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Development of Defect Textures in Smectic A Liquid Crystals: A Nonlinear Model†

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A smectic A liquid crystal is unstable against a dilative strain perpendicular to the layers. Above a certain threshold a characteristic undulation appears. Experimentally one observes highly nonlinear defect textures such as parabolic focal domains. Existing theories are linear and predict a one-dimensional sinusoidal undulation. It is controversial whether or not there is a second threshold for the two-dimensional pattern. A nonlinear model for the evolution of the undulation into defect textures is put forward. The mathematical description of the layer displacement starts with a nonlinear expression for the free energy and leads to a nonlinear partial differential equation of fourth order. To treat the problem analytically an approximate separation is performed. An "equivalent oscillator method" is developed to replace the problem with the well-known sine-Gordon equation. Solutions are found in terms of Jacobian elliptic functions in the complex domain, which have the desired two-dimensional periodicity as well as the weak singularities needed for the evolution of focal parabolae. The agreement with experiment is qualitative, but quite impressive. One predicts a one-dimensional pattern at threshold and a continuous transition to a two-dimensional texture without a second threshold.

INTRODUCTION

When a smectic A liquid crystal is subjected to a dilative strain perpendicular to the layers it displays a characteristic instability against undulation of the layers.[1–7]

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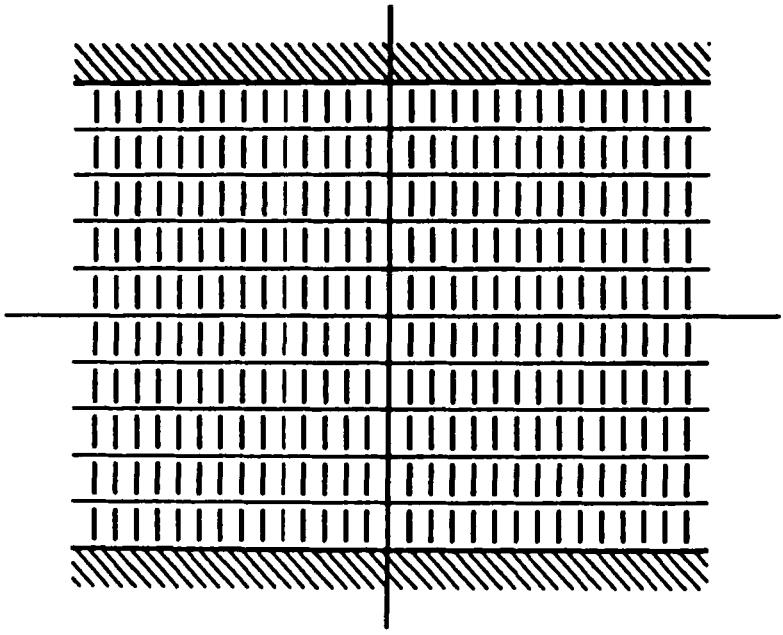

FIGURE 1 Homeotropic sample of a smectic A.

We consider a sample of a smectic A liquid crystal sandwiched between two parallel plates (Figure 1). The smectic layers are parallel to the plates. At the plates themselves, homeotropic boundary conditions are imposed by strong anchoring. Typically, the thickness of such a sample is a few hundred microns. When the distance between the plates is suddenly increased and thereby a dilative strain is imposed upon the smectic across its layers, an instability occurs. At first, the smectic responds to the strain by elastic expansion of the layer thickness. However, at a certain threshold dilation, on the order of a layer thickness (a few nanometers), the smectic can lower its energy by tilting of the layers with respect to the plates (Figure 2). Since a homogeneous tilt is prevented by the plates, the smectic layers tend to develop a zigzag pattern ultimately resulting in an undulation (Figure 3).

The pattern usually observed in a microscope is a two-dimensional grid more or less ordered or disordered, depending on the existence of a preferred direction in the plane of the layers. At higher dilations, the undulation develops into defect textures, the prominent one being a network of parabolic focal domains.[8,9]

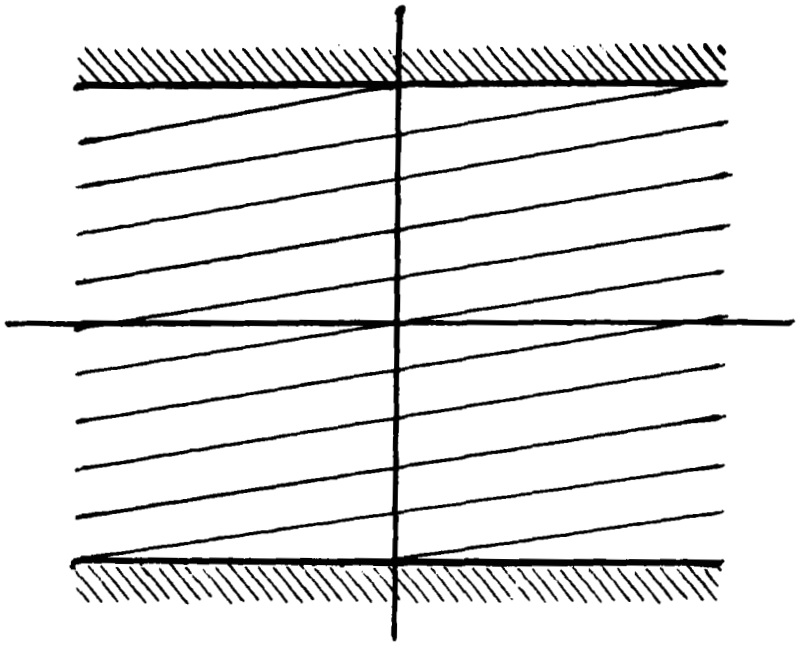

FIGURE 2 Homogeneously tilted smectic layers.

1. STATEMENT OF THE PROBLEM

Throughout this paper, we adopt for the geometry of the sample, the following conventions (Figure 3): the smectic is sandwiched between two plane parallel plates, assumed infinite, a distance $2d$ apart. The unperturbed smectic layers are parallel to the plates. Equivalently, the long molecular axes are on the average perpendicular to the plates. We call this orientation homeotropic; some authors prefer the designation perpendicular.[8]

We choose a righthanded, orthogonal cartesian coordinate system with origin O in the midplane between the plates, the x and y axes parallel, the z axis perpendicular to the plates.

The distortion of the layers will, conventionally, be described by a displacement field u in the z direction, normal to the unperturbed layers.

The elastic free energy density F of a smectic A liquid crystal, in

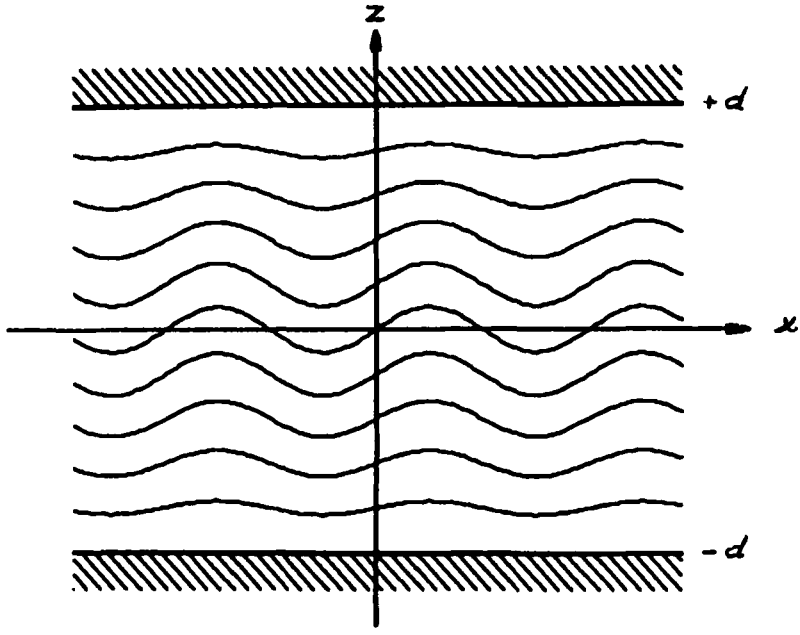

FIGURE 3 Undulation of smectic layers; also showing geometry of smectic sample.

an adequate nonlinear version, reads

$$F = \frac{1}{2} B\left(\frac{\partial u}{\partial z} - \left\{1 - \cos\left[\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2\right]^{1/2}\right\}\right)^2 + \frac{1}{2} K_1\left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right]^2 + \frac{1}{2} K_3\left[\left(\frac{\partial^2 u}{\partial x \partial z}\right)^2 + \left(\frac{\partial^2 u}{\partial y \partial z}\right)^2\right] \quad (1.1)$$

where B is the bulk elasticity modulus and K_1, K_3 are the Frank splay and bend elasticity moduli, respectively.

As usual, we introduce the characteristic lengths λ_1 and λ_3 defined by

$$\lambda_1^2 = K_1/B, \quad \lambda_3^2 = K_3/B \quad (1.2)$$

For the sake of convenience, and anticipating the results, we introduce the plane gradient operator

$$\partial = \frac{\partial}{\partial x} - i\frac{\partial}{\partial y} \quad (1.3)$$

and abbreviate the z-derivative by the subscript 3:

$$u_3 = \frac{\partial u}{\partial z} \tag{1.4}$$

The reduced, or dimensionless, free energy density f then becomes

$$f = \frac{F}{B} = \frac{1}{2}[u_3 - (1 - \cos|\partial u|)]^2 + \frac{1}{2}\lambda_1^2[\partial^2 u]^2 + \frac{1}{2}\lambda_3^2[\partial u_3]^2 \tag{1.5}$$

The permeation force G, or its dimensionless counterpart g, is given by the functional derivative

$$g = \frac{G}{B} = -\frac{\delta f}{\delta u} \tag{1.6}$$

which yields explicitly

$$g = -\lambda_1^2\partial^4 u + [1 - \lambda_3^2\partial^2]u_{33} - 2\,sin\,|\partial u| \cdot \partial u_3 - [\cos 2\,|\partial u| + (u_3 - 1)\cos|\partial u|]\partial^2 u \tag{1.7}$$

Expanding the cosine terms to second order in ∂u, we get the slightly simpler, but sufficiently adequate nonlinear expression

$$g = -\lambda_1^2\partial^4 u + [1 - \lambda_3^2\partial^2]u_{33} - 2(\partial u) \cdot (\partial u_3) + [u_3 - \frac{1}{2}(\partial u)^2]\partial^2 u + [(\partial u)\cdot\partial]^2 u \tag{1.8}$$

As in the linear case, the bend term $\lambda_3^2\partial^2 u_{33}$ is irrelevant and may be discarded. Then of course, the subscript *1* may be dropped from $\lambda_1 = \lambda$.

In equilibrum, we have

$$g = 0 \tag{1.9}$$

so that, finally we arrive at the equation

$$\lambda^2\partial^4 u + u_3\partial^2 u - u_{33} + 2(\partial u)\cdot(\partial u_3) - \frac{3}{2}(\partial u)^2(\partial^2 u) = 0 \tag{1.10}$$

An analytical solution of this nonlinear partial differential equation is far beyond our capabilities. One possible avenue to a solution is a straightforward brute force attempt to solve it numerically on a computer. While such an approach might be quite tedious and not easy to interpret, it may yield interesting results. At the very least, it should serve as a check for the approximation we propose.

2. QUASI-SEPARATION

In order to reduce the partial differential equation (1.10) to a tractable ordinary differential equation, we shall try to modify the method that works so well for the linear approximation.[9,10] That is to say, we represent the displacement as a superposition of a homogeneous dilative perturbation and a periodic response, and then try to separate the variables. The separation is only approximate; therefore we refer to it as "quasi-separation".

Thus, we assume for the displacement the form

$$u = \alpha z + U(x,y)Z(z) \tag{2.1}$$

where α is the imposed homogeneous dilation. Moreover, we assume

$$Z(z) = \mathrm{cn}(pz|n) \tag{2.2}$$

where $\mathrm{cn}(t|n)$ is the Jacobian elliptic function cosine amplitude (or elliptic cosine, for short) of argument t and parameter n.[11] Here p is the z-component of the wave vector defined so that a quarter period of the cn function is

$$pd = K(n) \tag{2.3}$$

where $K(n)$ is the complete elliptic integral of the first kind of parameter n.

The function $Z(z)$ was chosen as the elliptic cosine, since, in the first place, it is a straightforward generalization of the circular cosine valid in the linear approximation. Moreover, experimental observations indicate that most of the effect is concentrated in the middle of the sample. That fits well the shape of the cn function.

We take derivatives of Z with respect to z and obtain

$$Z' = p \,\mathrm{sn}\,\mathrm{dn} = -p[(1-n) - (1-2n)Z^2 - nZ^4]^{1/2} \quad (2.4)$$

$$Z'' = -p^2\mathrm{cn}(\mathrm{dn}^2 - n\mathrm{sn}^2) = -p^2Z[(1-2n) + 2nZ^2] \quad (2.5)$$

with the obvious abbreviations

$$\mathrm{sn} = \mathrm{sn}(pz|n), \quad \mathrm{cn} = \mathrm{cn}(pz|n), \quad \mathrm{dn} = \mathrm{dn}(pz|n) \quad (2.6)$$

We substitute this into Eq. (1.10) and obtain

$$\lambda^2 Z\partial^4 U + \alpha Z\partial^2 U + p^2 Z[(1-2n) + 2nZ^2]U - pZ[(1-Z^2) \times$$

$$\times (1 - n + nZ^2)]^{1/2}[U\partial^2 U + 2(\partial U)^2] - \frac{3}{2} Z^3(\partial U)^2(\partial^2 U) = 0 \quad (2.7)$$

Temporarily we introduce the dimensionless variable,

$$x_{\mathrm{new}} = x/\lambda, \quad y_{\mathrm{new}} = y/\lambda, \quad h = U/\lambda \quad (2.8)$$

However, without risking confusion, we can henceforth drop the label "new" and use the dimensionless variable.

For the time being, we shall ignore the variable y and interpret the derivatives as total derivatives with respect to x; we shall also denote them by primes. We shall come back to this point in Section 6.

Carrying out these manipulations we arrive at the equation

$$\text{(I)} \quad h'''' + \alpha h'' + \lambda^2 p^2(1 - 2n + 2nZ^2)h$$

$$\text{(II)} \quad -\lambda p[(1-Z^2)(1 - n + nZ^2)]^{1/2}(hh'' + 2h'^2) \quad (2.9)$$

$$\text{(III)} \quad -\frac{3}{2} Z^2 h' h'' = 0$$

The first line (I) of Eq. (2.9) corresponds to the linear approximation which it exactly reproduces for $n = 0$.

The second line (II) breaks the symmetry in a way reminiscent of squint.[12,13] These terms seem to be quite intractable and undesirable. However, it turns out that the derivatives h', h'' are expected to be

large precisely where h is small. But there, the linear approximation is perfect.

More specifically, in the midplane $Z^2 = 1$ irrespective of n, and thus line (II) vanishes exactly. At the boundaries, on the other hand, the solution is constrained to be trival: $u = 0 =$ constant. Consequently, there is no point in "improving" on the linear approximation.

Line (III) is nonexistent at the boundaries, since $Z^2 = 0$. In the midplane, it is precisely $-\frac{3}{2} h'^2 h''$, since $Z^2 = 1$ irrespective of the parameter n.

Let us see this in detail. At the boundaries, where $Z^2 = 0$, we have

$$h'''' + \alpha h'' + \lambda^2 p^2 (1 - 2n) h - \lambda p (1-n)^{1/2} (h h'' + 2h'^2) = 0 \quad (2.10)$$

Apart from the nonlinear term that has already been discussed, all that happens is a minor renormalization of λp. Moreover, one can safely assume that the parameter n will not be very difficult from zero and will never reach $\frac{1}{2}$.

For the midplane, where $Z^2 = 1$, we get

$$h'''' + \alpha h'' + \lambda^2 p^2 h - \frac{3}{2} h'^2 h'' = 0 \quad (2.11)$$

Thus, we have the original linear terms with the correction $-\frac{3}{2} h'^2 h''$. One can rewrite (2.11) in the form

$$h'''' + (\alpha - \frac{3}{2} h'^2) h'' + \lambda^2 p^2 h = 0 \quad (2.12)$$

in order to emphasize that the effect of the nonlinearity is to renormalize, and thus to effectively reduce, the dilation α.

In order to handle Eq. (2.9), one should in principle make some kind of adiabatic approximation. One may justifiably assume that the undulation varies much more rapidly within the (xy)-plane than it does in the perpendicular z-direction. As an alternative, one could choose to replace Z^2 by some effective value, such as, say, the root mean square $<Z^2>$. Clearly, all these versions do not differ significantly from each other.

Our physical intuition tells us that what happens in the midplane dominates all the rest. So we choose to focus our attention to the midplane and set $Z^2 = 1$. Thus, we deal with Eq. (2.11).

The standard approach to an equation like (2.11) is to apply perturbation theory to the linearized version. We are, however, interested in large deviations from linearity, such as the observed defect textures. We claim that such features cannot be obtained from perturbation theory. A more radical, nonperturbative approach is called for.

3. SINE-GORDON EQUATION

The pendulum equation, also known as the sine-Gordon equation is a tested tool for the qualitative and semi-quantitative study of strong nonlinearities.[14,15]

The pendulum, or sine-Gordon equation is

$$\phi'' + \gamma \sin \phi = 0 \tag{3.1}$$

where γ is a positive or negative constant. Another related equation is the sinh-Gordon equation

$$\chi'' + \gamma \sinh \chi = 0 \tag{3.2}$$

However, the substitution

$$\chi = -i\phi \tag{3.3}$$

reproduces Eq. (3.1). Thus both equations can be simultaneously covered by studying the pedulum equation in the complex domain.

We find the first integral of Eq. (3.1):

$$\phi'^2 = 2\epsilon + 2\gamma \cos \phi \tag{3.4}$$

where ϵ is an integration constant representing the total energy of the pendulum.

We take derivatives of Eq. (3.1)

$$\phi''' + \gamma \cos \phi \phi' = 0 \tag{3.5}$$

$$\phi'''' + \gamma \cos \phi \phi'' - \gamma \sin \phi \phi'^2 = 0 \tag{3.6}$$

In view of Eq. (3.1) this can also be written as

$$\phi'''' + \gamma \cos\phi\phi'' + \phi'^2\phi'' = 0 \tag{3.7}$$

Eq. (3.7) clearly displays the two kinds of nonlinearities introduced by replacing the harmonic oscillator by a pendulum. In the first place, we have the replacement $1 \rightarrow \cos\phi$. Secondly, we find the term, $\phi'^2\phi''$ which is of the same type as the nonlinear term in Eq. (2.11). Yet, notice that it has the wrong sign.

To remedy this deficiency, we use a kind of Lagrange multiplier method and add to Eq. (3.7) zero in the form

$$-\mu\phi''\left(\frac{1}{2}\phi'^2 - \gamma\cos\phi - \epsilon\right) = 0 \tag{3.8}$$

where μ is some arbitrary multiplier. Hence we obtain

$$\phi'''' + (1 + \mu)\gamma \cos\phi\phi'' + \left(1 - \frac{\mu}{2}\right)\phi'^2\phi'' - \mu\epsilon\gamma \sin\phi = 0 \tag{3.9}$$

Many other equivalent versions are possible.

For a small disturbance we have

$$\phi \ll 1\text{: } \sin\phi \rightarrow \phi, \quad \cos\phi \rightarrow 1 \tag{3.10}$$

and Eq. (3.9) becomes

$$\phi'''' + (1 + \mu)\gamma\phi'' - \mu\epsilon\gamma\phi + \left(1 - \frac{\mu}{2}\right)\phi'^2\phi'' = 0 \tag{3.11}$$

We now return to Eq. (2.10) and, respecting the angular topology of the "modular" variable h, we identify

$$2\pi h \equiv \phi \tag{3.12}$$

Thus, we rewrite Eq. (2.10) in the form

$$\phi'''' + \alpha\phi'' + \lambda^2 p^2\phi - \frac{3}{8\pi^2}\phi'^2\phi'' = 0 \tag{3.13}$$

To identify Eq. (3.11) with Eq. (3.13) we must set:

$$(1 + \mu)\gamma = \alpha \tag{3.14}$$

$$-\mu\epsilon\gamma = \lambda^2 p^2 \tag{3.15}$$

$$1 - \frac{\mu}{2} = -\frac{3}{8\pi^2} \tag{3.16}$$

whence

$$\gamma = \frac{\alpha}{1 + \mu} \tag{3.17}$$

$$\epsilon = \frac{\mu + 1}{\mu}\frac{\lambda^2 p^2}{\alpha} \tag{3.18}$$

$$\mu = 2 + \frac{3}{4\pi^2} \simeq 2.076 \simeq 2 \tag{3.19}$$

The threshold dilation α_1 can be obtained from Eq. (3.4) by setting $\phi' = 0$ at $\phi = 0$:

$$\epsilon_1 = \epsilon(\phi = 0, \phi' = 0) = -\gamma\cos 0 = -\gamma \tag{3.20}$$

Substituting this into Eq. (3.18) we get

$$\left(\frac{\alpha_1}{\lambda p}\right)^2 = \frac{(\mu + 1)^2}{\mu} \tag{3.21}$$

In order to reproduce the threshold dilation value known from the linear approximation,

$$\alpha_1^{\text{lin}} = 2\lambda p \tag{3.22}$$

we have to set

$$\mu = 1 \tag{3.23}$$

Then, Eq. (3.9) becomes

$$\phi'''' + 2\gamma \cos\phi\phi'' - \epsilon\gamma \sin\phi + \frac{1}{2}\phi'^2\phi'' = 0 \tag{3.24}$$

If, on the other hand, we take the value of μ given by Eq. (3.19), then

$$\alpha_1 = 2.14\lambda p \simeq 2\lambda p \tag{3.25}$$

Hence we conclude that the theory is rather insensitive to the value of μ.

Moreover, it turns out that μ can be effectively eliminated from the final results and replaced by α_1 as a parameter.

Summarizing, we see that the problem has been reduced to solving the pendulum equation

$$\phi'' + \frac{\alpha}{1 + \mu} \sin \phi = 0 \tag{3.26}$$

4. EQUIVALENT OSCILLATOR METHOD

Our approach might be called the "equivalent oscillator method". Let us illustrate this in the linear case.

We look for an equivalent oscillator for the system described by the equation

$$h'''' + \alpha h + \lambda^2 p^2 h = 0 \tag{4.1}$$

The equation of a linear, that is to say *harmonic* oscillator is, of course,

$$\phi'' + \gamma\phi = 0 \tag{4.2}$$

We find the first integral and the derivatives of Eq. (4.2):

$$\phi'^2 + \gamma\phi^2 = 2\epsilon \tag{4.3}$$

$$\phi''' = \gamma\phi' = 0 \tag{4.4}$$

$$\phi'''' + \gamma\phi'' = 0 \tag{4.5}$$

From Eqs. (4.2) and (4.5) we substitute

$$\phi'''' = -\gamma\phi'' = \gamma^2\phi \tag{4.6}$$

and, to make the analogy complete, we identify

$$2\pi h \equiv \phi \tag{4.7}$$

Thus, we get from Eq. (4.1)

$$\gamma^2\phi - \alpha\gamma\phi + \lambda^2 p^2\phi = 0 \tag{4.8}$$

Hence, of course, we retrieve the well known characteristic equation for the wave vector k of the undulation h defined by Eq. (4.1):

$$\gamma^2 - \alpha\gamma + \lambda^2 p^2 = 0 \tag{4.9}$$

with the solutions

$$k_{\pm}^2 = \gamma_{\pm} = \frac{\alpha \pm (\alpha^2 - 4\lambda^2 p^2)^{1/2}}{2} \tag{4.10}$$

which yields for the threshold dilation

$$\alpha_1 = \alpha_1{}^{\text{lin}} = 2\lambda p \tag{4.11}$$

This, of course, reproduces the whole linear theory of the undulation instability.

The usual elementary method of assuming the unknown function h (or ϕ) in a sinusoidal, cosinusoidal or exponential form is a shortcut of the present method. The shortcut presupposes that the correct form of the solution is known in advance. That is a trivial and transparent matter in the linear case. Yet, in the more interesting and more complicated nonlinear cases this is by no means so.

Essentially, our problem will be solved if we can find the right kind of equivalent oscillator. That is in general a highly nontrivial task. Since, for a *vanishing* amplitude, the harmonic oscillator osulates *all* oscillators, it is one of the most degenerate and pathological physical systems. Therefore, it is very hard to guess how to extrapolate and reconstruct the original. Fortunately, however, many physical systems have some common features represented by any anharmonic oscillator, such as a ϕ^4 system (the anharmonic oscillator proper), the sine-Gordon system (the pendulum), the double sine-Gordon system, or any other system of this type. Their important common feature is a convergent potential including a ϕ^4 term.

The next simplest system after a harmonic oscillator is a *simple pendulum*. This is also a very well known solvable system, but it is tremendously richer and more interesting than the harmonic oscillator. This is one reason for our choice of the pendulum to represent our system.

From the point of view of the physics involved, there is an other, more profound reason to choose the sine-Gordon equation. Our starting point, Eq. (1.1) or Eq. (1.5), clearly shows that ∂u is a modular variable, or in plain English, an angle. So it is plausible that the layer displacement u itself could be modular, or at least, in part so. As a matter of fact, that is perfectly reasonable, particularly in the bulk of a sample of finite thickness. The smectic layers see a mean field which tends to keep them at the right level. A displacement by one layer thickness restores an unstressed state, perhaps at the expense of creating an edge dislocation which might be a straight pair or a finite loop.

If there is a system where the Frenkel-Kontorova dislocation model makes sense, it is certainly a smectic. But the sine-Gordon equation is the continuum approximation to the Frenkel-Kontorova model. So we do have a strong physical motivation to adopt the sine-Gordon model. It seems to reproduce the observed physics quite well, which is probably a modest understatement. Moreover, as we have already pointed out, it is a nice, easy and versatile mathematical tool to work with.

5. SOLUTION

We are now ready to solve the pendulum equation

$$\phi'' + \gamma \sin \phi = 0 \tag{5.1}$$

corresponding to Eq. (3.26).

The first integral

$$\epsilon = \frac{1}{2}\phi'^2 - \gamma \cos \phi \tag{5.2}$$

has an obvious interpretation as the energy analog of the system described by Eq. (5.1).

From Eq. (5.2) we have

$$\int_0^{\phi} \frac{d\phi}{(2\epsilon + 2\gamma \cos \phi)^{1/2}} = x - x_0 \tag{5.3}$$

Here x_0 is an arbitrary integration constant corresponding to the choice of the origin. It will be dropped henceforth.

The substitutions

$$\cos \phi = 1 - 2 \sin^2 \frac{\phi}{2} \tag{5.4}$$

and

$$\phi = 2\psi \tag{5.5}$$

lead to

$$\left(\frac{2}{\gamma + \epsilon}\right)^{1/2} \int_{\psi=0}^{\phi/2} \frac{d\psi}{(1 - \overline{m} \sin^2 \psi)^{1/2}} = x \tag{5.6}$$

where the parameter $\overline{m}$ is defined by

$$\overline{m} = \frac{2\gamma}{\gamma + \epsilon} \tag{5.7}$$

We rewrite Eq. (5.6) in the standard form

$$\left(\frac{\gamma + \epsilon}{2}\right)^{1/2} x = F\left(\frac{\phi}{2} \,\middle|\, \overline{m} = \frac{2\gamma}{\gamma + \epsilon}\right) \tag{5.8}$$

where $F(u|m:)$ is the incomplete Jacobian elliptic integral of the first kind of argument u and parameter $\overline{m}$.[11]

Inversion of Eq. (5.8) yields

$$\frac{\phi}{2} = \mathrm{am}\left[\left(\frac{\gamma + \epsilon}{2}\right)^{1/2} x \,\middle|\, \overline{m} = \frac{2\gamma}{\gamma + \epsilon}\right] \tag{5.9}$$

where $\mathrm{am}(u|\overline{m})$ is the Jacobian elliptic function amplitude of argument u and parameter $\overline{m}$. We take the sine of both sides of Eq. (5.9) so

that we get

$$\sin\frac{\phi}{2} = \mathrm{sn}\left[\left(\frac{\gamma+\epsilon}{2}\right)^{1/2} x \;\middle|\; \bar{m} = \frac{2\gamma}{\gamma+\epsilon}\right] \tag{5.10}$$

where $\mathrm{sn}(u|\bar{m})$ is the Jacobian elliptic function sine amplitude (or elliptic sine) of argument u and parameter $\bar{m}$.

We now take a closer look at the parameter $\bar{m}$ defined by Eq. (5.7). We substitute for γ and ϵ from Eqs. (3.17) and (3.18) and obtain

$$\bar{m} = \frac{\dfrac{2\alpha}{\mu+1}}{\dfrac{\alpha}{\mu+1} - \dfrac{\mu+1}{\mu}\dfrac{\lambda^2 p^2}{\alpha}} = \frac{2}{1 - \dfrac{(\mu+1)^2}{\mu}\left(\dfrac{\lambda p}{\alpha}\right)^2} \tag{5.11}$$

Eq. (3.21) makes it possible to eliminate the undetermined multiplier μ by introducing instead the physical parameter α_1, so that

$$\bar{m} = \frac{2}{1-(\alpha_1/\alpha)^2} \tag{5.12}$$

Clearly, under normal circumstances

$$\bar{m} > 1 \tag{5.13}$$

Therefore, we must introduce the reciprocal parameter

$$m = 1/\bar{m} \tag{5.14}$$

by the transformation[11]

$$\mathrm{sn}\,(u|\bar{m}) = m^{1/2}\,\mathrm{sn}\,(\bar{m}^{1/2}u|m = 1/\bar{m}) \tag{5.15}$$

which yields

$$\sin\frac{\phi}{2} = \left(\frac{\gamma+\epsilon}{2\gamma}\right)^{1/2} \mathrm{sn}\left(\gamma^{1/2}x \;\middle|\; m=\frac{\gamma+\epsilon}{2\gamma}\right) \tag{5.16}$$

or, with the substitution (5.12):

$$\sin\frac{\phi}{2} = \left(\frac{1-(\alpha_1/\alpha)^2}{2}\right)^{1/2} \mathrm{sn}\left[\left(\frac{\alpha}{\mu+1}\right)^{1/2} x \,\middle|\, m = \frac{1-(\alpha_1/\alpha)^2}{2}\right] \tag{5.17}$$

We must now take a closer look at the parameter m. The behavior of m as a function of $(\alpha/\alpha_1)^2$ is shown in Figure 4.

In the first place, we notice that negative values for the dilation α (corresponding to compression) are included as well as positive ones. However, the coefficient

$$\gamma = \frac{\alpha}{\mu + 1} > 0 \tag{5.18}$$

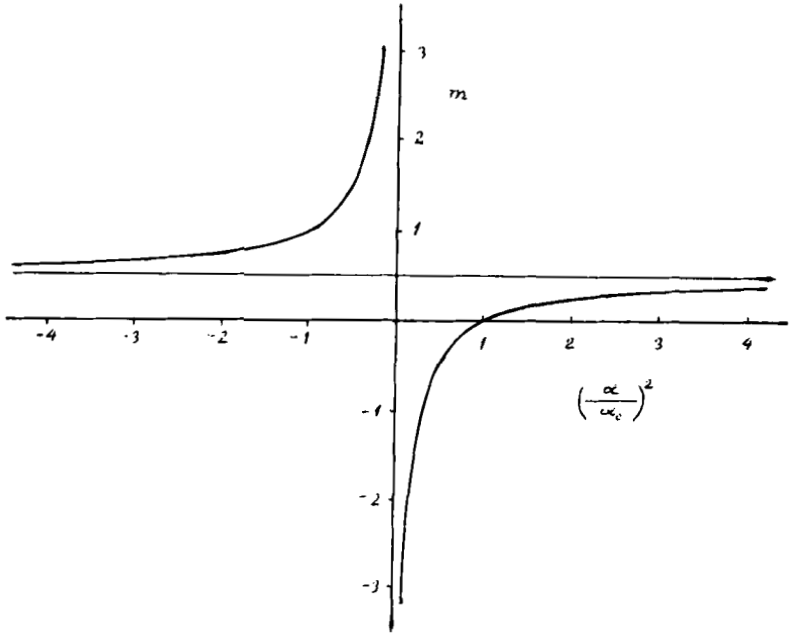

FIGURE 4 Parameter m as function of the square of the relative dilation $(\alpha/\alpha_1)^2$.

in Eq. (5.1) must be positive; incidentally, this is also obvious from Eq. (5.16). Since negative values for μ are forbidden by Eq. (3.21), this implies a positive dilation α. For a negative γ, Eq. (5.1) describes "oscillations on top of a hill," that is to say, around the unstable equilibrium. This then makes the dilation unambiguously positive. An undulation instability in compression is thus excluded, in agreement with experiment.

For dilations below threshold, $\alpha < \alpha_1$, Eq. (5.17) yields for $\sin(\phi/2)$ imaginary values. The undulation becomes real, and exactly sinusoidal with a vanishing amplitude, precisely at the threshold dilation $\alpha = \alpha_1$. Thus we retrieve the correct linear limit. The parameter m increases from zero at threshold α_1 to 1/2 for an infinite dilation $\alpha \to \infty$. The amplitude of ϕ then reaches $\pi/2$, whence the amplitude of h becomes $h_{\max} = 1/4$, and thus finally, the maximum layer displacement is $u_{\max} = \lambda/4$.

In general, the amplitude can be found from Eq. (5.17) or from the first integral (5.2) as

$$\phi_{\max} = \arccos\,(\alpha_1/\alpha)^2 \tag{5.19}$$

An experimental determination of the amplitude $\phi_{\max}$ as a function of the dilation α could perhaps be used to determine the right kind of potential. However, it is almost certain, that by the time the amplitude becomes this big, defects will have already been created.

6. TWO-DIMENSIONAL INTERPRETATION

The original equations, such as Eqs. (1.5), (1.10), or (2.7) were written so that $\partial = \partial/\partial x - i\partial/\partial y$ could be interpreted as a two-dimensional operator in the complex plane, the latter representing the physical (xy)plane. One cannot raise any objection against a two-dimensional interpretation of the result.

Accordingly, in Eq. (5.17) we pass from the real variable x to the complex variable z:

$$x \to z = x + iy \tag{6.1}$$

For $\mathrm{sn}(z|m)$ we have the formula

$$\mathrm{sn}(x + iy|m) = \frac{\mathrm{sn}(x|m)\mathrm{dn}(y|\bar{m}) + i\mathrm{cn}(x|m)\mathrm{dn}(x|m)\mathrm{sn}(y|\bar{m})\mathrm{cn}(y|\bar{m})}{\mathrm{cn}^2(y|\bar{m} + \mathrm{sn}^2(x|m)\mathrm{sn}^2(y|\bar{m})} \tag{6.2}$$

where

$$\tilde{m} = 1 - m \tag{6.3}$$

is the coparameter of the elliptic function.[11]

We perform the substitution (6.1) in Eq. (5.17), take the real part and find

$$\sin\frac{\phi}{2} = \left(\frac{1-(\alpha_1/\alpha)^2}{2}\right)^{1/2} \mathrm{Re}\,\mathrm{sn}\left[\left(\frac{\alpha}{\mu+1}\right)^{1/2} z \,\middle|\, m = \frac{1-(\alpha_1/\alpha)^2}{2}\right] \tag{6.4}$$

At threshold, $\alpha = \alpha_1$, we have

$$m = 0, \qquad \tilde{m} = 1 \tag{6.5}$$

so that Eq. (6.4) becomes

$$\sin\frac{\phi}{2} = 0 \cdot \sin\left[\left(\frac{\alpha}{\mu+1}\right)^{1/2} x\right] \cdot \cosh\left[\left(\frac{\alpha}{\mu+1}\right)^{1/2} y\right] \tag{6.6}$$

The cosh does not matter, since it diverges only at infinity and the amplitude is strictly zero.

In this limiting case, the period and coperiod of the elliptic function are, respectively, given by the complete elliptic integrals of the first kind

$$K_x = K(0) = \pi/2, \qquad K_y = K(1) \to \infty \tag{6.7}$$

Consequently, we have a one-dimensional undulation with the (physical, or dimensional) period Λ_1 given by

$$\left(\frac{\alpha_1}{\mu+1}\right)^{1/2} \frac{\Lambda_1}{4\lambda} = \frac{\pi}{2} \tag{6.8}$$

and hence

$$\Lambda_1 = \mu^{1/4} 2\pi(\lambda/p)^{1/2} \tag{6.9}$$

The factor $\mu^{1/4}$ is of order unity in any case. Since the linear theory should be strictly valid at threshold, Eq. (6.9) could perhaps serve to determine μ. Then we would have $\mu = 1$.

Above the threshold, that is for $\alpha > \alpha_1$, both periods decrease with increasing dilation α. While K_x decreases very slowly, K_y decreases rapidly, so that a finite rectangular pattern is established. The change is continuous. Hence, we predict *no second threshold* α_2 for the "square" pattern.

The condition for a truly square pattern is the equality of the periods in the x and y directions:

$$\Lambda_x = \Lambda_y \tag{6.10}$$

Hence we get an equation for the parameter m:

$$4K(m) = 2K(1-m) \tag{6.11}$$

The solution of this equation is

$$m_\square = 0.02943\ 72515 \tag{6.12}$$

which corresponds to

$$2K(m_\square) = K(1-m_\square) \simeq 3.1651\ldots = 1.0075\ldots\pi \tag{6.13}$$

The corresponding periods are well within experimental error equal to the period given by the linear approximation.

The dilation $\alpha_\square$ corresponding to $m_\square$ is

$$\alpha_\square = 1.031\ \alpha_1 \tag{6.14}$$

It is more interesting that for a parameter m exceeding $m_\square$, Λ_y is smaller than Λ_x:

$$m > m_\square: \qquad \Lambda_y < \Lambda_x \tag{6.15}$$

This prediction is in perfect agreement with experiment.

7. DEFECT TEXTURES

The elliptic sine function $\mathrm{sn}(z|m)$ has a simple pole at the points

$$z \equiv x + iy = 4rK(m) + i(2s+1)K(\tilde{m}) \tag{7.1}$$

where r and s are integers.

For the angular coordinate ϕ representing the layer displacement, we have, according to Eq. (6.4):

$$\phi = 2 \arcsin\left\{\left(\frac{1 - (\alpha_1/\alpha)^2}{2}\right)^{1/2} \times \right.$$
$$\left. \times \operatorname{Re} \operatorname{sn}\left[\left(\frac{\alpha}{\mu + 1}\right)^{1/2} z \,\middle|\, m = \frac{1 - (\alpha_1/\alpha)^2}{2}\right]\right\} \quad (7.2)$$

Clearly, there are regions where the argument of the arcsin exceeds unity and the angle ϕ becomes imaginary. These regions are bounded by closed lines defined by the condition

$$\phi = \pi \pmod{2\pi} \quad (7.3)$$

One these lines $\partial\phi$, the plane gradient of ϕ diverges, and hence the surface $\phi = \phi(z)$ becomes vertical; this can be seen in Figure 5.

Since $\sin\alpha = \sin(\pi - \alpha)$, the surface $\phi = \phi(z)$ matches up with

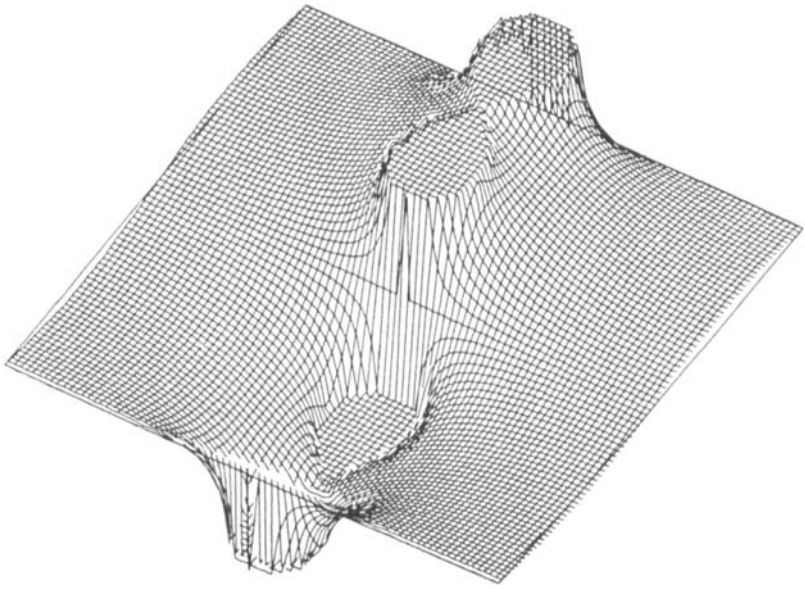

FIGURE 5a Aspects of the surface $\phi = \phi(z)$, Eq. (7.2); the "figure eight" contours corresponds to $\phi = \pi \pmod{2\pi}$.

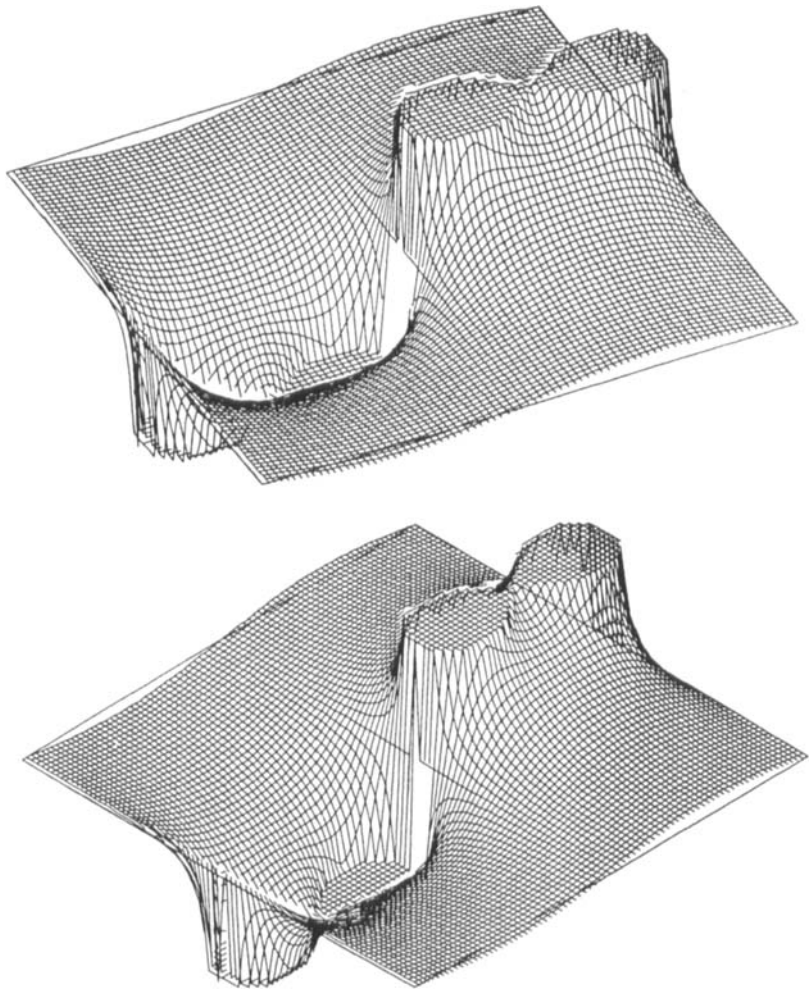

FIGURE 5b, c Continued

its mirror image with respect to the plane $\phi = \pi$, that is $\phi = 2\pi - \phi(z)$ as shown in Figure 6.

If we could take this result at face value and extend it throughout the bulk of the smectic sample, it would mean that the smectic layers joined up into a single periodic warped surface in three dimensions akin to the kind known from fermiology.

This, of course, cannot be true, since our calculation is valid only for the midplane and the extrapolation would violate the boundary conditions at the plates.

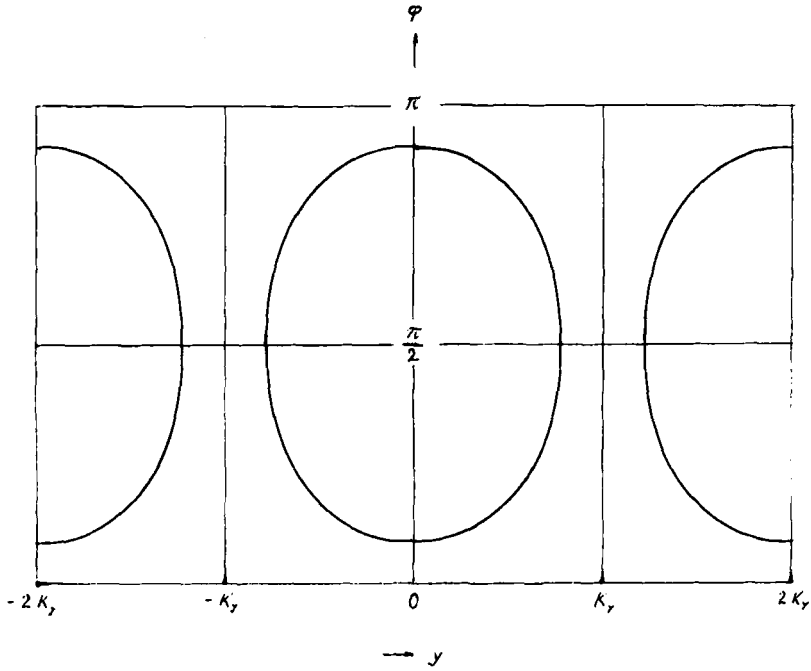

FIGURE 6 Matching of mirror images $\phi = \phi(z)$ and $\phi = \pi - \phi(z)$.

Nevertheless, at least for the region in the middle of the sample, our calculation should not be totally wrong. In fact the periodic regions of large localized displacements are similar to the pinching of layers needed for the development of parabolic focal domains.[8] So our calculation definitely indicates a trend toward the formation of this kind of defect texture.

It is also possible that in some region of limited thickness the layers actually do join up as indicated by our calculation. The result should be an intricate defect texture including a network of dislocations and disclinations. There are hints that such a network has been observed at Bell Laboratories.[16]

At this point it is still hard to say how seriously all this can be taken, but there may be a grain of truth in it.

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