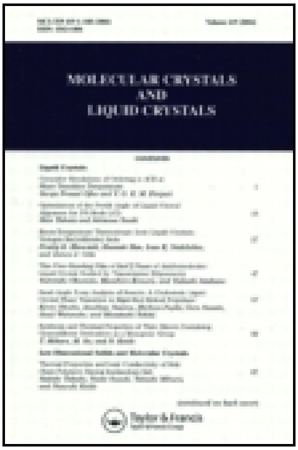

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STATIC DOMAIN WALL SOLUTIONS FOR SMECTIC C LIQUID CRYSTALS

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The continuum theory for smectic C liquid crystals proposed by Leslie et al. [1] is used to discuss static domain wall solutions in infinite samples in both cylindrical and planar geometry under applied fields. As the azimuthal magnetic field strength increases in an infinite sample of concentric, cylindrical layers arranged with a fixed inner radius, two critical values may occur where the solution changes some of its properties. The application of these results to the possible experimental determination of some of the elastic constants is discussed. The occurrence of domain walls may indicate the relative magnitudes of the combinations of the constants $A_{12} - A_{21}$ and $A_{12} + A_{21} + 2A_{11}$ and, in a special case, can indicate when $A_{12} \approx A_{21}$.

Keywords: domain walls; smectic *C*; smectic elastic constants

INTRODUCTION

Liquid crystals consist of elongated rigid molecules for which the long molecular axes locally adopt a preferred direction described by the unit vector **n**, called the director. Smectic *C* liquid crystals are layered structures for which the director **n** makes an angle θ with respect to the layer normal. The smectic tilt angle θ is here taken to be constant and the layers are assumed to be equidistant. To describe a smectic *C* liquid crystal de Gennes introduced a unit layer normal **a** and a unit vector **c**, which is

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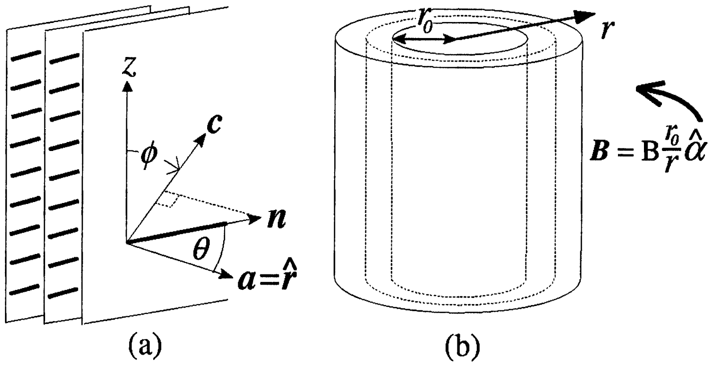

FIGURE 1 The director **n** makes an angle θ with the layer normal **a** as shown in (a). The z axis coincides with the axis of the concentric cylinders with inner radius r_0 shown in (b). The local arrangement of the equidistant cylindrical layers is depicted in (a) where **a** coincides with the radial direction $\widehat{\mathbf{r}}$. The orientation angle of the c-director **c** within the smectic planes is denoted by ϕ.

the unit orthogonal projection of **n** onto the smectic layers (see de Gennes and Prost [2]). The orientation of **n** can be deduced from the orientation angle ϕ of **c** measured within the smectic planes (see Fig. 1(a)). The continuum theory proposed by Leslie *et al.* [1,3] is used in this article. We summarise some applications of this theory to domain wall solutions in cylindrical and planar geometries and extend earlier work.

CYLINDRICAL LAYERS

For an infinite sample in which layers form concentric cylinders and are arranged with a fixed inner radius $r_0 > 0$, (see Fig. 1(b)), it is convenient to introduce the cylindrical polar coordinate system (r, α, z) with base vectors $\widehat{\mathbf{r}}$, $\widehat{\boldsymbol{\alpha}}$, $\widehat{\mathbf{z}}$; r measures the radial distance and $\widehat{\mathbf{r}}$ coincides with the layer normal **a**. The z-axis is coincident with the common axis of the cylinders and α is the usual polar angle. In the geometry of Figure 1 we seek solutions for the orientation angle $\phi = \phi(r)$ of the c-director where

$$\mathbf{a} = \widehat{\mathbf{r}}, \quad \mathbf{c} = \widehat{\boldsymbol{\alpha}} \sin \phi + \widehat{\mathbf{z}} \cos \phi, \tag{1}$$

and the director **n** is given by

$$\mathbf{n} = \mathbf{a} \cos \theta + \mathbf{c} \sin \theta = \widehat{\mathbf{r}} \cos \theta + \widehat{\boldsymbol{\alpha}} \sin \theta \sin \phi + \widehat{\mathbf{z}} \sin \theta \cos \phi. \tag{2}$$

As outlined in articles [4,5], for this solution the bulk energy, w_b, is

$$w_b = \frac{1}{2r^2}\{(A_{12}+A_{11})\sin^4\phi + (A_{21}+A_{11})\cos^4\phi - A_{11}\} + \frac{1}{2}B_3\{\phi'(r)\}^2. \quad (3)$$

The elastic constants A_{11}, A_{12}, A_{21} and B_3, are related to those introduced by the Orsay Group [6], except that here $A_{11} = -\frac{1}{2}A_{11}^{Orsay}$, and are interpreted physically in Carlsson *et al.* [7]. The first bracket of terms in (3) is connected with the bending of the layers and B_3 is associated with a reorientation of the director within the layers as an observer travels from layer to layer. Among other related inequalities, these constants satisfy (cf. [4,7])

$$A_{12}, A_{21}, B_3 > 0, \qquad A_{12} + A_{21} \pm 2A_{11} > 0. \quad (4)$$

Apart from the contribution $-A_{11}/r^2$, the A_{ij} constants enter the bulk energy in the two combinations $A_{12} + A_{11}$ and $A_{21} + A_{11}$. To satisfy $(4)_4$ these two combinations cannot both be negative and so there are three possibilities which can occur: both combinations can be positive or they are of opposite sign.

For a magnetic field **B** the magnetic energy, w_m, is taken as

$$w_m = -\frac{1}{2}\frac{\Delta\chi}{\mu_0}(\mathbf{n}\cdot\mathbf{B})^2, \qquad \mathbf{B} = B\frac{r_0}{r}\hat{\boldsymbol{\alpha}}, \quad (5)$$

where μ_0 is the permeability of free space, $\Delta\chi$ is the magnetic susceptibility of the liquid crystal, and B is the magnetic field strength at $r = r_0$. It will be assumed here that $\Delta\chi > 0$, indicating that the director has a preference to align parallel to **B**. This field may be achieved by passing an electric current along a wire situated along the z-axis. The total energy W over a sample region $\boldsymbol{\Omega}$ is

$$W = \int_{\boldsymbol{\Omega}} (w_b + w_m) r \, dr d\alpha dz. \quad (6)$$

The governing equilibrium equation derived from the aforementioned continuum theory is (Atkin and Stewart [4, Eq. (72)])

$$B_3\left[r^2\frac{d^2\phi}{dr^2} + r\frac{d\phi}{dr}\right] - 2(A_{12}+A_{21}+2A_{11})\sin^3\phi\cos\phi$$
$$+ \left[2(A_{21}+A_{11}) + \frac{\Delta\chi}{\mu_0}B^2 r_0^2 \sin^2\theta\right]\sin\phi\cos\phi = 0. \quad (7)$$

Introducing a new variable s defined by $s = \ln(r/r_0)$, and setting

$$a = \frac{1}{B_3}\left(A_{12} - A_{21} - \frac{\Delta\chi}{\mu_0}B^2 r_0^2 \sin^2\theta\right), \; b = \frac{1}{2B_3}(A_{12}+A_{21}+2A_{11}), \quad (8)$$

Eq. (7) may be rewritten in the more amenable form

$$\frac{d^2\psi}{ds^2} = a\sin\psi - b\sin(2\psi), \qquad \text{where} \qquad \psi = 2\phi. \tag{9}$$

From (4) it follows that $b > 0$ while the sign of a is indeterminate.

PLANAR LAYERS

Equation (9) arises when an electric field is applied to an infinite sample at an angle α $\left(0 < \alpha < \frac{\pi}{2}\right)$ to planar aligned layers of smectic C. Taking axes with the layers parallel to the xy-plane and the layer normal parallel to the z-axis an appropriate solution is

$$\mathbf{a} = (0,0,1),\ \mathbf{c} = (\cos\phi(z), \sin\phi(z), 0),\ \mathbf{E} = E_0(\cos\alpha, 0, \sin\alpha), \tag{10}$$

where $E_0 = |\mathbf{E}|$ is the electric field strength. The relevant bulk and electric energies are then (see [8, Eqs. (2),(3)])

$$w_b = \frac{1}{2}B_3\{\phi'(z)\}^2, \tag{11}$$

$$w_e = -\frac{1}{2}\epsilon_0\epsilon_a(\mathbf{n}\cdot\mathbf{E})^2 = -\frac{1}{2}\epsilon_0\epsilon_a E_0^2(\sin\alpha\cos\theta + \cos\alpha\sin\theta\cos\phi)^2, \tag{12}$$

where $\epsilon_0 > 0$ is the permittivity of free space and ϵ_a is the dielectric anisotropy of the liquid crystal. The governing equilibrium equation reduces to (9) ([8, Eq. (6)] when $\phi = \phi(z)$) with $\psi = \phi$ and the constants a and b set to

$$a = \epsilon_0\,\epsilon_a\,E_0^2 B_3^{-1}\sin\alpha\cos\alpha\sin\theta\cos\theta, \tag{13}$$

$$b = -\epsilon_0\,\epsilon_a\,E_0^2 B_3^{-1}\cos^2\alpha\sin^2\theta, \tag{14}$$

so that in the case when $\epsilon_a > 0$, we have $a > 0$ and $b < 0$.

For a ferroelectric smectic C* liquid crystal, Eq. (9) arises in the static solution in the problems considered by Maclennan *et al.* [9] and Anderson and Stewart [10].

We now outline solutions of (9) for general constants a and b.

DOMAIN WALL SOLUTIONS

When discussing the solutions of Eq. (9) it is necessary to consider separately the two cases (i) $|a| \leq 2|b|$ and (ii) $|a| > 2|b|$. Constant solutions are $\psi = 0$ and $\psi = \pi$ in both cases and in case (i) there is an additional constant solution $\psi_0 = \cos^{-1}(a/2b)$. Multiplying Eq. (9) by $d\psi/ds$ and integrating gives

$$\frac{d\psi}{ds} = \pm\sqrt{b\cos(2\psi) - 2a\cos\psi + c}, \tag{15}$$

where c is a constant of integration. Typical phase portraits obtained by varying c in (15) for fixed values of a and b are shown in Figure 2. It is possible to select solutions based on these phase portraits such that they match up with each other continuously as a and b change.

We begin by considering case (i) when the phase portraits are given by Figure 2(b) where $|a| < 2b$ and $b > 0$. For the case of an inner cylinder $r = r_0$ ($s = 0$) on which a strong anchoring boundary condition is imposed which conflicts with the angle ψ_0, it is necessary to consider variable solutions. A solution of (9) which satisfies

$$\psi(0) = 0, \qquad \psi \to \psi_0, \qquad \frac{d\psi}{ds} \to 0 \quad \text{as } s \to \infty, \tag{16}$$

and corresponds to the bold trajectory marked in Figure 2(b) is

$$\psi(s) = 2\tan^{-1}\left\{\tan\left(\frac{\psi_0}{2}\right)\tanh\left(\sqrt{\frac{b}{2}}\sin(\psi_0)s\right)\right\}, \tag{17}$$

which displays a domain wall [5]. The same type of solution arose in the work by Schiller *et al.* [11] on a static domain wall in a planar aligned sample of non-chiral smectic C under the influence of an electric field using an earlier simplified theory. The solution $\psi(s)$ is an increasing function of s for any values of a and b satisfying $|a| < 2b$ (see Fig. 3, $k = 0.5$). When $B = 0$ the strict inequality $|a| < 2b$ is equivalent to the combined restrictions $A_{12} + A_{11} > 0$ and $A_{21} + A_{11} > 0$. A measurement of ψ_0 leads to a comparison of the relative magnitudes of the quantities $A_{12} - A_{21}$ and $A_{12} + A_{21} + 2A_{11}$ (cf. Eqs. (18) and (19)). The solution (17) is physically feasible since it is expected that there may be a 'winding out' of the director across the cylindrical layers as an observer travels outwards from the inner radius. This type of alignment is known to be related to the elastic constant B_3 [7] which appears in the definitions of a and b.

When the magnetic field is increased it is necessary to consider all values of a and $b > 0$, and therefore attention now turns to case (ii). It proves convenient to introduce the parameter k defined by

$$k(B) = -\frac{a}{2b} = \frac{\Delta\chi\mu_0^{-1}B^2r_0^2\sin^2\theta + A_{21} - A_{12}}{A_{12} + A_{21} + 2A_{11}}, \tag{18}$$

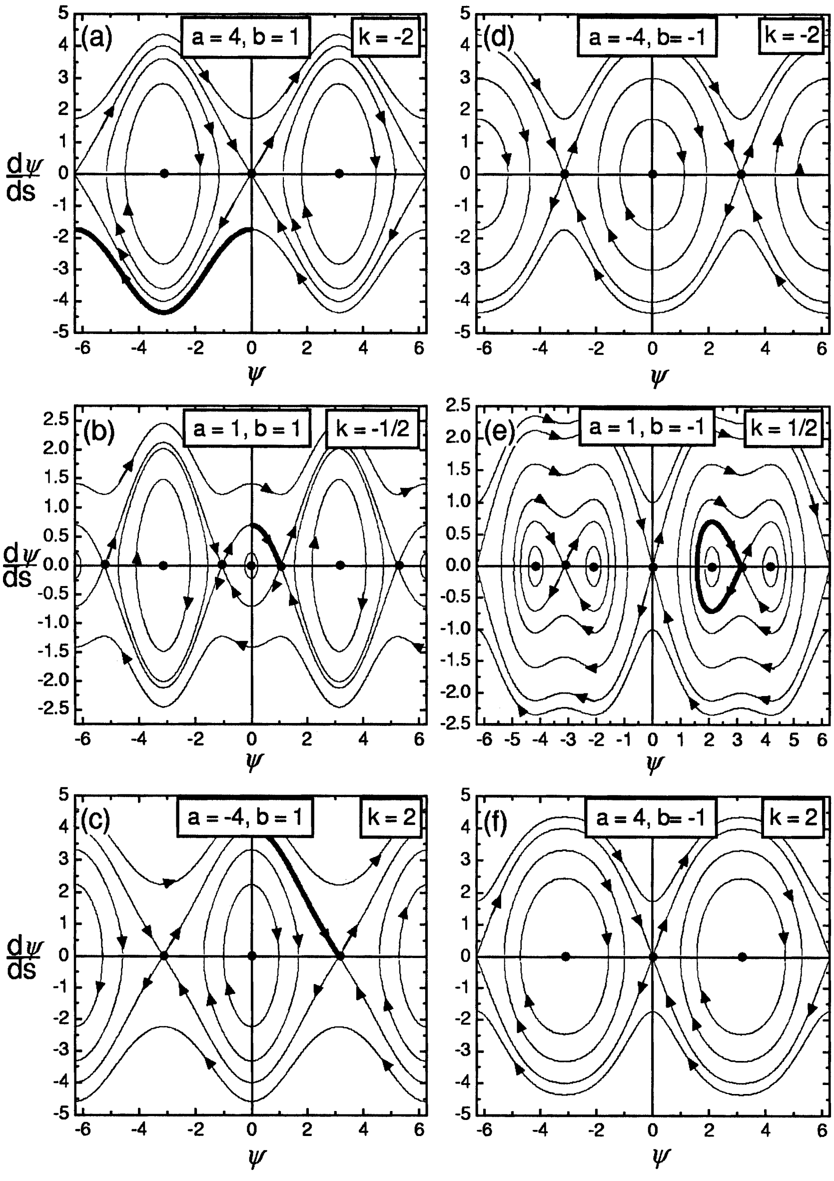

FIGURE 2 Phase portraits constructed from equation (9)for particular values of a and b, with the corresponding value of k defined by Eq. (18). The arrows indicate the direction of s increasing.

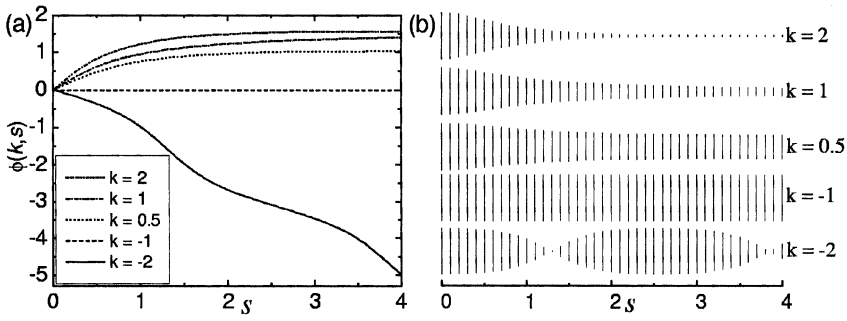

FIGURE 3 Solutions $\phi(k,s)$ for values of k obtained from ϕ_1 to ϕ_5 in equations (20) to (24) when $b = 1$.(a) The case for $k = 2$ represents the bold trajectory marked on Figure 2(c). Solutions for $k = 1, 0.5$ are typical of the bold trajectory presented in Figure 2(b). $k = -1$ represents the solution $\phi \equiv 0$. $k = -2$ corresponds to the bold trajectory in Figure 2(a). (b) Schematic representation of the c-director as s increases: the vertical direction is the z-direction and the lines represent the c-director as it twists into the page.

which is independent of B_3. For a given material, k depends only upon B, the magnitude of the magnetic field. For $\Delta\chi > 0$, $k(B)$ increases as B increases. The value of k when $B = 0$ is

$$k(0) = \frac{A_{21} - A_{12}}{A_{12} + A_{21} + 2A_{11}}. \tag{19}$$

In terms of k, $\psi_0 = \cos^{-1}(-k)$ for $|k| < 1$, explicit forms of the solutions which correspond in the special cases to the bold curves in Figure 2 for $b > 0$ can be obtained from (9) and (15). These forms are combined with solutions for the cases $k = -1$ and $k = 1$. The five solutions for the c-director orientation angle $\phi(= \psi/2)$ which match up continuously as the parameters a and b change are

$$\phi_1(k,s) = -n\pi - \tan^{-1}\left\{\sqrt{\frac{k+1}{k-1}}\tan\left(\sqrt{\frac{b}{2}}\sqrt{k^2-1}\,s\right)\right\},$$

$$\text{when } \frac{\pi(2n-1)}{\sqrt{2b(k^2-1)}} < s < \frac{\pi(2n+1)}{\sqrt{2b(k^2-1)}}, \quad k < -1, \tag{20}$$

$$\phi_2(k,s) = 0, \quad k = -1, \tag{21}$$

$$\phi_3(k,s) = \tan^{-1}\left\{\sqrt{\frac{1+k}{1-k}}\tan h\left(\sqrt{\frac{b}{2}}\sqrt{1-k^2}\,s\right)\right\}, \quad |k| < 1, \tag{22}$$

$$\phi_4(k,s) = \tan^{-1}(\sqrt{2b}\,s), \quad k = 1, \tag{23}$$

$$\phi_5(k,s) = \tan^{-1}\left\{\sqrt{\frac{k}{k-1}}\sinh(\sqrt{2b}\sqrt{k-1}\,s)\right\}, \quad k > 1, \tag{24}$$

where, in the definition of ϕ_1, $n = 0, 1, 2, \ldots$ the solution ϕ_3 corresponds to the form given in Eq. (17). Figure 3 shows the possibility of all five solutions for $\phi(k,s)$, for the indicated values of k, for $0 \le s \le 4$, in the particular case when $b = 2$, this arbitrary positive value being chosen to show the typical qualitative features of the full solutions. The solutions $\phi(k,s)$ constructed in this manner are indicative of the behaviour for $-\infty < k < \infty$ with $s \ge 0$. For $k > -1$, ϕ reorients from $\phi(k,0) = 0$ to $\phi_0(k)$ as $s \to \infty$, where

$$\phi_0(k) = \begin{cases} \frac{1}{2}\cos^{-1}(-k) & \text{if } |k| \le 1 \\ \frac{\pi}{2} & \text{if } k > 1. \end{cases} \tag{25}$$

For $\Delta\chi > 0, k(B)$ increases and so if, for a given material, $k(0) < -1$, there is the possibility of critical fields B_{c_1} and B_{c_2} occurring when $k(B_{c_1}) = -1$ and $k(B_{c_2}) = 1$. Explicitly,

$$B_{c_1}^2 = -\frac{2\mu_0(A_{21} + A_{11})}{\Delta\chi\, r_0^2 \sin^2\theta}, \qquad B_{c_2}^2 = \frac{2\mu_0(A_{12} + A_{11})}{\Delta\chi\, r_0^2 \sin^2\theta}. \tag{26}$$

The critical strength B_{c_1} coincides with the threshold for the Freedericksz transition threshold obtained for a sample confined between concentric circular cylinders in the limit as the outer radius tends to infinity, as discussed by Atkin and Stewart [4, Eqn. (85)]. It is always the case that $B_{c_2} > B_{c_1}$.

For the planar layer problem where $b < 0$ in the case when $0 \le k < 1$ we observe the following novel solution corresponding to the homoclinic orbit marked in bold in Figure 2(e) (in this case $\phi = \psi$):

$$\phi(k,z) = 2\tan^{-1}\left\{\sqrt{\frac{k}{1-k}}\cos h(\sqrt{-2b(1-k)}z + c)\right\}, \tag{27}$$

where c is a constant. In this geometry, $k = -a/2b = k(\alpha)$, by (13) and (14). The condition $0 \le k < 1$ is equivalent to $0 \le \alpha < \tan^{-1}(2\tan\theta)$ which includes the case $\alpha = \theta$ when $k = 1/2$ (see the bold trajectory in Fig. 2(e), where $c = 0$, $\phi(\frac{1}{2}, 0) = \frac{\pi}{2}$ and $\phi \to \pi$ as $z \to \infty$).

DISCUSSION

One motivation of the current work is to provide situations which may lead to the experimental determination of the elastic constants A_{ij}. These constants arise naturally in problems involving cylindrical layers through their rôle in the energy due to bending. The above results supplement the critical fields derived in earlier studies of Freedericksz transitions in samples with cylindrical layers in wedge and concentric cylindrical geometries [4,7]. There is currently little available experimental data on the constants A_{ij}. The wedge configuration has been achieved experimentally by Findon and Gleeson [12,13]. Using the theoretical results from [7], Findon and Gleeson established values for the elastic constant combination $A_{21}+A_{11}$ for the compound M3 (see [12] for the chemical structure of M3). Further, it was found that $A_{21}+A_{11}<0$. In view of inequalities (4) this means that $A_{11}<0$ and $A_{12}+A_{11}>0$, so that for this material both critical thresholds B_{c_1} and B_{c_2} exist and, since $k(0)<-1$, all the solutions (20) to (24) arise as B increases from zero. Since the solution ϕ_3 passes continuously to ϕ_5 as B increases through B_{c_2}, this second threshold is not expected to be observable as a critical phenomenon.

When $A_{21}+A_{11}>0$ only a subset of (20) to (24) will arise. If $A_{12}+A_{11}>0$, only B_{c_2} can occur and the complete solution is given by equations (22) to (24) where $\phi\to\pi/2$ as $B\to\infty$, similar in effect to the well known post-Freedericksz transition effect.

Measurement of the angle ϕ_0 $(=\psi_0/2)$ may also lead to some information on the constants A_{ij}. When $A_{21}+A_{11}>0$ and $A_{12}+A_{11}>0$ the domain wall solution (17) is possible in the absence of external fields. The observation of such a wall would lead to the measurement of the angle ϕ_0, which is present at the free boundary of a large sample, relative to the orientation of the wall at the surface of the cylinder. From this measurement, using (8) and the result $\cos(\psi_0)=a/2b$,

$$A_{12}-A_{21}=\cos(\psi_0)[A_{12}+A_{21}+2A_{11}]. \tag{28}$$

If $\psi_0=\frac{\pi}{2}$, that is there is a $\frac{\pi}{4}$ domain wall in ϕ, then $A_{12}\approx A_{21}$. When external fields are applied the observed value of ϕ_0 is altered (see Fig. 3) allowing further measurements of these constants.

The stability of solution (17) with no external field has been discussed by the authors [14] and it was found necessary to impose some restrictions on the values of the parameters a and b.

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