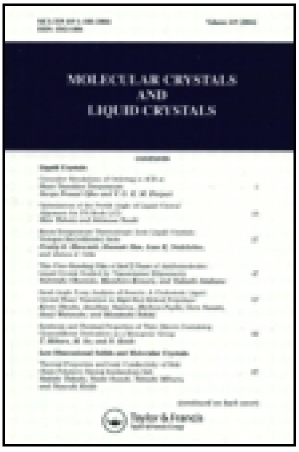

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Front Propagation in the Time-Dependent Landau-Ginzburg Model

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Front Propagation in the Time-Dependent Landau–Ginzburg Model

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Exact traveling-wave solutions of the time-dependent Landau-Ginzburg equation for a system undergoing first-order phase transition are found. These are two general types of solutions: domain walls which interpolate between two minima in the potential and relaxation modes which interpolate between a minimum and a maximum in the potential. The solutions are found in the presence of an external field. An estimation of the parameters of the solutions for *N*-[*p*-methoxybenzylidine]-*p*-butylaniline (MBBA) is performed.

Keywords: Nematic liquid crystal, nonlinear equation

1. INTRODUCTION

We consider the behaviour of transition regions in one-dimensional multistable media, described by the time-dependent Landau–Ginzburg equation (TDLG)

$$\gamma S_t - D S_{xx} = -\frac{\partial F}{\partial S} \tag{1}$$

where γ is a positive frictional coefficient associated with dissipative effects, S is the order parameter and F is the free energy density associated with the homogeneous situation. The coefficient D associated with the interfacial free energy is necessarily positive otherwise a one-phase state would never be stable. We are interested in a class of bounded solutions interpolating between zeros of $\partial F/\partial S$. There are two general types of topological solutions. Solutions interpolating between two minima of $F(S)$ are called domain walls (or transition regions). Solutions interpolating between a local maximum and a minimum of $F(S)$ will be called relaxation modes.[1] While domain walls propagate with a velocity uniquely determined by the parameters in Equation (1), relaxation modes have a continuum of possible velocities. The analysis of the velocity-selection mechanism for relaxation modes has been presented by Aronson and Weinberger[2] (see also Refs. 1 and 3).

The TDLG equation was analysed in relation to the kinetics of phase transitons,[4–6] the propagation of signals in electric circuits,[7] and the combined effects of population growth and diffusion.[8,9] In general, the nonlinear differential equations with dissipation are analysed by Fife.[10]

For the free energy density

$$F(S) = A_1 S + \tfrac{1}{2} A_2 S^2 + \tfrac{1}{3} A_3 S^3 + \tfrac{1}{4} A_4 S^4 \tag{2}$$

the model in Equation (1) describes structural phase transition in nematics in the presence of magnetic field $\vec{H}$ (so that $A_1 = -\frac{1}{2}\Delta\chi_{\max} H^2 < 0$).[11]

The TDLG equation is a good mathematical description of the nonlinear physical problems since it has, as particular solutions, profiles that move with a constant velocity and conserve their initial shape for a long time. In order to look for a traveling-wave solution of Equation (1) we change variables to a system of coordinates which moves along with the wave,

$$S(x, t) = S(x - vt) = S(z) \tag{3}$$

where v is the propagation velocity. Using Equation (3) we can rewrite Equation (1) as

$$S_{zz} + \Gamma S_z = \frac{\partial F}{\partial S} \tag{4}$$

where $\Gamma = \gamma v / D$. Equation (4) represents Newton's second law for particle of unit mass moving in a potential field $-F(S)$ under the influence of a frictional force with coefficient Γ. The bounded waves travel from right to left (for $v < 0$) or form left to right (for $v > 0$) and we have three possibilities for their asymptotic behaviour (see Figure 1) either between

$$S(x = \pm\infty) = S_2 \quad \text{and } S(x = \mp\infty) = S_1 \tag{5}$$

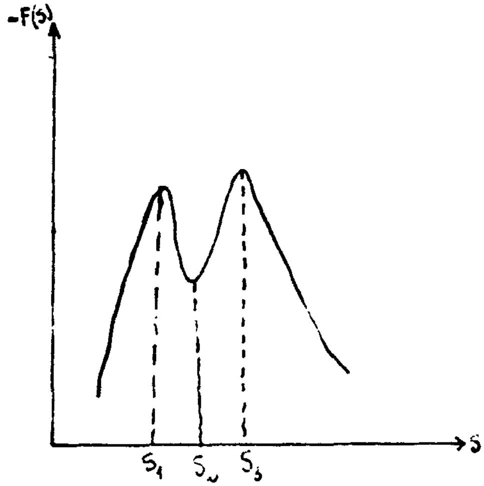

FIGURE 1 A typical potential for the mechanical problem defined by Equation (4).

or between

$$S(x=\pm\infty)=S_2 \quad \text{and } S(x=\mp\infty)=S_3 \tag{6}$$

or, finally, between

$$S(x=\pm\infty)=S_1 \quad \text{and } S(x=\mp\infty)=S_3 \tag{7}$$

Solutions (5), (6) which interpolate between two adjacent roots of $\partial F/\partial S$ (called relaxation modes) are not unique and can be both monotonic and non-monotonic. Solutions (7) which interpolate between S_1 and S_3 (called domain walls) are monotonic and unique in the sense that their velocity is uniquely determined by the form of the potential $-F(S)$ and by the boundary conditions.

Travelling-wave solutions of Equation (1) have the form of moving fronts and are responsible for the relaxation of the system to an equilibrium state defined by the boundary conditions. Usually, one considers the boundary conditions $S_x(x=\pm\infty, t=\infty)=0$ which correspond to zero energy flux at the boundaries.[1] This means that the energy loss by the system is due to dissipation, and that the energy exchange can take place anywhere between the boundary.

Our purpose is to find exact solutions of TDLG for first-order phase transitions (isotropic-nematic) and discuss the influence of an external magnetic field.

In Sec. 2 we briefly describe Landu-de Gennes theory of the isotropic-nematic transition in presence of an external field. In Sec. 3 the travelling-wave solutions of the TDLG equation are presented. In Sec. 4 the estimation of the parameters of new solutions of MBBA are performed, while we summarize the conclusions in Sec. 5.

2. LANDAU-DE GENNES THEORY OF THE ISOTROPIC-NEMATIC TRANSITION

In the absence of the megnetic field, the free energy density for the isotropic-nematic transition is given by[11]

$$F(S)=\tfrac{1}{2}A_2S^2+\tfrac{1}{3}A_3S^3+\tfrac{1}{4}A_4S^4 \tag{8}$$

The coefficient A_2 is assumed to be a $(T-T^*)$ where T is the temperature and T^* the supercooling limit, while $A_3<0$ and $A_4>0$ are constants. When $A_3=0$, $A_4<0$ describes first order phase transitions (in this case a stabilizing sixth-order term $A_6S^6/6$ with $A_6>0$ is required) and $A_4>0$ second-order phase transitions. If $A_3\neq 0$ the transition remains first order even for $A_4>0$.

Solutions of $\partial F/\partial S=0$ are well known,

$$\begin{aligned} S_1^0&=0\\ S_2^0&=\tfrac{3}{4}S_c(1-\Phi)\\ S_3^0&=\tfrac{3}{4}S_c(1+\Phi)\end{aligned} \tag{9}$$

Here $S_c = -2A_3/3A_4$ and $\Phi = (1 - 4A_2A_4/A_3^2)^{1/2} = [1 - 8(T - T^*)/9(T_c - T^*)]^{1/2}$. The equilibrim value of the order parameter S jumps discontinuously from 0 to S_c as the temperature decreases to $T_c = T^* + 2A_3^2/9aA_4$. The equilibrium expressions for S are

$$S_1^0 = 0 \qquad T > T_c$$
$$S_3^0 = \tfrac{3}{4}S_c(1 + \Phi) \qquad T < T_c \tag{10}$$

The supercooled metastable state is S_1^0 for $T^* < T < T_c$ while the superheated metastable state is S_3^0 for $T_c < T < T^+ = T^* + \frac{9}{8}(T_c - T^*)$.

In the presence of a magnetic field, the free energy density is given by Equation (2). For small values of A_1, the solutions of $\partial F/\partial S = 0$ are given by

$$S_1 = S_1^0 + \varepsilon_1 = -\frac{A_1}{A_2}$$
$$S_2 = S_2^0 + \varepsilon_2 = \tfrac{3}{4}S_c(1 - \Phi) + \frac{8A_1}{9A_4S_c^2\Phi(1 - \Phi)} \tag{11}$$
$$S_3 = S_3^0 + \varepsilon_3 = \tfrac{3}{4}S_c(1 + \Phi) - \frac{8A_1}{9A_4S_c^2\Phi(1 + \Phi)}$$

Note that these formulae are valid for small values of A_1. We see that when $A_1 \to 0$ the formulas (11) reduce to (9).

3. TRAVELLING-WAVE SOLUTIONS

We consider Equation (4) for $F(S)$ defined by Equation (2)

$$S_{zz} + \Gamma S_z - A_1 - A_2S - A_3S^2 - A_4S^3 = 0 \tag{12}$$

where $A_1 < 0$, $A_2 > 0$, $A_3 < 0$, $A_4 > 0$. We look for solutions in the form

$$S(z) = B_{ij} \pm C_{ij} \quad \tanh \alpha z \quad i = 1, 2, 3; j = 2, 3 \quad j > i \tag{13}$$

where $B_{ij} = (S_i + S_j)/2$, $C_{ij} = (S_j - S_i)/2$ with S_i, S_j given by (11).

A. Domain Walls

Domain walls are solutions of Equation (12), which interpolate between S_1 and S_3. Thus, for $S(-\infty) = S_1$ and $S(\infty) = S_3$,

$$S_{13}(z) = B_{13} + C_{13} \quad \tanh \alpha z \tag{14}$$

while for $S(-\infty) = S_3$ and $S(\infty) = S_1$,

$$S_{31}(z) = B_{13} - C_{13} \quad \tanh \alpha z \tag{15}$$

Substituting Equation (14) into Equation (12) we obtain

$$\alpha=\left(\frac{A_4}{2}\right)^{1/2}C_{13}$$

$$\Gamma=3\left(\frac{A_4}{2}\right)^{1/2}(S_c-2B_{13});\quad v=\frac{3D}{\gamma}\left(\frac{A_4}{2}\right)^{1/2}(S_c-2B_{13}) \tag{16}$$

Substituting Equation (15) into Equation (12) we obtain

$$\alpha=\left(\frac{A_4}{2}\right)^{1/2}C_{13}$$

$$\Gamma=-3\left(\frac{A_4}{2}\right)^{1/2}(S_c-2B_{13});\quad v=-\frac{3D}{\gamma}\left(\frac{A_4}{2}\right)^{1/2}(S_c-2B_{13}) \tag{17}$$

Thus, the domain wall solutions are given by

$$S(z)=B_{13}\pm C_{13}\quad \tanh\alpha z \tag{18}$$

where

$$\alpha=\left(\frac{A_4}{2}\right)^{1/2}C_{13} \tag{19}$$

$S(z)$ has a uniquely determined velocity

$$v=\pm\frac{3D}{\gamma}\left(\frac{A_4}{2}\right)^{1/2}(S_c-2B_{13}) \tag{20}$$

For $A_1=0$, $B_{13}=C_{13}=S_3^0/2$, the domain wall solutions become

$$S^0(z)=\frac{S_3^0}{2}(1\pm\tanh\alpha z)=\tfrac{3}{8}S_c(1+\Phi)(1\pm\tanh\alpha z) \tag{21}$$

where

$$\alpha=\left(\frac{A_4}{2}\right)^{1/2}\frac{S_3^0}{2}=\frac{3}{8}\left(\frac{A_4}{2}\right)^{1/2}S_c(1+\Phi) \tag{22}$$

and

$$\Gamma=\pm 3\left(\frac{A_4}{2}\right)^{1/2}(S_c-S_3^0)=\pm\left(\frac{A_4}{2}\right)^{1/2}S_c(1-3\Phi) \tag{23}$$

$$v=\pm\frac{3D}{4\gamma}\left(\frac{A_4}{2}\right)^{1/2}S_c(1-3\Phi) \tag{24}$$

When A_1 continuously changes from zero to an arbitrarily small value the domain wall solutions deform continuously from Equation (21) at Equation (18). For $A_1 = A_{1c}$ defined by

$$S_1 = S_2$$

the local minimum S_1 of $F(S)$ disappears and we no longer have travelling domain walls which become travelling relaxation modes.

B. Relaxation Modes

Relaxation modes are solutions of Equation (12) which interpolate between two adjacent roots of $\partial F/\partial S$. So,

$$S(z) = B_{23} \pm C_{23} \quad \tanh \alpha z \tag{25}$$

Substituting Equation (25) into Equation (12) we obtain

$$\alpha = \left(\frac{A_4}{2}\right)^{1/2} C_{23}$$

$$\Gamma = \pm 3\left(\frac{A_4}{2}\right)^{1/2}(S_c - 2B_{23}); \quad v = \pm\frac{3D}{\gamma}\left(\frac{A_4}{2}\right)^{1/2}(S_c - 2B_{23}) \tag{26}$$

For $A_1 = 0$, $B_{23} = (3/4)S_c$ and $C_{23} = (3/4)S_c\Phi$, the relaxation modes solutions become

$$S^0(z) = \tfrac{3}{4}S_c(1 \pm \Phi \tanh \alpha z) \tag{27}$$

where

$$\alpha = \frac{3}{4}\left(\frac{A_4}{2}\right)^{1/2}, \quad S_c\Phi = -\frac{A_3\Phi}{2(2A_4)^{1/2}}$$

$$\Gamma = \pm\frac{A_3}{(2A_4)^{1/2}}, \quad v = \pm\frac{D}{\gamma}\frac{A_3}{(2A_4)^{1/2}} \tag{28}$$

Other relaxation mode which interpolate between S_1 and S_2 is given by

$$S(z) = B_{12} \pm C_{12} \tanh \alpha z \tag{29}$$

Analogously we obtain:

$$\alpha = \left(\frac{A_4}{2}\right)^{1/2} C_{12}$$

$$\Gamma = \pm 3\left(\frac{A_4}{2}\right)^{1/2}(S_c - 2B_{12}); \quad v = \pm\frac{3D}{\gamma}\left(\frac{A_4}{2}\right)^{1/2}(S_c - 2B_{12}) \tag{30}$$

For $A_1 = 0$, $B_{12} = C_{12} = S_2^0/2$, so that the relaxation modes solutions are

$$S(z) = \frac{S_2^0}{2}(1 \pm \tanh \alpha z) = \tfrac{3}{8}S_c(1 - \Phi)(1 \pm \tanh \alpha z) \qquad (31)$$

where

$$\alpha = \left(\frac{A_4}{2}\right)^{1/2} \frac{S_0^2}{2} = \frac{3}{4}\left(\frac{A_4}{2}\right)^{1/2} S_c(1 - \Phi) \qquad (32)$$

$$\Gamma = \pm 3\left(\frac{A_4}{2}\right)^{1/2} (S_c - S_2^0) = \pm \frac{3}{4}\left(\frac{A_4}{2}\right)^{1/2} S_c(1 + 3\Phi) \qquad (33)$$

$$v = \pm \frac{3D}{4\gamma}\left(\frac{A_4}{2}\right)^{1/2} S_c(1 + 3\Phi) \qquad (34)$$

Although the form of relaxation modes solutions (25) and (29) is the same as those for domain wall solutions (18), they have different properties. Unlike the solution (18), which is a unique travelling wave, the solutions (25) and (29) represent-particular fronts belonging to a family $S(z, v)$ parameterized by the velocity v which is a continuous parameter. The relaxation modes $S(z; v)$ can be both monotonic (like the solutions (25) and (29)) for a velocity greater than a certain critical value v_c and non-monotonic for $v < v_c$[1,3]. For $v = v_c$ the relaxation mode is asymptotically stable. In fact, there exist infinitely many other travelling relaxation modes for which we do not obtain explicit solutions. This problem was discussed in Refs. (1)–(3). The smallest velocity v_c for which travelling relaxation modes are monotonic is given by[1]

$$v_c = 2\frac{D}{\gamma}\left[-\left.\frac{\partial^2 F}{\partial S^2}\right|_{S=S_2} \right]^{1/2} \qquad (35)$$

The velocity v_c increases with the increase of the external field.

4. THE RESULTS FOR MBBA

In the following the measured values[12] of $a = 0.090\,\mathrm{J.cm^{-3}K^{-1}}$, $A_3 = -0.591\,\mathrm{J.cm^{-3}}$, $A_4 = 1.228\,\mathrm{J.cm^{-3}}$, $T^* = 318.3\,\mathrm{K}$ and $T_c = 319\,\mathrm{K}$ for N-[p-methoxybenzylidine]-p-butylaniline (MBBA) will be used for the estimation of the parameters of solutions. In Table I we show the calculated results for $S_3^0/2$ (see Equation (21)), $3S_c/4$ (see Equation (27)), $S_2^0/2$ (see Equation (31)), α and Γ as functions of temperature for MBBA in the absence of the magnetic field ($A_1 = 0$). In the same table the critical values of A_1 (i.e., the values for which the local minimum S_1 of $F(S)$ disappears and we no longer have travelling domain walls) are also shown. At $T = T_c = 319\,\mathrm{K}$ the propagation velocity of the domain wall solutions cancel out. In this case we can obtain the solution by directly integrating Equation (4):

$$\frac{dS}{dz} = \sqrt{F(S) + C}$$

TABLE I

The Parameters of Solutions for MBBA in the Absence of Magnetic Field

	Domain wall solutions Eqs. (21) ÷ (23)			Relaxation mode Eqs. (27), (28)				Relaxation mode Eqs. (31) ÷ (33)			
T	$S_3^0/2$	α	Γ	$3S_c/4$	$3S_c\Phi/4$	α	Γ	$S_2^0/2$	α	Γ	A_{1c}
318.0	0.2327	0.1824	±0.3400	0.2406	0.2249	0.1762	±0.3771	0.0079	0.0062	±0.7171	−0.0001
318.5	0.2242	0.1757	±0.3000	0.2406	0.2078	0.1629	±0.3771	0.0164	0.0129	±0.6771	−0.0003
318.6	0.2150	0.1685	±0.2565	0.2406	0.1893	0.1484	±0.3771	0.0256	0.0201	±0.6386	−0.0007
318.7	0.2047	0.1604	±0.2083	0.2406	0.1688	0.1323	±0.3771	0.0359	0.0281	±0.5854	−0.0012
318.8	0.1930	0.1512	±0.1532	0.2406	0.1454	0.1139	±0.3771	0.0476	0.0373	±0.5303	−0.0018
318.9	0.1790	0.1403	±0.0875	0.2406	0.1174	0.0920	±0.3771	0.0616	0.0483	±0.4646	−0.0026
319.0	0.1604	0.1257	0	0.2406	0.0802	0.0629	±0.3771	0.0802	0.0629	±0.3771	−0.0033

TABLE II

The Parameters of Solutions for MBBA with $A_1 \neq 0$

		Domain wall solutions Eqs. (15), (16)		Relaxation mode Eqs. (25), (26)		Relaxation mode Eqs. (29), (30)	
T	A_1	α	Γ	α	Γ	α	Γ
318.8	−0.0014	0.1431	±0.2505	0.1341	±0.3041	0.0090	±0.5539
	−0.0016	0.1418	±0.2641	0.1369	±0.2937	0.0049	±0.5572
	−0.0018	0.1407	±0.2782	0.1407	±2782	0	±0.5662
318.9	−0.0022	0.1327	±0.2331	0.1247	±0.2815	0.0081	±0.5145
	−0.0024	0.1320	±0.2467	0.1276	±0.2730	0.0045	±0.5192
	−0.0026	0.1313	±0.2603	0.1313	±0.2603	0	±0.5276
319	−0.0029	0.1257	±0.2162	0.1168	±0.2693	0.0089	±0.4848
	−0.0031	0.1257	±0.2312	0.1206	±0.2622	0.0052	±0.4919
	−0.0033	0.1257	±0.2462	0.1257	±0.2462	0	±0.5079

where C is an integration constant. The critical values of A_1 increase with temperature, so that the magnetic field must increase for cancelling the local minimum S_1 of $F(S)$. For $A_1 = 0$, the relaxation modes are two pairs of kinks and anti-kinks which travel with a non-zero velocity but the velocity of the relaxation mode which interpolates between S_2 and S_3 is constant with temperature, while the velocity of the relaxation mode which interpolates between S_1 and S_2 decrease with increasing temperature.

The results for α and Γ as functions of temperature for MBBA in the presence of a magnetic field are given in Table II. The domain wall solutions disappear (become identical with the relaxation mode which interpolate between S_2 and S_3) for critical values of A_1. It is evident that for critical values of A_1 the values of α for the relaxation mode which interpolate between S_1 and S_2 cancel out.

5. CONCLUSION

Note that the travelling-wave solutions (18), (25) and (29) of Equation (12) satisfy the restrictive assumption of Ref. (13). Following this procedure we look for solutions of Equation (12) in the form

$$S_z = \sum_{k=0}^{n} a_k S^{k/2} \tag{36}$$

Substituting Equation (36) into Equation (12), integrating once with respect to z and equating the coefficients of equal powers of S we obtain

$$a_4 = \mp\left(\frac{A_4}{2}\right)^{1/2}; \quad a_3 = 0, \; a_2 = (2A_4)^{1/2} B_{ij};$$

$$a_1 = 0; \quad a_0 = \mp\left(\frac{A_4}{2}\right)^{1/2}(B_{ij}^2 - C_{ij}^2) \tag{37}$$

so that

$$S_z = a_4[S(z)]^2 + a_2 S(z) + a_0$$

For $A_1 = 0$ we obtain for domain wall solutions

$$a_4 = \mp\left(\frac{A_4}{2}\right)^{1/2}; \quad a_2 = \pm\frac{3}{4}\left(\frac{A_4}{2}\right)^{1/2} S_c(1+\Phi); \quad a_0 = 0 \tag{38}$$

and for relaxation modes solutions

$$a_4 = \mp\left(\frac{A_4}{2}\right)^{1/2}; \quad a_2 = \mp\frac{A_3}{(2A_4)^{1/2}}; \quad a_0 = \mp\frac{A_2}{(2A_4)^{1/2}}$$

$$a_4 = \mp\left(\frac{A_4}{2}\right)^{1/2}; \quad a_2 = \pm\frac{3}{4}\left(\frac{A_4}{2}\right)^{1/2} S_c(1-\Phi); \quad a_0 = 0 \tag{39}$$

These results are compatible with those of Ref. (1).

We have solved the TDLG equation for systems undergoing first-order phase transitions in the presence of an external field (for small values of A_1). These solutions were particularized for the case $A_1 = 0$ (in absence of the field). Two types of solutions have been found. Solutions interpolating between two minima of $F(S)$ are called domain walls and solutions interpolating between a local maximum and a minimum of $F(S)$ are called relaxation modes. The relaxation modes behave in a qualitatively different way to domain walls. While domain walls propagate with a unique velocity determined by the parameters of the system, relaxation modes propagate with arbitrary velocities. The relaxation modes are monotonic for a velocity greater than a critical value v_c given by Equation (35). The value of v_c increases with the curvature of the potential $F(S)$ at the unstable equilibrium state (local maximum) and does not depend on the characteristics of $F(S)$ around the stable state. For $v = v_c$ the relaxation modes are stable in the sense of Lyapunov[1], thus the monotonic relaxation modes traveling with $|v| \approx v_c$ from an attracting invariant set. This direct procedure of solving the TDLG equation is compatible with the procedure used in Refs. (1) and (2).

We have also estimated the parameters of solutions for MBBA in the two cases ($A_1 = 0$ and $A_1 \neq 0$). The critical values of A_1, the value for which domain walls disappear, increase with temperature. It is important to note that for $A_1 = 0$ the velocity of the relaxation mode which interpolates between S_2 and S_3 is constant with temperature while the velocity of the relaxation mode which interpolates between S_1 and S_2 decrease with increasing temperature.

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