PHYSICAL REVIEW E VOLUME 56, NUMBER 3 SEPTEMBER 1997

Forces in an inhomogeneously ordered nematic liquid crystal: Stable and metastable states

A. Borštnik and S. Žumer
Department of Physics, University of Ljubljana, 1000 Ljubljana, Slovenia

(Received 30 December 1996; revised manuscript received 8 April 1997)

Forces on plates separated a few nanometers and immersed in an isotropic liquid crystal are examined within a continuum approximation. The surface induced partial ordering of a liquid crystal is described using Landau–de Gennes phenomenological theory. Phase diagrams are presented to show the effect of surface coupling parameters, distance between the plates, and temperature on the stability and metastability of nematic and isotropic phases. Special attention is paid to the appearance of metastable phases. For selected examples we study distance and temperature dependences of the force. Values of surface coupling parameters are chosen in agreement with the results of recent experiments. For large distances between the plates the force scales with the second power of the surface coupling parameters and becomes an exponentially decreasing function of distance characterized with the nematic correlation length. [S1063-651X(97)03608-8]

PACS number(s): 61.30.−v

I. INTRODUCTION

Observations of forces in nematic films were performed by Horn, Israelachvili, and Perez [1] more than 15 years ago but later most attention was paid to the electro-optical properties, ordering, and dynamics of confined nematic liquid crystals, while forces on objects immersed in liquid crystals have usually been left aside. The ordering in thin nematic films within the Landau–de Gennes approximation was investigated by Sheng [2] and later studied by several others [3,4]. In a more detailed theoretical study, based on the same approach, Poniewierski and Sluckin [5] give a brief discussion of forces in the case of partial nematic order. Later more efforts were devoted to fluctuation (Casimir) forces in the completely ordered nematic phase [6]. The interest in experimental analysis of forces has been renewed by the investigations of Moreau *et al.* [7] devoted to presmectic phenomena in lyotropic systems. The recent preliminary results of Muševič, Slak, and Blinc [8] who used the atomic force microscope (AFM) to probe forces in partially ordered nematic liquid crystal above the nematic isotropic phase transition stimulated us to perform a detailed theoretical study of forces resulting from a nonhomogeneous surface-induced nematic ordering. Particular interest is paid to the stability and metastability of confined nematic and isotropic phases.

The structure of this paper is the following. In Sec. II we present a model of our confined nematic liquid crystal. We use a Landau–de Gennes phenomenological approach with a surface interaction which adds to the free energy of a bulk liquid crystal a linear and quadratic term in the order parameter. In Sec. III we present calculations of the order parameter. We show a phase diagram in which it can be seen how the regions of stability and metastability of the nematic and isotropic phase depend on the surface coupling parameters and temperature. Section IV deals with forces. Calculated spatial and temperature dependences of forces are presented for various surface coupling parameters.

II. DESCRIPTION OF THE MODEL

Ordering of molecules in a microconfined liquid crystal is strongly influenced by the vicinity of surfaces. In the nematic phase the most significant effect is the orientational anchoring of molecules at the confining surface. Such enforcing of a preferred surface orientation of molecules leads in any nontrivial geometry to a spatially dependent director field. Further, the presence of the surface directly and indirectly, via deformations in the director field, influences orientational fluctuations of molecules and thus modifies the degree of order and biaxiality. In the surface layer molecules are also positionally anchored so that their mobility is reduced [9–11]. The surface layer at flat substrates promotes the pretransitional formation of several smectic layers [12,13]. In the isotropic phase, the most significant effect of the substrate is the induction of the orientational order extending beyond the surface layer. Since this ordering is weaker than in the nematic phase and is also localized to the vicinity of interfaces, the effect of deformed director field and smectic layering is less pronounced. All these ordering effects result in particular contributions to forces on the substrates.

In our study we focus our attention on the isotropic phase. To be able to concentrate on the effect of surface induced orientational ordering, we limit our discussion to surfaces which prefer perpendicular orientation of molecules, which is usually, in the literature, termed homeotropic anchoring. In an experiment homeotropic anchoring can be achieved by a proper preparation of substrates. Further we assume that no smectic layers are formed in the film. Since the formation of smectic layers depends on the type of liquid crystal, one can choose pentylcyanobiphenyl (5CB) in which layers are not found in the isotropic phase, instead of 8CB or 12CB, in which pretransitional smectic layering is often observed [12,13]. Homeotropic anchoring makes the director field perpendicular to the surfaces and therefore the ordering of liquid crystal can be sufficiently described with a scalar order parameter. In the case of non-homeotropic anchoring (planar or tilted anchoring [14]), the director is spatially dependent, which requires the use of a tensor order parameter [15–17]. Several experiments indicate that the ordering of molecules in the surface layer significantly differs from the ordering of other molecules [18–20]. Therefore we expect that forces between substrates, when the liquid crystal film reduces to the surface layers, strongly depend on molecular details. To

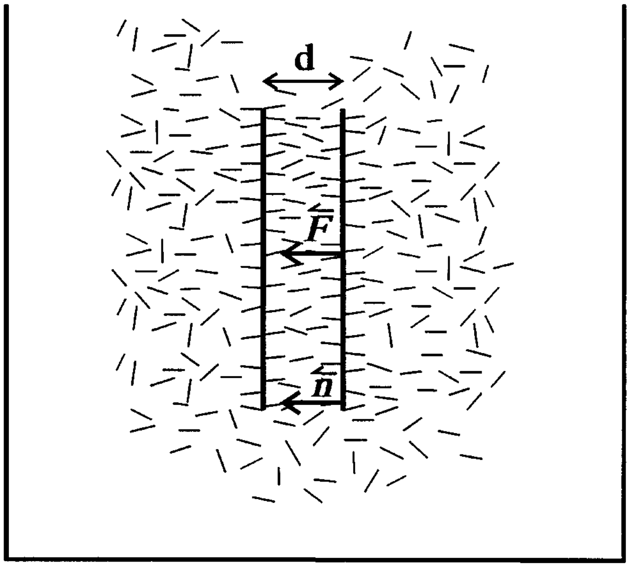

FIG. 1. A scheme of the model. Two large parallel plates are immersed in an isotropic liquid crystal. The anchoring of the molecules is homeotropic, which makes the director perpendicular to the plates. Force F is perpendicular to the plates as well.

quantitatively understand the ordering of molecules at the substrates, one should first know in detail molecular interactions and then perform a molecular dynamics study. On the other hand, if one is not interested in details occurring in the surface layer, studies of the surface induced ordering in confined liquid crystals [20–22] indicate that a combination of a phenomenological continuum approximation and an extra surface layer of molecular thickness and constant order gives a good description of the liquid crystal ordering. The typical thickness of the nematic film in our study will be of the order of 10 nm. Therefore we leave the properties of the surface layer for future discussions and simply consider them as parts of the substrate. So the thickness of our nematic film, where we use a continuum approximation, is for two surface layers smaller than the real intersubstrate distance. Further we must stress that our analysis is performed within a mean-field approximation. We expect that fluctuation forces yield only a minor correction to mean-field values and can therefore be left for further considerations.

Our model system consists of two infinite parallel plates immersed in an isotropic liquid crystal. A scheme of the arrangement is presented in Fig. 1. The anchoring of the liquid crystal molecules on the plates tends to orient the molecules perpendicular to the plates. We describe the ordering of the liquid crystal by a scalar order parameter Q and use a Landau–de Gennes phenomenological approach to determine its spatial dependence and to calculate the free energy of the system. We determine the force between the plates by differentiating the free energy of the liquid crystal with respect to the interplate distance.

In a standard way the free energy density of liquid crystal is expanded in series of order parameter Q and its derivative $\vec{\nabla}Q$ [23],

$$f=\tfrac{1}{2}a(T-T^*)Q^2+\tfrac{1}{3}bQ^3+\tfrac{1}{4}cQ^4+\tfrac{3}{2}L_1(\vec{\nabla}Q)^2. \qquad (1)$$

We use a single elastic constant approximation (corresponding to $L_2=0$ in [23]) with temperature independent constants $a,\ b,\ c,\ L_1$, and T^*.

The two plates influence the ordering of the liquid crystal by an interfacial coupling. To describe this *surface coupling* we add to the bulk free energy density an extra term, characterized by constants G and Q_s [24],

$$G(Q-Q_s)^2\delta(|\vec{r}-\vec{R}_s|). \qquad (2)$$

This coupling term tends to equalize the order parameter of the liquid crystal at the surface of the plates with the preferred value given by Q_s. The constant G determines how strongly the surface induces its preferred ordering.

The order parameter Q varies only in the direction perpendicular to the plates (x), so that the free energy density can be written as

$$\begin{aligned} f=&\frac{1}{2}\,a\Delta TQ^2+\frac{1}{3}\,bQ^3+\frac{1}{4}\,cQ^4+\frac{3}{2}\,L_1\left(\frac{\partial Q}{\partial x}\right)^2\\ &+G(Q-Q_s)^2[\delta(x)+\delta(x-d)]. \end{aligned} \qquad (3)$$

Here d is the distance between the plates. When minimizing the free energy functional $F=\int f\,dV$ the following differential equation and boundary condition are found:

$$\begin{aligned} &\frac{\partial^2 Q}{\partial x^2}-\frac{a\Delta T}{3L_1}\,Q-\frac{b}{3L_1}\,Q^2-\frac{c}{3L_1}\,Q^3=0,\\ &\left(\frac{\partial Q}{\partial x}\right)_{x=0,\ x=d}=\pm\frac{2G}{3L_1}\,[Q(x=0,\ x=d)-Q_s]. \end{aligned} \qquad (4)$$

Signs $+$ and $-$ correspond to $x=0$ and d, respectively.

We use a one dimensional relaxation method to calculate the order parameter.

III. CALCULATIONS OF THE ORDER PARAMETER

To get a feeling for the magnitude of the effects in a nematic liquid crystal, the values of constants, corresponding to a typical nematic liquid crystal, $a=0.18\times10^6$ J/m^3 K, $b=-2.3\times10^6$ J/m^3, $c=5.02\times10^6$ J/m^3, $L_1=3\times10^{-12}$ J/m, and $T^*=313.5$ K [25] will be used in further calculations. Coupling constants Q_s and G will vary between 0 and 1 and 1×10^{-5} and 5×10^{-4} J/m^2, respectively. These values are in good agreement with the latest experiments [20,21].

Within the Landau–de Gennes approach the temperature of the nematic-isotropic phase transition (T_{NI}) of a bulk nematic liquid crystal depends on constants a,b,c, and supercooling temperature of the isotropic phase T^*, and can be expressed as $T_{\mathrm{NI}}=T^*+2b^2/9ac\simeq T^*+1.3$ K. The superheating temperature of the bulk nematic phase $T^*+b^2/4ac$ is approximately 0.16 K above T_{NI}. The transition temperature of our confined liquid crystal depends on, in addition to constants a,b,c,T^*, the surface coupling constants Q_s and G and on distance between the plates (d).

Stable and metastable phases. The differential equation [Eq. (4)] with its boundary condition has in the vicinity of phase transition temperature two solutions. The solution with $Q\sim0$ describes the isotropic phase with partial surface in-

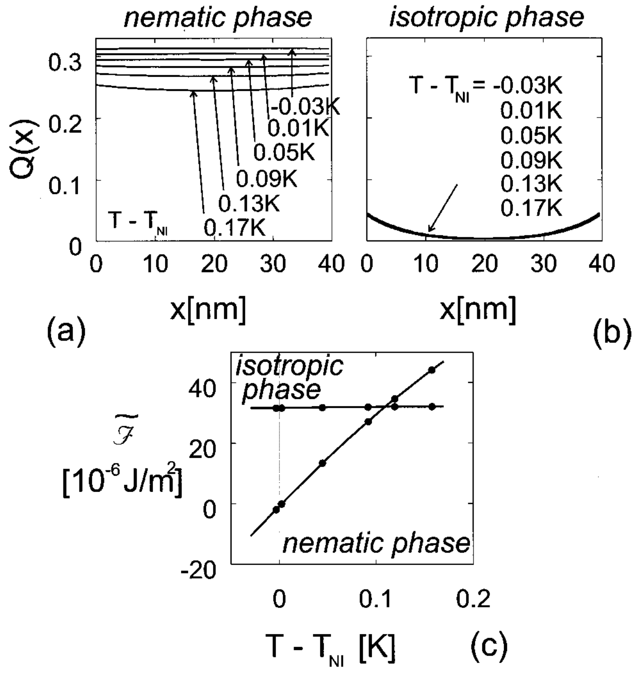

FIG. 2. Spatial dependences of the order parameter Q for a liquid crystal between the two plates. Q_s, G, and d are equal to 0.3, 0.000 11 J/m^2, and 40 nm, respectively. (a) Solutions of the differential equation (4) (for various temperatures) which correspond to the nematic phase. (b) Solutions of the differential equation (4) (for various temperatures) which correspond to the isotropic phase. (c) Free energy of the liquid crystal per unit area ($\tilde{\mathcal{F}}$) for the curves in (a) and (b). Dots correspond to the values of temperature used in (a) and (b).

duced order while the other solution with $Q \sim 0.3$ corresponds to the nematic phase. The solution having lower value of the free energy defines the *stable* phase while the other one corresponds to the *metastable* phase. At a temperature of the phase transition both free energies are equal.

Solutions for the order parameter profile $Q(x)$ at different temperatures are presented in Fig. 2 [(a) nematic phase and (b) isotropic phase]. The distance between the plates d and coupling constants Q_s and G are taken to be 40 nm, 0.3, and 1.1×10^{-4} J/m^2, respectively. To discriminate between stable and metastable solutions, we present in Fig. 2(c) the free energy of the liquid crystal per unit area for all curves shown in Figs. 2(a) and 2(b). One can see that for $T - T_{\mathrm{NI}} < 0.11$ K the free energy of the nematic phase is lower than that of the isotropic phase while for $T - T_{\mathrm{NI}} > 0.11$ K the reverse is true. Both phases have the same value of free energy for $T = T_{\mathrm{NI}} + 0.11$ K, which therefore yields the temperature of phase transition for our particular choice of surface coupling parameters.

Phase diagram. Conditions for the appearance of stable and metastable phases depend on temperature, distance between the plates, and surface coupling parameters Q_s and G. In Fig. 3 the corresponding four dimensional phase space is projected on two dimensional phase diagrams for various values of temperature. The distance between the plates is fixed to 20 nm.

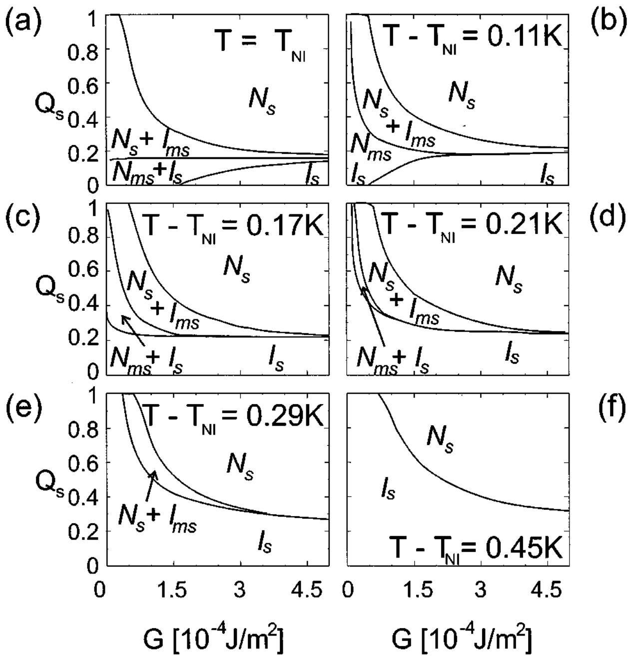

FIG. 3. Phase diagrams in which Q_s, G, and temperature are varied. Distance between the plates (d) is set to 20 nm. Regions of stability and metastability of the nematic and the isotropic phase are marked in the figure. Symbols N_s and I_s denote stable nematic and isotropic phase, respectively, while N_{ms} and I_{ms} denote metastable nematic and isotropic phase, respectively.

One can see that for temperatures that are close to the transition temperature of a bulk liquid crystal T_{NI} [Figs. 3(a)–3(c)], regions with only one possible state, nematic or isotropic, and regions with two possible states, one of them being stable and the other one metastable, can be found in the Q_s-G diagram. As temperature is increasing, the regions with two possible states are becoming narrower. At $T = T_{\mathrm{NI}} + 0.29$ K the region with stable isotropic and metastable nematic phase disappears. Further increase of temperature for another 0.16 K leads to the disappearance of the region with stable nematic and metastable isotropic phase while the line of phase transition, which separates nematic and isotropic phase, still exists. In our two parameter presentation of the phase diagram the critical point, where this line of phase transition ends, appears at values of G far from the interval of our interest. If temperature is raised above $T_{\mathrm{NI}} + 0.64$ K the line of nematic-isotropic phase transition disappears and only the isotropic phase exists for all values of Q_s and G. In a three dimensional (Q_s, G, T) phase diagram the phase transition surface ends with a critical line characterized by $T \sim$ const.

Surface values of the order parameter. To show what values of order parameter correspond to certain points in the phase diagram the order parameter of the liquid crystal at the surface of the plates is presented as a function of temperature for $Q_s = 0.3$ in Figs. 4(a) and 4(b) and $Q_s = 0.1$ in Figs. 4(c) and 4(d). Values of the parameter G vary in the range of 1×10^{-5} J/m$^2 < G < 5 \times 10^{-4}$ J/m^2. Figures 4(a) and 4(c) correspond to the liquid crystal in the nematic phase while Figs. 4(b) and 4(d) correspond to the isotropic phase. Notice that in Fig. 4(b) only two curves are drawn. This happens because liquid crystal cannot exist in the isotropic phase for $Q_s = 0.3$, $G > 1 \times 10^{-4}$ J/m^2, and temperatures that are close to T_{NI}.

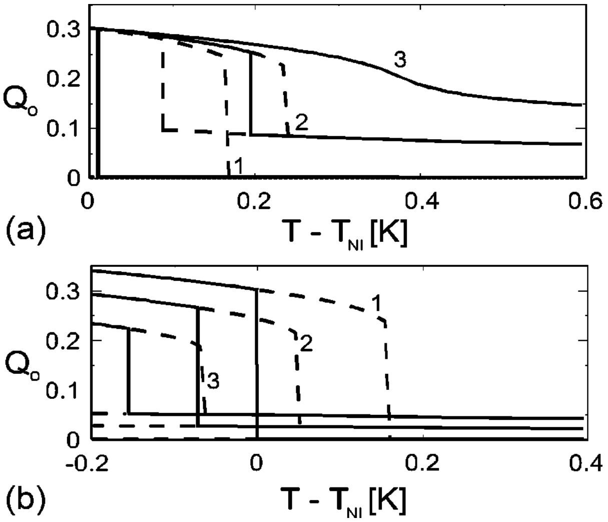

FIG. 4. The order parameter of the liquid crystal at the surface of the plates (Q_0) as a function of temperature for different values of surface coupling constants Q_s and G. In (a) Q_s is equal to 0.3, while in (b) Q_s is equal to 0.1. Labels 1,2,3 correspond to values of $G = 1\times10^{-5}$, 2.1×10^{-4}, and 5.1×10^{-4} J/m^2, respectively. The distance between the plates is equal to 20 nm. Dashed lines correspond to the metastable state.

As can be seen in Fig. 4(a), for some values of $G < 4\times10^{-4}$ J/m^2, the stable surface value of the order parameter is not a continuous function of temperature. The temperature at which the discontinuity appears is the phase transition temperature. For $G = 5\times10^{-4}$ J/m^2, there is no phase transition because this value of G corresponds to a point lying above the surface in the Q_s, T, G phase diagram. It is interesting to note that in the case of $Q_s = 0.3$ [Fig. 4(a)] transition temperature increases with increasing values of G while in the case of $Q_s = 0.1$ [Fig. 4(b)] the transition temperature decreases with increasing values of G. This effect can be explained in the following way. $Q_s = 0.3$ is bigger than the bulk value of Q at T_{NI} thus the surface tends to increase the ordering of the liquid crystal. On the other hand $Q_s = 0.1$ is smaller than the bulk value of Q at T_{NI} and the surface tends to decrease the liquid crystal ordering.

A change of distance between the plates has a similar effect on the ordering of the liquid crystal as a change in coupling constant G. This becomes obvious if we compare Fig. 4(a) with Fig. 5. In Fig. 5 the order parameter value at the surface of the plates is presented as a function of temperature. Different curves correspond to different values of distance between the plates d. We can see that for $d > 15$ nm the order parameter of the liquid crystal is not a continuous function of temperature. As in Fig. 4, the discontinuity of the stable surface value of the order parameter shows the position of the phase transition.

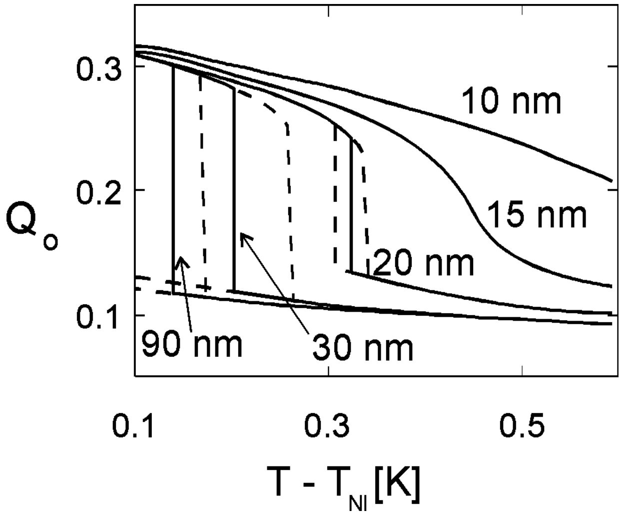

FIG. 5. The order parameter of the liquid crystal at the surface of the plates (Q_0) as a function of temperature for different values of distance between the plates d. Surface coupling constants Q_s and G are equal to 0.4 and 2.1×10^{-4} J/m^2, respectively. Dashed lines correspond to the metastable states.

IV. CALCULATIONS OF FORCE

Force exerted by the liquid crystal on the surfaces of a nematic film is defined in the following way: $\vec{F} = -\Delta A/\Delta\vec{d}$, where ΔA is the amount of work which has to be performed by the liquid crystal in order to move one of the surfaces for $\Delta\vec{d}$. ΔA is related to the free energy of the system $\mathcal{F}$ by the well known thermodynamic relation $\Delta A = \Delta\mathcal{F} + S\Delta T$, where S is the entropy of the system. Taking into account this relation and limiting the description to an isothermal process, we get the following expression for the force:

$$\vec{F} = -\frac{\partial\mathcal{F}}{\partial\vec{d}}. \tag{5}$$

Since the force on the substrates of a thin nematic film is always pointing in the direction perpendicular to the surfaces, arrows in Eq. (5) can be omitted. According to the above convention negative values of force correspond to the attraction and positive to the repulsion of the plates. One finds for the force per unit surface area

$$\tilde{F} = \frac{F}{\mathcal{A}} = -\frac{1}{\mathcal{A}}\frac{\partial\mathcal{F}}{\partial d} = -\frac{\partial}{\partial d}\int_0^d f(x,d)dx + f_{\mathrm{bulk}}, \tag{6}$$

where both the integral range and the free energy density of the confined liquid crystal $f(x,d)$ [Eq. (3)] depend on d and $\mathcal{A}$ denotes the surface area. f_{bulk}, which depends only on temperature, is equal to zero above bulk T_{NI}.

We would like to point out that since the two plates are immersed in a liquid crystal, a change of the distance between the plates does not affect the total volume of liquid crystal.

High temperature and large distance approximation. For temperatures far above nematic-isotropic phase transition ($\Delta T = T - T^* \gg 1$ K) or for large distances between the plates ($d \gg \xi_0 = \sqrt{3L_1/a\Delta T}$) the order parameter becomes much smaller than 1. In this case the quadratic and the cubic term in Eq. (3) become negligible and one can find an analytical

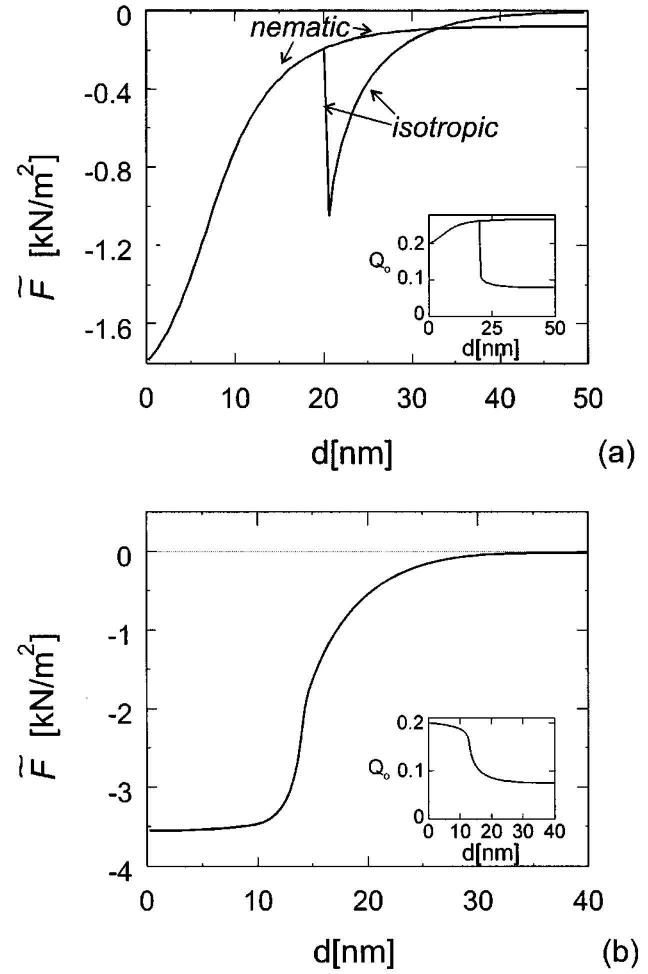

FIG. 6. Force between the plates per unit area ($\widetilde{F}$) and order parameter at interfaces (Q_0), inset, as a function of distance between the plates. Surface coupling constants Q_s and G are 0.2 and 3.6×10^{-4} J/m^2, respectively. Temperature of liquid crystal is $T_{\rm NI}$+0.005 K in (a) and is $T_{\rm NI}$+0.17 K in (b). In (a) the distance where the phase transition occurs is equal to 500 nm.

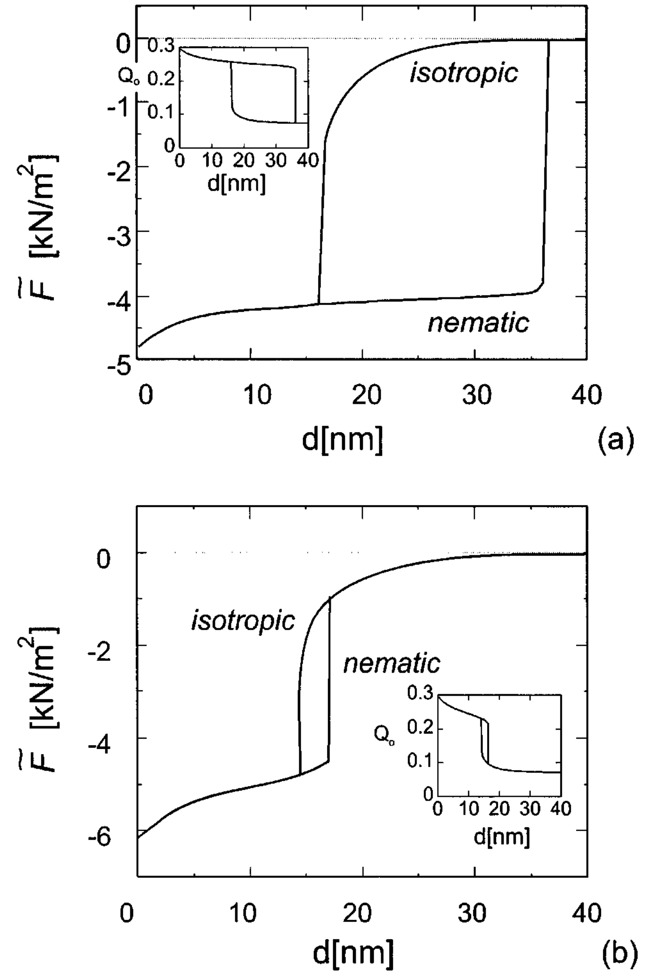

FIG. 7. Force between the plates per unit area ($\widetilde{F}$) and order parameter at interfaces (Q_0), inset, as a function of distance between the plates (d). Surface coupling constants Q_s and G are 0.3 and 2×10^{-4} J/m^2, respectively. Temperature of liquid crystal is $T_{\rm NI}$+0.2 K in (a) and $T_{\rm NI}$+0.26 K in (b). The distance at which the phase occurs in cases (a) and (b) is equal to 19 and 14.8 nm, respectively.

solution of the differential equation (4). Inserting this solution into Eq. (6) one finds the following asymptotic expression for the force per unit area:

$$\widetilde{F}_{\rm asy} = -\frac{8}{3L_1} G^2 Q_s^2 e^{-d\sqrt{(a/3L_1)\Delta T}}. \qquad (7)$$

Spatial dependence of the force. In Figs. 6 and 7 we present typical spatial dependences of the force per surface area ($\widetilde{F}$). As insets to the figures the corresponding dependences of the order parameter of the liquid crystal at the interfaces (Q_0) are shown. We have concentrated our attention on the vicinity of $T_{\rm NI}$ and selected values of surface coupling parameters in a range used in explaining surface induced ordering in Sec. III. Exploration of forces for other values of parameters is left for future studies.

The temperature of liquid crystal in Fig. 6(a) is slightly (0.005 K) above $T_{\rm NI}$ while the surface coupling constants Q_s and G are 0.2 and 3.6×10^{-4} J/m^2, respectively. For $d=20$ nm the set of parameters chosen corresponds to a point in the phase diagram [Fig. 3(a)] in a region of a stable nematic phase, slightly above the region of two possible states, stable nematic and metastable isotropic phase. As we can see in Fig. 6(a) for $d>21$ nm the liquid crystal can be found either in stable nematic or metastable isotropic phase. For $d<21$ nm the metastable isotropic phase of the liquid crystal does not exist and at $d=21$ nm $\widetilde{F}$ is a discontinuous function of d. We would like to point out that the hysteresis loop is not closed. This happens because $T_{\rm NI}+0.005$ K is lower than the highest superheating temperature of the nematic phase in a bulk liquid crystal. Therefore the metastable nematic phase exists also for large values of d yielding a nonzero attractive force. Namely, when the distance between the plates is increased for large d, the order parameter profile close to the plates does not change [see the inset $Q_0(d)$] so one can imagine that some amount of liquid crystal from the region outside is moved in the region between the plates and its order parameter value is increased from zero to Q of a bulk liquid crystal in the nematic phase. Therefore the free energy increases proportionally to d and leads to a long range attraction force which does not depend on d.

For plots in Fig. 6(b) the surface coupling constants Q_s and G have the same values as in the case of Fig. 6(a) but here the temperature $T_{\mathrm{NI}}+0.17$ K is set higher so that for $d=20$ nm the corresponding point in the phase diagram [Fig. 3(c)] is in the region of isotropic phase. The knee of the curve at $d=12$ nm is a consequence of a nonmonotonous decrease of the order parameter profile with respect to d [see the inset $Q_0(d)$ in Fig. 6(b)]. It corresponds to the phase transition from the nematic to the isotropic phase.

In Fig. 7(a) the parameter Q_s is set to 0.3, which is 50% larger than in the case treated in Fig. 6. G and T are selected to be 2×10^{-4} J/m^2 and $T_{\mathrm{NI}}+0.2$ K, respectively. In the phase diagram [Fig. 3(d)] for $d=20$ nm this corresponds to a point lying in the region of two possible states $(N_{\mathrm{ms}}+I_s)$. This helps us understand why for $d>36$ nm only a curve corresponding to the isotropic phase exists while for the interval 16 nm$<d<$36 nm either the nematic or the isotropic phase is present. For $d<16$ nm there is only one curve, corresponding to the nematic phase. The discontinuities of the order parameter at $d=16$ and 36 nm [see inset $Q_0(d)$] manifest in the discontinuities of the $\widetilde{F}$ curves.

To obtain results in Fig. 7(b) the same surface coupling constants, $Q_s=0.3$ and $G=2\times10^{-4}$ J/m^2, are used as in Fig. 7(a). The temperature is raised for 0.06 K and set to $T_{\mathrm{NI}}+0.26$ K. The hysteresis loop of the force has become narrower. The nematic-isotropic phase transition occurs in the region of the hysteresis loop, somewhere between 14 and 16 nm. For d smaller than 14 nm the liquid crystal is in the nematic phase while for $d>16$ nm only the isotropic phase exists.

Focusing on the curves corresponding to the isotropic phase in Figs. 6 and 7 one can see that in the limit of large d the absolute value of the force is an exponentially decreasing function of d. We have found out that the correlation length is equal to 6 nm and is independent of the surface coupling parameters. These results are in accordance with the large distance approximation [Eq. (7)], which determines exponential decrease of force with respect to d with correlation length inversely proportional to the square root of ΔT and approximately equal to 6 nm for temperatures close to T_{NI}.

Temperature dependence of the force. In Fig. 8(a) we present the temperature dependence of the force in the isotropic phase for several values of Q_s. Surface coupling $G=2\times10^{-4}$ J/m^2 has the same value as the one in Fig. 7. Distance between the plates is 10 nm. The graph is plotted in the logarithmic scale. In Fig. 8(b) a part of Fig. 8(a), plotted in an ordinary scale, is presented in order to show a detailed behavior of the curve. In Fig. 8(b) one can see that force corresponding to $Q_s=0.1$ is a monotonous function of temperature, indicating that for this value of the surface coupling constant the liquid crystal is in the isotropic phase for all the temperatures above T_{NI}. Even if d is increased to 20 nm, $Q_s=0.1$ still induces isotropic phase of the liquid crystal for all temperatures above T_{NI}, which can be seen in the phase diagram (Fig. 3), where the line $Q_s=0.1$ lies beneath the line of phase transition for all values of T. For $Q_s\geqslant0.2$ the behavior of the force is more heterogeneous. For temperatures close to T_{NI}, where values of order parameter are close to those of a bulk nematic liquid crystal, the force is an increasing function of temperature. For $Q_s=0.2$ at a certain temperature a phase transition from the nematic to the isotropic phase occurs. It is accompanied by the jump in the value of the force. For $Q_s=0.3$, 0.4 the change from the nematiclike to the isotropiclike behavior is continuous, but relatively sharp, occurring within the temperature range of a few tenths of a degree. In this range the absolute value of force reaches its maximum value. For temperatures well above the phase transition ($T-T_{\mathrm{NI}}\gg1$ K) the liquid crystal is in the isotropic phase. One can see in Fig. 8(a) that force is an approximately exponentially decreasing function of temperature. Curves corresponding to different values of Q_s only differ by a constant scaling factor, proportional to Q_s^2. This is in accordance with the high temperature expansion formula [Eq. (7)], which describes the force as a product of a scaling factor proportional to the squares of surface coupling constants and a surface coupling independent exponential function of a square root of $T-T^*$.

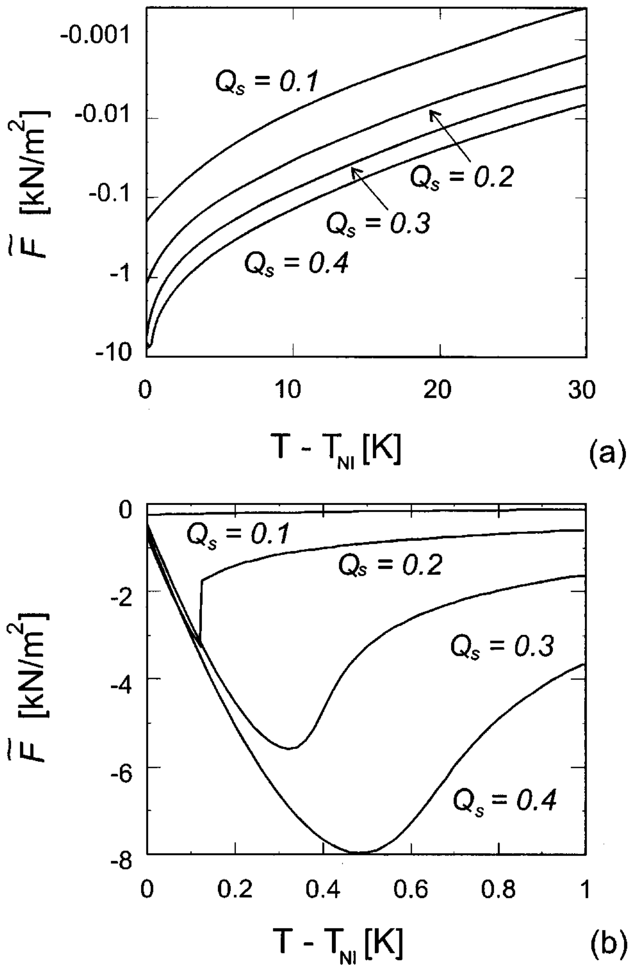

FIG. 8. (a) Force between the plates per unit area ($\widetilde{F}$) as a function of temperature for various values of Q_s. Graph is plotted in the logarithmic scale. Surface coupling constant G and distance between the plates d are 2×10^{-4} J/m^2 and 10 nm, respectively. (b) A part of (a) with temperature scale expanded in order to show a detailed structure of the curve.

V. CONCLUSION

We investigate ordering and forces in a liquid crystal at temperatures above the nematic-isotropic phase transition of a bulk material confined by two parallel plates. We limit our discussion to cases where the typical distance between the plates is much larger than one molecular layer so that we leave the properties of the surface layer for future considerations. Using Landau–de Gennes continuum theory we first calculate the phase diagram to localize regions of the stability and metastability of nematic and partially ordered isotropic phases. The main goal of our study is to show how the force between the parallel plates depends on the distance between the plates, temperature of liquid crystal, and on surface parameters. In the range of our interest the force often can have two different values, which manifests in a hysteresis loop in a force versus distance diagram, and jumps in the dependences on distance. The size of the hysteresis loop decreases with temperature and at a certain temperature it disappears. At large distances between the plates, where the liquid crystal can be found in the isotropic phase only, the absolute value of force approaches zero exponentially, with a correlation length independent of surface coupling parameters. Similarly, when observing the temperature dependence of the force at higher temperatures, one finds out that curves corresponding to different values of Q_s exhibit the same behavior.

A comparison of our predictions with the results of the preliminary experiments performed by Muševič, Slak, and Blinc [8] show that the observed behavior of forces can be explained within the Landau–de Gennes formalism.

ACKNOWLEDGMENTS

Financial support from the Ministry of Science and Technology of Slovenia (Grant No. J1-7067/790-96) and the European Community (Grant No. EC ICIT-CT96-0744) is gratefully acknowledged.

---

[1] R. G. Horn, J. N. Israelachvili, and E. Perez, J. Phys. (France) **42**, 39 (1981).
[2] P. Sheng, Phys. Rev. A **26**, 1610 (1982).
[3] J. C. Tarczon and K. Miyano, J. Chem. Phys. **73**, 1994 (1980).
[4] D. W. Allender, G. L. Henderson, and D. L. Johnson, Phys. Rev. A **24**, 1086 (1981).
[5] A. Poniewierski and T. J. Sluckin, Liq. Cryst. **2**, 281 (1987).
[6] A. Adjari, L. Peliti, and J. Prost, Phys. Rev. Lett. **66**, 1481 (1991); B. D. Swanson and L. B. Sorensen, Phys. Rev. Lett. **75**, 3293 (1995).
[7] L. Moreau, P. Richetti, and P. Barois, Phys. Rev. Lett. **26**, 3556 (1994); P. Richetti, L. Moreau, P. Barois, and P. Kekichef, Phys. Rev. E **54**, 1749 (1996).
[8] I. Muševič, G. Slak, and R. Blinc (unpublished).
[9] N. Vrbančič, M. Vilfan, R. Blinc, J. Dolinšek, G. P. Crawford, and J. W. Doane, J. Chem. Phys. **103**, 8726 (1993).
[10] J. Dolinšek, O. Jarh, M. Vilfan, S. Žumer, R. Blinc, J. W. Doane, and G. P. Crawford, J. Chem. Phys. **95**, 2154 (1991).
[11] G. P. Crawford, D. K. Yang, S. Žumer, D. Finotello, and J. W. Doane, Phys. Rev. Lett. **66**, 723 (1991).
[12] B. M. Ocko, Phys. Rev. Lett. **64**, 2160 (1990).
[13] G. S. Iannacchione, J. T. Mang, S. Kumar, and D. Finotello, Phys. Rev. Lett. **73**, 2708 (1994).
[14] B. Jérôme, Rep. Prog. Phys. **54**, 391 (1991).
[15] T. J. Sluckin and A. Poniewierski, Phys. Rev. Lett. **55**, 2907 (1985).
[16] H. G. Galabova, D. W. Allender, and J. Chen, Phys. Rev. E **55**, 1627 (1997).
[17] Y. L'vov, R. M. Hornreich, and D. W. Allender, Phys. Rev. E **48**, 1115 (1993).
[18] T. Moses and Y. R. Shen, Phys. Rev. Lett. **67**, 2033 (1991).
[19] W. Chen, L. J. Martinez-Miranda, H. Hsiung, and Y. R. Shen, Phys. Rev. Lett. **62**, 1860 (1989); Mol. Cryst. Liq. Cryst. **179**, 419 (1990).
[20] G. P. Crawford, R. Ondris-Crawford, S. Žumer, and J. W. Doane, Phys. Rev. Lett. **70**, 1838 (1993).
[21] G. P. Crawford, R. J. Ondris-Crawford, J. W. Doane, and S. Žumer, Phys. Rev. E **53**, 3647 (1996).
[22] Y. K. Fung, A. Borštnik, S. Žumer, D.-K. Yang, and J. W. Doane, Phys. Rev. E **55**, 1637 (1997).
[23] E. B. Priestely, P. J. Wojtowitz, and P. Sheng, *Introduction to Liquid Crystals* (Plenum, New York, 1974), p. 143.
[24] M. Nobili and G. Durand, Phys. Rev. A **46**, R6174 (1992).
[25] H. J. Coles, Mol. Cryst. Liq. Cryst. Lett. **49**, 67 (1978).