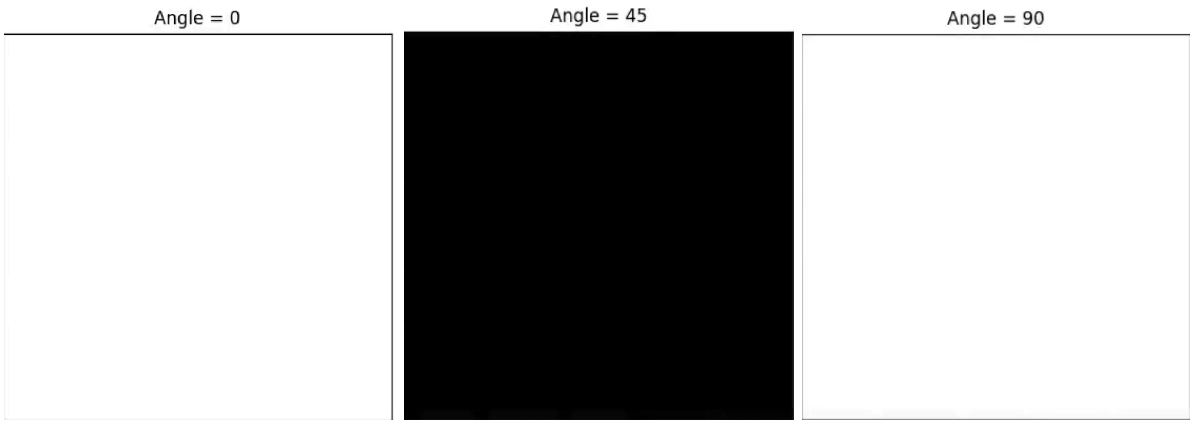

Figure 6: The resulting cross polarized images for different angles of rotation of the sample. When the directors are diagonal, angle = 0 or some multiple of 90°, there is an admittance of light. When the sample is in phase with one of the polarizers there is a blockage of light.

For the frames in between these extremes, some amount of light propagates through the sample. As the angle approaches an integer multiple of 90 degrees, the intensity increases until it reaches a peak intensity at 90 degrees.

On the other hand, consider an LC sample that is a single column of LCs. If there is a small polar rotation between the director of each consecutive coordinate, and we assume that the LCs are orthogonal to the propagation of light (theta = 90°) then it would be expected that the same principle should apply. Specifically, the twist of the director spiral will determine whether light can propagate through the cross polarizers. By looking at the intensity of cross polarized light from subsections of the sample, a column of light and dark patterns can be created, where each point on the column is found by considering the LCs from the origin of the light to that coordinate in the sample. This column is shown on the right, with light propagating from the top of the page down. The total twist of the director throughout the column is 360°, which is why the perceived light returns to 0 intensity at the bottom of the column. Additionally, when the director has rotated a full 180°, halfway through the column, the perceived light is also 0 intensity. This is because LC directors are headless. The light spots in between are the equivalent of rotating the polarization of the light such that it can pass through the second polarizer.

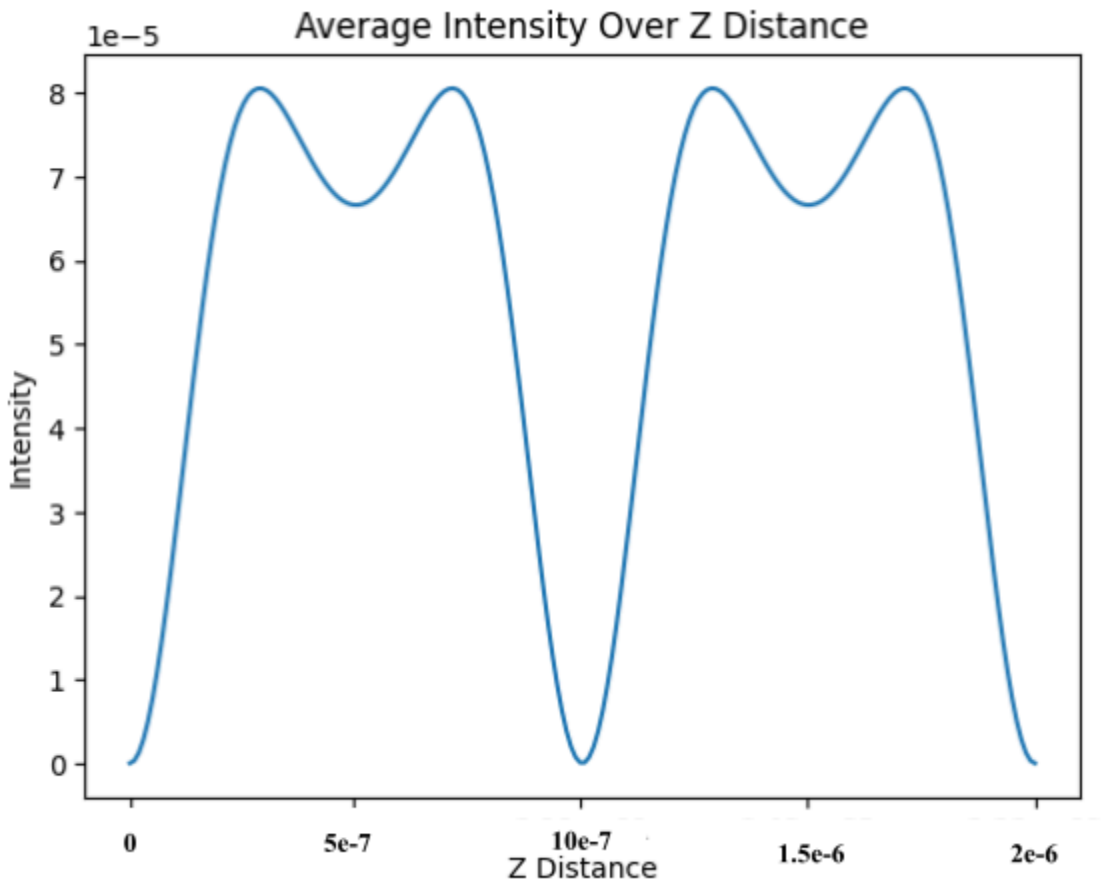

Figure 7: The cross polarized light intensity at a particular distance into a LC sample of unit length and width

This polarity rotation holds true for all LC samples, but becomes more complicated with defects. Defects are isotropic regions within the sample that occur due to boundary conditions. As LC samples approach a nematic form, there are local regions that cannot conform to such an orientation due to structural constraints. These regions have interesting optical properties. In general, defects are associated with light and dark brushes on the cross polarized image.

Each defect has a spin that is determined by the number of rotations of the director for one rotation around the defect. In other words, if a unit circle was centered at the defect, then one could walk counterclockwise along the perimeter. If this walker keeps their orientation constant, they do not turn as they walk, then they would see the director turning relative to them as they progress.

The number of ways that this rotation could occur is limited by the constraint that the director must return to its original orientation after one loop around the defect. Hence defects can have ±1/2 spin, corresponding to the director rotating 180° around the defect loop. Additionally, defects can have any integer multiple of 1/2 spin.

Beginning with 1/2 spin defects, these can either have a positive or negative spin. The fundamental difference between a positive and negative spin is that the phi component of the orientation is rotated 180°. This can be seen in the below plots of the director field for a +1/2 and a -1/2 spin defect. Again (theta = 90°), but now the sample is not in the nematic phase. Notice that each vector must be rotated 180° inorder to change the sign of the spin.

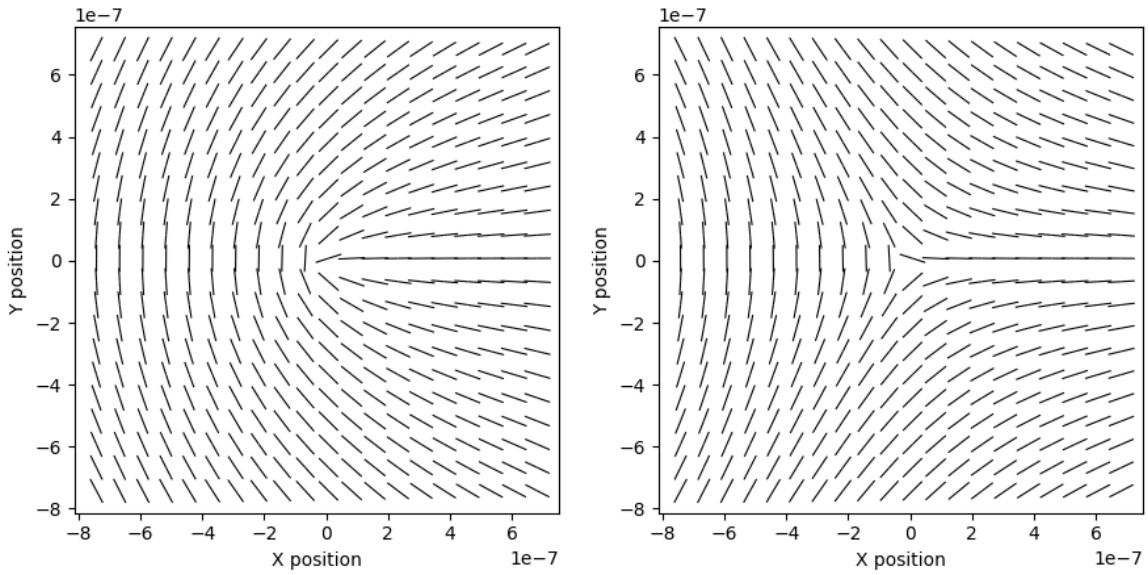

Figure 8: The director field plot on the left shows a +1/2 spin defect and on the right is a -1/2 spin defect.

One drawback of the cross polarized image is that it does not show the sign of the spin. Take for example, the cross polarized images of the two director field plots above. Seen in the two figures below, these images are the same for no sample rotation. Only when the sample is turned a small amount can we see the direction that the brushes turn. This theme of spinning brushes holds true for a full rotation of the LC sample.

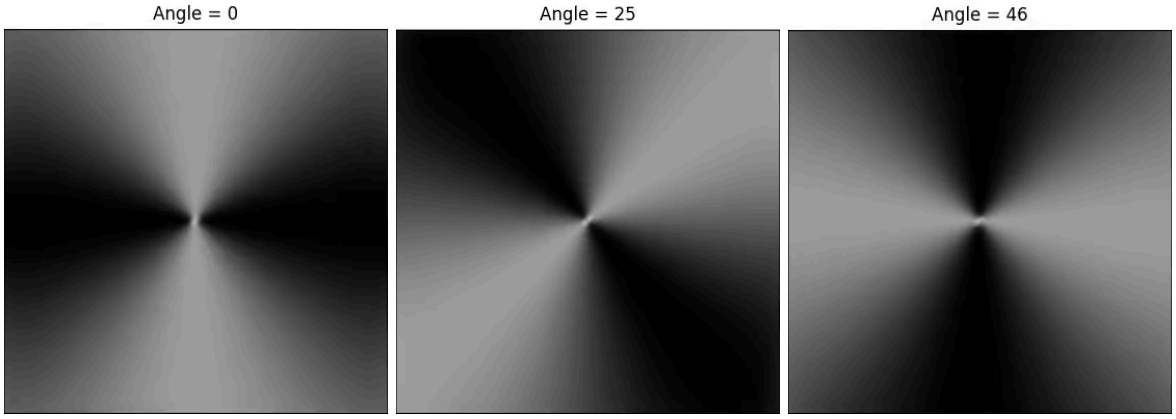

Figure 9: Cross polarized images for the +1/2 spin defect taken for 3 rotations of the LC sample.

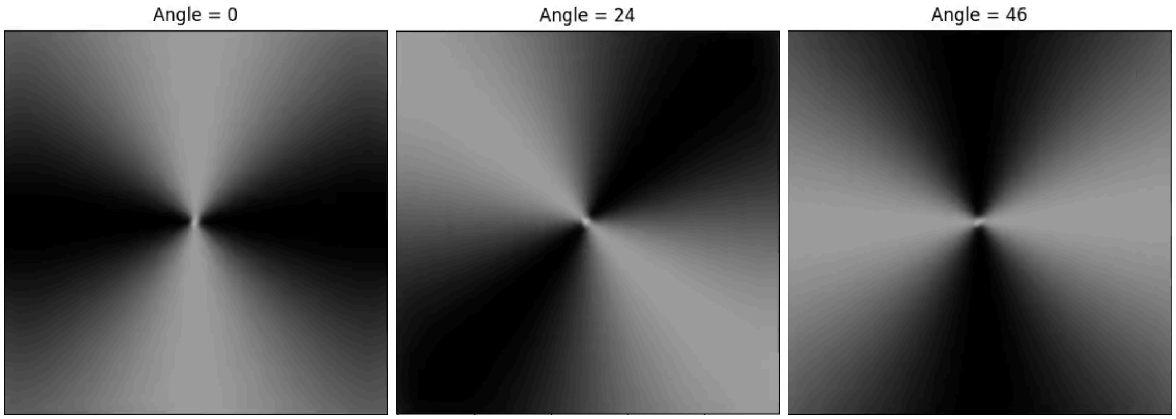

Figure 10: Cross polarized images for the -1/2 spin defect taken for 3 rotations of the LC sample.

By rotating the cross polarizers and observing the direction of spin of the brushes, one can determine the sign of the defect. That is, the +½ defect spins counterclockwise, while the -½ defect spins clockwise. The rate of rotation is constant throughout the entire 360 degrees of rotation. Due to the spin of the defect, the image is rotated by twice the cross polarizer rotation. Similar effects also occur for higher spin defects, as shown below.

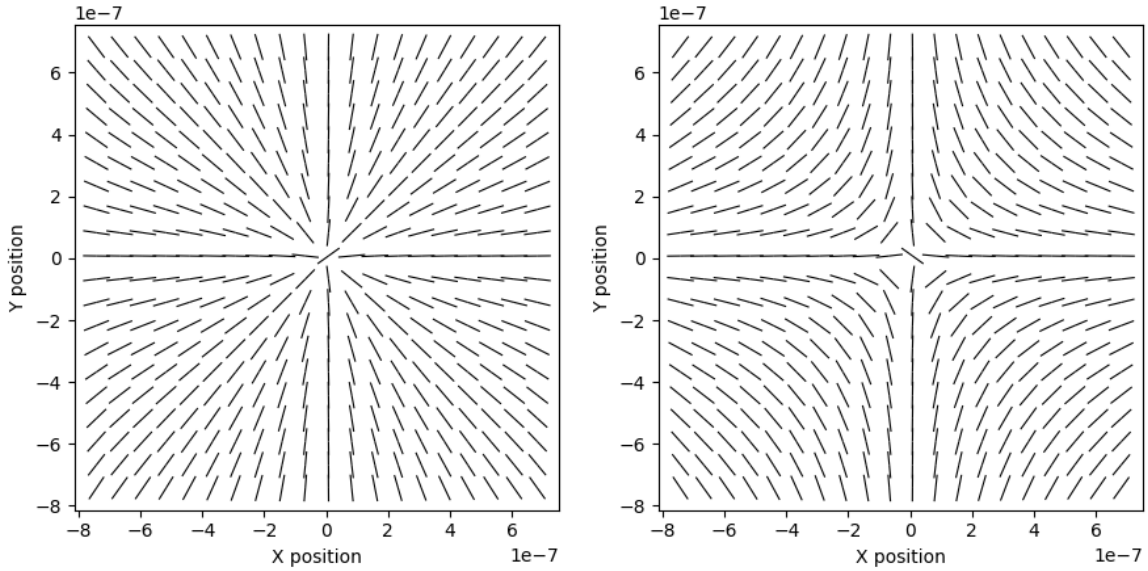

Figure 11: The director field plot on the left shows a +1 spin defect and on the right is a -1 spin defect.

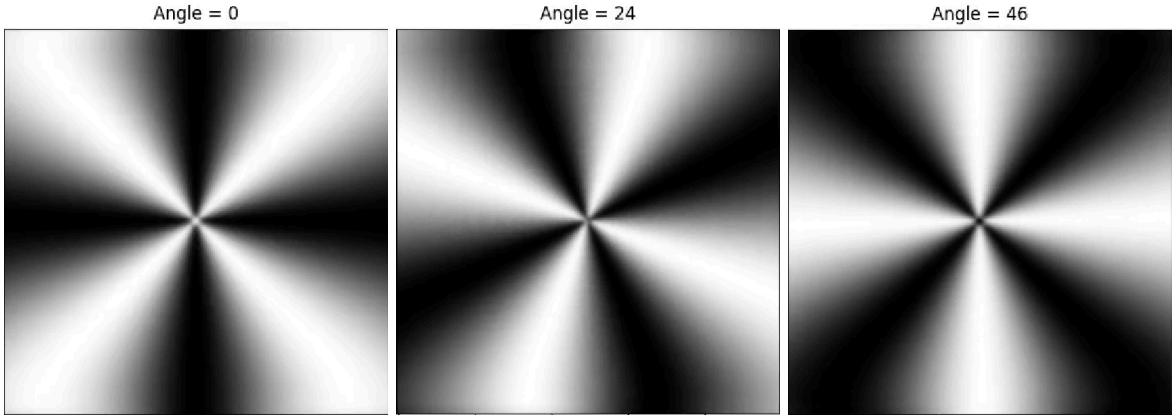

Figure 12: Cross polarized images for the +1/2 spin defect for 3 rotations of the LC sample.

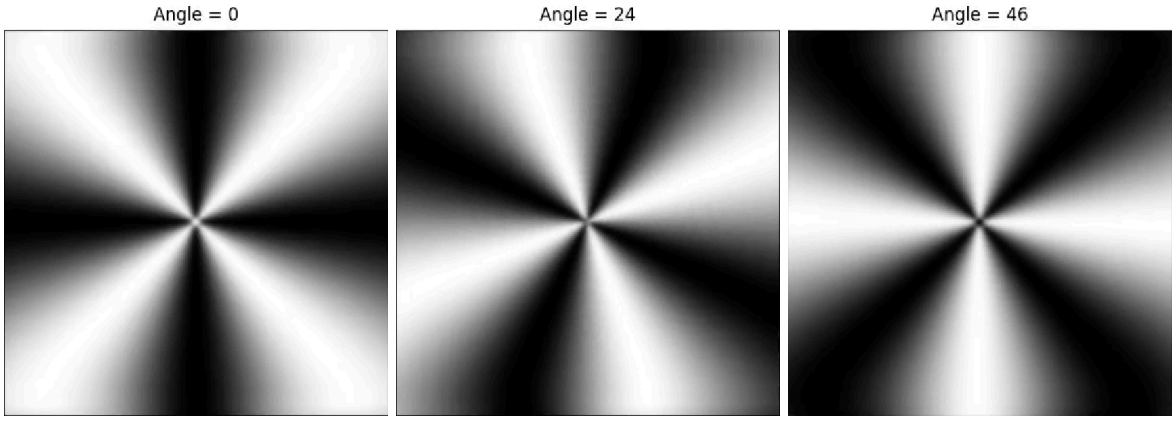

Figure 13: Cross polarized images for the -1/2 spin defect taken for 3 rotations of the LC sample.

Having a higher spin results in more defect brushes. Specifically the number of brushes is four times the number of the spin. Another observation from the higher spin is that it rotates slower than lower spins. For a polarizer rotation of 45 degrees, the ½ spin defects made a full 90 degree rotation, while the 1 spin defects made a 45 degree rotation. A further observation of these defect structures is that the center is ill defined in the images. This is because of the discretization of the sample leading to poor resolution.

Conclusion

This study has investigated the complex interplay between light propagation and the structural dynamics of liquid crystals (LCs) using the Jones Matrix Formalism. By exploring the transition between nematic and isotropic phases, the project has highlighted the crucial role of molecular orientation in determining the optical properties of LCs, such as anisotropy and birefringence. The results obtained through simulations underscore the ability of LCs to manipulate polarized light, which is critical for applications ranging from simple displays to intricate optical devices.

The implementation of the Jones Matrix Formalism within a Python environment has proved to be a robust method for visualizing and analyzing the interaction between light and LCs. By simulating the effect of varying director field orientations, this study has not only confirmed theoretical predictions but also provided a visualization of LC behavior under different conditions.

Moving forward, further research could focus on enhancing the computational efficiency of these simulations and expanding their applicability to other types of complex materials, such as 3D defects, thereby broadening our understanding of light-matter interactions in advanced technological applications.