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Fluctuation-induced interaction in a hybrid nematic liquid-crystal cell

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Abstract. We discuss the thermal Casimir effect in a thin hybrid nematic cell, and we analyse the enhancement of the fluctuation-mediated force due to the frustrating effect of competing surface interactions. The force exhibits a non-algebraic and non-monotonic dependence on the distance, and it dominates the total structural interaction in the system. Similar behaviour is found in the Fréedericksz cell, characterized by a bulk destabilizing external force.

1. Introduction

In the past decade, the theoretical understanding of the pseudo-Casimir effect in liquid crystals has expanded considerably. The pioneering analysis of the interaction induced by thermal fluctuations of the orientational and positional order [1] has been followed by studies of the influence of the substrate's roughness [2], anchoring [3], and heterophase nature of ordering in wetting geometries [4]. By now, it has become quite clear that the physics of liquid crystals can provide a variety of model systems that are very illuminating as regards the theory of the fluctuation-induced interaction in general.

In this study, we examine the pseudo-Casimir force in a nematic liquid crystal in the so-called hybrid geometry usually characterized by perpendicular orientation of the preferred molecular alignment at the two plates that constitute the nematic cell. In section 2 we show that in a thin enough cell, hybridity acts as a destabilizing force which enhances the fluctuation-mediated interaction. This analysis is complemented by a brief discussion of the phenomenon in the Fréedericksz cell where the substrate-induced alignment is destabilized by a bulk external force (section 3). In section 4 we summarize the results.

2. Hybrid-aligned cell

Although the hybridity of a nematic cell refers primarily to the mismatch of the easy axes at the plates, the corresponding anchoring strengths are always different too. This implies that the director configuration in the cell is uniform and dictated exclusively by the strongest anchoring provided that its thickness is smaller than the difference between the extrapolation lengths that characterize the strength of the anchoring at the plates [5, 6].

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In the following, we focus on the fluctuation-induced interaction in a thin cell with infinitely strong homeotropic anchoring at one plate and planar anchoring of finite strength at the other (figure 1). This leaves us with a single characteristic length—the planar extrapolation length λ.

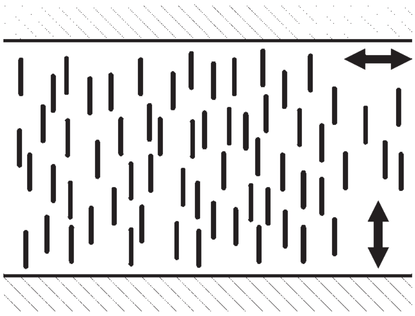

Figure 1. A thin hybrid cell with strong homeotropic anchoring (lower plate) and planar anchoring of finite strength (upper plate).

The Hamiltonian of the nematic ordering consists of the Frank elastic energy and of the Rapini–Papoular surface interaction at the planar plate [7], and in the one-constant approximation it reads

$$H[\boldsymbol{n}] = \frac{K}{2}\left\{\int\left[(\boldsymbol{\nabla}\cdot\boldsymbol{n})^2 + (\boldsymbol{\nabla}\times\boldsymbol{n})^2\right]\,\mathrm{d}V + \lambda^{-1}\int(\boldsymbol{n}\cdot\boldsymbol{k})^2\,\mathrm{d}S\right\} \tag{1}$$

where $\boldsymbol{n}$ is the director field and $\boldsymbol{k}$ is the normal to the plates [7]. Of course, the surface integral should be evaluated only at the planar plate.

We limit the discussion to harmonic fluctuations around the uniform structure, which is expected to give a quantitatively correct description of the system unless d is very close to $d_c = \lambda$. Within the harmonic approximation, the director field is given by $\boldsymbol{n} = \left(n_x, n_y, 1 - (n_x^2 + n_y^2)/2\right)$, and the Hamiltonian of each of the two fluctuating modes reduces to

$$H[n_i] = \frac{K}{2}\left[\int(\nabla n_i)^2\,\mathrm{d}V - \lambda^{-1}\int n_i^2\,\mathrm{d}S\right] \tag{2}$$

where n_i is either n_x or n_y. The negative sign of the surface term is a clear signature of the destabilizing effect of the hybridity.

To calculate the fluctuation-induced interaction, one must evaluate the partition function of each of the two fluctuating degrees of freedom:

$$\exp(-F/k_\mathrm{B}T) = \int\mathcal{D}n_i\ \exp(-H[n_i]/k_\mathrm{B}T) \tag{3}$$

where k_B is the Boltzmann constant and T is the temperature. Due to the in-plane translational invariance of the system, we can Fourier decompose the fluctuating fields in the two transverse directions, which reduces the system to an ensemble of independent one-dimensional harmonic oscillators. Using the analogy between the statistical mechanics of planar systems and the quantum mechanics [8], one eventually arrives at

$$F = \frac{k_\mathrm{B}TS}{2\pi}\int_0^\infty \ln\left(-\frac{1}{q\lambda}\sinh(qd) + \cosh(qd)\right)q\,\mathrm{d}q \tag{4}$$

which implies that the structural force defined by

$$\mathcal{F} = -\left(\frac{\partial F}{\partial d}\right)_{S,V} \tag{5}$$

reads

$$\mathcal{F} = \frac{k_B T S}{\pi} \int_0^\infty \frac{q^2 \, dq}{(q\lambda - 1)(q\lambda + 1)^{-1} \exp(2qd) + 1}. \tag{6}$$

Although this integral cannot be computed analytically, one can derive the approximate behaviour of the pseudo-Casimir force both in extremely thin cells and in the vicinity of the structural transition from the uniform to the distorted structure. In the first case, the effect of the destabilizing surface field is not very prominent, and we find that

$$\mathcal{F}(d/\lambda \ll 1) \approx \frac{k_B T S}{2\pi} \left[\frac{3\zeta(3)}{8d^3} + \frac{\ln 2}{\lambda d^2} \right] \tag{7}$$

where ζ is the Riemann zeta function and $\zeta(3) = 1.202\ldots$. The leading term is the usual d^{-3}-repulsion found in systems characterized by mixed (Dirichlet/Neumann) boundary conditions [1, 2], which correspond to a cell bounded by a strong-anchoring plate and a zero-anchoring plate. This is the zeroth-order description of the hybrid cell in the limit of small d/λ. The second term proportional to d^{-2} describes the effect of a finite destabilizing surface interaction, which enhances fluctuations at the planar substrate and amplifies the repulsion between the plates.

In the vicinity of the structural transition, the destabilizing effect of the planar substrate is much stronger, and a significant departure from the usual long-range force is expected. Indeed it turns out that for $d/\lambda \to 1$, the fluctuation-induced force diverges logarithmically:

$$\mathcal{F}(d/\lambda \to 1) \approx -\frac{3k_B T S}{2\pi\lambda^3} \ln\big(3(1 - d/\lambda)\big). \tag{8}$$

Both approximations agree very well with the numerically calculated pseudo-Casimir force (figure 2). As predicted, the force is characterized by non-algebraic and non-monotonic dependence on the reduced thickness, and the destabilizing-field-induced part of the force controls the total interaction at d/λ larger than 0.44. Let us note at this point that in real systems, the pretransitional behaviour of the force is probably somewhat different from our predictions because of the anharmonic fluctuations which have not been taken into account in the present study.

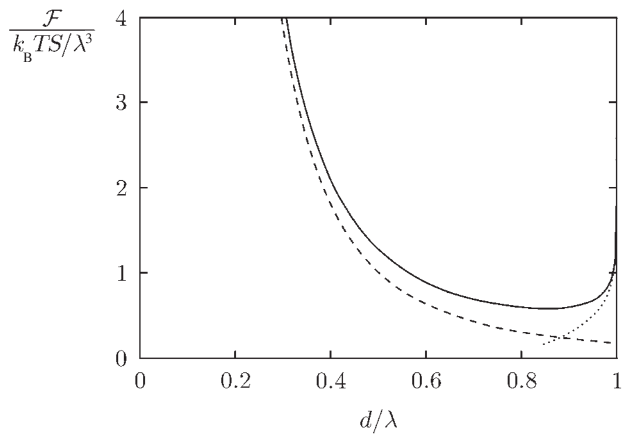

Figure 2. Fluctuation-induced force in the hybrid cell versus the reduced distance (solid line). Also plotted are the small-d expansion (dashed line) and the logarithmic divergence at the transition (dotted line).

It is not difficult to see that the fluctuation-induced force is the most important source of the structural interaction in the uniform configuration. Below the critical thickness, the mean-field free energy of the system consists solely of the surface contribution and is equal to $KS/2\lambda$, the penalty for the maximum deviation from the planar orientation. This is obviously independent of the thickness of the cell, so the mean-field force between the plates is zero.

3. The Fréedericksz cell

Let us now briefly discuss the fluctuation-induced interaction in another liquid-crystalline system characterized by macroscopic frustration—the Fréedericksz cell [7]. In such a cell, the liquid crystal is trapped between identical parallel substrates and subjected to a static magnetic field which favours a molecular orientation different from the easy axis of the surface interaction. As long as the external field is weak enough, the equilibrium director configuration is uniform and dictated by the anchoring.

We analyse the fluctuation-induced interaction in a liquid-crystalline material with negative anisotropy of the magnetic susceptibility such that the substrate-aligned state is destabilized by a magnetic field applied *along* the easy axis. In the one-constant approximation, the two director modes are degenerate and their Hamiltonian reads

$$H[n_i] = \frac{K}{2}\int_{-d/2}^{d/2}\left[(\nabla n_i)^2 - \xi^{-2}n_i^2\right]\,\mathrm{d}V. \tag{9}$$

where n_i is either of the two modes and $\xi = \sqrt{K\mu_0/|\chi_\mathrm{a}|B^2}$ is the so-called magnetic coherence length. The transition from the substrate-aligned to the field-aligned configuration occurs when the total energy of the lowest normal mode drops to 0: in the strong-anchoring limit, $d_\mathrm{c} = \pi\xi$ [7].

Just like in the hybrid cell, the interaction free energy of fluctuations can be calculated using the analogy between the statistical mechanics of planar systems and quantum mechanics, and the result is

$$F = -\frac{k_\mathrm{B}TS}{2\pi}\left\{\frac{\zeta(3)}{4d^2} - \int_0^{\xi^{-1}}\left[\ln\sin(qd) + \frac{qd}{2}\right]q\,\mathrm{d}q\right\}. \tag{10}$$

The leading term corresponds to the usual long-range attraction between like plates [1]. The influence of the magnetic field is entirely described by the integral, which consists of two contributions of quite different origin. To understand the difference between them, one should realize that the magnetic field actually plays a double role:

(a) Within the cell, it destabilizes the director fluctuations around the substrate-aligned state. This gives rise to the first part of the integrand which turns out to diverge at the transition.
(b) In the surrounding field-aligned medium the fluctuations are stabilized by the magnetic field and the second part of the integral describes the corresponding change of the reference bulk free energy.

The exact functional dependence of the fluctuation-induced force on the reduced distance between the plates is shown in figure 3. At small d/ξ, the field-induced correction to the d^{-3}-attraction is attractive and given by $-k_\mathrm{B}TS/4\pi\xi^2 d$. At distances comparable to the critical thickness, the constant attraction due to the difference between the bulk free energies of the substrate-aligned configuration and the field-aligned configuration becomes more important although the total fluctuation-induced interaction does not really flatten out. In the vicinity of the structural transition, the interaction diverges logarithmically as $\ln\sin(d/\xi)$—just like in the hybrid cell.

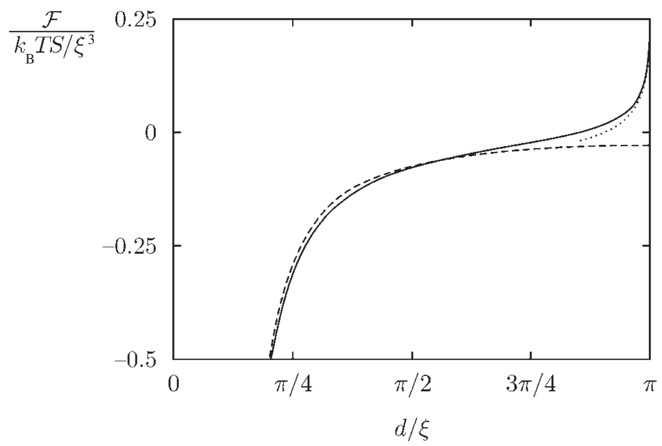

Figure 3. Field-induced pseudo-Casimir force in the Fréedericksz cell as a function of the reduced distance (solid line) and its analytical approximations: small-d expansion (dashed line) and pretransitional divergence (dotted line).

There is, however, an important difference between the two systems discussed: in the Fréedericksz cell, the magnetic field generates a strong and thickness-independent attraction between the plates because as far as the magnetic energy is concerned, the substrate-aligned configuration is very unfavourable compared to the bulk field-aligned configuration. This means that in this system, the fluctuation-induced interaction is to be sought by a method sensitive to variations of the force superposed onto a strong attractive background.

4. Conclusions

We have analysed the fluctuation-induced force in a hybrid nematic cell thin enough to be characterized by a uniform rather than a distorted director structure. We have shown that the macroscopic frustration due to competing surface interaction gives rise to a strong amplification of the force, particularly prominent in the vicinity of the structural transition from the uniform to the distorted configuration. The system studied can also serve as a paradigm for severely constrained liquid crystals, such as liquid crystals in porous glasses, aerogels, and polymer networks, where the fluctuation-induced interaction is expected to play an important role.

The universality of the pretransitional behaviour of a liquid-crystalline system in the vicinity of a structural transition has been illustrated by another well-known model geometry—the Fréedericksz cell. In this cell, the director fluctuations are destabilized by a bulk external field rather than by a surface interaction like in the hybrid cell, yet the fluctuation-induced force exhibits identical repulsive divergence at the structural transition.

Acknowledgments

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