Nonlinear effects in liquid crystals

S. I. Ben-Abraham
Department of Physics, Ben-Gurion University of the Negev, 84 120 Be'er-Sheva', Israel
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The effects of nonlinearity in nematic liquid crystals subject to electric and magnetic fields are emphasized. For the Fréedericks transition, the distortion profile is calculated exactly. For the domain modes, the torque equation can be approximated to a high degree by the nonlinear sine-Gordon equation. An exact two-dimensional periodic solution is found whose consequences are in good quantitative agreement with all experimental observations. The possibility of a first-order transition to a vortex pattern is predicted.

INTRODUCTION

Applied electric, magnetic, and thermal fields induce in liquid crystals a variety of flow patterns with striking optical properties.[1,2] The first and best known of these patterns is the Williams domain mode,[3] but a number of other vortex patterns or domain modes are now well established.[4] Our basic understanding of the physical mechanism involved comes from Helfrich's conduction-induced alignment theory.[5] His treatment, however, is essentially one-dimensional and linear. Penz and Ford have substantiated Helfrich's theory by solving the stationary electromagnetohydrodynamic boundary value problem.[4,6,7] Recently, Penz modified the solution to include dynamic effects, invoking the principle of selective amplification.[8] In either case, the equations are linearized, and thus the treatment is, of necessity, limited to small perturbations. A linearized theory can, of course, yield no values for the amplitudes. Yet the interesting domain modes appear with finite amplitudes at well-defined thresholds. Thus the validity of the theory is still open to question.

It seems that nonlinearity plays a crucial role in stabilizing the domain patterns. Therefore in this work attention is focused upon the effects of nonlinearity. In this paper, the distortion profiles, i.e., the director angle as a function of the coordinates are calculated. It should be emphasized that analytic rather than numerical solutions are sought.

Section I deals with the exactly solvable case of the Fréedericks transition. The mathematical details are postponed to the appendixes. The Williams domain mode is the subject of Sec. II, which constitutes the main body of this paper. A version of the one-elastic-constant approximation reduces the rather complicated torque equation to the sine-Gordon equation, which, in this instance, is exactly solvable yet retains the essential nonlinear features of the problem. Section III extends the results to homeotropic domain patterns. In Sec. IV, the form of the solutions, as well as ways to improve on the predictions are discussed. Moreover, it is shown that the model predicts domain contraction with increasing voltage and a first-order transition to the domain modes.

I. FRÉEDERICKS TRANSITION

As an example of a complete treatment of a nonlinear problem we present the exact solution for the well-known Fréedericks transition.[9] Saupe[10] calculated the critical field and the distortion amplitude but failed to calculate the distortion profile. We shall do so now. After the completion of this report, it came to my attention that Deuling[11] has treated the same problem. Nevertheless, I present my results, since they seem to be more compact and also for reference purposes in what follows.

A. Case 1: Splay-bend (n_x, H_y)

Consider a nematic liquid crystal of thickness d sandwiched between two plane-parallel plates. To fix ideas, we assume that the nematic molecules in the undisturbed sample are aligned along some well-defined "easy" direction parallel to the plates. Such an easy direction can be readily established by rubbing the plates. A magnetic field $\vec{H}$ and/or an electric field $\vec{E}$ applied perpendicular to the plates will, generally speaking, change the orientation pattern. We shall calculate the director angle ϕ as a function of the distance from one of the plates.

We introduce a Cartesian coordinate system with the x axis parallel to the easy direction, the y axis parallel to the field, and the z axis perpendicular to both.

The differential equation for the director angle ϕ is, in the magnetic case,

$$\frac{d^2\phi}{dy^2} = -\frac{\Delta\chi H^2 + k(d\phi/dy)^2}{k_{11}\cos^2\phi + k_{33}\sin^2\phi}\sin\phi\cos\phi, \qquad (1.1)$$

where

$$\Delta\chi = \chi^{\parallel} - \chi^{\perp}, \quad \Delta k = k_{33} - k_{11}; \tag{1.2}$$

k_{11} and k_{33} are the splay and bend moduli, respectively, and $\chi^{\parallel}$ and $\chi^{\perp}$ are the magnetic susceptibilities parallel and perpendicular to the easy director axis. In the presence of an electric field, $\Delta\chi H^2$ must obviously be replaced by $\Delta\chi H^2 + \Delta\epsilon E^2$, where

$$\Delta\epsilon = \epsilon^{\parallel} - \epsilon^{\perp}, \tag{1.2'}$$

and where $\epsilon^{\parallel}$ and $\epsilon^{\perp}$ are the parallel and perpendicular permittivities.

We make Eq. (1.1) dimensionless by introducing a characteristic (or "coherence") length λ_y defined by

$$\lambda_y^2 = k_{11}/\Delta\chi H^2 \tag{1.3}$$

and substituting

$$\eta = y/\lambda_y. \tag{1.4}$$

Moreover, we set

$$\kappa = (k_{33} - k_{11})/k_{11}. \tag{1.5}$$

Then, (1.1) becomes

$$\frac{\partial^2\phi}{\partial\eta^2} = \frac{1 + \kappa(\partial\phi/\partial\eta)^2}{1 + \kappa\sin^2\phi}\sin\phi\cos\phi\,. \tag{1.6}$$

This equation can be solved by standard procedure. The solution is

$$\kappa\sin\phi = \gamma\,\mathrm{sp}/(1 - \gamma^2\mathrm{sp}^2)^{1/2}, \tag{1.7}$$

where sp is an abbreviation for a generalized Jacobian sine-amplitude function,

$$\gamma^2 = \kappa\sin^2\phi_0/(1 + \kappa\sin^2\phi_0), \tag{1.8}$$

and ϕ_0 is the maximum value of the director angle. The details of the calculation and the relevant definitions are postponed to Appendixes A and B.

B. Case 2: Twist (n_x, H_x, H_z)

The geometry is almost the same as for case 1, except that now the magnetic field is in the xz plane, i.e., parallel to the plates $\vec{H} = (H\cos\alpha, 0, H\sin\alpha)$. The distortion is pure twist.

Now the differential equation for the director angle becomes

$$\frac{d^2\phi}{dy^2} = -\frac{\Delta\chi H^2}{k_{22}}\cos(\alpha - \phi)\sin(\alpha - \phi), \tag{1.9}$$

where k_{22} is the twist modulus.

If the magnetic field is in the z direction, then $\alpha = \frac{1}{2}\pi$, and we have

$$\frac{d^2\phi}{dy^2} = -\frac{\Delta\chi H^2}{k_{22}}\sin\phi\cos\phi. \tag{1.10}$$

This is the one-dimensional sine-Gordon equation. It has to be solved subject to the boundary conditions

$$\phi(0) = \phi(d) = 0. \tag{1.11}$$

The solution is well known to be

$$\sin\phi = \sin\phi_0\,\mathrm{sn}(\eta\backslash\phi_0), \tag{1.12}$$

where η is defined by (1.3, 4) except that k_{11} is replaced by the twist modulus k_{22}, and $\mathrm{sn}(\eta\backslash\phi_0)$ is the Jacobian sine-amplitude function of argument η and modular angle ϕ_0.

For arbitrary α, we introduce the substitution

$$\psi = \phi - \alpha, \tag{1.13}$$

which again reduces (1.9) to the sine-Gordon equation

$$\frac{d^2\psi}{dy^2} = +\frac{\Delta\chi H^2}{k_{22}}\cos\psi\sin\psi, \tag{1.14}$$

now subject to the boundary conditions

$$\psi(0) = \psi(d) = -\alpha. \tag{1.15}$$

Again, the solution is

$$\sin\psi = \sin\psi_0\,\mathrm{sn}(\eta - \eta_0\backslash\psi_0)\,, \tag{1.16}$$

with

$$\eta_0 = F(\arcsin(\sin\alpha/\sin\psi_0)\backslash\psi_0) = \int_0^{\arcsin(\sin\alpha/\sin\psi_0)} d\theta(1 - \sin^2\psi_0\sin^2\theta)^{-1/2}, \tag{1.17}$$

where $F(\phi\backslash\psi_0)$ denotes the elliptic integral of the first kind, of argument ϕ and modular angle ψ_0.

C. Case 3: Bend-splay (n_y, H_x)

In this case we have homeotropic boundary conditions, i.e., the easy direction is perpendicular to the plates. This can be achieved, for instance, by treating the plates with lecithin. Otherwise, this case is analogous to case 1, except that k_{11} and k_{33} have interchanged their roles.

Figure 1 shows plots of ϕ vs $2y/d$ for 4-4′-azoxydianisole (PAA) for all three cases. The curve corresponding to twist can also be used to compare the exact solution to the one-constant approximation ($\kappa = 0$). It becomes clear how to correct the results of the one-constant approximation. For case 1, the exact curve starts off steeper and ends up flatter. Of course that could have been anticipated, since at the boundary k_{11} dominates, while further on k_{33} becomes more important. For case 3, the converse is true. Figure 1 shows also an ordinary sinusoidal curve to facilitate comparison with the linear approximation.

The corresponding curves for N-(p-methoxybenzilidene) p'-butylaniline (MBBA) are not shown, since because of the small difference between the elastic moduli, the curves appear to be almost indistinguishable at the given scale. Hence we conclude that the one-constant approximation will be excellent for MBBA.

II. WILLIAMS DOMAINS

If the nematic sample contains free charge carriers, i.e., impurity ions, the phenomena become much more complicated and interesting. In the geometry of case 1, with an electric field $\vec{E}=(0, E_y, 0)$ applied across the sample, one observes stripes parallel to the z direction. This pattern has become known as Williams domains. We shall not describe the physical model, which is by now familiar and is described in Refs. 1–5. Rather, we focus attention on the specifically nonlinear aspects of the problem.

We are again dealing with a nematic liquid crystal sandwiched between two plane-parallel electrodes across which an electric field $\vec{E}$ is applied. A magnetic field $\vec{H}$ may also be present. To fix ideas, we assume that the nematic molecules in the undisturbed sample are aligned along a well-defined easy direction. We work in the geometry of case 1. Helfrich[5] has shown that the problem is planar in the xy plane.

We choose to calculate the director angle ϕ. Once that is known, other quantities of interest may be computed, and perhaps a self-consistent calculation might even be attempted. For that purpose our solution should serve as the best available trial function.

To begin with, we write the torque densities

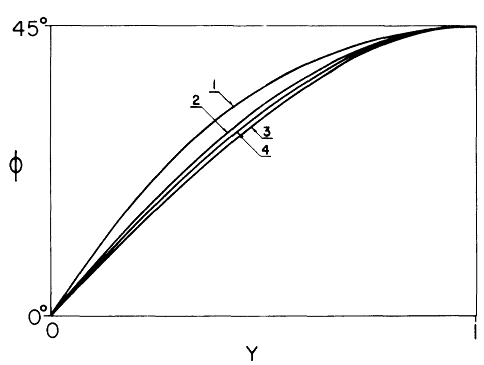

FIG. 1. Director angle ϕ vs reduced distance $Y=2y/d$ for the Fréedericksz transition in PAA. Curve 1: splay-bend ($\kappa_1=1.43$); 2: twist ($\kappa_2=0$); 3: bend-splay ($\kappa_3=0.59$); and 4: linear approximation [$\phi=\phi_0\sin(\frac{1}{2}\pi Y)$]. The amplitude was arbitrarily chosen as $\phi_0=45°$. Curve 2 represents also the one-constant approximation, which for $\phi_0=45°$ should be worst. The corresponding plots for MBBA ($\kappa_1=0.189$, $\kappa_3=-0.159$) are virtually indistinguishable from curve 2.

m_z^S, m_z^P, m_z^H produced, respectively, by viscous shear, dielectric polarization, and magnetic field. According to Helfrich,[5]

$$m_z^S=(\kappa/2\eta)[(\Delta\sigma/\sigma)\epsilon-\Delta\epsilon]E_y^2\sin 2\phi, \quad (2.1)$$

$$m_z^P=\tfrac{1}{2}\Delta\epsilon[(E_y^2-E_x^2)\sin 2\phi-2E_xE_y\cos 2\phi], \quad (2.2)$$

$$m_z^H=-\tfrac{1}{2}\Delta\chi H_x^2\sin 2\phi. \quad (2.3)$$

Here we have introduced the notations

$$\omega=\omega^{\parallel}c^2+\omega^{\perp}s^2,\quad \Delta\omega=\omega^{\parallel}-\omega^{\perp},$$
$$\eta=\eta^{\parallel}c^2+\eta^{*}c^2s^2+\eta^{\perp}s^2, \quad (2.4)$$
$$c=\cos\phi,\quad s=\sin\phi.$$

The symbol ω represents the permittivity ϵ, the conductivity σ, the susceptibility χ, or the shear-torque coefficients $k^{\parallel}=k_1$, $k^{\perp}=k_2$; the viscosity coefficients were denoted by η. For κ and η, parallel ($\parallel$) and perpendicular ($\perp$) refer to the orientation of the velocity gradient with respect to the easy director axis; i.e., in standard notation, $\eta^{\parallel}=\eta_2$, $\eta^{\perp}=\eta_1$.

The distortion torque density is

$$m_z^D=(k_{33}c^2+k_{11}s^2)\frac{\partial^2\phi}{\partial x^2}+(k_{11}c^2+k_{33}s^2)\frac{\partial^2\phi}{\partial y^2}$$
$$+2\Delta k\frac{\partial^2\phi}{\partial x\partial y}-kcs\left[\left(\frac{\partial\phi}{\partial x}\right)^2-\left(\frac{\partial\phi}{\partial y}\right)^2\right]$$
$$+\Delta k(c-s)\frac{\partial\phi}{\partial x}\frac{\partial\phi}{\partial y}. \quad (2.5)$$

The equilibrium of torques yields the equation

$$m_z^D+m_z^S+m_z^P+m_z^H=0. \quad (2.6)$$

Clearly, this is a rather complicated nonlinear partial differential equation. It should be solved subject to the boundary conditions

$$\phi(y=0)=\phi(y=d)=0. \quad (2.7)$$

The solution must, moreover, be consistent with the hydrodynamic and electrodynamic field equations. For the linearized case, Penz and Ford have found just a solution.

It is reasonable to assume that the essential qualitative features of the linearized solution should remain valid at least for moderately large director angles. Therefore we shall postulate that the periodicity conditions derived and discussed by Penz and Ford hold in general, except, perhaps, for minor modifications in the period ratios. In other words, we postulate solutions $\phi(x,y)$ periodic in x and y.

To reduce the problem to manageable size, we introduce a modified one-constant approximation. That is, we set

$$k_x = k_{33}c^2 + k_{11}s^2 = \text{const},$$
$$k_y = k_{11}c^2 + k_{33}s^2 = \text{const}, \quad (2.8)$$
$$\Delta k = 0, \quad \omega = \text{const},$$

but nevertheless admit $\Delta\omega \neq 0$. Even the ordinary one-constant approximation is known to be useful in much simpler cases, so probably this is the best we can do. After completing the solution one can find appropriate mean values for the coefficients. Moreover, the terms neglected because of $\Delta k = 0$ are very small anyway. Consistently we may also set $E_x = 0$. Equation (2.6) then becomes

$$k_x \frac{\partial^2\phi}{\partial_{x^2}} + k_y \frac{\partial^2\phi}{\partial_{y^2}} = A \sin\phi \cos\phi, \quad (2.9)$$

with

$$A = -\Delta\epsilon^{\text{eff}} E_y^2 + \Delta\chi H_x^2,$$
$$\frac{\Delta\epsilon^{\text{eff}}}{\epsilon} = \frac{k}{\eta}\left(\frac{\Delta\epsilon}{\epsilon} + \frac{\Delta\sigma}{\sigma}\right) + \frac{\Delta\epsilon}{\epsilon}. \quad (2.10)$$

The stability of the uniform orientation pattern depends crucially on the sign of A. Helfrich[5] has already discussed this point. With the appropriate values we get for PAA: $\Delta\epsilon/\epsilon \approx -0.03$, $\Delta\epsilon^{\text{eff}}/\epsilon \approx +0.10$; and for MBBA: $\Delta\epsilon/\epsilon \approx -0.15$, $\Delta\epsilon^{\text{eff}}/\epsilon \approx +0.15$. Thus the conductivity clearly governs the instability.

Now we introduce the characteristic (or "coherence") lengths

$$\lambda_x = (2k_x/|A|)^{1/2}, \quad \lambda_y = (2k_y/|A|)^{1/2}, \quad (2.11)$$

and substitute

$$\xi = x/\lambda_x, \quad \eta = y/\lambda_y. \quad (2.12)$$

Then Eq. (2.9) becomes the two dimensional sine-Gordon or Frenkel-Kontorova equation

$$\frac{\partial^2\phi}{\partial\xi^2} + \frac{\partial^2\phi}{\partial\eta^2} \pm 2\sin\phi \cos\phi = 0. \quad (2.13)$$

Equation (2.12) has the obvious trivial solutions

$$\phi = n\pi/2, \quad n = 0, \pm 1, \pm 2, \ldots, \quad (2.14)$$

corresponding to perfect alignment along x (for even n) and along y (for odd n).

An exact periodic solution to (2.13), vanishing at $y = 0$, is[12]

$$\sin\phi = \pm \frac{2k\,\text{sn}((1+k^2)^{1/2}\xi, k)\,\text{sn}((1+k^2)^{1/2}\eta, k)}{1 + k^2\,\text{sn}^2((1+k^2)^{1/2}\xi, k)\,\text{sn}^2((1+k^2)^{1/2}\eta, k)},$$
$$k \in (-\infty, +\infty), \quad (2.15)$$

where $\text{sn}(u, k)$ is the Jacobian elliptic function sine amplitude of argument u and module k. (Unfortunately, k happens to be a much-used letter, but we prefer to adhere to established standards.)

For $|k| > 1$, Eq. (2.15) may be transformed into

$$\sin\phi = \frac{2l\,\text{sn}((1+l^2)^{1/2}\xi/l^2, l)\,\text{sn}((1+l^2)^{1/2}\eta/l^2, l)}{1 + l^2\,\text{sn}^2((1+l^2)^{1/2}\xi/l^2, l)\,\text{sn}^2((1+l^2)^{1/2}\eta/l^2, l)},$$
$$l = 1/k \in \{-1, +1\}. \quad (2.16)$$

For either case, the director angle amplitude is given by

$$\sin\phi_0 = 2k/(1+k^2) = 2l/(1+l^2). \quad (2.17)$$

Thus for each value of the module there are two solutions, one stable, the other unstable. For $A \gtrless 0$, the stable solution corresponds to $|k| \gtrless 1$, respectively. We shall not dwell upon this point here.

The function $\text{sn}(u, k)$ is periodic with the real period $4K$, where K is the complete elliptic integral of the first kind of module k. According to the boundary conditions (2.7), the sample thickness must be a half-period in y. We use these boundary conditions, taking into account (2.10), (2.11), and (2.12). With the inessential simplification $H_x = 0$ we obtain the equations

$$nK(1+k^2)^{-1/2} = (\Delta\epsilon^{\text{eff}}/8k_y)^{1/2} E_y d,$$
$$nl^2 L(L + l^2)^{-1/2} = (\Delta\epsilon^{\text{eff}}/8k_y)^{1/2} E_y d, \quad (2.18)$$
$$n = 0, 1, 2,$$

for the two sets of solutions, respectively. Here K and L denote the complete elliptic integral of the first kind of module k, l, respectively. The first of Eqs. (2.18) then implies, for $n = 1$, $k = 0$, a critical voltage.

$$V^{\text{cr}} = E_y d = \pi(2k_y/\Delta\epsilon^{\text{eff}})^{1/2}. \quad (2.19)$$

Inserting the proper values, we predict $V^{\text{cr}} = 6.8$ V for PAA and $V^{\text{cr}} = 4.5$ V for MBBA. The observed values are[2] 7 and[13] 5 V, respectively.

The dispersion relations (2.18) are plotted in Fig. 2, which shows V/V^{cr} vs the modular angle α and vs the amplitude ϕ_0. Figure 3 shows an example of a map of $\phi = \phi(\xi, \eta)$ for $\phi_0 = 45°$. The dependence of the modular angle α and the module $k = \sin\alpha$ (or $l = \sin\alpha$) upon the amplitude ϕ_0 is shown in Fig. 4.

It can be seen that according to the present model integral multiples of the critical voltage, $V_n = nV^{\text{cr}}$, are again thresholds. At these thresholds new modes appear and thus instabilities are to be expected.

It must be emphasized that the module k is the same for the elliptic functions of both ξ and η. Thus the boundary conditions in the y direction impose periodicity in the x direction. This effect is essentially nonlinear. A whole class of nonli-

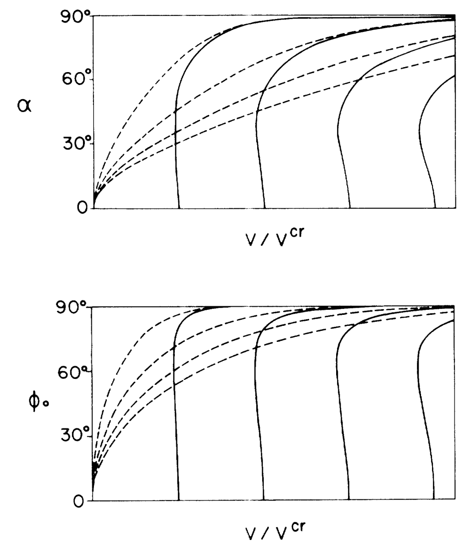

FIG. 2. (a) Modular angle α and (b) director angle amplitude ϕ_0 vs reduced voltage $V/V^{cr} = E/E^{cr}$. The first four stable (solid line) and unstable (dashed line) modes are shown.

near equations, of which the sine-Gordon equation is a typical example, exhibits effects of this kind.[14,15]

This seems to be a paradox, since the problem has translational symmetry in the x direction. Yet this is just the common phenomenon of broken symmetry, familiar even within the context of liquid crystals. After all, the symmetry argument cannot be carried too far, since in the real sample there are of course boundary conditions in the x direction which may well uniquely determine the origin, albeit in an uncontrolled manner.

Penz[8] claims that the x period is determined by the "fastest-growing solution." Although I have

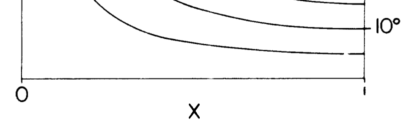

FIG. 3. Height map of the function $\phi(X=\xi/\xi_0, Y=\eta/\eta_0)$, for amplitude $\phi_0 = 45°$. (ξ_0, η_0) are the coordinates of the crest. The coordinate scales are not necessarily equal, since in general $\lambda_x \neq \lambda_y$.

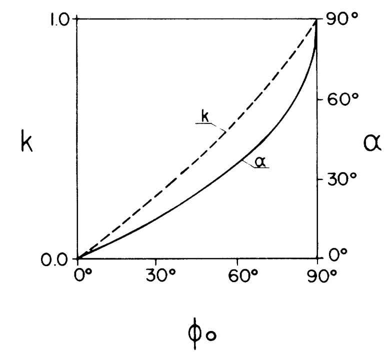

FIG. 4. Module k and modular angle α vs director angle amplitude ϕ_0.

not yet studied this point in detail, I believe that these two aspects may well be reconciled. Our solution holds for the steady state at high amplitudes and predicts their saturation. Penz's linear dynamic solution describes the buildup of the pattern and should be adequate at least at the beginning, when the distortions are still small. It is quite plausible that the fastest growing solution will tend to that stationary one which is stable.

III. HOMEOTROPIC DOMAINS

Greubel and Wolff,[16] as well as Schiekel and Fahrenschon,[17] have observed domain patterns under homeotropic boundary conditions, i.e., with an easy direction perpendicular to the capacitor plates. Penz and Ford[4] suggested that this pattern be called the homeotropic domain mode. This situation corresponds to case 3 of the Freedericks transition.

This time the y axis of the Cartesian coordinate system is parallel to the applied electric and magnetic fields and to the easy direction, while the mutually perpendicular x and z axes are parallel to the plates but may be rotated through an arbitrary angle. The director angle deviation ϕ is from the y axis.

We again start with the torque densities

$$m_z^S = (\kappa'/2\eta')[(\Delta\sigma'/\sigma')\epsilon' - \Delta\epsilon']E_y^2 \sin 2\phi, \qquad (3.1)$$

$$m_z^P = \tfrac{1}{2}\Delta\epsilon'[(E_y^2 - E_x^2)\sin 2\phi - 2E_xE_y\cos 2\phi], \qquad (3.2)$$

$$m_z^H = -\tfrac{1}{2}\Delta\chi H_y^2 \sin 2\phi, \qquad (3.3)$$

$$m_z^D = (k_{11}c^2 + k_{33}s^2)\frac{\partial^2\phi}{\partial x^2} + (k_{33}c^2 + k_{11}s^2)\frac{\partial^2\phi}{\partial y^2} + 2\Delta k'\frac{\partial^2\phi}{\partial x\partial y} - \Delta k' cs\left[\left(\frac{\partial\phi}{\partial x}\right)^2 - \left(\frac{\partial\phi}{\partial y}\right)^2\right] + \Delta k'(c^2 - s^2)\frac{\partial\phi}{\partial x}\frac{\partial\phi}{\partial y}. \qquad (3.4)$$

The parameters are defined as before, except that the prime denotes the interchange $(\|) \rightarrow (\perp)$, $(11) \rightarrow (33)$. Clearly, keeping this modification in mind, the arguments of Sec. II hold exactly.

It is worthwhile to note that the problem as formulated now has rotational symmetry around the y axis as well as translational symmetry in any direction within the xz plane. Nevertheless, one observes well-defined parallel domains. This is even more paradoxical than the static Williams domain pattern. The explanation obviously must be that in laboratory practice these symmetries are never exact. Minute deviations from symmetry determine the establishment of some particular pattern. In this sense then, the fastest-growing solution comes into play.

IV. FURTHER DISCUSSION

According to Fig. 2, the domain pattern sets in with a relatively high director amplitude which hardly changes with further increases in the applied voltage, until the next higher instability is reached. Our model predicts values of ϕ_0 above 60°, which should be compared to 45° from optical and resistance measurements, as reported by Penz.[2] The rather too high value of ϕ_0 is clearly an artifact of our approximation in which all coefficients ω were taken to be constant [cf. Eq. (2.8)]. Carroll[18] has shown how to correct this deficiency. Very roughly speaking, one should replace in the results $\sin\phi$ by $\tan\phi$. If such an approach is to be taken seriously, we predict $\phi_0^{cr} = 41°$. Moreover, we find that ϕ_0 remains always less than 45°. At any rate, the data are rather uncertain and the calculated value of ϕ_0 should not be taken too seriously.

We also note that at the threshold amplitude $\phi_0 \approx 62°$, $k \approx \sin 37°$, and consequently the sn function is still virtually indistinguishable from an ordinary sine function (cf. Fig. 1). Hence the linear analysis should not be in significant error. This ought to be the ultimate justification for the calculations by Penz and Ford.[4,6,7] Hence our stipulation of their periodicity conditions is sustained.

An interesting novel feature of the dispersion relations (2.18) is the S shape of the stable curve, with a minimum of V/V^{cr} at $V \approx 0.955 V^{cr}$ and $\phi_0 \approx 62°$. Hence it follows that in the present approximation the transition becomes of *first order*, albeit only weakly. This does not seem to be supported by experiment and is probably an artifact of the introduced simplifications.

APPENDIX A: SOLUTION OF EQ. (1.6)

To solve the equation

$$\frac{d^2\phi}{d\eta^2} = -\frac{1+\kappa(d\phi/d\eta)^2}{1+\kappa\sin^2\phi}\sin\phi\cos\phi, \quad \text{(A1)}$$

we observe that

$$(\phi'^2)' = 2\phi'\phi'', \quad \text{(A2)}$$

where the primes denote derivatives with respect to the argument η. We also substitute

$$s = \sin\phi, \quad ds = \cos\phi\, d\phi. \quad \text{(A3)}$$

Thus we obtain

$$\frac{d\phi'}{1+\kappa\phi'^2} = -\frac{2s\,ds}{1+\kappa s^2} = -\frac{d(s^2)}{1+\kappa s^2}. \quad \text{(A4)}$$

A trivial integration yields

$$1+\kappa\phi'^2 = C/(1+\kappa s^2). \quad \text{(A5)}$$

The integration constant is determined from the condition that the director amplitude ϕ_0 be an extremum value,

$$\phi = \phi_0, \quad \phi' = 0. \quad \text{(A6)}$$

Thus

$$C = 1+\kappa\sin^2\phi_0. \quad \text{(A7)}$$

Then

$$\phi'^2 = (\sin^2\phi_0 - \sin^2\phi)/(1+\kappa\sin^2\phi), \quad \text{(A8)}$$

and hence

$$d\eta = d\phi\left(\frac{1+\kappa\sin^2\phi}{\sin^2\phi_0 - \sin^2\phi}\right)^{1/2}. \quad \text{(A9)}$$

Now we substitute

$$\sin\phi = \sin\phi_0 \sin\psi. \quad \text{(A10)}$$

Then

$$\eta - \eta_0 = \int_0^\psi d\psi\left(\frac{1+\kappa\sin^2\phi_0\sin^2\psi}{1-\sin^2\phi_0\sin^2\psi}\right)^{1/2}. \quad \text{(A11)}$$

The nonessential integration constant η_0 only fixes the origin and can be discarded. The right-hand side can be evaluated in terms of the elliptic integral of the third kind, $\Pi(n;\Phi\backslash\alpha)$ in standard notation.[19,20] Thus we finally obtain (cf. formula 284.02 of Ref. 19.)

$$\eta = (1+\kappa\sin^2\phi_0)^{-1/2}\,\Pi(n;\Phi\backslash\alpha), \quad \text{(A12)}$$

with the substitutions

$$\sin\Phi = \sin\phi(1+\kappa\sin\phi_0)^{1/2}/\sin\phi_0(1+\kappa\sin^2\phi)^{1/2},$$
$$n = \kappa\sin^2\phi_0/(1+\kappa\sin^2\phi_0), \quad \text{(A13)}$$
$$\sin^2\alpha = (1+\kappa)\sin^2\phi_0/(1+\kappa\sin^2\phi_0).$$

Actually, Eq. (A11) is better suited for numerical computations.

The director angle takes its maximum value ϕ_0 midway through the slab, where $y = \frac{1}{2}d$. Substituting into (A12)

$$\eta = \tfrac{1}{2}(\Delta\chi/k_n)^{1/2}Hd, \quad \phi = \phi_0 \quad \text{(A14)}$$

we get an equation determining ϕ_0 as a function of H:

$$\tfrac{1}{2}(\Delta\chi/k_{11})^{1/2}Hd = (1+\kappa\sin^2\phi_0)^{-1/2}\Pi(n\backslash\alpha), \quad (A15)$$

where

$$\Pi(n\backslash\alpha) = \Pi(n;\tfrac{1}{2}\pi\backslash\alpha) \quad (A16)$$

is the complete elliptic integral of the third kind.[19,20] This exactly reproduces Saupe's result [Eq. (5) of Ref. 10].

APPENDIX B: INVERSION

Equation (A12) determines η as a function of ϕ. However, we are interested in the inverse function $\phi(\eta)$.

Consider the elliptic integral of the third kind

$$v = \Pi(n;\Phi\backslash\alpha) = \int_0^\Phi \frac{d\phi}{(1-n\sin^2\phi)(1-\sin^2\alpha\sin^2\phi)^{1/2}}. \quad (B1)$$

We define an elliptic function of the third kind as the inverse function

$$\Phi = \mathrm{ap}(n;v\backslash\alpha). \quad (B2)$$

This is an analog and a generalization of the Jacobian function $\mathrm{am}(v\backslash\alpha)$. Indeed, for $n=0$

$$\mathrm{ap}(0;v\backslash\alpha) = \mathrm{am}(v\backslash\alpha). \quad (B3)$$

We further define the function

$$\mathrm{sp}(n;v\backslash\alpha) = \sin\,\mathrm{ap}(n;v\backslash\alpha). \quad (B4)$$

In an analogous fashion one could define the functions cp, dp, etc. Again we have

$$\mathrm{sp}(0;v\backslash\alpha) = \mathrm{sn}(v\backslash\alpha). \quad (B5)$$

With these definitions we obtain from (A12)

$$\frac{\sin\phi}{\sin\phi_0} = \frac{\mathrm{sp}(n;(1+\kappa\sin^2\phi_0)^{1/2}\eta\backslash\alpha)}{[(1+\kappa\sin^2\phi_0)-\kappa\sin^2\phi_0\,\mathrm{sp}^2(n;(1+\kappa\sin^2\phi_0)^{1/2}\eta\backslash\alpha)]^{1/2}}, \quad (B6)$$

or, in a form easy to remember,

$$\kappa\sin\phi = \gamma\,\mathrm{sp}/(1-\gamma^2\,\mathrm{sp}^2)^{1/2}, \quad (B7)$$

where, of course, sp takes the arguments indicated in (B6) and $\gamma = n^{1/2}$.

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