



THE KINETICS OF NON-LINEAR ORIENTATIONAL DEFORMATIONS IN NEMATIC LIQUID CRYSTALS IN A UNIFORM MAGNETIC FIELD†

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The non-linear kinetic equation describing the evolution of the orientational structural of nematic liquid crystals is investigated. The equilibrium structures are described and their stability and the behaviour of the solutions for long times are investigated. The super-slow evolution (for example, in a very intense magnetic field) of the irregular structure to a regular stable structure is described. © 1997 Elsevier Science Ltd. All rights reserved.

1. FORMULATION OF THE PROBLEM

Continuing our investigations of extremely non-linear equations of the theory of the elasticity of nematic liquid crystals (NLC) [1–3], we will consider the non-linear evolution in a magnetic field of the deformed orientational structure containing, moreover, a large number of π -walls, and kinks while preserving the overall topological charge. The orientational structure of the NLC becomes particularly unstable in regions of large dimensions, and also in weak magnetic fields.

The equations of the theory of the elasticity of NLC express the balance of moments related to the rotation of the local anisotropy (director) vector $\mathbf{l}(x, y, z)$ due to the action of an external magnetic field \mathbf{H} and neighbouring parts of the medium. The equilibrium equations were first obtained from the variational principle [4, 5]

$$\delta F = 0, \quad \mathbf{l}^2 = 1$$

$$F = \frac{1}{2} \int_V [K_1 (\operatorname{div} \mathbf{l})^2 + K_2 (\mathbf{l} \operatorname{rot} \mathbf{l})^2 + K_3 |\mathbf{l} \times \operatorname{rot} \mathbf{l}|^2 - \chi_{ik} H_i H_k] dv \quad (1.1)$$

Here F is the Oseen–Frank elastic energy. The value of F varies over the gradients of the local vector $\nabla \mathbf{l}$ while the length of the latter remains unchanged. The coefficients K_1 , K_2 and K_3 characterize the transverse bending (K_1), the longitudinal bending (K_3) and the twisting (K_2) of the vector lines of the field $\mathbf{l}(x, y, z)$. The diamagnetic tensor $\chi_{ik} = \chi_{\perp} \delta_{ik} + (\chi_{\parallel} - \chi_{\perp}) l_i l_k$ has two components—the longitudinal susceptibility (χ_{\parallel}) and the transverse susceptibility (χ_{\perp}) of the NLC.

We will consider the case of the bending of an orientational structure when the two-dimensional vectors \mathbf{l} and \mathbf{H} lie in the same (x, y) plane at all instants of time t . Then $\mathbf{l} \operatorname{rot} \mathbf{l} = 0$ and no twisting of the structure occurs. By considering the non-equilibrium case, in the moment-balance equation, a term proportional to the velocity of rotation of the director \mathbf{l} is usually added, which is responsible for rotational friction. It then takes the form

$$\mathbf{l} \times [K_1 \operatorname{grad} \operatorname{div} \mathbf{l} - K_3 \operatorname{rot} \operatorname{rot} \mathbf{l} + \chi_a \mathbf{H}(\mathbf{H})] = \gamma \mathbf{l} \times \dot{\mathbf{l}}, \quad \chi_a = \chi_{\parallel} - \chi_{\perp} \quad (1.2)$$

The variational form of the kinetic equation will be considered in Section 4. Here χ_a is the diamagnetic anisotropy and γ is the rotational viscosity. Strictly speaking, the inertial term $\sim \dot{\mathbf{l}}$, related to the molecular moments of inertia, and also the hydrodynamic term $\sim \operatorname{rot} \mathbf{v}$, can be omitted since they are unimportant for large dimensions of the region S .

Equation (1.2) is extremely non-linear, so its general analysis is difficult. In the one-dimensional case $\mathbf{l} = \mathbf{l}(y, t)$ for a constant magnetic field it can be represented in the form of an equation in a single scalar function α —the angle of mutual orientation of the vectors \mathbf{l} and \mathbf{H} . We then have

$$2\gamma \dot{\alpha} = 2K_1 \alpha''_{yy} - \chi_a H^2 \sin 2\alpha - 2\Delta K [(a'_y)^2 \sin 2\alpha - \alpha''_{yy} \sin^2 \alpha] \quad (1.3)$$

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$$\alpha = \arccos(\mathbf{IH})H^{-1}, \quad H = \text{const}, \quad \Delta K = K_3 - K_1$$

The evolution equation can be analysed in this form. It was investigated in the linearized form previously in [1].

We will refine the problem. In the case of an infinitely extended region we will consider only solutions that are periodic in y with period h . If the region S is a plane-parallel layer $0 \leq y \leq h$, Eq. (1.3) corresponds to the case when the field is orthogonal to its boundaries. We will specify the orientation of the vector \mathbf{l} on its boundaries so that it is orthogonal to the magnetic-field vector \mathbf{H}

$$\alpha(0, t) = \pi/2, \quad \alpha(h, t) = \pi/2 \pm N\pi, \quad N = 0, 1, 2, \dots \quad (1.4)$$

2. EQUILIBRIUM STABLE AND METASTABLE ORIENTATIONAL STRUCTURES (FIELDS)

We will begin with a description of equilibrium structures. For equilibrium states ($\alpha = 0$) the evolution equation (1.3) becomes an equation describing the static orientational deformations of the NLC structure, which arises due to the action of the walls and magnetic field

$$(1 - p \sin^2 \alpha) \alpha''_{yy} - [p(\alpha'_y)^2 + m^2] \sin \alpha \cos \alpha = 0 \quad (2.1)$$

$$p = 1 - K_1 / K_3, \quad m^2 = H^2 \chi_a K_3^{-1}$$

The first integral of this equation is well known

$$\alpha'_y = \pm \left(\frac{m^2 \sin^2 \alpha - C}{1 - p \sin^2 \alpha} \right)^{1/2} \quad (2.2)$$

(C is the constant of integration). Equation (2.2) has two families of solutions. When $C > 0$ the solutions describe states without preliminary deformation—when there is no magnetic field we have $\alpha = \text{const}$. The case $C < 0$ covers the presence of a non-uniform field and also as $H \rightarrow 0$, i.e. due to the boundary conditions, dissimilar orientation on the boundaries. In the first case the deformations begin from zero only as a result of bifurcation when a certain threshold is reached.

It is clear that, in the first case, which we will now consider, on the boundaries $y = 0$ and $y = h$ the same values of the angle α or of the complementary angle $\beta = \pi/2 - \alpha$ must be specified

$$\alpha(0) = \alpha(h) = \pi/2 \quad \text{or} \quad \beta(0) = \beta(h) = 0 \quad (2.3)$$

The solution of Eq. (2.2) is expressed in terms of an elliptic integral of the third kind [6]

$$\begin{aligned} h - y &= m^{-1} \sqrt{(1-p)(1-n)} \Pi(n, k, \chi), \quad n = k^2 p \\ k^{-2} &= 1 + (1-p) \text{tg}^2 \alpha_m, \quad \sin \alpha_m = C / m^2, \quad \alpha_m = \min \alpha \\ \sin \chi &= \frac{1}{k \sqrt{1-p}} \frac{\cos \alpha}{\sqrt{1 + (K_3 / K_1) p \cos^2 \alpha}} = \frac{k^{-1} (1-p)^{-1/2} \sin \beta}{\sqrt{1 + (K_3 / K_1) p \sin^2 \beta}} \end{aligned} \quad (2.4)$$

The parameter k , related to the constant of integration, represents the “amplitude” of the deformation α_m , where α_m is the minimum angle (between the vectors \mathbf{H} and \mathbf{l}), reached in the middle of the layer $y = h/2$, corresponding to the greatest deformation. The value of the related “amplitude” of the deformation is found from the dispersion equation

$$hm / \sqrt{1-p} = 2\sqrt{1-n} \Pi(n, k), \quad \Pi(n, k) = \Pi(n, k, \pi/2) \quad (2.5)$$

It follows from boundary condition (2.3) when $y = 0$.

In this equation k occurs as the unique arbitrary constant of integration. The parameters m and p are expressed solely in terms of the characteristics of the medium, the magnetic field H and the layer thickness h .

It is significant that Eq. (2.5) does not have a solution for all k . By virtue of the properties of the complete elliptic integral of the third kind $\Pi(n, k)$ we have $\Pi(n, 0) = \pi/2$, $\Pi(n, k) \geq \Pi(n, 0)$. Using this inequality in (2.5) and taking into account the fact that $n = 0$ when $k = 0$, we initially obtain the inequality

$$hm \geq \pi\sqrt{1-p}, \quad m^2 = H^2\chi_a K_3^{-1}$$

After elementary algebra, taking into account the fact that χ_a, K_3 and p are positive quantities, we can write

$$Hh \geq \mu_c, \quad \mu_c = \pi\sqrt{K_3^{-1}\chi_a(1-p)} \tag{2.6}$$

This inequality denotes that a non-trivial solution is obtained (deformations occur) if the product Hh reaches and exceeds the threshold μ_c .

Equation (2.5) corresponds to the special case when the maximum value of the angle β is reached once—in the middle of the layer, in the interval $0 \leq y \leq h$. The boundary conditions (2.3) will obviously be satisfied if, for zero values at the ends, their value is reached inside the interval an integer number of times: i.e. the section h/N corresponds to the interval $0 \leq \chi \leq \pi/2$, where $N = 1, 2, 3, \dots$. The value $N = 1$ corresponds to condition (2.5). It can be written in general form as

$$hm = (2N\sqrt{1-n}\sqrt{1-p})\Pi(n, k) \tag{2.7}$$

For fixed values of m and p we obtain a series of monotonically increasing curves of $\Pi(n, k) = N\pi/2$ (for different values of N). The dispersion equation (2.5) defines N values of k_N , to which correspond N solutions of Eq. (2.2), satisfying the zero boundary conditions (2.3).

To estimate the gradient properties of these solutions we start from the expression for the first integral (2.2), in which we must take into account the representation of the constant C in terms of α_m , according to (2.5). The angular gradient takes its greatest value (in absolute value) at the ends of the sections $y_N = 0, h/N$, where $\alpha = \pi/2$. From (2.2) we obtain

$$\max(\alpha'_y)^2 = \frac{N^2 m^2 \cos^2 \alpha_m}{h^2(1-p)} = \frac{N^2 m^2}{h^2(k_N^{-2} - p)} = \frac{N^2 m^2 k_N^2}{(1-n)h^2} \tag{2.8}$$

It is clear that large values of the gradients correspond to large values of the numbers k_N . It can be seen that k_N is a decreasing sequence. The greatest value of k_1 is found from Eq. (2.5), and it is greater the greater the value of the product Hh compared with the threshold μ_c . Hence, the spectrum of the numbers k_N occupies a strip from 0 to k_1 .

The explicit dependence $\alpha(y)$ or $\beta(y)$ can be determined for limiting values of the parameters k and $n = k^2 p$. For small k and p , taking $n \approx 0$, we obtain

$$h - y = \frac{\sqrt{1-p}}{m} \Pi(0, k, \chi) = \frac{\sqrt{1-p}}{m} F(k, \chi) \tag{2.9}$$

where F is an elliptic integral of the second kind, for which there is the inversion formula

$$\sin \chi = \operatorname{sn} \left[\frac{m}{\sqrt{1-p}}(h - y), k \right] \tag{2.10}$$

Using (2.4), by putting $n = 0$ in it, we can change to the angle α or β , which gives the final relation

$$\frac{\cos \alpha}{\sqrt{1 + (K_3 / K_1)p \cos^2 \alpha}} = k\sqrt{1-p} \operatorname{sn} \left[\frac{m}{\sqrt{1-p}}(h - y), k \right] \tag{2.11}$$

For $p = 0$ (when $n = 0$ irrespective of k) this formula, and also (2.10), become exact for any k . For $k = 1$ the elliptic sine changes to a hyperbolic tangent, and we arrive at a regular system of kinks (π -walls), concentrated around points with coordinates $y_i = 0, h/N, 2h/N, \dots$. We have

$$\beta_s = 2 \operatorname{arctg} \left[\frac{m}{\sqrt{1-p}} (y - y_l) \right] - \pi + s\pi, \quad s = \pm 1 \tag{2.12}$$

The profile of a kink in general is given by the formula

$$\beta = B_s(\xi), \quad \xi = m(y - y_l) / \sqrt{1-p} \tag{2.13}$$

To construct asymptotic solutions describing the interaction of the kinks, we require the following formulae

$$B_s(\xi) = s\pi - s\rho(p)e^{-\xi} + O(e^{-2\xi}), \quad \xi \rightarrow +\infty \tag{2.14}$$

$$\rho(p) = \frac{1}{\sqrt{2}} \left(\frac{1-\sqrt{p}}{1+\sqrt{p}} \right)^{1/4} \exp \left[2\sqrt{p} \operatorname{arctg} \left(\frac{1-\sqrt{p}}{1+\sqrt{p}} \right)^{1/2} - \frac{\pi}{4} \right]$$

which describe the asymptotic properties of a kink. Here s is the topological charge.

3. THE STABILITY OF THE EQUILIBRIUM SOLUTIONS

We will investigate the kinetic equation (1.3), linearized in the region of the equilibrium solutions (n is the number of a solution).

Suppose $\alpha = \alpha_n + \psi$, where ψ is a small quantity. Equation (1.3) can then be written in the form

$$\gamma_1 \psi_t = A_n \psi, \quad \gamma_1 = \gamma / K_1 \tag{3.1}$$

$$A_n \psi = \psi''_{yy} (1 - p \sin^2 \alpha_n) - 2\psi'_y p(\alpha_n)'_y \sin \alpha_n \cos \alpha_n - \\ - \psi \{ 2p \sin \alpha_n \cos \alpha_n (\alpha_n)''_{yy} + [p(\alpha_n)'_y]^2 + m^2 \} \cos 2\alpha_n \}$$

The following result (previously known for $p = 0$) is important when using the theory of regular attractors [7] in the problem in question. Since the attractor describes the behaviour of the solutions of the kinetic equation as $t \rightarrow +\infty$ this enables the physically realizable limiting regimes to be described at long times.

Lemma. For the Dirichlet conditions for “almost all” values of the parameter m (with the exception of a denumerable set), all the equilibrium solutions $\alpha_n(y)$ are hyperbolic, i.e. the operator A_n has an empty kernel.

For periodic conditions the kernel A_n consists only of the function $(\alpha_n)'_y$.

Note. This denotes that the equilibrium solutions almost always give non-degenerate extrema of the system energy, i.e. non-degenerate maxima, minima or saddle points.

Proof. We will use the well-known scheme in [8]. For the Dirichlet case, we can verify by direct substitution that the function

$$2m^2 \partial \alpha_n(y, m^2) / \partial (m^2) - y(\alpha_n)'_y = \psi \tag{3.2}$$

satisfies the equalities $A_n \psi \equiv 0$, $\psi(0) = 0$. But we see from (2.2) that for “almost all” m the second condition $\psi(h) = 0$ is not satisfied, which it was also required to prove. The assertion is well-known for periodic conditions [9].

For the case of the Dirichlet boundary conditions (1.4) all the non-trivial non-constant solutions for which $(\alpha_n)'_y$ has more than one root, are unstable, i.e. an eigenvalue $q > 0$ exists for the problem $A_n \psi = q\psi$ and correspondingly solutions $\psi(y, t)$ (3.1) that increase exponentially with time.

The proof is carried out using the well-known scheme in [9, p. 138, 139].

4. SOME GENERAL PROPERTIES OF THE KINETIC EQUATION AND THE RELAXATION OF A NON-EQUILIBRIUM STRUCTURE

For systems of limited dimensions h when the non-linearities $m^2 \sin^2 \beta$ are “not too large”, the description of the behaviour of the solutions of Eq. (1.3) follows directly from the theorem on attractors of gradient-like dynamical systems [7–11]. Equation (1.3) with boundary conditions (1.5) or (2.4) can in fact be represented in the functional form

$$\delta D / \delta \beta' = -\delta L / \delta \beta \tag{4.1}$$

where the functionals of “dissipation” D and “energy” L have the form (we have changed from the angle α to the angle β)

$$D = \frac{\gamma_1}{2} \int_0^h (\beta'_y)^2 dy, \quad L = \int_0^h \left[\frac{1}{2} (1 - p \cos^2 \beta) (\beta'_y)^2 + m^2 \sin^2 \beta \right] dy \tag{4.2}$$

It follows from (4.1) that L is a Lyapunov functional which does not increase along the trajectory of the dynamical system

$$D = -\partial L / \partial t \tag{4.3}$$

Moreover $L \geq 0$.

These properties and the lemma proved above enable the general theory [7–11] to be employed.

All the trajectories of the dynamical system converge to equilibria, where, for “almost all” (see [9]) of the initial data $\beta(y, 0)$ the corresponding trajectory $\beta(y, t)$ approaches a certain stable equilibrium as $t \rightarrow +\infty$.

This stable equilibrium is unique for the case of the Dirichlet conditions (1.4) with $N \neq 0$. For (2.3), if the magnetic field is below the threshold, this is a trivial solution for $\beta \equiv 0, \alpha = \pi/2$. If the field is above the threshold, this half-wave is a non-trivial solution of (2.2) with $C > 0$ and the least period.

There are exactly two such half-waves corresponding to different signs in front of the root in (2.2). If we consider condition (1.4) with $N \neq 0$, a certain monotonic solution with $C < 0$ will be an equilibrium solution.

For periodic boundary conditions, “almost all” trajectories will converge at an exponential rate to the trivial equilibria $\beta_n \equiv n\pi$ ($n = 0, \pm 1, \pm 2, \dots$). The relaxation time for this process of approaching equilibrium can be estimated using (4.3). We will assume that the solution β is attracted to the equilibrium β_n . We will select small neighbourhoods V_n of the equilibrium solutions β_n such that in V_n Eq. (1.3) can be linearized. Inside V_n we then have (see Section 3)

$$\begin{aligned} \gamma_1 \psi' &= A_n \psi, \quad \psi = \beta - \beta_n, \quad \beta_n + \psi(t_0) \in V_n \\ \|\psi\|^2 &= \int_0^h \psi^2 dy, \quad \|\psi(t)\| \leq \|\psi(t_0)\| \exp[-\lambda_n \gamma_1^{-1} (t - t_0)], \quad t \geq t_0 \end{aligned}$$

Here λ_n is the least positive eigenvalue A_n .

Thus, the relaxation time inside V_n is proportional to $\lambda_n \gamma_1^{-1}$. The instant t_0 of falling inside V_n can be estimated from relation (4.3)

$$\int_0^{t_0} D[\beta(s)] ds = L[\beta(0)] - L[\beta(t_0)] \leq L_0 = L[\beta(0)]$$

Since we have $D \geq \delta > 0$ outside V_n , this gives

$$t_0 \leq L_0 \delta^{-1} = L[\beta(0)] (\min D[\beta])^{-1}, \quad \beta \in V_n, \quad n = 0, \pm 1, \pm 2, \dots$$

According to this method of estimating the relaxation time for limited h and m^{-1} , the solution for the initial data of the “common position” after a limited time t_0 , (β_0, m, h) falls in a small neighbourhood of V_n of a certain equilibrium (they are all described in Section 2).

This analysis is insufficient, however, when the dimensionless parameter $\varepsilon = (mh)^{-1}$ is small. Long-lived structures made up of kinks then occur which relax, in the final analysis, to equilibrium solutions,

as described above. Here the relaxation time becomes exponentially long, $\ln \tau = O(mh)$. Hence, in the case of a small parameter the attractor analysis (1.3) has to be supplemented, since it is sometime difficult to detect a slow evolution by numerical methods. However, an asymptotic analysis is possible, carried out below in Sections 5 and 6, which describes both the occurrence of a kink structure from certain natural initial states and its slow evolution.

We obtain below a formula for the relaxation time $\tau = \tau(m, p, h)$, which gives its explicit dependence on the problem parameters. Here it turns out that the unstable equilibria solutions (1.3) with a large number of extrema (i.e. with a period $d \ll h$ for large h) decay much more rapidly than the solution with a small number of extrema, when $d = O(h)$, and that the latter correspond to the special case of irregular kink structures. A similar pattern is obtained when $h \sim 1$, but for large characteristic scales m^{-1} , since the conversion of the spatial scale converts these situations into one another.

5. THE THEORY OF THE GROWTHS OF DEFECTS (THE FORMATION OF "WALLS")

We will consider the process by which spatial gradients are localized with the formation of kinks, which arise from smooth orientational fields after a high magnetic field is switched on for ($Hh \gg \mu_c$). The latter can be the result of thermal fluctuations in an initially small field for a thicker layer, when the orientational structure is unstable. In a high field H the part played by thermal fluctuations may be fairly small and the evolution of the orientational field can be described by the equilibrium equation (1.3).

We will show that with certain limitations on the initial data, the process by which a kink structure arises can be described analytically and the corresponding relaxation time can be obtained.

We mean by a growth process the increase in the spatial gradient at the centre of the kink, i.e. the growth of a local twist in the structure. For (1.3) the formal-asymptotic theory, like the simpler equations, has been investigated previously. We will therefore simply present the main results [12, 13].

The process can be described for "smooth" initial data

$$\beta(y, 0) = \psi(Y), \quad Y = \delta y, \quad \delta \ll 1 \tag{5.1}$$

The same results are also obtained for given $\beta(y, 0)$ of the form $\psi(Y) + \delta_1 \psi_1(y)$, $||\psi_1|| < C$, where δ_1 is a small quantity.

We will write the asymptotic expansion in δ

$$\beta = \beta_0(Y, t) + \delta^2 \beta_1(Y, t) + \dots \tag{5.2}$$

where the principal term satisfies the equation

$$\gamma_1 \partial \beta_0 / \partial t = -m^2 \sin 2\beta_0, \quad \beta_0|_{t=0} = \psi(Y)$$

while the corrections β_0, β_1 are found from the linear equations [13]. We have

$$\text{tg} \beta_0 = [\text{tg} \psi(Y)] \exp(-2\gamma_1^{-1} m^2 t)$$

Expansion (5.2) is correct for times of the order of $\tau_1 = t \sim \gamma_1^{-1} \ln(\delta^{-1})$, and this is necessary for the defect to grow. Expansion (5.2) can be justified using comparison theorems [14].

In particular, this leads to the following conclusions.

1. If the initial configuration of the twist $\psi(Y) = \beta(y, 0)$ from (4.1) lies in one of the open intervals $I_n = [(n - 1/2)\pi]$ for integer n , no kinks (defects) can arise: if $\psi(Y) \in I_n$ for all Y , we have $\lim \beta(y, t) = n\pi, t \rightarrow +\infty$.

2. If property 1 is not satisfied, the curve $\beta = \psi(Y)$ will intersect one of the straight lines $\beta = (n - 1/2)\pi$ at least twice for certain n . The growth time is of the order of $\gamma_1^{-1} \ln(\delta^{-1})$ and the kinks grow at points y_i where $\psi(\delta y_i) = (n - 1/2)\pi$ for certain n .

It follows from these considerations that the structures investigated below in Section 6, may arise from smooth initial data. Generally speaking, for given ψ of general form, a non-periodic (random) sequence of defects arises.

6. INTERACTION OF KINKS AND ANTIKINKS. SUPERSLOW RELAXATION OF NON-EQUILIBRIUM UNORDERED STRUCTURES TO EQUILIBRIUM STRUCTURES

As calculations from Section 5 show, a structure with sharp boundaries arises from the initially smooth structure; they can be described using kink profiles $B_s(y-y_i)$ (see Section 2). Here the charge $s = \pm 1$ depends on the sign of the derivative $\partial\beta/\partial y(y, 0)|_{y=y_i}$ of the initial given structure (for $s = -1$ we will call the solution B_s an antikink). Further evolution of the structure occurs, generally speaking, much less slowly than it occurred from the initial unordered state $\beta(y, 0)$ and can be described using kink interaction theory.

This theory was initially developed by Ostrovskii and his co-workers for non-dissipative media.† The mechanism by which soliton (kink) interaction forces occur is physically related to their interaction due to the exponentially falling “tails” (see formula (2.14)).

The theory of the interaction of kinks ($s = 1$) and antikinks ($s = -1$) in a dissipative medium has also been developed [12, 15, 16]. It is a rigorous theory [15–16] for the case of the Ginzburg–Landau type equations

$$u'_t = u''_{xx} + a^2(u - u^3) \tag{6.1}$$

In this case, for large values of h , long-lived structures occur consisting of kink–antikink chains, where each kink ($s = 1$) is followed by an antikink ($s = -1$), and they are separated by “large” distances d_i . The quantity $\lambda = \exp(-cad)$ is in fact the small parameter in the theory, since the interaction forces here are exponentially small and are attractive forces.

The theory is correct so long as $\lambda \ll 1$, i.e. so long as the kinks do not converge. We know from computational experiments and also from other considerations [17], that if a kink and an antikink converge, they “annihilate” one another and (in case (6.1)) a locally almost constant section arises where $u \approx 1$ or $u \approx -1$.

The main difference between problem (1.3) and equations of the type (6.1) previously investigated is that here it is possible for kinks of the same charge to interact, when the closest neighbour of a kink is again a kink. This is due to the fact that the non-linearity is periodic in β , so that after a step “upwards” from zero to π a step “upwards” from π to 2π may again follow.

Such situations have not been considered. Below we propose a simple formally asymptotic method which enables the interaction of kinks with any succession of topological charges to be described. Note that the existing method [16] can only be applied to a regular sequence of unlike charges.

For simplicity we will first consider the case of periodic boundary conditions.

Suppose we have $N = 2n$ kinks and antikinks with coordinates $q_1(t), \dots, q_N(t)$. We will assume that at the initial instant $d = \min|q_i - q_{i+1}| \gg 1$. The small parameter in the asymptotic form described below is the quantity $\lambda = \exp(-md/\sqrt{1-p})$, and the system of equations which arises is correct so long as $\lambda \ll 1$. We will formally assume, taking the periodicity into account, that $q_{N+1} = q_1, q_N = q_0$.

We introduce an auxiliary shear function $\theta(y) \in C^\infty$, where the carrier $\theta(y)$ coincides with $(-1, 1)$, $0 \leq \theta \leq 1$ and θ increases monotonically. We will introduce neighbourhoods V_i and W_i

$$V_i(c) = \{y: |y - r_i| \leq c\}, \quad W_{i+1} = (r_i + c, r_{i+1} - c), \quad r_i = (q_i + q_{i+1})/2 \tag{6.2}$$

where c is a certain constant. We now introduce the ansatz

$$\begin{aligned} \beta &= \varphi_0[\mathbf{q}(t), y] + \varphi_1[\mathbf{q}(t), y] + \dots, \quad \mathbf{q} = (q_1, q_2, \dots, q_N) \\ \varphi_0(\mathbf{q}, y) &= \begin{cases} B_i[a(y - q_i)], & y \in W_i \\ B_i[a(y - q_i)](1 - \theta_i) + B_{i+1}[a(y - q_{i+1})]\theta_i, & y \in V_i \end{cases} \\ B_i(\xi) &= B_{s_i}(\xi) + n_i\pi, \quad a = m(1 - p)^{-1/2} \end{aligned} \tag{6.3}$$

where the correction φ_1 is of the order of λ . The integer numbers n_i define the asymptotic form of the kink as $\xi \rightarrow \infty$, and the numbers $s_i = \pm 1$ are the topological charges. Although the ansatz (6.3) depends

†GORSHKOV, K. A. and OSTROVSKII, L. A., Interaction of solitons in non-integrable systems. The direct perturbation method. Preprint No. 47, Inst. Appl. Physics, Academy of Sciences of the U.S.S.R., Gor’kii, 1981.

on the choice of the shear function θ and the constant c , as we will see below the resultant equations for $q_i(t)$ are independent of the choice of the function θ and the constant c as $d \rightarrow \infty$.

Substituting (6.3) into (1.3) we obtain the following linear equation for the correction

$$A(q)\varphi_1 = R(\varphi_0, y, \dot{q}, q) \tag{6.4}$$

An expression for R will be described below; A is a Schrödinger-type linear operator with variable coefficients. These coefficients only vary appreciably in limited neighbourhoods q_i , which are separated by considerable intervals, where $A \approx (1 - p)d^2/dy^2 - m^2$.

Thus, we have N local potential wells separated by "large" distances. The spectrum of such operators is known [16]. Using simple estimates it can be shown [16] that there are N small eigenvalues of the order of λ or less, while the remaining eigenvalues are negative and are separate from zero. Here the eigenfunctions corresponding to the N small values are linear combinations of the functions $B'_i(y)$, concentrated in the neighbourhoods q_i . Consequently, in order to ensure that the corrections φ_1 are small ($O(\lambda)$) it is sufficient to satisfy the condition

$$\langle R, B'_i \rangle = \int_0^h R(q, \dot{q}, y) B'_i[a(y - q_i)] dy = 0 \tag{6.5}$$

for each i . The derivative B'_i here and below is taken with respect to the argument $\xi = a(y - q_i)$. These equations also give a system of equations of the kink motion.

To simplify the expression for R and to write in explicit form, we will represent R in the form $R = S + Q$. The contribution of S is concentrated around the coordinates q_i in the regions W_i and decays exponentially with distance from q_i . Up to terms $O(\lambda)$ we have

$$S = a\gamma_1 \sum_{j=1}^N B'_j \frac{dq_j}{dt} \tag{6.6}$$

Conversely, the contribution of Q is non-zero only in neighbourhoods V_i . We have

$$Q = \sum_{j=1}^N Q_j + O(\lambda), \quad \text{supp } Q_j = V_j \tag{6.7}$$

$$Q_j = \rho(p)(1 - p)\{s_j(Q'_j - 2aQ'_j) \exp[a(q_j - y)]\} + s_{j+1}(Q'_{j+1} + 2aQ'_{j+1}) \exp[a(y - q_{j+1})] \tag{6.8}$$

The function $\rho = \rho(p)$ was defined in (2.14).

We will now simplify conditions (6.5) and obtain an explicit system for $q_i(t)$. We will first calculate $\langle S, B'_i \rangle$. The contribution of all terms in (6.6), apart from the term $i = j$, is of the order of λ or less. Thus, we have (the integral is evaluated using the well-known scheme described in [12])

$$\langle S, B'_i \rangle = \gamma_1 \frac{dq_i}{dt} \left[\int_{-\infty}^{\infty} (B'(\xi))^2 d\xi + O(\lambda) \right] = \gamma_1 \frac{dq_i}{dt} [p^{-1/2} \arcsin \sqrt{p} + O(\lambda)] \tag{6.9}$$

When calculating $\langle Q, B'_i \rangle$ only the terms $j = i - 1$ and $j = i$ are important. This means physically that each kink interacts only with neighbouring kinks.

Taking into account the fact that the carrier Q_j lies in the region V_j , we can replace the function B'_i by its asymptotic form (the exponential tail). Then, we have from (6.6) and (6.7)

$$B'_i \approx s_j \rho(p) \exp[\mp a(y - q_i)]$$

where the minus sign corresponds to the region V_j , while the plus sign corresponds to the region V_{i-1} .

Integrating by parts, taking the properties of $\chi(y)$ into account, we have

$$J_j = \int_{V_j} Q_j B'_j dy = \pm 2ap^2(p)(1 - p)s_i s_j \exp[-a|q_i - q_j|], \quad j = i, i - 1$$

where the plus sign is taken for $j = i$ and the minus sign is taken for $j = i - 1$.

We finally have the following system of equations (apart from corrections that vanish as $\lambda \rightarrow 0$)

$$\gamma_1 C(p) dq_i / dt = 2ap^2(1-p)s_i[s_{i+1} \exp(a(q_i - q_{i+1})) - s_{i-1} \exp(a(q_{i-1} - q_i))] \tag{6.10}$$

Each of these equations resembles the classical equation of a Tod chain except that the first derivative is on the left. For a kink-antikink chain, when $s_i = -s_{i+1}$ always, it converts into the well-known equations obtained previously [16].

Equations (6.10) have a dissipative form, which follows directly from the possibility of writing them in a form analogous to (4.1) (\bar{D} is the dissipation and \bar{L} is the energy)

$$\partial \bar{D} / \partial \dot{q}_i = -\partial \bar{L} / \partial q_i \tag{6.11}$$

$$\bar{D} = \frac{\gamma_1 C(p)}{2} \sum_{i=1}^N \left(\frac{dq_i}{dt} \right)^2, \quad \bar{L} = p^2 a(1-p) \sum_{i=1}^N s_i s_{i+1} \exp[a(q_i - q_{i+1})]$$

(we recall that $s_{N+1} = s_1, q_{N+1} = q_1$).

The energy \bar{L} decreases along the trajectories (6.10). Hence it follows that kinks of the same charge tend to recede from one another while those of different charge converge. Hence, there is an analogy with ordinary charges. Formally (6.10) and (6.11), which give the asymptotic energy of the system of kinks and their evolution, are correct so long as $d = \min |q_i - q_{i+1}| \gg 1$.

The analysis of Eqs (6.10) is analogous to that carried out earlier for other cases [16]. For periodic boundary conditions the total charge of the system of kinks is zero. System (6.10) can have equilibrium states consisting of chains of kinks of different charges. As in the case of (6.1), they are all unstable. The decay of these unstable structures occurs as follows. In the case of the "common position" there are always two kinks of different charges (signs), closest to one another. Since the interaction force is exponential, one of the exponential functions in (6.10) is much greater than all the remaining ones. The kinks thereby converge in a time of the order of $\exp(ad)$, where d is their initial distance apart.

This is a very slow process. Since only d becomes a quantity of the order of unity, the process of kink collision is speeded up, and it can be modelled on a computer (here it is clear that the remaining kinks have no effect on this collision).

We know [17] that the result will be the annihilation of two kinks and the occurrence of a new system of defects with zero total charge, but a smaller number of kinks. This continues until, after a time of the order of $\exp(ad)$, all the kinks are annihilated and a defect-free state occurs (for the case of periodic conditions). It can be seen that this conclusion agrees with the general theory outlined in Section 4.

This approach can be extended to the Dirichlet condition (2.3).

The formally asymptotic approach described here can also be used in the case of conditions (1.4). In order to satisfy these conditions it is sufficient to introduce two boundary layers with the help of two kinks $B_s[a(y - y_0)], B_{s_1}[a(y - y_1)]$, where y_0 and y_1 are chosen so as to satisfy the following boundary conditions

$$B_{s_0}(-ay_0) = \psi_0, \quad B_{s_1}[a(h - y_1)] = \psi_1$$

(we recall that we have changed to the angle $\beta, \psi_0 = \beta(0), \psi_1 = \beta(h)$).

As a result, a chain of kinks arises where the two extreme kinks are attached. Here it is appropriate to introduce a non-integer defect charge. Thus, for "internal" kinks we assume $s = \pm 1$, as above, while for boundary kinks we find s using the relations

$$s_0 = (\psi_0 - n_0\pi)/\pi, \quad s_1 = (n_1\pi - \psi_1)/\pi$$

The charge is then conserved when readjustment of the structure occurs. These readjustments amount of the fact, as a result of collisions between kinks of different charge, a structure slowly arises (exponentially slowly) consisting of the least number of kinks having the same total charge as the initial configuration.

An important difference between this and the case of periodic conditions is the possibility of stable structures of kinks (of two boundary kinks in case (2.3)).

For the case of conditions (1.4) a "short ladder" of kinks of the same charge occurs. We recall that, according to Section 6, after the initial period of kink growth, N_0 kinks occur, where N_0 is the number of intersections between $\beta = \psi(Y)$ and the straight lines $\beta = (n - 1/2)\pi$. If this number is greater than

N from (1.4), then after initial growth an exponentially prolonged readjustment of the structure will begin leading to a structure consisting of the least number of kinks, ensuring a total charge of N ($N = 0$ for conditions (2.3)).

7. CONCLUSION

Thus, we have described the evolution of an initially weakly non-uniform structure to a stable equilibrium structure for the non-linear kinetic equation (1.3). This evolution occurs in two stages. The first is a comparatively rapid stage and is accompanied by a growth of local gradients and concludes with the formation, generally speaking, of an irregular structure of kinks (described by the ansatz from Section 6, Eqs (6.3)).

The relaxation time corresponding to this stage is described by the formula

$$\tau_1 \sim c\gamma_1^{-1} \ln(m \min_i |\beta'_i(y_i, 0)|)$$

Kinks and antikinks can be formed at points where the curve $\beta = \beta(y, 0)$, which gives the initial data, intersects the straight lines $\beta = (n - 1/2)\pi$, $n = 0, \pm 1, \pm 2, \dots$

However, everything depends on the values of the parameter $\epsilon_d = (md)^{-1}$, where $d = \min_i |q_i - q_{i+1}|$. If this parameter is small (the field strength H is high or d is large) and there are points of intersection y_i , further evolution occurs over an exponentially long period, since the equilibrium state is connected with a very high energy level. In this case the superslow evolution mentioned reduces to convergence of kinks of different charge s and their mutual annihilation until a stable regular structure occurs.

This structure here is either two boundary kinks plus a trivial solution (see (2.3)), or a small ladder of kinks or simply a trivial solution. Note that numerical methods may be ineffective for small ϵ_d in view of the huge value of τ_2 (this superslow evolution may not be noticed in a numerical experiment).

We note an analogy with electromagnetism, namely, the overall topological charge is conserved in the evolution described.

The corresponding relaxation time τ_2 is given by the formula $\ln \tau_2 = O(m\bar{d})$, where \bar{d} is the characteristic distance between kinks.

If ϵ_d is not small (the field strength H is close to the threshold), there is practically no second stage and, according to Section 4, a stable equilibrium structure (described in Sections 2 and 3) is immediately formed comparatively rapidly. In this case the usual numerical methods are effective.

A similar analysis can also be carried out in the two-dimensional case, which is extremely important, since there are then no simple foreseeable formulae for the equilibrium solutions.

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REFERENCES

1. AERO, E. L. and BULYGIN, A. N., Linear mechanics of liquid-crystal media. *Fiz. Tverd. Tela*, 1971, 13, 6, 1701–1714.
2. AERO, E. L., Magneto-optical effects in nematic liquid crystals and Fredericks transitions in non-uniform fields. *Opt. Spektrosk.*, 1988, 65, 2, 342–348.
3. AERO, E. L. and ZAKHAROV, A. V., Elastic deformation of liquid crystals, their stability and use in technology. In *Advances in Science and Technology Ser. Complex and Special Divisions of Mechanics*. Vsesoyuzh. Inst. Nauchn. Tekhn. Inform., Moscow, 1988, 3, 163–237.
4. AERO, E. L., Plane boundary-value problems for the sine-Helmholtz equation in the theory of elasticity of liquid crystals in non-uniform magnetic fields. *Prikl. Mat. Mekh.*, 1996, 60, 1, 79–87.
5. BULYGIN, A. N. and SHALTYKO, L. G., Elastic deformations of nematic liquid-crystal media. *Kristallografiya*, 1983, 28, 2, 405–408.
6. ABRAMOWITZ, M. and STEGUN, I., *Handbook of Special Functions*. Dover, New York, 1975.
7. BABIN, A. V. and VISHIK, M. I., Regular attractors of semigroups and evolution equations. *J. Math. Pure et Appl.*, 1983, 62, 4, 441–491.
8. HENRY, D., Some infinite-dimensional Morse–Smale systems defined by parabolic differential equations. *J. Different. Equat.*, 1985, 59, 2, 165–205.
9. HENRY, D., *Geometric Theory of Semilinear Parabolic Equations*. Springer, Berlin, 1982.
10. LADYZHENSKAYA, O. A., Obtaining minimum global attractors for the Navier–Stokes equation and other partial differential equations. *Usp. Mat. Nauk*, 1987, 42, 6, 25–60.
11. CHUYESHOV, I. D., Global attractors in non-linear equations of mathematical physics. *Usp. Mat. Nauk*, 1993, 48, 3, 135–162.
12. MOLOTKOV, I. A. and VAKULENKO, S. A., *Concentrated Non-linear Waves*. Izd. Leningr. Gos. Univ., Leningrad, 1988.
13. RUBINSTEIN, J., STERNBERG, P. and KELLER, J. B., Fast reaction slow diffusion and curve shortening. *SIAM Journal Appl. Math.*, 1989, 49, 1, 116–133.
14. SMOLLER, J. A., *Shock Waves and Reaction–Diffusion Equations*. Springer, New York, 1983.

15. NISHIURA, Y. and FUJII, H., *SLEP Method to the Stability of Singular Perturbed Solutions with Multiple Internal Transition Layers in Reaction-Diffusion Systems*, Dynamics of Infinite Dimensional Systems: NATO ASI V. F37, eds S. N. Show and J. K. Hale. Springer, Berlin, 1987, pp. 211–230.
16. FUSCO, G., A geometric approach to the dynamic of $u_t = \varepsilon^2 u_{xx} + f(u)$ for small ε . *Lecture Notes in Physics*, Vol. 359, *Problems Involving Change of Type*. Springer, Berlin, 1990, pp. 53–73.
17. FIFE, P. and McLEOD, J. B., The approach of solutions of nonlinear diffusion equations to travelling front solutions. *Arch. Rat. Mech. Analysis*, 1977, **65**, 4, 335–361.

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