Expansion in width for domain walls in nematic liquid crystals in an external magnetic field

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The improved expansion in width is applied to curved domain walls in uniaxial nematic liquid crystals in an external magnetic field. In the present paper we concentrate on the case of equal elastic constants. We obtain an approximate form of the director field up to second order in the magnetic coherence length. [S1063-651X(99)13408-1]

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I. INTRODUCTION

Liquid crystals are probably the best materials for experimental and theoretical studies of topological defects. A variety of defects, relatively simple experiments in which one can observe them, and soundness of theoretical models of dynamics of relevant order parameters make liquid crystals unique in this respect. The literature on topological defects in liquid crystals is enormous, therefore we do not attempt to review it here. Let us only point out Refs. [1-3] where one can find lucid introductions to the topic as well as collections of references.

Our paper is devoted to dynamics of domain walls in uniaxial nematic liquid crystals in an external magnetic field. Static planar domain walls were discussed for the first time in Ref. [4]. We would like to approximately calculate the director field of a curved domain wall. We use a method, called the improved expansion in width, whose general theoretical formulation has been given in Refs. [5,6]. Appropriately adapted expansion in width can also be applied to disclination lines [7].

The expansion in width is based on the idea that transverse profiles of the curved domain wall and of a planar one differ from each other by small corrections which are due to the curvature of the domain wall. We calculate these corrections perturbatively. Formally, we expand the director field in a parameter which gives the width of the domain wall, that is the magnetic coherence length ξ_m in the case at hand, but in fact terms in the expansion involve the dimensionless ratios ξ_m/R_i , where R_i are (local) curvature radia of the domain wall. Therefore, our expansion is expected to provide a good approximation when the curvature radia of the domain wall are much larger than the magnetic coherence length. For the planar domain walls the perturbative solution reduces to just one term which coincides with a well-known exact solution. As we shall see below, the improved expansion in width is not quite straightforward-certain consistency conditions appear and a special coordinate system is used-but that should be regarded as a reflection of nontriviality of evolution of the curved domain walls. Nevertheless, several first terms in the expansion can be calculated without much difficulty, and the whole approach looks quite promising.

In the present paper we consider the simplest and rather elegant case of equal elastic constants. In order to take into account the differences of values of the elastic constants for real liquid crystals one can use, for example, the following two strategies: a perturbative expansion with respect to deviations of the elastic constants from their mean value, or the expansion in width generalized to the unequal constants case. In the former approach, the equal constant approximate solution obtained in the present paper can be used as the starting point for calculating corrections. The case of unequal elastic constants we will discuss in a subsequent paper.

The plan of our paper is as follows. We begin with a general description of domain walls in uniaxial nematic liquid crystals in Sec. II. Next, in Sec. III, we introduce the special coordinate system comoving with the domain wall. Section IV contains the presentation of the improved expansion in width. In Sec. V we discuss consecutive terms in the expansion up to the second order in ξ_m . Several remarks related to our work are collected in Sec. V.

II. DOMAIN WALLS IN NEMATIC LIQUID CRYSTALS

In this section we recall basic facts about domain walls in uniaxial nematic liquid crystals [1,2]. We fix our notation and sketch background for the calculations presented in the next two sections.

We parametrize the director field $\vec{n}(\vec{x},t)$ by two angles $\Theta(\vec{x},t)$, $\Phi(\vec{x},t)$:

$$\vec{n} = \begin{pmatrix} \sin \Theta \cos \Phi \\ \sin \Theta \sin \Phi \\ \cos \Theta \end{pmatrix}.$$
(1)

In this way we get rid of the constraint $\vec{n}^2 = 1$.

We assume that the splay, twist and bend elastic constants are equal $(K_{11}=K_{22}=K_{33}=K)$. In this case the Frank-Oseen-Zöcher elastic free energy density can be written in the form

$$\mathcal{F}_e = \frac{K}{2} (\partial_\alpha \Theta \ \partial_\alpha \Theta + \sin^2 \Theta \ \partial_\alpha \Phi \ \partial_\alpha \Phi). \tag{2}$$

Our notation is as follows: $\alpha = 1,2,3$, $\partial_{\alpha} = \partial/\partial x^{\alpha}$, x^{α} are Cartesian coordinates in the usual three-dimensional space \mathbb{R}^3 ; $\vec{x} = (x^{\alpha})$. In formula (2) we have abandoned a surface term which is irrelevant for our considerations.

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In order to have stable domain walls it is necessary to apply an external magnetic field \vec{H}_0 [1,2]. We assume that \vec{H}_0 is constant in space and time. Without any loss in generality we may take

$$\vec{H}_0 = \begin{pmatrix} 0 \\ 0 \\ H_0 \end{pmatrix}.$$

Then the magnetic field contribution to the free energy density of the nematic is given by the following formula:

$$\mathcal{F}_m = -\frac{1}{2}\chi_a H_0^2 \cos^2\Theta.$$
(3)

Here χ_a is the anisotropy of the magnetic susceptibility. It can be either positive or negative. For concreteness, we assume that $\chi_a > 0$. Our calculations can easily be repeated if $\chi_a < 0$. The ground state of the nematic is double degenerate: $\Theta = 0$ and $\Theta = \pi$ give the minimal total free energy density $\mathcal{F} = \mathcal{F}_e + \mathcal{F}_m$. It is due to this degeneracy that the stable domain walls can exist.

The dynamics of the director field is mathematically described by the equation

$$\gamma_1 \frac{\partial \vec{n}}{\partial t} + \frac{\delta F}{\delta \vec{n}} = \vec{0},\tag{4}$$

where

$$F = \int d^3x \, \mathcal{F}.$$

The constant γ_1 is the rotational viscosity of the liquid crystal, and $\delta / \delta \vec{n}$ denotes the variational derivative with respect to \vec{n} . Equation (4) is equivalent to the following equations for the Θ and Φ angles:

$$\gamma_1 \frac{\partial \Theta}{\partial t} = K \Delta \Theta - \frac{K}{2} \sin(2\Theta) \partial_\alpha \Phi \partial_\alpha \Phi - \frac{1}{2} \chi_a H_0^2 \sin(2\Theta),$$
(5)

$$\gamma_1 \sin^2 \Theta \,\frac{\partial \Phi}{\partial t} = K \partial_\alpha (\sin^2 \Theta \,\partial_\alpha \Phi), \tag{6}$$

where $\Delta = \partial_{\alpha} \partial_{\alpha}$.

The domain walls arise when the director field is parallel to the magnetic field \vec{H}_0 in one part of the space and antiparallel to it in another. In between there is a layer—the domain wall—across which \vec{n} smoothly changes its orientation from the parallel to \vec{H}_0 to the opposite one, that is Θ varies from 0 to π or vice versa. The angle Φ does not play an important role. The ansatz

$$\Phi = \Phi_0 \tag{7}$$

with constant Φ_0 trivially solves Eq. (6). Then, Eq. (5) is the only equation we have to solve. In the following we assume the ansatz (7), hereby restricting the class of domain walls we consider. It is clear from formula (2) that domain walls with varying Φ have higher elastic free energy than the walls with constant Φ .

Let us recall the static planar domain wall [1,2]. We assume that it is parallel to the $x^1=0$ plane. Then

$$\Theta = \Theta_0(x^1), \quad \Phi_0 = \text{const},$$
 (8)

where

$$\Theta_0|_{x^1 \to -\infty} = 0, \quad \Theta_0|_{x^1 \to +\infty} = \pi.$$
(9)

One could also consider the "antidomain wall" obtained by interchanging 0 and π on the right-hand side (RHS) of boundary conditions (9). Equation (5) is now reduced to the following equation:

$$K\Theta_0'' = \frac{1}{2}\chi_a H_0^2 \sin(2\Theta_0), \qquad (10)$$

where primes denote d/dx^1 . This equation is well-known in soliton theory as the sine-Gordon equation, see, e.g., Ref. [8]. It is convenient to introduce the magnetic coherence length ξ_m ,

$$\xi_m = (K/\chi_a H_0^2)^{1/2}.$$
 (11)

The functions

$$\Theta_0(x^1) = 2 \arctan\left(\exp\frac{x^1 - x_0^1}{\xi_m}\right) \tag{12}$$

with arbitrary constant x_0^1 obey Eq. (10) as well as the boundary conditions (9). The planar domain walls (8) are homogeneous in the $x^1=0$ plane. Their transverse profile is parametrized by x^1 . Width of the wall is approximately equal to ξ_m , in the sense that for $|x^1-x_0^1| \ge \xi_m$ values of Θ_0 differ from 0 or π by exponentially small terms.

The planar domain wall solution (8) contains the two arbitrary constants: Φ_0 and x_0^1 . The arbitrariness of Φ_0 is due to the assumption that the elastic constants are equal. Then, the free energy density \mathcal{F} is invariant with respect to the transformations $\Phi \rightarrow \Phi + \text{const.}$ If the elastic constants are not equal this invariance is lost, and in the case of planar domain walls Φ_0 can take only discrete values $n\pi/2$, n = 0,1,2,3. The constant x_0^1 appears because of invariance of Eqs. (5), (6) with respect to the translations $x^1 \rightarrow x^1 + \text{const.}$

Notice that $\Theta_0(x_0^1) = \pi/2$. Hence, at $x^1 = x_0^1$ the director \vec{n} is perpendicular to \vec{H}_0 . In fact, the boundary conditions (9) imply that for any domain wall there's a surface on which $\vec{n} \cdot \vec{H}_0 = 0$. Such surface is called the core of the domain wall. The magnetic free energy density \mathcal{F}_m has the maximum on the core.

The planar domain wall (8), (12) plays a very important role in our approach. In a sense, it is taken as the zeroth order approximation to the curved domain walls. The trick consists in using the special coordinate system comoving with the curved domain wall. This coordinate system encodes shape and motion of the domain wall regarded as a surface in the space. Internal dynamics of the domain wall, in particular orientation of the director inside the domain wall, is then calculated perturbatively in the comoving reference frame with the function (12) taken as the leading term.

III. THE COMOVING COORDINATES

The first step in our construction of the perturbative solution consists in introducing the coordinates comoving with the domain wall. The two coordinates (σ^1, σ^2) parametrize the domain wall regarded as a surface in the \mathbb{R}^3 space, and one coordinate, say ξ , parametrizes the direction perpendicular to the domain wall. For convenience of the reader we quote below main definitions and formulas [6].

We introduce a smooth, closed or infinite surface *S* in the usual \mathbb{R}^3 space. It is supposed to lie close to the domain wall, and its shape mimics the shape of the domain wall. In particular we may assume that *S* coincides with the core at certain time t_0 . Points of *S* are given by $\vec{X}(\sigma^i, t)$, where σ^i (i=1,2) are the two intrinsic coordinates on *S*, and *t* denotes the time. We allow for motion of *S* in the space. The vectors $\vec{X}_{,k}$, k=1,2, are tangent to *S* at the point $\vec{X}(\sigma^i, t)$ (we use the notation $f_{,k} \equiv \partial f/\partial \sigma^k$). They are linearly independent, but not necessarily orthogonal to each other. At each point of *S* we also introduce a unit vector $\vec{p}(\sigma^i, t)$ perpendicular to *S*, that is,

$$\vec{p} \cdot \vec{X}_{,k} = 0, \quad \vec{p}^2 = 1.$$

The triad $(\tilde{X}_{,k}, \vec{p})$ forms a local basis at the point \tilde{X} of S. Geometrically, the surface S is characterized by the induced, positive definite metric tensor

$$g_{ik} = \vec{X}_{,i} \cdot \vec{X}_{,k}$$

and by the extrinsic curvature coefficients

$$K_{il} = \vec{p} \cdot \vec{X}_{,il},$$

where i,k,l=1,2. They appear in Gauss-Weingarten formulas

$$\vec{X}_{,ij} = K_{ij}\vec{p} + \Gamma^l_{ij}\vec{X}_{,l}, \quad \vec{p}_{,i} = -g^{jl}K_{li}\vec{X}_{,j}.$$
 (13)

The matrix (g^{ik}) is by definition the inverse of the matrix (g_{kl}) , i.e., $g^{ik}g_{kl} = \delta_l^i$, and Γ_{ik}^l are Christoffel symbols constructed from the metric tensor g_{ik} . The two eigenvalues k_1, k_2 of the matrix (K_j^i) , where $K_j^i = g^{il}K_{lj}$, are called the extrinsic curvatures of *S* at the point \vec{X} . The corresponding main curvature radia are defined as $R_i = 1/k_i$.

The comoving coordinates $(\sigma^1, \sigma^2, \xi)$ are introduced by the following formula:

$$\vec{x} = \vec{X}(\sigma^i, t) + \xi \vec{p}(\sigma^i, t), \qquad (14)$$

where ξ is the coordinate in the direction perpendicular to the surface *S*. In the comoving coordinates this surface is given by the simple condition $\xi = 0$. We will use the compact notation: $(\sigma^1, \sigma^2, \xi) = (\sigma^{\alpha})$, where $\alpha = 1,2,3$ and $\sigma^3 = \xi$. The coordinates (σ^{α}) are just a special case of curvilinear coordinates in the space \mathbb{R}^3 . In these coordinates the metric tensor $(G_{\alpha\beta})$ in \mathbb{R}^3 has the following components:

$$G_{33}=1, \quad G_{3k}=G_{k3}=0, \quad G_{ik}=N_{i}^{l}g_{lr}N_{k}^{r},$$

where

$$N_i^l = \delta_i^l - \xi K_i^l,$$

i,k,l,r=1,2. Simple calculations give

$$\sqrt{G} = \sqrt{g}N$$

where $G = \det(G_{\alpha\beta})$, $g = \det(g_{ik})$, and $N = \det(N_k^i)$. For N we obtain the following formula:

$$N = 1 - \xi K_i^i + \frac{1}{2} \xi^2 (K_i^i K_l^l - K_l^i K_l^i).$$

Components $G^{\alpha\beta}$ of the inverse metric tensor in \mathbb{R}^3 have the form

$$G^{33}=1, G^{3k}=G^{k3}=0, G^{ik}=(N^{-1})^i_r g^{rl}(N^{-1})^k_l,$$

where

$$(N^{-1})_{r}^{i} = \frac{1}{N} [(1 - \xi K_{l}^{l}) \delta_{r}^{i} + \xi K_{r}^{i}].$$

We see that dependence on the transverse coordinate ξ is explicit, while σ^1, σ^2 appear through the tensors g_{ik}, K_r^l which characterize the surface *S*.

The comoving coordinates (σ^{α}) have, in general, certain finite region of validity. In particular, the range of ξ at fixed (σ^1, σ^2) is determined from the condition G > 0. It is clear that it increases with decreasing extrinsic curvature coefficients K_i^l , reaching infinity for the planar domain wall for which $K_j^i = 0$. We assume that the surface *S* (hence also the domain wall) is not curved too much. Then, that region is large enough, so that outside it there are only exponentially small tails of the domain wall which give negligible contributions to physical characteristics of the domain wall.

The comoving coordinates are utilized to write Eq. (5) in the form suitable for calculating the curvature corrections. Let us start from the Laplacian $\Delta \Theta$. In the new coordinates it has the form

$$\Delta \Theta = \frac{1}{\sqrt{G}} \frac{\partial}{\partial \sigma^{\alpha}} \left(\sqrt{G} G^{\alpha \beta} \frac{\partial \Theta}{\partial \sigma^{\beta}} \right).$$

The time derivative on the left-hand side (LHS) of Eq. (5) is taken under the condition that all x^{α} are constant. It is convenient to use time derivative taken at constant σ^{α} . The two derivatives are related by the formula

$$\frac{\partial}{\partial t}\bigg|_{x^{\alpha}} = \frac{\partial}{\partial t}\bigg|_{\sigma^{\alpha}} + \frac{\partial \sigma^{\beta}}{\partial t}\bigg|_{x^{\alpha}} \frac{\partial}{\partial \sigma^{\beta}}$$

where

$$\frac{\partial \xi}{\partial t}\Big|_{x^{\alpha}} = -\vec{p} \cdot \dot{\vec{X}}, \quad \frac{\partial \sigma^{i}}{\partial t}\Big|_{x^{\alpha}} = -(N^{-1})^{i}_{k}g^{kr}\vec{X}_{,r} \cdot (\dot{\vec{X}} + \xi\dot{\vec{p}}),$$

the overdots stand for $\partial/\partial t|_{\sigma^i}$. Let us also introduce the dimensionless coordinate

$$s = \xi/\xi_m$$
.

Now we can write Eq. (5) transformed to the comoving coordinates (σ^i , s) [with the ansatz (7) taken into account]:

$$\frac{\gamma_{1}}{K}\xi_{m}^{2}\left(\frac{\partial\Theta}{\partial t}\Big|_{\sigma^{\alpha}}-\frac{1}{\xi_{m}}\vec{p}\cdot\vec{X}\frac{\partial\Theta}{\partial s}\right)$$
$$-(N^{-1})_{k}^{i}g^{kr}\vec{X}_{,r}\cdot(\vec{X}+\xi_{m}s\vec{p})\frac{\partial\Theta}{\partial\sigma^{i}}$$
$$=\frac{\partial^{2}\Theta}{\partial s^{2}}-\frac{1}{2}\sin(2\Theta)+\frac{1}{N}\frac{\partial N}{\partial s}\frac{\partial\Theta}{\partial s}$$
$$+\xi_{m}^{2}\frac{1}{\sqrt{g}N}\frac{\partial}{\partial\sigma^{j}}\left(G^{jk}\sqrt{g}N\frac{\partial\Theta}{\partial\sigma^{k}}\right).$$
(15)

Equation (15) is the starting point for our construction of the expansion in width.

IV. THE IMPROVED EXPANSION IN WIDTH

We seek the domain wall solutions of Eq. (15) in the form of expansion with respect to ξ_m , that is,

$$\Theta = \Theta_0 + \xi_m \Theta_1 + \xi_m^2 \Theta_2 + \cdots . \tag{16}$$

Inserting formula (16) in Eq. (15) and keeping only terms of the lowest order ($\sim \xi_m^0$) we obtain the following equation:

$$\frac{\partial^2 \Theta_0}{\partial s^2} = \frac{1}{2} \sin(2\Theta_0), \qquad (17)$$

which coincides with Eq. (10) after the rescaling $x^1 = \xi_m s$. Its solutions

$$\Theta_{s_0}(s) = 2 \arctan[\exp(s-s_0)],$$

have essentially the same form as the planar domain walls (12), but now *s* gives the distance from the surface *S*. This surface will be determined later. We shall calculate the curvature corrections to the simplest solution

$$\Theta_0(s) = 2 \arctan[\exp(s)]. \tag{18}$$

Because already Θ_0 interpolates between the ground state solutions 0 and π , the corrections Θ_k , $k \ge 1$ should vanish in the limits $s \to \pm \infty$.

Equations for the corrections Θ_k , $k \ge 1$ are obtained by expanding both sides of Eq. (15) and equating terms proportional to ξ_m^k . These equations can be written in the form

$$\hat{L}\Theta_k = f_k, \tag{19}$$

with the operator \hat{L}

$$\hat{L} = \frac{\partial^2}{\partial s^2} - \cos(2\Theta_0) = \frac{\partial^2}{\partial s^2} + \frac{2}{\cosh^2 s} - 1.$$
(20)

The last equality in Eq. (20) can be obtained, e.g., from Eq. (17): inserting Θ_0 given by formula (18) on the LHS of Eq. (17) we find that $\sin(2\Theta_0) = -2 \sinh s / \cosh^2 s$ and $\cos(2\Theta_0) = 1 - 2 / \cosh^2 s$. The expressions f_k on the RHS of Eqs. (19) depend on the lower orders contributions Θ_l , l < k. Straightforward calculations give

$$f_1 = \partial_s \Theta_0 \left(K_r^r - \frac{\gamma_1}{K} \vec{p} \cdot \dot{\vec{X}} \right), \tag{21}$$

$$f_2 = -\sin(2\Theta_0)\Theta_1^2 + s\partial_s\Theta_0K_j^iK_i^j + \partial_s\Theta_1\left(K_r^r - \frac{\gamma_1}{K}\vec{p}\cdot\vec{X}\right),$$
(22)

$$f_{3} = \frac{\gamma_{1}}{K} (\partial_{t} \Theta_{1} - g^{kr} \vec{X}_{,r} \cdot \dot{\vec{X}} \partial_{k} \Theta_{1}) - 2 \sin(2\Theta_{0}) \Theta_{1} \Theta_{2}$$

$$- \frac{2}{3} \cos(2\Theta_{0}) \Theta_{1}^{3} + s \partial_{s} \Theta_{1} K_{j}^{i} K_{i}^{j}$$

$$- \frac{1}{2} s^{2} \partial_{s} \Theta_{0} K_{r}^{r} [(K_{i}^{i})^{2} - 3K_{j}^{i} K_{i}^{j}] - \frac{1}{\sqrt{g}} \partial_{j} (\sqrt{g} g^{jk} \partial_{k} \Theta_{1})$$

$$+ \partial_{s} \Theta_{2} \left(K_{r}^{r} - \frac{\gamma_{1}}{K} \vec{p} \cdot \dot{\vec{X}} \right)$$
(23)

and

$$f_{4} = \frac{\gamma_{1}}{K} (\partial_{t}\Theta_{2} - sg^{ik}\dot{\vec{p}} \cdot \vec{X}_{,k}\partial_{i}\Theta_{1}) - \frac{\gamma_{1}}{K}g^{jk}\vec{X}_{,k} \cdot \dot{\vec{X}}(\partial_{j}\Theta_{2} + sK_{j}^{i}\partial_{i}\Theta_{1}) - \sin(2\Theta_{0}) \left(\Theta_{2}^{2} + 2\Theta_{1}\Theta_{3} - \frac{1}{3}\Theta_{1}^{4}\right) - 2\cos(2\Theta_{0})\Theta_{1}^{2}\Theta_{2} + s\partial_{s}\Theta_{2}K_{j}^{i}K_{i}^{j} + s^{3}\partial_{s}\Theta_{0} \left[(K_{r}^{r})^{4} + \frac{1}{2}(K_{s}^{r}K_{r}^{s})^{2} - 2(K_{r}^{r})^{2}K_{j}^{i}K_{i}^{j} \right] - \frac{s^{2}}{2}\partial_{s}\Theta_{1}K_{r}^{r}((K_{i}^{i})^{2} - 3K_{j}^{i}K_{i}^{j}) - \frac{1}{\sqrt{g}}\partial_{j}(\sqrt{g}g^{jk}\partial_{k}\Theta_{2}) - \frac{2s}{\sqrt{g}}\partial_{j}(\sqrt{g}K^{jk}\partial_{k}\Theta_{1}) + sg^{jk}(\partial_{j}K_{r}^{r})\partial_{k}\Theta_{1} + \partial_{s}\Theta_{3} \left(K_{r}^{r} - \frac{\gamma_{1}}{K}\vec{p} \cdot \dot{\vec{X}}\right),$$
(24)

where $\partial_t = \partial/\partial t$, $\partial_i = \partial/\partial \sigma^i$. We have taken into account the fact that Θ_0 does not depend on σ^i .

Notice that all Eqs. (19) for Θ_k are linear. The only nonlinear equation in our perturbative scheme is the zeroth order equation (17). It is very important to observe that the operator \hat{L} has a zero mode, that is, the function $\psi_0(s)$ which quickly vanishes in the limits $s \rightarrow \pm \infty$, and which obeys the equation

$$L\psi_0=0.$$

Inserting $\Theta_{s_0}(s)$ in Eq. (17), differentiating that equation with respect to s_0 , and putting $s_0=0$ we obtain (as the identity) that $\hat{L}\psi_0=0$ where

$$\psi_0(s) = \frac{1}{\cosh s}.\tag{25}$$

The presence of this zero mode is related to the invariance of Eq. (17) with respect to translations in *s*; therefore it is often called the translational zero mode. Let us multiply both sides of Eqs. (19) by $\psi_0(s)$ and integrate over *s*. Integration by parts gives

$$\int_{-\infty}^{\infty} ds \ \psi_0 \hat{L} \Theta_k = \int_{-\infty}^{\infty} ds \ \Theta_k \hat{L} \psi_0 = 0.$$

Hence, we obtain the consistency (or integrability) conditions

$$\int_{-\infty}^{\infty} ds \ \psi_0(s) f_k(s) = 0, \tag{26}$$

where f_k are given by formulas of the type (21)–(24). We shall see in the next section that these conditions play a crucial role in determining the curved domain wall solutions.

Using standard methods [9] one can obtain the following formulas for vanishing in the limits $s \rightarrow \pm \infty$ solutions Θ_k of Eqs. (19):

$$\Theta_k = G[f_k] + C_k(\sigma^i, t)\psi_0(s), \qquad (27)$$

where

$$G[f_k] = -\psi_0(s) \int_0^s dx \psi_1(x) f_k(x) + \psi_1(s) \int_{-\infty}^s dx \psi_0(x) f_k(x).$$
(28)

Here $\psi_0(s)$ is the zero mode (25) and

$$\psi_1(s) = \frac{1}{2} \left(\sinh s + \frac{s}{\cosh s} \right) \tag{29}$$

is the other solution of the homogeneous equation

 $\hat{L}\psi = 0.$

The second term on the RHS of formula (27) obeys the homogeneous equation $\hat{L}\Theta_k = 0$. It vanishes when $s \rightarrow \pm \infty$.

The solutions (27) contain the functions $C_k(\sigma^i, t)$ which are still arbitrary. Also $\vec{X}(\sigma^i, t)$ giving the comoving surface *S* has not been specified. It turns out that the conditions (26) are so restrictive that they essentially fix those functions. The extrinsic curvature coefficients K_l^i and the metric g_{ik} will follow from $\vec{X}(\sigma^i, t)$.

One can worry that $G[f_k]$, $k \ge 1$, given by formula (28) do not vanish when $s \to \pm \infty$ because the second term on the RHS of formula (28) is proportional to ψ_1 , which exponentially increases in the limits $s \to \pm \infty$. However, the integrals

$$\int_{-\infty}^{s} dx \,\psi_0 f_k$$

vanish in that limit due to the consistency conditions (26). Moreover, qualitative analysis of Eq. (15) shows that $f_k \sim (\text{polynomial in } s) \times \exp(-|s|)$ for large |s|, hence those integrals behave as (polynomial in $s) \times \exp(-2|s|)$ for large |s|. This ensures that all $G[f_k]$ exponentially vanish when $|s| \rightarrow \infty$.

V. THE APPROXIMATE DOMAIN WALL SOLUTIONS

In this section we discuss the approximate solutions obtained with the help of the perturbative scheme we have just described. We present formulas for the first two corrections Θ_1 and Θ_2 , an equation for $\vec{X}(\sigma^i, t)$ which determines motion of the surface *S*, as well as equations for the functions C_1, C_2 .

The zeroth order solution is already known, see formula (18). This allows us to discuss the consistency condition with k=1. Substituting f_1 from formula (21) and noticing that

$$\partial_s \Theta_0 = \frac{1}{\cosh s} = \psi_0(s)$$

we find that the consistency condition (26) is equivalent to

$$\frac{\gamma_1}{K}\vec{p}\cdot\dot{\vec{X}} = K_r^r.$$
(30)

This condition is in fact the equation for \tilde{X} . It is of the same type as Allen-Cahn equation [10], but in our approach it governs the motion of the auxiliary surface S.

Let us now turn to the perturbative corrections. After taking into account Allen-Cahn equation (30) we have $f_1=0$. Therefore, the total first order contribution has the form

$$\Theta_1 = \frac{C_1(\sigma^i, t)}{\cosh s}.$$
(31)

The second order contribution Θ_2 is calculated from formula (28) with f_2 given by Eq. (22). Using the results (30), (31) we obtain the following expression:

$$\Theta_2 = \psi_2(s) C_1^2(\sigma^i, t) + \psi_3(s) K_j^i K_i^j + \frac{C_2(\sigma^i, t)}{\cosh s}, \quad (32)$$

where

$$\psi_2(s) = -\frac{\sinh s}{2\cosh^2 s},$$

and

$$\psi_3(s) = \frac{1}{2}s \cosh s - \frac{s}{2 \cosh s} - \psi_1(s) \ln(2 \cosh s) + \frac{s^2 \sinh s}{4 \cosh^2 s} - \frac{1}{4 \cosh s} \int_0^s dx \frac{x^2}{\cosh^2 x}.$$

The integral in $\psi_3(s)$ can easily be evaluated numerically. Due to the consistency conditions, the functions C_1, C_2 in formulas (31), (32) are not arbitrary, see below.

The consistency condition (26) with k=2 does not give any restrictions—it can be reduced to the identity 0=0. More interesting is the next condition, that is the one with k=3. Inserting formula (23) for f_3 and calculating necessary integrals over s, we find that it can be written in the form of the following inhomogeneous equation for $C_1(\sigma^i, t)$

$$\frac{\gamma_1}{K} (\partial_t C_1 - g^{kr} \vec{X}_{,r} \cdot \dot{\vec{X}} \partial_k C_1) - \frac{1}{\sqrt{g}} \partial_j (\sqrt{g} g^{jk} \partial_k C_1) - K^i_j K^j_i C_1$$
$$= \frac{\pi^2}{24} K^r_r [(K^i_i)^2 - 3K^i_j K^j_i].$$
(33)

We have also used Allen-Cahn equation (30). Equation (33) determines C_1 provided that we fix initial data for it. Similarly, the consistency condition coming from the fourth order (k=4) is equivalent to the following homogeneous equation for C_2 :

$$\frac{\gamma_1}{K}(\partial_t C_2 - g^{kr}\vec{X}_{,r} \cdot \dot{\vec{X}}\partial_k C_2) - \frac{1}{\sqrt{g}}\partial_j(\sqrt{g}g^{jk}\partial_k C_2) - K^i_j K^j_i C_2$$
$$= 0. \tag{34}$$

Formulas (16), (18), (31), and (32) give a family of domain walls. To obtain one concrete domain wall solution we have to choose the initial position of the auxiliary surface S. Its positions at later times are determined from Allen-Cahn equation (30). We also have to fix the initial values of the functions C_1, C_2 , and to find the corresponding solutions of Eqs. (33),(34). Notice that we are not allowed to choose the initial profile of the domain wall because the dependence on the transverse coordinate s is explicitly given by formulas (18), (31), and (32). The choice of the initial data should not lead to large perturbative corrections at least in certain finite time interval. Therefore we require that at the initial time $\xi_m C_1 \ll 1, \ \xi_m^2 C_2 \ll 1, \ \xi_m K_i^i \ll 1.$ The domain wall is located close to the surface S because for large |s| the perturbative contributions exponentially vanish and the leading term 2 arctan(e^s) is close to one of the vacuum values $0, \pi$.

Notice that Eqs. (30), (33), and (34) imply that the planar domain wall ($K_j^i = 0$) cannot move, in contradistinction with relativistic domain walls for which uniform, inertial motions are possible.

In our approach the evolution of the domain wall is described in terms of the surface S, and of the functions C_1, C_2 which can be regarded as fields defined on S. In some cases Eqs. (30), (33), (34) for S, C_1 , and C_2 can be solved analytically, one can also use numerical methods. Anyway, these equations are much simpler than the initial Eq. (5).

The presented formalism is invariant with respect to changes of the coordinates σ^1, σ^2 on *S*. In particular, in a vicinity of any point \vec{X} of *S* we can choose the coordinates in such a way that $g_{ik} = \delta_{ik}$ at \vec{X} . In these coordinates Eq. (30) has the form

$$\frac{\gamma_1}{K}v = \frac{1}{R_1} + \frac{1}{R_2},$$
(35)

where v is the velocity in the direction \vec{p} perpendicular to S at the point \vec{X} , and R_1, R_2 are the main curvature radia of S at that point.

As an example, let us consider cylindrical and spherical domain walls. If S is a straight cylinder of radius R then $R_1 = \infty$, $R_2 = -R(t)$, $v = \dot{R}$ and Eq. (35) gives

$$R(t) = \sqrt{R_0^2 - \frac{2K}{\gamma_1}(t - t_0)},$$
(36)

where R_0 is the initial radius. The origin of the Cartesian coordinate frame is located on the symmetry axis of the cylinder *S* (which is the *z* axis), \vec{p} is the outward normal to *S*, and $s = \left[\sqrt{r^2 - z^2} - R(t)\right]/\xi_m$, where *r* is the radial coordinate in R^3 . As σ^1, σ^2 we take the usual cylindrical coordinates *z*, ϕ . Equations (33), (34) reduce to

$$\frac{\gamma_1}{K}\partial_t C_1 - \left(\partial_z^2 C_1 + \frac{1}{R^2}\partial_\phi^2 C_1\right) - \frac{1}{R^2}C_1 = \frac{\pi^2}{12}\frac{1}{R^3}, \quad (37)$$

$$\frac{\gamma_1}{K}\partial_t C_2 - \left(\partial_z^2 C_2 + \frac{1}{R^2}\partial_\phi^2 C_2\right) - \frac{1}{R^2}C_2 = 0.$$
(38)

If at the initial time t_0 the functions C_1, C_2 have constant values $C_1(0), C_2(0)$ all over the cylinder, then

$$C_{1}(t) = \frac{\pi^{2}}{12R(t)} \ln[R_{0}/R(t)] + \frac{R_{0}}{R(t)}C_{1}(0),$$

$$C_{2}(t) = \frac{R_{0}}{R(t)}C_{2}(0).$$
(39)

General solutions of Eqs. (37),(38) can be found by splitting C_1, C_2 into Fourier modes, but we shall not present them here.

The case of spherical domain wall is quite similar. Now *S* is the sphere of radius *R* and $R_1 = R_2 = -R$, $v = \dot{R}$. Equation (35) gives

$$R(t) = \sqrt{R_0^2 - \frac{4K}{\gamma_1}(t - t_0)},$$
(40)

The origin is located at the center of the sphere, $s = [r - R(t)]/\xi_m$, and \vec{p} is the outward normal to *S*. As σ^k we take the usual spherical coordinates. Then, Eqs. (33),(34) can be written in the form

$$\frac{\gamma_1}{K}\partial_t C_1 - \frac{1}{R^2} \left(\frac{1}{\sin\theta} \partial_\theta (\sin\theta\partial_\theta C_1) + \frac{1}{\sin^2\theta} \partial_\phi^2 C_1 \right) - \frac{2}{R^2} C_1$$
$$= \frac{\pi^2}{6} \frac{1}{R^3}$$
(41)

and

$$\frac{\gamma_1}{K}\partial_t C_2 - \frac{1}{R^2} \left(\frac{1}{\sin\theta} \partial_\theta (\sin\theta\partial_\theta C_2) + \frac{1}{\sin^2\theta} \partial_\phi^2 C_2 \right) - \frac{2}{R^2} C_2$$
$$= 0. \tag{42}$$

General solution of these equations can be obtained by expanding C_1, C_2 into spherical harmonics. In the particular case when C_1, C_2 are constant on the sphere *S*, the solutions $C_k(t)$ have the same form (39) as in the previous case except that now R(t) is given by formula (40). In both cases our approximate formulas are expected to be meaningful as long as $R(t)/\xi_m \ge 1$.

Because we have found the transverse profile of the domain wall explicitly, we can express the total free energy Fby geometric characteristics of the domain wall. One should insert our approximate solution for Θ in formulas (2) and (3) for \mathcal{F}_e and \mathcal{F}_m , and to perform integration over s. The volume element d^3x is taken in the form

$$d^3x = \xi_m \sqrt{G} d^2\sigma ds.$$

For simplicity, let us consider curved domain walls for which

$$C_1 = 0 = C_2$$

Straightforward calculation gives

$$F = -\frac{K}{2} \frac{V}{\xi_m^2} + \frac{2K}{\xi_m} |S| - \frac{\pi^2}{6} K \xi_m \int d^2 \sigma \sqrt{g} \\ \times \left(\frac{1}{R_1^2} + \frac{1}{R_2^2} - \frac{1}{R_1 R_2} \right) + (\text{terms of the order } \xi_m^3) ,$$
(43)

where |S| denotes the area of the surface S, and V is the total volume of the liquid crystalline sample. The first term on the RHS of this formula is a trivial bulk term which appears because the smallest value of the magnetic free energy density has been chosen to be equal to $-K/(2\xi_m^2)$. The proper domain wall contribution starts from the second term. This term gives the main contribution of the domain wall to F. One can think about the corresponding constant free energy $2K/\xi_m$ per unit area. The third term on the RHS of formula (43) represents the first perturbative correction. It is of the order $(\xi_m/R_i)^2$ when compared with the main term, and within the region of validity of our perturbative scheme it is small. One can easily show that this term is negative or zero. Hence, it slightly diminishes the total free energy. In this sense, the domain walls have negative rigidity-bending them without stretching (i.e., with |S| kept constant) diminishes the free energy.

VI. REMARKS

We would like to add several remarks about the expansion in width and the approximate domain wall solutions it yields. (1) In the approach presented the dynamics of the curved domain wall in the three-dimensional space is described in terms of the comoving surface *S* and of the functions C_k , $k \leq 1$, defined on *S*. The profile of the domain wall has been explicitly expressed by these functions, the transverse coordinate ξ , and the geometric characteristics of *S*. The surface *S* and the functions C_k obey Eqs. (30),(33),(34) which do not contain ξ . In particular cases these equations can be solved analytically, and in general one can look for numerical solutions. Such numerical analysis is much simpler than it would be in the case of the initial equation (5) for the angle Θ , precisely because one independent variable has been eliminated.

(2) We have used ξ_m as the formal expansion parameter. This may seem unsatisfactory because it is a dimensionful quantity, hence it is hard to say whether its value is small or large. What really matters is smallness of the corrections $\xi_m \Theta_1, \xi_m^2 \Theta_2$. This is the case when $\xi_m C_1 \ll 1, \xi_m^2 C_2 \ll 1$, and $\xi_m K_i^i \ll 1$, as it follows from formulas (16), (31), and (32).

(3) Notice that an assumption that *S* coincides with the core for all times in general would not be compatible with the expansion in width. If we assume that $C_1=0=C_2$ at certain initial time t_0 , Eq. (33) implies that $C_1 \neq 0$ at later times (unless the RHS of it happens to vanish). Then, it follows from formulas (16), (18), and (31) that $\Theta \neq \pi/2$ at s=0, that is, on *S*.

(4) In the present work we have neglected effects which could come from perturbations of the exponentially small tails of the domain wall. For example, consider a domain wall in the form of an infinite straight cylinder flattened from two opposite sides. Its front and rear flat sides have vanishing curvatures, and according to Eq. (35) they do not move. In our description the flattened domain wall shrinks from the edges where the mean curvature $1/R_1 + 1/R_2$ does not vanish. Now, in reality the front and rear flat parts interact with each other. This interaction is exponentially small only if the two parts are far away from each other. We have neglected it altogether assuming the exact 2 arctan(e^s) asymptotics at large *s*. In this sense, our approximate solution takes into account only the effects of curvature.

(5) Finally, let us mention that the dynamics of the domain walls in nematic liquid crystals can also be investigated with the help of another approximation scheme, called the polynomial approximation. In the first paper [11] it has been applied to the cylindrical domain wall, and in the second one to a planar soliton. Comparing the two approaches, the polynomial approximation is much cruder than the expansion in width. It also contains more arbitrariness, e.g., in choosing a concrete form of boundary conditions at $|s| \rightarrow \infty$. On the other hand, that method is much simpler and it can be useful for rough estimates.

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