Research

Domain Patterns in Quenched Confined Nematic Liquid Crystals

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Abstract:
This study explores the Imry-Ma theorem and the Kibble-Zurek mechanism in the context of quenched confined nematic liquid crystals (NLCs). The Imry-Ma theorem explains domain formation under the influence of random fields, while the Kibble-Zurek mechanism describes defect dynamics during fast enough symmetry breaking phase transitions. We demonstrate that considering both mechanisms one could explain the equilibrium domain structure observed in NLCs confined within a plane-parallel cell.

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1. Introduction

1.1. Context and importance

The interplay between theoretical frameworks and experimental observations is essential for understanding complex systems like nematic liquid crystals. Liquid crystals (LC) , with their unique combination of fluidity and ordered molecular alignment, are sensitive to impurities and external influences, making them an excellent platform for exploring the effects of disorder on structural properties and phase transitions (Kléman et al., 2003). For simplicity we limit to thermotropic rod-like LC molecules whose local orientational order is at the mesoscopic scale described by the nematic director field $\vec{n}$ which points along the average orientation. Here the states $\pm\vec{n}$ are physically equivalent. In thermotropic LCs phase behavior is controlled by varying temperature. At relatively high temperatures LC display liquid-like order, forming the so-called isotropic (I) phase. Thermotyropic nematic liquid crystal (NLC) phase represents the simplest LC phase which can be reached starting from the isotropic phase by lowering temperature. The equilibrium nematic (N) phase exhibits long range orientational order in which $\vec{n}$ is homogeneously aligned alog a single symmetry breaking direction.

Of our interest is recent experimental study (Pišljar et al., 2024) in which domain-type is observed in NLC confined with a plane-parallel cell of thickness h, where the confining substrates enforce the so-called isotropic tangential anchoring. In the latter case nearby LC molecules prefer to lie within the confining plate where all directions are equivalent. However, the experimental study shows that in equilibrium a domain-type nematic structure exists, where the characteristic domain size $\xi_d \propto h$.

Below we demonstrate that such behavior could be explained using universal Imry-Ma (Imry & Ma, 1975) and Kibble-Zurek (Kibble, 1976; Zurek, 1985) mechanism which are valid for phases which are reached via a continuous-symmetry breaking phase transition (Sethna, 1992).

1.2. Theoretical background

The Imry-Ma (IM) theorem, first introduced in the context of magnetism, provides a foundational framework for studying the impact of disorder on long-range order which is reached via a continuous symmetry breaking phase transition. It predicts that random fields can destabilize order in systems described by continuous symmetry breaking phase transitions, leading to the formation of domains whose sizes depend on the strength of the disorder (Imry & Ma, 1975). Initially formulated for ferromagnets, the theorem has since been adapted to other systems, including liquid crystals (Ranjkesh et al., 2014). Furthermore, if a continuous symmetry breaking phase transition is fast enough it could temporarily exhibit domain-like structure due to the finite speed of information propagation. The resulting size of initially formed domains is determined by the Kibble-Zurek (KZ) mechanism (Zurek, 1985) which was originally derived in cosmology (Kibble, 1976).

1.3. Application to liquid crystals

In confined nematic liquid crystals, domains could be temporarily formed in a fast enough (Zurek, 1985) I-N phase transition. Namely, in such cases in distant parts of LC symmetry is in general broken in different directions because of finite information velocity propagation (Kibble, 1976). In bulk NLC domains grow with time and terminate in a single domain which exhibits the lowest parallel cell of thickness h, whose non-treated confining plates do not favor any in-plane direction. We claim that a domain pattern, formed slightly after the nematic phase was reached, could be imprinted into confining plates due to the memory effects (Kléman et al., 2003; Kralj & Sluckin, 1994). Namely, it is well known that LC molecules nearby a confining plate could be »frozen-in« orientationally if LC-substrate interaction is stronger that LC-LC configuration. In the following we show that the combination of IM argument and KZ mechanism could qualitatively explain recent experimental observations (Pišljar et al., 2024).

2. Material and Methods

2.1. Theoretical framework for Imry-Ma theorem

The Imry-Ma theorem explains the emergence of domain structures in systems experiencing continuous symmetry breaking, particularly in the presence of random fields(Imry & Ma, 1975). The elastic energy term, which enforces homogeneity, plays a critical role in this process. The key term enforcing homogeneity in field-type theories is approximated by a single elastic modulus, given by (Kléman et al., 2003)

$$f_e \sim \frac{K}{2}|\nabla \vec{n}|^2 \quad , \tag{1}$$

where K is the nematic elastic constant and $\nabla \vec{n}$ represents the spatial gradient of the director field $\vec{n}$. This energy term drives the system toward minimizing distortions and maintaining uniform alignment. When geometrical constraints are enforced, elastic energy becomes sensitive to characteristic distances within the system, such as the domain size ξ_d. It roughly holds

$$f_e \sim \frac{K}{2}\left(\frac{1}{\xi_d}\right)^2 \quad . \tag{2}$$

Equation (2) highlights how smaller domains increase elastic energy, favoring larger domains in the absence of competing forces.

2.2. Influence of random fields

Random fields disrupt the uniform alignment enforced by the elastic term. In our illustration we present a random-type disorder by spatially randomly varying local random field direction $\vec{u}$. This local field enforces a preferred local alignment on the director field $\vec{n}$. In NLCs the energy contribution from the random field could express as (Bradač et al., 2011)

$$f_i \sim -WSP_2\ (\vec{n}.\vec{u}) \ , \tag{3}$$

here, W is the random field strength, S represents the degree of molecular order, and the second Legendre polynomial $P_2(x) = (3x^2 - 1)/2$ is dependent on the alignment between $\vec{n}$ and $\vec{u}$. The random field leads to the formation of domains, as it introduces localized disruptions to the system. In the continuation we assume that W is spatially constant and orientations of unit vectors $\vec{n}$ are randomly distributed.

The balance between elastic energy (f_e) and random field energy (f_i) determines the characteristic domain size. The resulting domain size ξ_d is given by (Ranjkesh et al., 2014)

$$\xi_d \sim \frac{1}{W^{\frac{2}{4-d}}} \quad , \tag{4}$$

where d is the dimensionality of the system. This equation shows that stronger random fields lead to smaller domains, while larger elastic constants promote larger domain sizes what is illustrated in **Figure 1**.

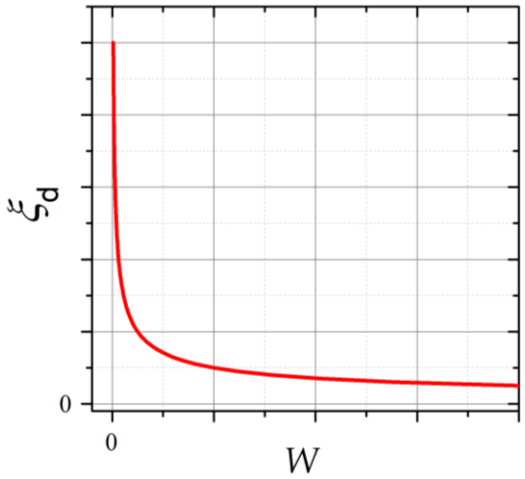

Figure 1. Dependence of domain size ξ_d on the strength of a random field W in *d*=3 systems. The graph illustrates how an increasing random field strength impacts the characteristic domain size.

2.3. *Kibble-Zurek mechanism*

The Kibble-Zurek mechanism provides a framework for understanding how defects form during continuous phase transitions. As the system is cooled through its critical temperature T_c, the relaxation time τ and coherence length ξ diverge. These quantities are close to T_c expressed as (Zurek, 1985)

$$\tau = \tau_0 |r|^{-\eta} \quad , \tag{5}$$

$$\xi = \xi_0 |r|^{-\nu} \quad , \tag{6}$$

where $r = (T - T_c)/T_c$, η and ν are critical exponents and τ_0, ξ_0 are values of τ and ξ_0 deep below the phase transition. In NLCs it roughly holds $\eta = 1$ and ν=1/2 (Bradač et al., 2011) what we consider in the continuation. In the classical KZ approach one assumes that the quench is realized linearly in time, i.e. $r = -t/\tau_Q$, where τ_Q is the characteristic quench time. At the freeze – out time t_z, the system transitions from an adiabatic to a non–adiabatic regime as shown in **Figure 2a**. It is defined by (Zurek, 1985)

$$t_z \sim \tau_0 |r_z|^{-1} \tag{7}$$

and the corresponding coherence length at freeze-out is:

$$\xi_z \sim \xi_0 |r_z|^{-\frac{1}{2}} \quad . \tag{8}$$

One assumes that the maximal cluster size formed by fluctuations is frozen-in at the time $|t_z|$ above T_c and remains frozen-in till the time $-|t_z|$ below T_c. The largest frozen-in domains, given by ξ_z, in this modelling then represent the so-called *protodomains*, which, below T_c, nucleate individual domains whose orientational distribution is randomly distributed. From description above it follows (Bradač et al., 2011; Zurek, 1985) that the characteristic size of protodomains $\xi_p \sim \xi_z$ exhibits the following scaling law in NLCs:

$$\xi_p \sim \xi_0 (\tau_Q/\tau_0)^{1/4}. \tag{9}$$

Faster cooling rates result in higher defect densities, while slower rates allow the system to form fewer defects. It roughly holds that the defect density when the protodomains are formed scales as $n \propto 1/\sqrt{\tau_Q}$ on varying τ_Q, see **Figure 2b**.

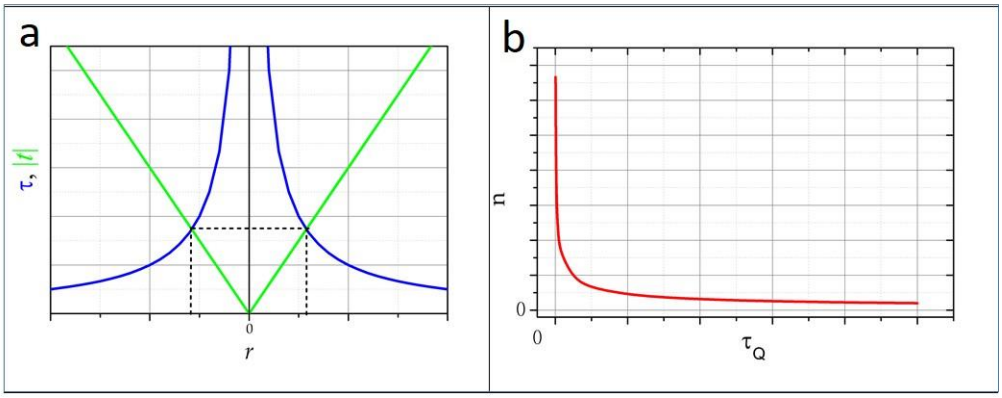

Figure 2. a: Dynamics of the system as a function of temperature. The blue color shows the change in the relaxation time (τ) as a function of the change in temperature. The green color shows how the system temperature changes over time (t). The dashed line shows the part where the system goes through the freeze-out process, **b**: Defect density n at the time when protodomains are formed as a function of the characteristic quench time τ_Q.

3. Results

In the following we apply the KZ and IM approaches to explain experimental observation reported in (Pišljar et al., 2024) with respect to typical domain length ξ_d as a function of the confining cell thickness h.

We describe the essential free energy contributions of the confined NLC as

$$F = \int \frac{K}{2} |\nabla \vec{n}|^2 dV - \int WSP_2 \ (\vec{n}.\vec{u}) \, dA. \tag{10}$$

In the first term the integration is performed over the LC body. In the 2nd term we consider conditions at the confining boundaries. We assume that the conditions at both substrates are identical and that they do not enforce any preferred direction within the confining plates in the isotropic phase. Therefore, this term begins to contribute in the nematic phase where it enforces a locally preferred direction due to the reasons explained below.

We assume that the system is quenched into the nematic phase with the characteristic quench rate τ_Q. Consequently, a domain-type structure is formed where the initial size of domains is estimated by ξ_p given by Eq.(9). Next, we assume that the pattern of LC molecules at the confining plates becomes frozen-in due to stronger LC-substrate interactions with respect to LC-LC coupling. Note that this phenomenon is not possible in the isotropic phase because the thermal fluctuations are two strong. After the pattern is imprinted at the substrates it remains relative stable which is supported by several observations (Kralj & Sluckin, 1994). Therefore, soon after the quench a domain-type pattern, which depends on τ_Q, is frozen-in at the confining substrates which effectively acts as a local random-field. In Eq.(10) we approximate this randomness by randomly distributed values of surface imposed unit vectors $\vec{u}$. Note that the average separation between two neighboring sites enforcing different orientations is given by ξ_p.

Our goal is to obtain an estimate on the characteristic size ξ_d of stable domains where they reflect the compromise between the elastic and random-field penalties. For this purpose we use similar approaches used in standard IM approach and apply it to our system.

With this in mind the average elastic penalty F_e reads

$$F_e \sim K/(2\xi_d^2)Ah \tag{11}$$

where A stands for the confining substrate area. On the other hand the average surface interaction penalty F_i of the systems reads

$$F_i \sim -WS < P_2 > A, \tag{12}$$

where <....> determines the average. Using the standard IM approach we assume that $< P_2 >$ depends on the domain size and that it is averaged out in very large domains. In finite domains it holds $< P_2 > \sim 1/\sqrt{N}$, wher N stands for the number of random sites within each domain. It roughly holds $N \sim (\xi_d/\xi_p)^2$ since the confining plates are two dimensional. Taking this into account one obtains from the »compromise« condition $F_i \sim F_e$ an estimate for a stable domain size:

$$\xi_d \sim h\frac{d_e}{\xi_p}, \tag{13}$$

where $d_e = K/W$ is commonly referred to as the surface coherence length.

4. Discussion

Our simple derivation suggests that stable domain pattern could be observed in confined LCs where the imposed disorder is enabled by memory effects. Because disorder is in such a case enforced only by the confining plan-parallel surfaces the resulting domain size should linearly depend on the cell thickness. Note that this observation could be experimentally tested by changing the quench rate of the I-N phase transition. Our derivation suggests that $\xi_d \propto \frac{1}{\xi_p} \propto 1/\sqrt{\tau_Q}$.

5. Conclusions

Our study illustrates how knowledge in different branches of science could be transferred between disciplines. This transfer is possible even in strongly physically different systems if mathematical description is similar. In our study this transfer was possible because the unifying element was continuous symmetry breaking phase transition. In it we crossed from a phase exhibiting isotropic symmetry to a phase where the symmetry was broken along a single symmetry direction.

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