Smectic-A surface order in a nematic-substrate system

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Nematic liquid crystals in contact with a flat substrate are studied by means of the Landau–de Gennes formalism. It is assumed that the substrate provides homogeneous boundary conditions and that the nematic phase undergoes a first-order transition to the smectic-A phase in the bulk. Above the bulk transition temperature, a smectic-A film with layers perpendicular to the substrate can form if the surface field is sufficiently strong. This surface phase transition is found to be continuous in the mean-field approximation. Apart from the symmetry-breaking transition, an ordinary prewetting transition may occur. The effect of smectic layer fluctuations on the stability of the smectic film is discussed. It is suggested that the continuous surface transition can be a Kosterlitz-Thouless transition, where the defects are edge dislocations.

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I. INTRODUCTION

The ordering of liquid crystals (LC's) by surfaces still attracts a great deal of experimental and theoretical attention [1]. This is because of the practical importance of LC devices and a potential wealth of surface phenomena that can occur at LC interfaces. Apart from wetting transitions, observed also in simple fluids, there exists a possibility of surface transitions in which the LC close to the surface has different symmetry than in the bulk [2].

So far the most studied surface effects have concerned nematic order in nematogen-substrate systems [1,3]. Relatively less work has been devoted to the onset of smectic order near a limiting surface. It is known that smectic order can appear at the free surface of the isotropic phase or at the interface between the isotropic phase and a solid substrate, for some systems exhibiting a direct isotropic–smectic-A transition [4]. Theoretical models [5–7] confirm to some extent experimental observations. In both cases the onset of smectic order is compatible with the geometry of the system, i.e., smectic layers are parallel to the limiting surface.

In this paper we consider another possibility, when LC molecules prefer to lie on the substrate. Then smectic-A layers have to be perpendicular to it. We assume that the system undergoes a first-order nematic–smectic-A transition and that the substrate enhances the surface nematic order. It is interesting to see whether the increased nematic order at the surface can result in smectic-A surface ordering above the bulk nematic–smectic-A transition temperature. As far as we know this phenomenon has not yet been observed in real systems. However, very recent experimental studies of a bulk LC in an external electric field [8] show that it is possible to induce the nematic–smectic-A transition by changing the intensity of the field. The field couples directly to the nematic order parameter and the influence on the smectic order is indirect, through the coupling of the nematic and smectic order parameters [9]. We expect that a similar mechanism could be responsible for formation of smectic-A layers in the direction perpendicular to the substrate.

In the next section we define the model and present our results. In the last section we discuss the effect of fluctuations on the stability of the surface smectic-A phase and also the relation of the surface phase transition to the Kosterlitz-Thouless transition. Some details of the calculations are presented in the Appendix.

II. THEORY AND RESULTS

We study the problem outlined in the Introduction using a Landau–de Gennes formalism. It is assumed that the free-energy density of the bulk system depends on the nematic order parameter $\mathbf{Q}$, which is a traceless symmetric tensor, and the smectic order parameter ψ as follows [10]:

$$F = A\psi^2 + B\psi^4 + C\,\mathrm{Tr}\mathbf{Q}^2 + D\,\mathrm{Tr}\mathbf{Q}^3 + E(\mathrm{Tr}\mathbf{Q}^2)^2 + \psi^2[F\,\mathrm{Tr}\mathbf{Q}^2 + G(\hat{\mathbf{k}}\cdot\mathbf{Q}\cdot\hat{\mathbf{k}}) + H(\hat{\mathbf{k}}\cdot\mathbf{Q}\cdot\hat{\mathbf{k}})^2 + L(\mathbf{Q}\cdot\hat{\mathbf{k}})^2] , \quad (1)$$

where $\hat{\mathbf{k}}$ is normal to the smectic layers. The nematic and smectic-A phases are uniaxial and there is only one independent component of $\mathbf{Q}$, which measures the degree of orientational order with respect to the nematic direction $\hat{\mathbf{n}}$. Moreover, in the smectic-A phase, $\hat{\mathbf{k}} \| \hat{\mathbf{n}}$. It is convenient to rescale the order parameters and the free energy to reduce the number of independent coupling constants. After rescaling we have

$$F = (t+1)\eta^2 - 2\eta^3 + \eta^4 + (a_0 + a_1\eta + a_2\eta^2)\psi^2 + \psi^4 , \quad (2)$$

where η is the nematic order parameter, t measures the temperature, and for simplicity we have used the same symbols for the rescaled free-energy density and the smectic order parameter. All quantities appearing in Eq. (2) are dimensionless. As the smectic order cannot appear without the nematic order, a_0 must be positive. When the temperature is lowered the nematic order parameter increases, and this should favor smectic ordering;

thus we choose a negative a_1. Finally, a_2 can be either positive or negative with the restriction $a_2 > -2$, which is required by the stability condition for F. The nematic–smectic-A transition depends on a particular choice of a_0, a_1, and a_2. Here we study the case in which the system undergoes a first-order nematic-isotropic transition at $t_{NI}=0$ and then at $t_{NA}<0$, a first-order transition to the smectic-A phase. Other choices of the coupling constants can lead to a continuous nematic–smectic-A transition or to a direct first-order isotropic–smectic-A transition. We note that the same form of F was also used in Ref. [8] to describe the electrically induced isotropic-nematic–smectic-A transitions.

We further assume that the substrate provides homogeneous boundary conditions [3], which means that the nematic director favors some particular direction in the plane of the substrate. We choose the x axis along that direction and the z axis along the normal to the substrate. In the first approximation it seems reasonable to neglect the biaxiality of the system and assume that $Q_{xx}=\eta$, $Q_{yy}=Q_{zz}=-\eta/2$. However, in more detailed studies one should consider a third-order parameter $P=Q_{yy}-Q_{zz}$, which, in general, does not vanish in the surface layer. The surface free energy per unit area $\mathcal{F}$ is a functional of $\eta(z)$ and $\psi(z)$, with the boundary conditions $\eta(\infty)=\eta_N(t)$ and $\psi(\infty)=0$, where $\eta_N(t)$ is the bulk nematic order parameter at temperature $t_{NA}<t<t_{NI}$. $\mathcal{F}$ is given by

$$\mathcal{F}[\eta,\psi]=\frac{1}{\sqrt{L_1}}\int_0^\infty dz\left[\frac{1}{2}L_1\left[\frac{d\eta}{dz}\right]^2+\frac{1}{2}L_2\left[\frac{d\psi}{dz}\right]^2+F(\eta,\psi)-F_b\right]-h\eta(z=0)\ , \tag{3}$$

where L_1 and L_2 are the elastic constants, F_b corresponds to the bulk nematic at temperature t, h is the dimensionless surface field, and $\eta(z=0)$ is the surface nematic order parameter. It is assumed that $h>0$, i.e., the substrate enhances the nematic order parameter. There is no direct coupling between the substrate and $\psi(z=0)$ because smectic layers can form only perpendicular to the substrate, as a result of the homogeneous boundary conditions. However, such a term would be present in the case of the nematic director normal to the substrate. In general, one usually considers the surface contribution to $\mathcal{F}$ up to the second order in the order parameters, and then both $\eta(z=0)^2$ and $\psi(z=0)^2$ should appear. In this work we take into account only linear surface terms. Consequences of the inclusion of the second-order surface terms should be studied separately.

Minimization of $\mathcal{F}$ leads to the Euler-Lagrange equations

$$L_1\frac{d^2\eta}{dz^2}=\frac{\partial F}{\partial\eta}=2(t+1)\eta-6\eta^2+4\eta^3+(a_1+2a_2\eta)\psi^2\ , \tag{4a}$$

$$L_2\frac{d^2\psi}{dz^2}=\frac{\partial F}{\partial\psi}=2\psi(a_0+a_1\eta+a_2\eta^2+2\psi^2) \tag{4b}$$

together with the boundary conditions at $z=0$,

$$L_1\frac{d\eta}{dz}=-h\sqrt{L_1}\ , \tag{5a}$$

$$L_2\frac{d\psi}{dz}=0\ . \tag{5b}$$

Equations (4) and (5) always have a nematic solution with $\psi(z)=0$, which does not necessarily correspond to the global minimum of $\mathcal{F}$. If the surface field is sufficiently strong we may expect that another solution with $\psi(z)\neq 0$ appears at some t_s^* between t_{NI} and t_{NA}, i.e., a symmetry-breaking surface transition takes place and the translational symmetry of the system in the (x,y) plane is broken. In the case of a continuous surface transition to the state with $\psi(z)\neq 0$, t_s^* is equal to the mean-field transition temperature t_s. If the surface transition is first order, t_s^* corresponds to the stability limit of the solution with $\psi(z)=0$. In any case it is useful to first determine this stability limit. To do this, we seek the solution of the linearized Euler-Lagrange equations

$$L_1\frac{d^2\eta}{dz^2}=2(t+1)\eta-6\eta^2+4\eta^3\ , \tag{6a}$$

$$L_2\frac{d^2\psi}{dz^2}=2\psi(a_0+a_1\eta+a_2\eta^2)\ , \tag{6b}$$

satisfying boundary conditions (5). Equation (6a) can be solved analytically, but here we need only the first integral, which is

$$\frac{d\eta}{dz}=-\left[\frac{2\Delta F_N(\eta)}{L_1}\right]^{1/2}\ , \tag{7}$$

where $\Delta F_N(\eta)=F_N(\eta)-F_b$ and $F_N(\eta)=(t+1)\eta^2-2\eta^3+\eta^4$. Using (6a) and (7) we eliminate z from (6b) to get

$$2\Delta F_N(\eta)\psi''(\eta)+\Delta F_N'(\eta)\psi'(\eta)-2\frac{L_1}{L_2}(a_0+a_1\eta+a_2\eta^2)\psi(\eta)=0\ , \tag{8}$$

with the boundary conditions $\psi'[\eta(z=0)]=0$ and $\psi(\eta_N)=0$, where $\eta(z=0)$ is determined from (5a) and (7), and the nematic order parameter of the bulk system is $\eta_N(t)=(3+\sqrt{1-8t})/4$. From (8) we find that $\psi(\eta)\sim(\eta-\eta_N)^\beta$ for $\eta\to\eta_N$, where $\beta^2=2(L_1/L_2)(a_0+a_1\eta_N+a_2\eta_N^2)/F_N''(\eta_N)$ and we choose $\beta>0$. Hence, the solution of (8) can be expressed as $\psi(\eta)=(\eta-\eta_N)^\beta f(\eta)$, where $f(\eta)$ is a regular function at $\eta=\eta_N$. In fact, to determine the stability limit it is sufficient to find the function $r(\eta)=(\eta-\eta_N)\psi'(\eta)/\psi(\eta)$, which satisfies a Riccati equation,

$$(\eta-\eta_N)r'=-r^2+\left[1-\frac{(\eta-\eta_N)\Delta F_N'}{2\Delta F_N}\right]r+\frac{L_1}{L_2}\frac{(\eta-\eta_N)^2}{\Delta F_N}(a_0+a_1\eta+a_2\eta^2)\ . \tag{9}$$

Equation (9) can be easily solved numerically as an initial value problem with $r(\eta_N)=\beta$. We proceed as follows:

for a given temperature t the solution $r(\eta)$ of (9) is propagated until $r=0$ is obtained at some value of $\eta(z=0)$. Then the value of the surface field $h=h_s^*(t)$ at which the solution of the Euler-Lagrange equations with $\psi(z)=0$ becomes unstable is found from Eqs. (5a) and (7).

As the number of independent parameters is quite large, we fix the values of a_0,a_1,a_2 at $a_0=10.4833$, $a_1=-5.8718$, $a_2=0$, for which the nematic–smectic-A transition is first order at a temperature $t_{NA}=-2$. The order parameters at the transition are $\eta_N=1.7808$, $\eta_A=1.9$, $\psi_A=0.5801$. The surface phase diagram is studied in the (t,h) plane for a few values of the ratio L_2/L_1. In Fig. 1 we show $h=h_s^*(t)$ for $L_2/L_1=0,0.01,0.1,1,10$. Below each line the solution of Eqs. (4) with $\psi(z)=0$ is stable, i.e., it corresponds at least to a local minimum of $\mathcal{F}$. Above each line the surface layer exhibits the smectic-A order with smectic layers perpendicular to the substrate. In the plot t varies from t_{NA} to $t=-1$. The latter is the temperature at which the isotropic phase becomes unstable with respect to the onset of the nematic phase in a bulk system. In fact, the lines $h_s^*(t)$ extend up to t_{NI} for sufficiently high surface fields. It is instructive to compare the values of the surface field at which the smectic order appears close to the surface with some characteristic bulk field. To do this we add to F, given by Eq. (2), the term $-H\eta$, where H is a bulk field. By changing H at fixed a_0,a_1,a_2 we can change the order of the nematic–smectic-A transition. For our choice of parameters the tricritical point is at $\eta_{tcr}=1.7854$, $t_{tcr}=-0.7938$, $H_{tcr}=4.3751$.

The case $L_2/L_1=0$ has to be considered separately. Then Eq. (4b) becomes simply

$$\frac{\partial F}{\partial \psi}=2\psi(a_0+a_1\eta+a_2\eta^2+2\psi^2)=0\ , \tag{10}$$

which has either the solution $\psi=0$ or $\psi^2=-(a_0+a_1\eta+a_2\eta^2)/2$, depending on the value of η. Substitution of $\psi(\eta)$ into (4a) allows us to integrate the differential equation for $\eta(z)$ in the same manner as in one-order parameter problems. However, the profile $\psi(z)$ has a discontinuous derivative at η^*, for which $a_0+a_1\eta^*+a_2(\eta^*)^2=0$. Even though the case $L_2/L_1=0$ is, in some sense, singular, we can see that the instability lines in Fig. 1 do tend to the line with $L_2/L_1=0$ when the value of L_2/L_1 decreases.

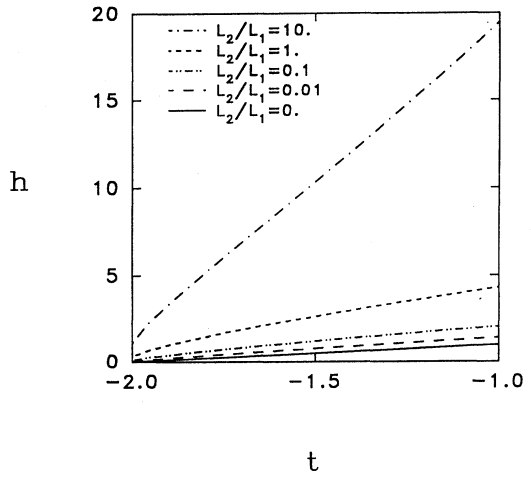

FIG. 1. Instability lines for a few values of L_2/L_1 in the (t,h) plane. To the left of each line there exists a smectic-A surface order with smectic layers perpendicular to the substrate.

To study surface transitions one usually introduces suitable surface order parameters. In our case they are adsorptions corresponding to η and ψ,

$$\Gamma_\eta=\int_0^\infty(\eta(z)-\eta_N)dz \tag{11a}$$

and

$$\Gamma_\psi=\int_0^\infty\psi(z)dz\ . \tag{11b}$$

At the symmetry-breaking surface transition Γ_ψ changes from zero above the transition temperature t_s to a nonzero value below t_s. It is interesting to study the relation between this surface transition and the prewetting transition, at which both Γ_η and Γ_ψ change discontinuously. To do this we have to solve the Euler-Lagrange equations. We have done that using a relaxation method for solving two-point boundary value problems [11]. Two boundary conditions are at $z=0$ [Eqs. (5a) and (5b)] and the other two are given at $z=\infty$. In practice the range of z is limited to $0\le z\le z_{max}$. If z_{max} is sufficiently large we can solve the Euler-Lagrange equations in the asymptotic limit $z\to\infty$, i.e.,

$$\xi_1^2\frac{d^2\eta}{dz^2}\approx\eta-\eta_N\ , \tag{12a}$$

$$\xi_2^2\frac{d^2\psi}{dz^2}\approx\psi\ , \tag{12b}$$

where $\xi_1^2=L_1/\partial^2F/\partial\eta^2\ (\eta_N,\psi=0)$ and $\xi_2^2=L_2/\partial^2F/\partial\psi^2\ (\eta_N,\psi=0)$. In this limit $\eta(z)-\eta_N$ and $\psi(z)$ decay exponentially with characteristic lengths ξ_1 and ξ_2, respectively, and the boundary conditions at $z=z_{max}$ can be expressed as follows [12]:

$$\xi_1\frac{d\eta}{dz}(z_{max})+\eta(z_{max})-\eta_N=0\ , \tag{13a}$$

$$\xi_2\frac{d\psi}{dz}(z_{max})+\psi(z_{max})=0\ . \tag{13b}$$

In the relaxation method a good initial approximation to the solution of the differential equations is necessary. In our case, the solution of Eqs. (4a) and (4b) with $L_2=0$ was always a good approximation, and the profiles $\eta(z)$ and $\psi(z)$ converged to the true solution after a few iterations.

The resulting phase diagrams in the (t,h) plane are shown in Figs. 2 and 3. First we have studied the case $L_2/L_1=0$ [Fig. 2(a)]. There are five possible behaviors of the system when the temperature is lowered from t_{NI} to t_{NA} at constant surface field.

(i) For small h the system has always the nematic symmetry down to t_{NA}.

(ii) The system undergoes a continuous symmetry-breaking surface transition at $t=t_s(h)$. However, the

thickness of the smectic-A film remains finite when t approaches t_{NA}^{+}. This corresponds to a partial wetting situation.

(iii) Apart from the symmetry-breaking transition there is an ordinary prewetting transition at $t=t_p(h)<t_s(h)$, at which both Γ_η and Γ_ψ jump to higher values. $\Gamma_\eta, \Gamma_\psi \to \infty$ when $t \to t_{NA}^{+}$ and the wetting by the smectic-A is complete.

(iv) If the surface field is higher than h_p^{cr}, at which the difference between the thin and thick films disappears, there is only a continuous transition at $t=t_s(h)$ and $\Gamma_\eta, \Gamma_\psi \to \infty$ when $t \to t_{NA}^{+}$.

(v) For rather high values of h the smectic-A surface order exists in the whole range $t_{NA} \le t \le t_{NI}$.

The phase diagram for $L_2/L_1=0.01$ is shown in Fig. 2(b). Again there are five possible behaviors of the system, depending on the value of h. However, they differ in some respects from those in the previous case. The line of the continuous surface transition terminates at a critical end point, which lies on the prewetting line instead of the nematic–smectic-A transition line $t=t_{NA}$. Thus, the prewetting line is divided into two parts. The lower part corresponds to the thin film–thick film transition with a symmetry change, i.e., Γ_ψ jumps from zero to a nonzero value. The upper part of the prewetting line corresponds to an ordinary thin film–thick film transition, in which the symmetry of the film does not change.

Figures 3(a) and 3(b) show the phase diagrams for $L_2/L_1=0.1$ and $L_2/L_1=1$, respectively. They differ from each other only quantitatively. At some value of L_2/L_1 between 0.01 and 0.1 the critical end point and the surface critical point, terminating the prewetting line, merge, and for higher values of L_2/L_1 there is a tricritical point on the line of the surface transition, shown in Figs. 3(a) and 3(b). Then there are only four possible behaviors of the system when t is lowered from t_{NI} to t_{NA}. Different from the previous cases, the thin film–thick film transition is simultaneously a symmetry-breaking transition.

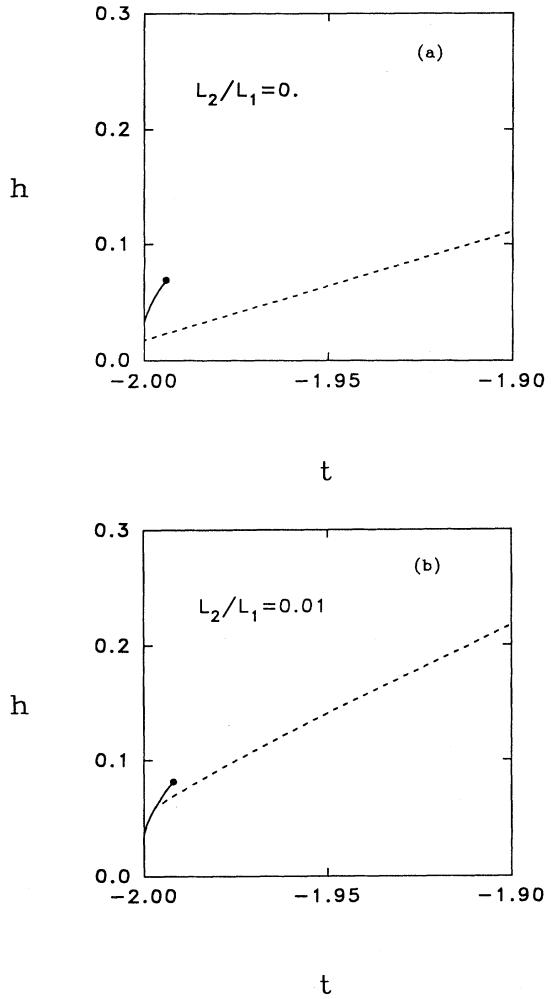

FIG. 2. Surface phase diagram in the (t,h) plane for (a) $L_2/L_1=0$ and (b) $L_2/L_1=0.01$. The dashed line corresponds to the continuous surface transition (see text), and the solid line to the prewetting transition, ending at a surface critical point.

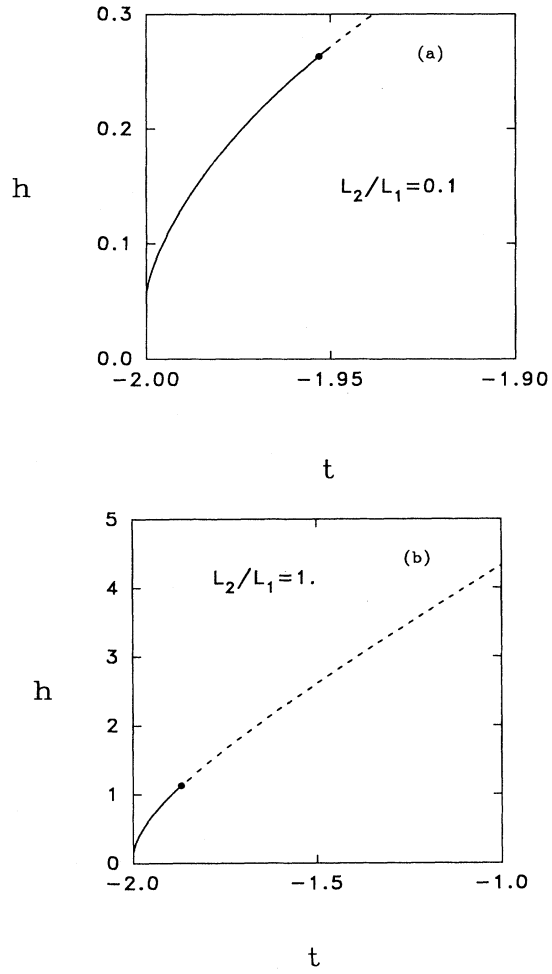

FIG. 3. Surface phase diagram in the (t,h) for (a) $L_2/L_1=0.1$ and (b) $L_2/L_1=1$. The meaning of the lines is the same as in Fig. 2. Note the presence of a tricritical point instead of the surface critical point and the critical end point.

III. DISCUSSION

We have studied a nematogen in contact with a solid substrate using a Landau–de Gennes description of the system. The temperature range of interest has been between the temperatures of the nematic-isotropic and nematic–smectic-A transitions. We have assumed that the substrate provides homogeneous boundary conditions and shown that this may result in smectic-A ordering close to the surface of the substrate. However, our considerations have been of the mean-field type. It is well known that in three dimensions smectic order does not exist in the thermodynamic limit because of the Landau-Peierls instability [9]. This means that fluctuations of smectic layers destroy the smectic order, i.e., $\langle u^2(\mathbf{r})\rangle \sim \ln L$, when the linear size of the system $L \to \infty$. This asymptotic behavior results from the form of the elastic free energy, which gives

$$\langle u^2(\mathbf{r})\rangle \sim k_B T \int d^d\mathbf{q}(Bq_\parallel^2 + Kq_\perp^4)^{-1} , \tag{14}$$

where B and K are the elastic constants of the compression and undulation modes, respectively, and $q_{\min} = 2\pi/L$. For $d=2$ the divergence of $\langle u^2(\mathbf{r})\rangle$ is larger than in $d=3$, as $\langle u^2(\mathbf{r})\rangle \sim L$ for $L \to \infty$. If a bulk field H coupling to the director is present, then a term proportional to $H^2 q_\perp^2$ has to be added in (14). This changes the asymptotic behavior for $L \to \infty$ as follows: $\langle u^2(\mathbf{r})\rangle \sim$ const for $d=3$ and $\langle u^2(\mathbf{r})\rangle \sim \ln L$ for $d=2$. The correlation function $G(\mathbf{r}) = \langle \exp\{iq_0[u(\mathbf{r}) - u(0)]\}\rangle$, where $2\pi/q_0$ is the smectic period, decays algebraically in $d=3$ if $H=0$ [13], which means quasi-long-range translational order. In $d=2$ the decay of the correlation function is also algebraic, provided that $H \neq 0$. The exponent characterizing that algebraic decay is proportional to the coherence length $\xi_H \sim K^{1/2}/H$; thus it diverges when $H \to 0$.

In our surface problem, as long as the smectic-A film is not macroscopically thick it should be treated as a quasi-two-dimensional system. Then the long wavelength contribution to $\langle u^2(\mathbf{r})\rangle$ is dominated by the modes with $\mathbf{q}$ lying in the plane of the substrate. This means that in the absence of an ordering field in that plane, the surface smectic order should be destroyed by the fluctuation effect. If a surface ordering field is present we expect a quasi-long-range smectic order close to the substrate, as for a three-dimensional bulk system. However, the exponent characterizing the algebraic decay of the correlation function depends on the strength of the surface field.

It is worth noting that the surface phase transitions above the nematic–smectic-A transition temperature, studied in this paper, resemble the surface phase transitions above the nematic-isotropic transition temperature, studied in Ref. [2] and more recently in Refs. [12,14], although the latter case corresponds to planar boundary conditions. Indeed, the phase diagrams shown in this paper and in Ref. [12] are very similar. This probably results from similarities between the free energies, which in both cases are functions of two order parameters with similar couplings. However, it is argued in Ref. [2] that the continuous isotropic-nematic surface transition, predicted by a mean-field calculation, is expected to be a Kosterlitz-Thouless defect-unbinding transition [15,16]. These defects are disclination lines in the director field. The low-temperature phase does not have true long-range orientational order but only quasi-long-range order. As we have argued, the smectic-A film should exhibit quasi-long-range translational order. Therefore, it is natural to ask whether the surface symmetry-breaking transition can be a defect-unbinding transition. To check this possibility we consider an isolated edge dislocation in the smectic-A phase [9]. Such a dislocation is made of a $+\frac{1}{2}$, $-\frac{1}{2}$ disclination pair and its strength is measured by an integer n, related to the Burgers vector b and the average layer thickness a_0 by $b = na_0$. In $d=3$ the edge dislocation forms a line and its energy per unit length, or the line tension τ, depends on b, but remains finite when the size of the system $L \to \infty$. This is, however, true only if there is no external field coupling to the director. In the Appendix we analyze the edge dislocation in the presence of an external field that fixes the orientation of smectic-A layers far from the dislocation. In that case τ does not have a thermodynamic limit but diverges as $\ln L$. This asymptotic behavior is the same as, for example, in the case of a disclination line in the nematic phase. The logarithmic divergence of τ with L suggests that in $d=2$ a continuous nematic–smectic-A transition in the presence of an external field is a defect-unbinding transition and the defects are edge dislocations.

Finally, we think that it could be interesting to study a LC-substrate system in the case where there is no stable bulk nematic phase and a direct isotropic–smectic-A transition occurs. It has been shown by Lelidis and Durand [8] that in such a case the electric field can induce a stable bulk nematic phase called a "nonspontaneous" nematic phase. We expect that a similar phenomenon may occur in the surface layer. If the substrate provides homogeneous boundary conditions, then above the isotropic–smectic-A transition temperature it could, in principle, be possible to observe two surface phase transitions: the isotropic-nematic transition and the nematic–smectic-A transition, apart from the prewetting transition. We intend to study this problem in the future.

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APPENDIX

We generalize the discussion of the edge dislocation presented in [9] to the case of an external field H parallel to the z axis. The dislocation line is at the origin along the z axis and the displacement u, along the z direction, depends only on x and z. The free-energy density is given by

$$F = \tfrac{1}{2}B\left\{\left[\frac{\partial u}{\partial z}\right]^2 + \lambda^2\xi_H^{-2}\left[\frac{\partial u}{\partial x}\right]^2 + \lambda^2\left[\frac{\partial^2 u}{\partial x^2}\right]^2\right\}, \tag{A1}$$

where $\lambda^2 = K/B$. One introduces a new field $\mathbf{m} = \nabla u$, which is single-valued and then expresses the Euler-

Lagrange equation in terms of $\mathbf{m}$,

$$-\frac{\partial m_z}{\partial z}+\lambda^2\xi_H^{-2}\frac{\partial m_x}{\partial x}+\lambda^2\frac{\partial^3 m_x}{\partial x^3}=0\ . \tag{A2}$$

The second equation

$$\nabla\times\mathbf{m}=\mathbf{J} \tag{A3}$$

relates $\mathbf{m}$ to the dislocation current $\mathbf{J}$, where $J_x=J_z=0$ and $J_y=-a_0 n\delta(x)\delta(y)$. From (A2) and (A3) one finds the Fourier transform of m_x,

$$m_x(\mathbf{q})=\frac{ina_0 q_z}{q_z^2+\lambda^2\xi_H^{-2}q_x^2+\lambda^2 q_x^4}\ ; \tag{A4}$$

hence, after integration over q_z,

$$m_x(x,z)=\frac{\pm na_0}{4\pi}\int dq_x\exp(iq_x x)\times\exp(-\lambda|z|\sqrt{\xi_H^{-2}q_x^2+q_x^4}) \tag{A5}$$

and

$$m_z(x,z)=\frac{\pm ina_0}{4\pi}\lambda\int dq_x\exp(iq_x x)\frac{\sqrt{\xi_H^{-2}q_x^2+q_x^4}}{q_x}\times\exp(-\lambda|z|\sqrt{\xi_H^{-2}q_x^2+q_x^4})\ . \tag{A6}$$

If $H=0$, then $\xi_H=\infty$ and

$$m_x(x,z)=\frac{\pm na_0}{4\sqrt{\pi\lambda|z|}}\exp(-x^2/4\lambda|z|)\ . \tag{A7}$$

However, for $H\neq 0$ the decay of m_x and m_z when $x\to\infty$ is much slower and we find, at $z=$const, that $m_x(x,z)\sim x^{-2}$ and $m_z(x,z)\sim x^{-1}$. To find the line tension τ we integrate F outside the dislocation core $-\xi<x$, $z<\xi$, where $\xi\sim na_0$ is a cut-off length. Integration over the stripe $\xi<x<+\infty$, $0<z<\xi$ gives a finite contribution to τ. Then we integrate over $-\infty<x<+\infty$, $\xi<z<L$ using Fourier representation (A5) and (A6), and performing the integral over z first. The term $(\partial m_x/\partial x)^2$ gives a finite contribution to τ in the limit $L\to\infty$. However, the contributions from m_x^2 and m_z^2 diverge. For example, the integral of m_x^2 gives

$$\int_{-\infty}^{+\infty}dx\int_{\xi}^{L}dz\,m_x^2(x,z)\sim\int_0^{\infty}\frac{dq_x}{\sqrt{\xi_H^{-2}q_x^2+q_x^4}}[\exp(-2\lambda L\sqrt{\xi_H^{-2}q_x^2+q_x^4})-\exp[-2\lambda\xi\sqrt{\xi_H^{-2}q_x^2+q_x^4}]\ . \tag{A8}$$

The last integral has a logarithmic divergence at $q_x=0$ when $L\to\infty$; hence it diverges as $\ln L$.

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