# PATTERN FORMATION IN LIQUID CRYSTALS: A THEORETICAL STUDY

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*Abstract*

*Liquid crystals are such a state of matter which has properties between those of conventional liquids and people of solid crystals. For example, a liquid may flow sort of a liquid, but its molecules could also be oriented in an exceedingly crystal-like way.*

*Liquid crystals are composites of organic, rod-shaped molecules that align in parallel, and therefore the common types utilized in electronic displays are nematic, cholesteric and smectic.*

*Liquid crystals are classified in many ways, molecules within the mesophases (mesogens) may be calamitic (rod-like), discotic (disc-like), amphiphilic, nonamphiphilic, metal containing, non-metal containing and low relative molecular mass or polymeric. Liquid crystals either show thermotropic behaviour or lyotropic behaviour.*

*Liquid crystal phases are generally cloudy in appearance, which suggests that they scatter light in much the identical way as colloids like milk. This light scattering could be a consequence of fluctuating regions of non-uniformity as small groups of molecules form and disperse. Most liquid compounds exhibit polymorphism, or a condition where over one phase is observed within the liquid crystalline state. The term mesophase is employed to explain the "subphases" of liquid materials. Mesophases are formed by changing the quantity of order within the sample, either by imposing order in barely one or two dimensions, or by allowing the molecules to own a degree of translational motion.*

*Anisotropy of liquid crystals could be a property not observed in other fluids. This anisotropy makes flows of liquid crystals behave more differentially than those of ordinary fluids. For instance, injection of a flux of a liquid between two close parallel plates (viscous fingering) causes orientation of the molecules to couple with the flow, with the resulting emergence of dendritic patterns. This anisotropy is additionally manifested within the interfacial energy (surface tension) between different liquid phases. This anisotropy determines the equilibrium shape at the coexistence temperature, and is so strong that typically facets appear. When temperature is modified; one phases grows, forming different morphologies betting on the activity. Since growth is controlled by heat diffusion, anisotropy in thermal conductivity favors growth in specific directions, which has also a bearing on the ultimate shape.*

*Keywords: Pattern formation, Liquid Crystals, Theoretical Study, Models, Oscillatory chemical kinetics, Autocatalytic reactions, Order parameter*

## Introduction

Pattern formation has been well studied in chemistry and chemical engineering, including both temperature and concentration patterns. The Brusselator model developed by Ilya Prigogine and collaborators is one such example that exhibits 'Turing instability'. Pattern formation in chemical systems often involves oscillatory chemical kinetics or autocatalytic reactions like Belousov–Zhabotinsky reaction or Briggs–Rauscher reaction. In industrial applications like chemical reactors; pattern formation can cause temperature hot spots, which might reduce the yield or create hazardous safety problems like a thermal runaway. The emergence of pattern formation is studied by mathematical modeling and simulation of the underlying reaction-diffusion system.

Similarly as in chemical systems, patterns can develop during weak ionized plasma of a positive column of a glow discharge. In such cases creation and annihilation of charged particles thanks to collisions of atoms corresponds to reactions in chemical systems. Corresponding processes are essentially non-linear and lead in an exceedingly discharge tube to formation of striations with regular or random character.

## Theoretical treatment of liquid crystals

Microscopic theoretical treatment of fluid phases can become quite complicated, because of the high material density, meaning that strong interactions, hard-core repulsions, and many-body correlations can't be ignored. In the case of liquid crystals, anisotropy interactions further complicates analysis. There are variety of fairly simple theories, however, they will have a minimum of the interference behavior of the phase transitions in liquid systems.

## Director

As we already saw above, the nematic liquid crystals are composed of rod-like molecules with the long axes of neighboring molecules aligned approximately to at least one another. To explain this anisotropic structure, a dimensionless unit vector n called the director, is introduced to represent the direction of preferred orientation of molecules within the neighborhood of any point. Because there's no physical polarity along the director axis, n and -n are fully equivalent.
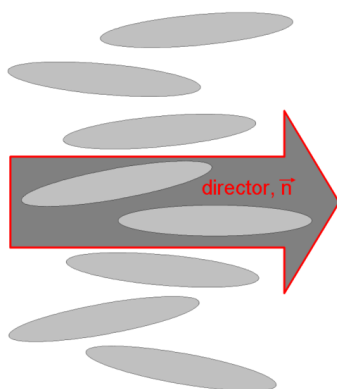
**Order parameter**



Figure: The *local nematic director*, which is also the *local optical axis*, is given by the spatial and temporal average of the long molecular axes

The description of liquid crystals involves an analysis of order. A second rank symmetric traceless tensor order parameter is employed to explain the orientational order of a nematic liquid, although a scalar order parameter is typically sufficient to explain uniaxial nematic liquid crystals. to create this quantitative, an orientational order parameter is typically defined supported the common of the second Legendre polynomial:

$$S = \langle P_2(\cos\theta) \rangle = \left\langle \frac{3\cos^2(\theta) - 1}{2} \right\rangle$$

where $\theta$ is that the angle between the liquid-crystal molecular axis and therefore the local director (which is that the 'preferred direction' in a very volume element of a liquid sample, also representing its local optical axis). The brackets denote both a temporal and spatial average. This definition is convenient, since for a very random and isotropic sample, $S = 0$, whereas for a perfectly aligned sample S=1. For a typical liquid sample, S is on the order of 0.3 to 0.8, and customarily decreases because the temperature is raised. Specifically, a pointy drop of the order parameter to 0 is observed when the system undergoes an activity from an LC phase into the isotropic phase. The order parameter may be measured experimentally in a very number of ways; for example, diamagnetism, birefringence, Raman scattering, NMR and EPR may be accustomed determine S.

The order of a liquid could even be characterized by using other even Legendre polynomials (all the odd polynomials average to zero since the director can point in either of two anti-

parallel directions). These higher-order averages are harder to live, but can yield additional information about molecular ordering.

A positional order parameter is additionally accustomed describe the ordering of a liquid. It's characterized by the variation of the density of the middle of mass of the liquid molecules along a given vector. In the case of positional variation along the *z*-axis the density $\rho(z)$ is often given by:

$$\rho(\mathbf{r}) = \rho(z) = \rho_0 + \rho_1 \cos(q_s z - \varphi) + \mathrm{L}$$

The complex positional order parameter is defined as $\psi(\mathbf{r}) = \rho_1(\mathbf{r})e^{i\varphi(\mathbf{r})}$ and $\rho_0$ the average density. Typically only the primary two terms are kept and better order terms are ignored since most phases is described adequately using sinusoidal functions. For an ideal nematic $\psi = 0$ and for a smectic phase $\psi$ will tackle complex values. The complex nature of this order parameter allows for several parallels between nematic to smectic phase transitions and conductor to superconductor transitions.

A simple model which predicts lyotropic phase transitions is that the hard-rod model proposed by chemist. This theory considers the amount excluded from the center-of-mass of 1 idealized cylinder because it approaches another. Specifically, if the cylinders are oriented parallel to at least one another, there's little volume that's excluded from the center-of-mass of the approaching cylinder (it can come quite near the opposite cylinder). If, however, the cylinders are at some angle to at least one another, then there's an oversized volume surrounding the cylinder which the approaching cylinder's center-of-mass cannot enter (due to the hard-rod repulsion between the 2 idealized objects). Thus, this angular arrangement sees a decrease within the net positional entropy of the approaching cylinder (there are fewer states available to it).

The fundamental insight here is that, whilst parallel arrangements of anisotropic objects cause a decrease in orientational entropy, there's a rise in positional entropy. Thus in some case greater positional order are entropically favorable. Thus in some case greater positional order are entropically favorable. This theory thus predicts that an answer of rod-shaped objects will undergo a activity, at sufficient concentration, into a nematic phase. Although this model is conceptually helpful, its mathematical formulation makes several assumptions that limit its applicability to real systems.

**Maier–Saupe mean theory**

This statistical theory, proposed by Alfred Saupe and Wilhelm Maier, includes contributions from a lovely intermolecular potential from an induced moment between adjacent rod-like liquid molecules. The anisotropic attraction stabilizes parallel alignment of neighboring molecules, and also the theory then considers a mean-field average of the interaction. Solved self-consistently, this theory predicts thermotropic nematic-isotropic phase transitions, according to experiment. Maier-Saupe mean theory is extended to high relative molecular mass liquid crystals by incorporating the bending stiffness of the molecules and using the strategy of path integrals in polymer science.

**McMillan's model**

McMillan's model, proposed by William McMillan, is an extension of the Maier–Saupe mean theory accustomed describes the physical change of a liquid from a nematic to a smectic A phase. It predicts that the physical change will be either continuous or discontinuous reckoning on the strength of the short-range interaction between the molecules. As a result, it allows for a triple crossroads where the nematic, isotropic, and smectic A phase meet. Although it predicts the existence of a triple crisis, it doesn't successfully predict its value. The model utilizes two order parameters that describe the orientational and positional order of the liquid. The primary is just the typical of the second Legendre polynomial and therefore the second order parameter is given by:

$$\sigma = \left\langle \cos\left(\frac{2\pi z_i}{d}\right)\left(\frac{3}{2}\cos^2(\theta_i) - \frac{1}{2}\right) \right\rangle$$

The values $z_i$, $\theta_i$, and $d$ are the position of the molecule, the angle between the molecular axis and director, and the layer spacing. The postulated potential energy of a single molecule is given by:

$$U_i(\theta_i, z_i) = -U_0\left(S + \alpha\sigma\cos\left(\frac{2\pi z_i}{d}\right)\right)\left(\frac{3}{2}\cos^2(\theta_i) - \frac{1}{2}\right)$$

Here constant α quantifies the strength of the interaction between adjacent molecules. The potential is then wont to derive the thermodynamic properties of the system assuming

equilibrium. It leads to two self-consistency equations that have to be solved numerically, the solutions of which are the three stable phases of the liquid.

**Elastic continuum theory**

In this formalism, a liquid material is treated as a continuum; molecular details are entirely ignored. Rather, this theory considers perturbations to a presumed oriented sample. The distortions of the liquid are commonly described by the Frank free energy density. One can identify three forms of distortions that might occur in an oriented sample: (1) twists of the fabric, where neighboring molecules are forced to be angled with relation to each other, instead of aligned; (2) splay of the fabric, where bending occurs perpendicular to the director; and (3) bend of the fabric, where the distortion is parallel to the director and molecular axis. All three of those forms of distortions incur an energy penalty. They're distortions that are induced by the boundary conditions at domain walls or the enclosing container. The response of the fabric can then be decomposed into terms supported the elastic constants love the three kinds of distortions. Elastic continuum theory is an efficient tool for modeling liquid devices and lipid bilayers.

**External influences on liquid crystals**

Scientists and engineers use liquids during a sort of applications, because external perturbation can cause significant changes within the macroscopic properties of the liquid crystal system. Both electric and magnetic fields won't induce these changes. The magnitude of the fields spread the speed at which the molecules align are important characteristics industry deals with. Special surface treatments may be employed in liquid devices to force specific orientations of the director.

**Electric and flux effects**

The ability of the director to align along an external field is caused by the electrical nature of the molecules. Permanent electric dipoles result when one end of a molecule incorporates a net charge while the opposite end contains a net charge. When an external force field is applied to the liquid, the dipole molecules tend to orient themselves along the direction of the sphere.

Though, a molecule doesn't form permanent dipole, it can still be influenced by an electrical field. In some cases, the sphere produces slight re-arrangement of electrons and protons in

molecules specified an induced electric doublet results. While not as strong as permanent dipoles, orientation with the external field still occurs.

The response of any system to an external electrical field is

$$D_i = \epsilon_0 E_i + P_i$$

where $E_i$, $D_i$ and $P_i$ are the components of the electric field, electric displacement field and polarization density. The electric energy per volume stored in the system is

$$f_{\text{elec}} = -\frac{1}{2} D_i E_i$$

(summation over the doubly appearing index $_i$). In nematic liquid crystals, the polarization, and electric displacement both depend linearly on the direction of the electric field. The polarization should be even in the director since liquid crystals are invariants under reflexions of $n$. The most general form to express $D$ is

$$D_i = \epsilon_0 \epsilon_\perp E_i + \left( \epsilon_\parallel - \epsilon_\perp \right) n_i n_j E_j$$

(summation over the index $_j$) with $\epsilon_\perp$ and $\epsilon_\parallel$ the electric permittivity parallel and perpendicular to the director $n$. Then density of energy is (ignoring the constant terms that do not contribute to the dynamics of the system)

$$f_{\text{elec}} = -\frac{1}{2} \epsilon_0 \left( \epsilon_\parallel - \epsilon_\perp \right) \left( E_i n_i \right)^2$$

(summation over $_i$). If $\epsilon_\parallel - \epsilon_\perp$ is positive, then the minimum of the energy is achieved when $E$ and $n$ are parallel. This means that the system will favor aligning the liquid crystal with the externally applied electric field. If $\epsilon_\parallel - \epsilon_\perp$ is negative, then the minimum of the energy is achieved when $E$ and $n$ are perpendicular (in nematics the perpendicular orientation is degenerated, making possible the emergence of vortices).

The difference $\Delta\epsilon = \epsilon_\parallel - \epsilon_\perp$ is called dielectrical anisotropy and is an important parameter in liquid crystal applications. There are both $\Delta\epsilon > 0$ and $\Delta\epsilon < 0$ commercial liquid crystals. 5CB and E7 liquid crystal mixture are two $\Delta\epsilon > 0$ liquid crystals commonly used. MBBA is a common $\Delta\epsilon < 0$ liquid crystal.

The effects of magnetic fields on liquid molecules are analogous to electric fields. Because magnetic fields are generated by moving electric charges, permanent magnetic dipoles are produced by electrons moving about atoms. When a force field is applied, the molecules will tend to align with or against the sphere. Non-particulate radiation, e.g. UV-Visible light, can influence light-responsive liquid crystals which mainly carry a minimum of a photo-switchable unit.

**Surface preparations**

In the absence of an external field, the director of a liquid is absolve to point in any direction. It's possible, however, to force the director to point in an exceedingly specific direction by introducing an out of doors agent to the system. As an example, when a skinny polymer coating (usually a polyimide) is spread on a glass substrate and rubbed in a very single direction with a cloth, it's observed that liquid molecules in-tuned therewith surface align with the rubbing direction. The currently accepted mechanism for this is often believed to be an epitaxial growth of the liquid layers on the partially aligned polymer chains within the near surface layers of the polyimide.

Several liquid chemicals also align to a 'command surface' which is successively aligned by field of polarized light. This process is named photoalignment.

**Fredericks transition**

The competition between orientation produced by surface anchoring and by field of force effects is commonly exploited in liquid devices. Consider the case during which liquid molecules are aligned parallel to the surface and an electrical field is applied perpendicular to the cell. At first, because the field increases in magnitude, no change in alignment occurs. However at a threshold magnitude of electrical field, deformation occurs. Deformation occurs where the director changes its orientation from one molecule to the following. The occurrence of such a change from an aligned to a deformed state is termed a Fredericks transition and might even be produced by the applying of a field of sufficient strength.

The Fredericks transition is essential to the operation of the many liquid displays due to the director orientation (and thus the properties) will be controlled easily by the appliance of a field.

**Reaction–diffusion system**

Reaction–diffusion systems are mathematical models corresponding to many physical phenomena. The foremost common is that the change in space and time of the concentration of 1 or more chemical substances: local chemical reactions within which the substances are transformed into one another, and diffusion which causes the substances to detached over a surface in space.

Reaction–diffusion systems are applied in chemistry. However, the system can even describe dynamical processes of non-chemical nature. Examples are found in biology, geology and physics (neutron diffusion theory) and ecology. Mathematically, reaction–diffusion systems take the shape of semi-linear parabolic partial differential equations. They'll be represented within the general form

$$\partial_t \mathbf{q} = \underline{\underline{\mathbf{D}}} \nabla^2 \mathbf{q} + \mathbf{R}(\mathbf{q}),$$

where $q(x, t)$ represents the unknown vector function, $D$ may be a square matrix of diffusion coefficients, and $R$ accounts for all local reactions. The solutions of reaction–diffusion equations display a large range of behaviours, including the formation of travelling waves and wave-like phenomena also as other self-organized patterns like stripes, hexagons or more intricate structure like dissipative solitons. Such patterns are dubbed "Turing patterns". Each function, that a reaction diffusion equation holds, represents of course a degree variable.

## *Conclusion*

Liquid crystals are discovered just a century ago, have wide application to electro-optic displays and thermography. Their physical properties have also made them fascinating materials for more fundamental research.

The name "liquid crystals" is really a misnomer for what are more properly termed "mesophases," that is, phases having symmetries intermediate between ordinary solids and liquids. There are three major classes of liquid crystals: nematics, smectics, and columnar mesophases. In nematics, although there's no correlation between positions of the rodlike molecules, the molecules tend to lie parallel along a standard axis; labeled by a unit vector (or director) n. Smectics are more ordered. The molecules are rodlike and are in layers. Different subtypes of smectics (labeled, for historical reasons, smectic A, smectic B,..) have layers that

are more or less organized. Within the smectic A phase, the layers are fluid and may glide easily over one another. Within the smectic B phase, the layers have hexagonal ordering and robust interlayer corrélations. Indeed, the smectic B phase is more a highly anisotropic plastic crystal than it's a liquid. Finally, columnar mesophases are obtained with disklike molecules. These molecules can pull together in columns which are themselves organized in an exceedingly two-dimensional array. There's no positional correlation between molecules in one column and molecules within the other columns.

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