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# Analytical approach to V-shaped characteristics in antiferroelectric liquid crystal displays

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Not only in ferroelectric liquid crystal displays (LCDs), but also in antiferroelectric LCDs, grey levels are possible by actively addressing the 'continuous director rotation mode'. For ferroelectric LCDs this was shown qualitatively and quantitatively in previous articles. In this article it is shown that an exact analytical approach is also possible for antiferroelectric LCDs. In two consecutive layers the director orientations are symmetric, and at zero voltage they are in a splayed state. The conditions on alignment layer thickness and interaction coefficients are related to those of ferroelectric liquid crystal but are easier to fulfill.

#### 1. Introduction

For antiferroelectric liquid crystals there has been discussion as to whether thresholdless V-shaped characteristics are possible [1]. In this discussion an approximate theory, the so-called uniform  $\varphi$ -theory, plays an important role [2], in which the orientation of the layer polarization is considered to be independent of the depth within the liquid crystal cell. This theory often gives a qualitative insight into what is happening. The so-called symmetrical up-state (SU) plays an important role in explaining V-shaped characteristics [3]. If one has applied a sufficiently strong positive voltage, and thus has set the liquid crystal in the ferroelectric up-state (FU) and then lets V gradually decrease, one first goes over to the SU-state, with the polarization in two successive layers symmetrical with respect to the field direction. If one succeeds in remaining in this state until V = 0, an alternating state (or antiferroelectric state) results, with both polarizations parallel to the electrodes. We shall call this state the continuous director rotation state (CDR) because it gives rise to the thresholdless V-shaped characteristics. If the liquid crystal does not remain in the SU-state but switches to the normal alternating state (NA) with both polarizations perpendicular to the electrodes, then the normal tri-state switching with thresholds and hysteresis is observed.

The careful study of the SU-state is thus important. We found that it is not necessary to use the (approximate)

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uniform  $\varphi$ -theory, but that an exact analytical solution is possible, at least in the bookshelf geometry, and if one neglects dielectric anisotropy. This is not always justified but we think its influence is negligible at the small voltages where V-shape characteristics take place.

The derivation of the equations of motion and of the stationary states always starts from an energy expression. Two approaches are used in the literature. Either one solves the problem with a computer program without avoiding complexity, or alternatively, one tries to find analytical solutions and so seeks to avoid non-essential complexity. Nakagawa [4] and De Meyere and Dahl [5] have studied the shape of the chevron structure and tried to develop the most general energy expression. Sabater and Oton [6, 7] also used a very general expression and include a chevron structure, bending and motion of the chevron tip, dielectric anisotropy, etc. The controversy over V-shaped switching in ferroelectrics and antiferroelectrics was not known at that time. In this respect the polar interaction with the alignment layers plays a crucial role, and this was not included by Sabater and Oton [6,7]. Fornier et al. [8] used a somewhat less general model but did briefly study the influence of polar interaction.

Mottram and Elston [9, 10] more or less follow our approach. They try to gain as much insight as possible using analytical solutions, and thus reduce the energy expression to its essential components. Even if they use computer solutions, they start from these simple energy expressions. We will later compare their results with ours. The energy expression we use is the Gibbs free energy (per unit area),

$$2G = \int \frac{1}{2} \alpha \left[ \left( \frac{\partial \varphi_1}{\partial x} \right)^2 + \left( \frac{\partial \varphi_2}{\partial x} \right)^2 \right] dx$$
$$+ \int A \cos(\varphi_1 - \varphi_2) dx + 2F_s$$
$$+ \int (-EP \cos \varphi_1 - EP \cos \varphi_2 - \varepsilon \varepsilon_0 E^2) dx$$

where  $\varphi_1$  and  $\varphi_2$  are the azimuthal angles of the directors in two successive layers. The term containing A describes the antiferroelectric interaction; Mottram and Elston [9] recognized that we were the first to use such an expression. The term containing  $\alpha$  supposes a single elastic constant ( $K_1 = K_2 = K_3$ ). This isotropic elasticity assumption also assumes that the elasticity may be taken as nematic-like within the smectic layer. The term  $F_s$ describes the interaction energy with the alignment layers and contains a non-polar and a polar interaction term:  $\gamma_1 \sin^2 \varphi \pm \gamma_2 \cos \varphi$  at the top and bottom alignment layer and for both  $\varphi_1$  and  $\varphi_2$ .

In deriving the Euler-Lagrange equations, it was proved in [11] that E may be considered as invariable, although it depends on  $\varphi_1$  and  $\varphi_2$  through Maxwell's equations. However the solutions of these Euler-Lagrange equations maximise G at constant potential over the cell. One may also treat E as a function of  $\varphi_1$ ,  $\varphi_2$ . One ends up with the same equations of motion but in an unnecessarily complicated form. Several authors prefer to follow the latter approach so their equations look more complicated than ours. In particular the term in  $E^2$  has no influence on the equation of motion provided one neglects anisotropy.

#### 2. Analytical solution

In figure 1 the situation of the SU-state is represented, and this assumes the bookshelf structure. The smectic layer planes are parallel to the figure plane. There is a bulk state with uniform orientations of the polarizations, and two surface layers where the polarizations tend to turn into the alignment layers. These are indicated between the dashed lines. Finally there are the two alignment layers with thickness  $d_a$  and the top and bottom electrodes indicated by the bold lines.

The non-stationary equations are [12–14], according to Euler–Lagrange,

$$\eta \frac{\partial \varphi_1}{\partial t} = \alpha \frac{\partial^2 \varphi_1}{\partial x^2} - EP \sin \varphi_1 + A \sin(\varphi_1 - \varphi_2) \quad (1 a)$$

$$\eta \frac{\partial \varphi_2}{\partial t} = \alpha \frac{\partial^2 \varphi_2}{\partial x^2} - EP \sin \varphi_2 + A \sin(\varphi_2 - \varphi_1) \quad (1 b)$$



Figure 1. The symmetrical up-state (SU). The smectic layer planes are parallel to the figure plane. In the bulk the orientation of the polarizations are uniform but at the surface they tend to point into the alignment layers. These surface layers are indicated by dashed lines. Finally the alignment layers with total thickness  $d_a$  are indicated and the top and bottom electrodes by the bold lines.

with the boundary conditions

$$\alpha \frac{\partial \varphi}{\partial x} = \gamma_1 \sin 2\varphi - \gamma_2 \sin \varphi \quad (\text{at bottom}) \qquad (2 a)$$

$$\alpha \frac{\partial \varphi}{\partial x} = -\gamma_1 \sin 2\varphi - \gamma_2 \sin \varphi \quad (\text{at top}) \qquad (2 b)$$

for both  $\varphi_1$  and  $\varphi_2$ . The parameters  $\gamma_1$ ,  $\gamma_2$ , A,  $\eta$  and  $\alpha$  are the non-polar and the polar interaction coefficient, the antiferroelectric interaction coefficient, the viscosity and the elastic constant respectively.

The symmetrical up-state is characterized by  $\varphi_2 = -\varphi_1$ for all x, and thus also in the surface layers. This also implies that the problem is one-dimensional since the polarization charges in consecutive layers are identical. The stationary equation,  $\partial \varphi / \partial t = 0$  with  $\varphi_1 = -\varphi_2 = \varphi$  is

$$\alpha \frac{\partial^2 \varphi}{\partial x^2} = EP \sin \varphi - A \sin 2\varphi \qquad (3a)$$

where

$$\varepsilon \varepsilon_0 E = D - P \cos \varphi \tag{3b}$$

with D independent of x. The uniform bulk solution,  $\varphi$  independent of x, obeys

$$(D - P \cos \varphi_{u})P = 2\varepsilon\varepsilon_{0}A \cos \varphi_{u}$$

$$D = P \cos \varphi_{u} \left( 1 + \frac{2\varepsilon\varepsilon_{0}A}{P^{2}} \right)$$
(4 a)

and

$$E_{\rm u} = \frac{2A}{P} \cos \varphi_{\rm u}. \tag{4b}$$

In the surface layers, we multiply equation (3 *a*) with  $\varepsilon \varepsilon_0 d\varphi/dx$ , giving rise to

$$\frac{\varepsilon\varepsilon_0 \alpha}{2} \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\mathrm{d}\varphi}{\mathrm{d}x}\right)^2$$

$$= (D - P\cos\varphi) \frac{\mathrm{d}}{\mathrm{d}x} (-P\cos\varphi) + 2A\varepsilon\varepsilon_0 \cos\varphi \frac{\mathrm{d}\cos\varphi}{\mathrm{d}x}$$

$$= \left[D - P\cos\varphi - \frac{2A\varepsilon\varepsilon_0}{P}\cos\varphi\right] \frac{\mathrm{d}}{\mathrm{d}x} (-P\cos\varphi)$$

$$= \left[D - P\cos\varphi - \frac{2A\varepsilon\varepsilon_0}{P}\cos\varphi\right] \frac{\mathrm{d}}{\mathrm{d}x}$$

$$\times \left[D - P\left(1 + \frac{2A\varepsilon\varepsilon_0}{P^2}\right)\cos\varphi\right] \frac{1}{1 + \frac{2A\varepsilon\varepsilon_0}{P^2}}$$

from which we obtain

$$(\varepsilon\varepsilon_{0}\alpha)^{1/2}\frac{\mathrm{d}\varphi}{\mathrm{d}x}$$

$$=\pm\frac{1}{\left(1+\frac{2A\varepsilon\varepsilon_{0}}{P^{2}}\right)^{1/2}}\left[D-P\left(1+\frac{2A\varepsilon\varepsilon_{0}}{P^{2}}\right)\cos\varphi\right]$$

$$=\pm P\left(1+\frac{2A\varepsilon\varepsilon_{0}}{P^{2}}\right)^{1/2}(\cos\varphi_{u}-\cos\varphi)$$
(5)

where the bulk equation (4a) has been taken into account. This equation can be solved analytically (see equations (8) of [13]), but for the stability investigations we need only an integral, i.e. the voltage over the cell. This voltage can be calculated from equations (3b) and (4a):

$$V = \frac{D}{\varepsilon_{a}\varepsilon_{0}}d_{a} + \int_{0}^{d} \frac{P}{\varepsilon\varepsilon_{0}}(\cos\varphi_{u} - \cos\varphi)\frac{1}{d\varphi/dx}d\varphi + \frac{2A}{P}d\cos\varphi_{u}.$$

In this equation  $\varepsilon_a$  is the isotropic dielectric constant of the alignment layers.

From equation (5) it then follows

$$V = \cos \varphi_{u} \left[ P \left( 1 + \frac{2\varepsilon\varepsilon_{0}A}{P^{2}} \right) \frac{d_{a}}{\varepsilon_{a}\varepsilon_{0}} + \frac{2A}{P} d \right]$$
$$- \left( \frac{\alpha}{\varepsilon\varepsilon_{0}} \right)^{1/2} \frac{1}{\left( 1 + \frac{2\varepsilon\varepsilon_{0}A}{P^{2}} \right)^{1/2}} (2\varphi_{u} - \varphi_{b} - \varphi_{t}). \quad (6)$$

In these equations  $\varphi_u$ ,  $\varphi_b$  and  $\varphi_t$  are the  $\varphi$ -values in the uniform bulk, the bottom surface and at the top surface respectively. In figure 2, two cases of  $\varphi$ -distributions and the corresponding  $\cos \varphi$  distributions are shown. These are qualitative figures, not calculated ones. In the first case the polarization is pointing out of the alignment layer at the bottom side, and pointing into the alignment layer at the top side. It is a case of weaker polar interaction. The voltage over the cell is considered to be positive. In the second case the polarization is pointing into the alignment layer at both sides. It is a case of stronger polar interaction and corresponds to V = 0 with the CDR state.

#### 3. Stability

If one begins in the ferroelectric-up state for a sufficiently strong positive voltage and then gradually lowers the voltage, a state of type 1 as represented in figure 2 is obtained. If one stays in this type 1 state up to V = 0, one does not end up in the CDR-state. It is only a solution of type 2, where both consecutive layers are in a splayed state, that is the CDR-state that gives rise to V-shaped characteristics.

If  $\varphi$  of the type 1 solution increases, the voltage V decreases but at a certain point starts to increase again. In [15] and also later in [2] it is clearly shown that then the weaker surface, in this case the bottom surface, jumps over to the type 2 situation, thus giving rise to a



Figure 2.  $\varphi$ -distributions and  $\cos \varphi$ -distributions at weak (1) and strong (2) polar interaction.

splayed state. We want this to happen before reaching V = 0. We therefore want to investigate when at V = 0 a type 1 solution becomes unstable and jumps over to a type 2 solution. This requires  $\varphi_b$  and  $d_a$  to be such that V is both zero and minimum as a function of  $\varphi$ . This implies that fV is a maximum, where f is arbitrary. Indeed

$$\frac{\mathrm{d}fV}{\mathrm{d}\varphi} = \frac{\mathrm{d}f}{\mathrm{d}\varphi}V + f\frac{\mathrm{d}V}{\mathrm{d}\varphi} = 0 + 0 = 0.$$

If f is negative, fV should be a maximum as a function of  $\varphi$ . It therefore follows that

$$y = \frac{2\varphi_{u} - \varphi_{b} - \varphi_{t}}{\cos \varphi_{u}}$$
$$= \left(\frac{\varepsilon\varepsilon_{0}}{\alpha}\right)^{1/2} \left(1 + \frac{2A\varepsilon\varepsilon_{0}}{P^{2}}\right)^{1/2} P$$
$$\times \left[\frac{d_{a}}{\varepsilon_{a}\varepsilon_{0}} \left(1 + \frac{2A\varepsilon\varepsilon_{0}}{P^{2}}\right) + \frac{2A}{P^{2}}d\right]$$
(7)

should be a maximum as a function of  $\varphi_b$ . It is possible, but difficult, to prove that  $\varphi$  at any x is a monotonous function of  $\varphi_b$ . This maximum can be found from equations (2 *a*) and (5) by a simple computer program:

$$\alpha \frac{\partial \varphi}{\partial x} = \gamma_1 \sin 2\varphi_{\rm b} - \gamma_2 \sin \varphi_{\rm b}$$
$$= -(\cos \varphi_{\rm u} - \cos \varphi_{\rm b}) \left(1 + \frac{2\varepsilon\varepsilon_0 A}{P^2}\right)^{1/2} \frac{P\alpha}{(\varepsilon\varepsilon_0 \alpha)^{1/2}} \quad (8)$$

from which we obtain  $\varphi_u$ , and from equations (2 b) and (5)

$$\alpha \frac{\partial \varphi}{\partial x} = -\gamma_1 \sin 2\varphi_t - \gamma_2 \sin \varphi_t$$
$$= (\cos \varphi_u - \cos \varphi_t) \left(1 + \frac{2\varepsilon\varepsilon_0 A}{P^2}\right)^{1/2} \frac{P\alpha}{(\varepsilon\varepsilon_0 \alpha)^{1/2}} \quad (9)$$

from which we obtain  $\varphi_t$  by iteration. If this maximum value of y is found as a function of

$$x = \left(\frac{\varepsilon\varepsilon_0}{\alpha}\right)^{1/2} \frac{\gamma_1}{P} \frac{1}{\left(1 + \frac{2\varepsilon\varepsilon_0 A}{P^2}\right)^{1/2}}$$
(10)

for various values of  $\gamma = \gamma_2/\gamma_1$ , we can find the stability criterion as shown in figure 3.

#### 4. Discussion

If the representative point (x, y) lies below the curve corresponding with a given  $\gamma = \gamma_2/\gamma_1$ , the liquid crystal will remain at V = 0 in the type 1 state, and thus will not give rise to V-shaped characteristics. If instead the



Figure 3. Stability criterion at V = 0 for antiferroelectric liquid crystals. The coordinates x and y are defined in equations (10) and (7), respectively.

representative point (x, y) lies above the curve corresponding with a given  $\gamma$ , the liquid crystal will end up in the type 2 state at V = 0, and thus give rise to V-shaped characteristics.

Note that figure 3 is exactly the same as the curves determined for a ferroelectric liquid crystal in [15], except that the parameters x and y have a different expression in the antiferroelectric case. The antiferroelectric case reduces to the ferroelectric case if one sets the antiferroelectric interaction coefficient A equal to zero. The main influence of A lies in the term proportional to d in the square brackets of equation (7), which puts the representative point (x, y) almost always above the corresponding curve, even for zero alignment layer thickness  $d_a$ . A numerical example will make this clearer. We take  $P = 100 \text{ nC cm}^{-2} = 10^{-3} \text{ Cm}^{-2}, \ \alpha = 4 \times 10^{-12} \text{ Nm}^{-1}$  $d = 10^{-6}$  m,  $d_a = 100$  nm  $= 10^{-7}$  m, A = 1500 N m<sup>-2</sup>,  $\varepsilon = \varepsilon_{a} = 5$ ,  $2A\varepsilon\varepsilon_{0}/P^{2} = 0.15$ ,  $\gamma_{1} = \gamma_{2} = 2.4 \times 10^{-4} \text{ N m}^{-1}$ which leads to x = 0.78, y = 20 = 43% contribution of  $d_{\rm a}$  and 57% contribution of d. From figure 3 one sees that  $y_{cr} = 3$ , so that we are far above  $y_{cr}$  and thus in the CDR state.

We conclude that V-shaped characteristics occur more easily in antiferroelectric liquid crystals than in ferroelectric liquid crystals.

In order to place this result in the context of the literature, we first need to discuss the work of Mottram and Elston [10]. They impose (infinitely) strong boundary conditions  $\varphi = n\pi$ , both polar and non-polar, and use a computer program to calculate minimum energy states. They find three types of solutions which we call: the splayed ferroelectric state ( $\varphi_1 = \varphi_2$ ), the splayed antiferroelectric state ( $\varphi_2 = -\varphi_1$ ) and the normal antiferroelectric

state with the polarizations perpendicular to the substrate. The splayed antiferroelectric state corresponds to the state we are investigating and which we called the SU state of both type 1 and 2. They find that the splayed antiferroelectric state is the most stable.

These discussions belong to the field of V-shaped characteristics. The earlier work on antiferroelectric switching did not deal with this since it was not yet discovered. Fukuda and coworkers [16] explain it as being associated with statistical fluctuations of the  $\varphi$ -orientation, but this is rejected by most non-Japanese authors [1]. Lagerwall, Clark and coworkers [1] support the splayed ferroelectric state. Ourselves and Mottram and Elston [10] are the only researchers proposing the antiferroelectric splayed state. Because their boundary conditions are infinitely strong, their result corresponds with our case  $\gamma = \gamma_2/\gamma_1 > 2$ . Our result is much more general, but the method only works if one supposes *a priori* that one follows the SU state. This can only be verified by computer simulations which were presented in [17, 18].

In this article we did not want to solve the controversies about V-shaped modelling. We only wanted to stress that for the SU state an analytical solution exists, and allows the parameter determination that permits V-shaped characteristics.

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