Radial fluctuations and nonisotropic disclinations in nematic liquid crystals

M. Simões, A. J. Palangana,* and A. E. Gonçalves
Departamento de Física, Universidade Estadual de Londrina, Campus Universitário, 86051-970, Londrina, PR, Brazil

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The aim of this paper is to study the role of the radial symmetry in the profile of anisotropic disclinations of the nematic liquid crystals. It will be shown that when radial fluctuations are allowed a macroscopic term appears. This term preserves the known topology of these disclinations but changes their angular structure and the distribution of elastic energy. Furthermore, it is shown that one of the isotropiclike disclinations predicted by the usual approach is forbidden by the radial fluctuations.

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I. INTRODUCTION

According to Frank [1–4], planar polar disclinations of nematic materials would be described by the profile

$$\varphi = S\chi + \varphi_0, \tag{1}$$

where φ is the angle of the director with the $\vec{e}_x$ direction, χ is the polar angle (See Fig. 1), and $S = n/2$, $n = \pm 1, \pm 2, \ldots,$ is the strength of the disclination. The validity of Eq. (1) [5] depends upon two basic assumptions: the director lies on a plane perpendicular to the disclination line and the elastic constants are assumed as the same (isotropic condition). Both assumptions have been subject of intense study and it was found that they are idealizations of the real experimental situation [5–10]. The planar disclinations are not usually found in nematic materials because, in order to avoid a singularity, the director always escapes into the third dimension [5,6]. Furthermore, it was found that when the elastic constants are not considered the same, the solution given by Eq. (1) becomes an approximation of a more complex solution [7]. An important aspect of the approximation given by Eq. (1) is that it has the same topological properties of the anisotropic solution. The anisotropy of the elastic constants stretches and shrinks the solution given by Eq. (1), but does not change its general character: when we turn round a closed path, the director always returns to the same initial orientation. In fact, this compactness condition is the essence of the topological properties of the polar disclinations.

The basic equations describing the anisotropic version of the Eq. (1) were proposed by Dzyaloshinskii [7]. In his study he realized that the polar disclinations have radial symmetry and imposed it by removing a radial derivative from the Frank free energy, getting an elastic energy that only deals with of the angular dependence of the problem. Furthermore, the compactness of the solution was used as a boundary condition of the differential equation determining the polar configuration. Since then, this solution has been considered as the anisotropic version of the Eq. (1).

In this paper we will regard a slight different approach to the same problem. We will not force the radial symmetry directly on the Frank free energy, but we will consider it as a limit to be imposed on the Euler-Lagrange equation. The advantage of this procedure, is that the radial fluctuations are not eliminated from the beginning, allowing the study of their effects during the calculations. When this procedure is applied to the limit of vanishing small radial fluctuations, we discover that the equation describing the director configuration preserves the topological properties of the Eq. (1), but it is considerably different from the one proposed by Dzyaloshinskii. In the next two sections the equation for the configuration of the director will be deduced and the differences between our approach and the usual one will be emphasized. At the conclusion some comments about our approach will be presented.

II. ANISOTROPIC POLAR DISCLINATIONS

Consider the two-dimensional elastic free energy proposed by Dzyaloshinskii [7] to study polar disclinations

$$F = \frac{1}{2}(K_{33}+K_{11}) \int \{(1+a)(\vec{\nabla}\times\vec{n})^2 + (1-a)(\vec{\nabla}\cdot\vec{n})^2\} dV, \tag{2}$$

where $a = (K_{33}-K_{11})/(K_{33}+K_{11})$ measures the elastic anisotropy, K_{11} is the splay elastic constant and K_{33} is the bend elastic constant. Using the polar geometry described in Fig. 1 one can show that

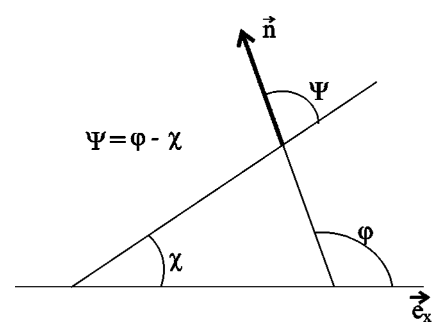

FIG. 1. Geometry and variables used in the analytical definition of the disclinations.

*Permanent address: Departamento de Física, Universidade Estadual de Maringá, Campus Universitário, Maringá, Paraná, Brazil.

$$\vec{\nabla}\cdot\vec{n}=\partial_r n_r+\frac{1}{r}(\partial_\chi n_\chi+n_r)$$

$$=-n_\chi\partial_r\psi+\frac{1}{r}n_r(\partial_\chi\psi+1), \tag{3}$$

$$(\vec{\nabla}\times\vec{n})_S=\partial_r n_\psi+\frac{1}{r}(-\partial_\chi n_r+n_\psi)$$

$$=n_r\partial_r\psi+\frac{1}{r}n_\psi(\partial_\chi\psi+1), \tag{4}$$

where $n_r=\cos\psi$, $n_\psi=\sin\psi$, $\psi(\chi)=\varphi(\chi)-\chi$, and the index S means that the corresponding operator is restricted to acting on the surface of the planar configuration.

So,

$$F=\frac{1}{2}(K_{33}+K_{11})\int \mathcal{F}dV \tag{5}$$

with

$$\mathcal{F}=(1+a\cos 2\psi)(\partial_r\psi)^2+\frac{1}{r^2}(1-a\cos 2\psi)(\partial_\chi\psi+1)^2$$

$$+\frac{2a}{r}\sin 2\psi(\partial_\chi\psi+1)(\partial_r\psi), \tag{6}$$

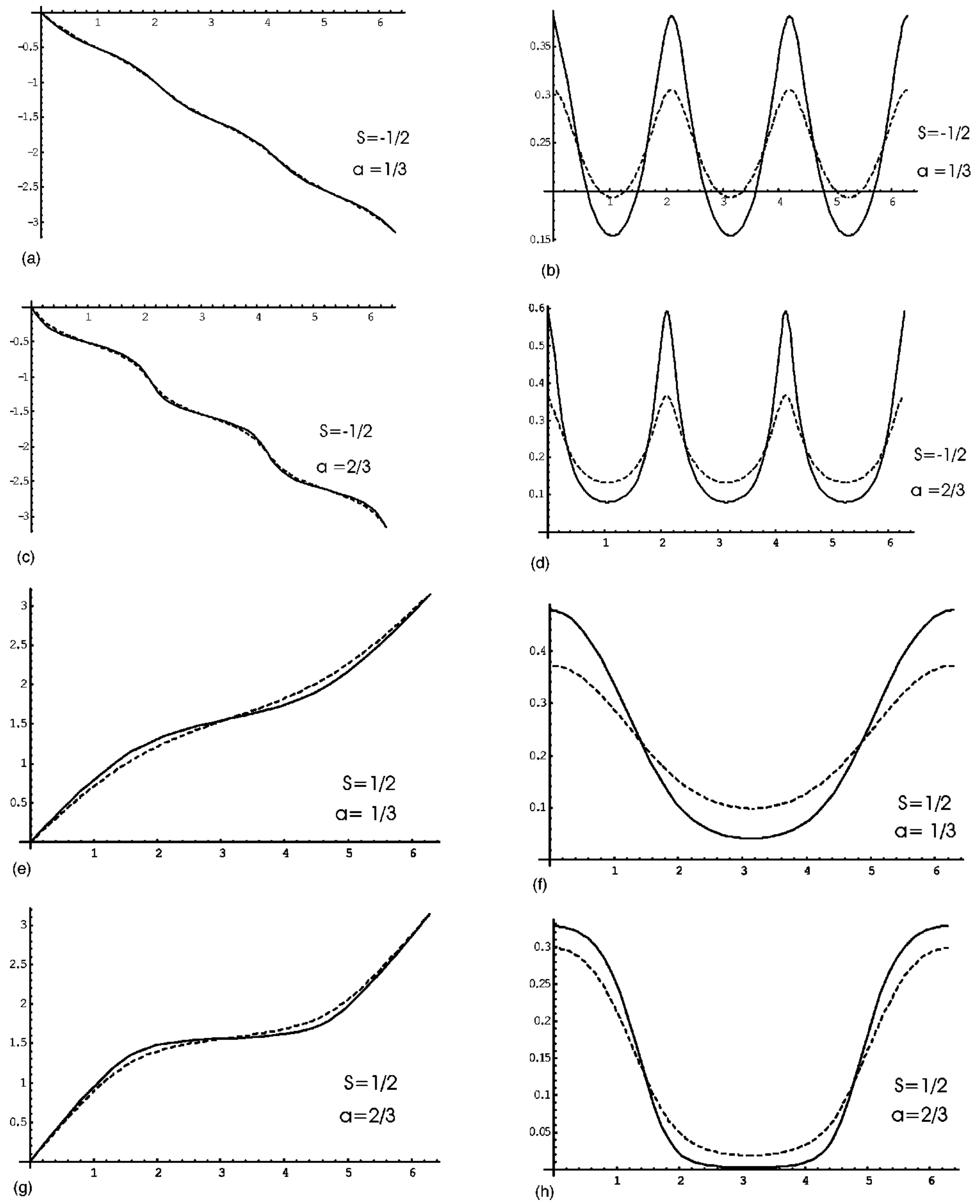

FIG. 2. Profile of the function $\varphi(\chi)$ and the density of energy F for the disclinations $S=-1/2$ and $S=1/2$ and anisotropies $K_{33}=2K_{11}$ ($a=0.33$) and $K_{33}=4K_{11}$ ($a=0.66$) at a fixed distance r from the origin. The variable φ gives the angular orientation of the director and the variable χ gives the angular position, as described in Fig. 1. The continuous line corresponds to the results that follow from Eq. (9) and the dashed lines correspond to the results that follow from Dzyaloshinskii solution. Arbitrary unities were used for the density of energy. (a) and (c) correspond to the profile of the disclination $S=-1/2$, and (b) and (d) correspond to the angular distributions of free energy, F. Observe that the two approaches have a strong difference in the angular distribution of free energy. (e), (g), (f), and (h) describe, for $S=1/2$, the same physics as the preceding four figures.

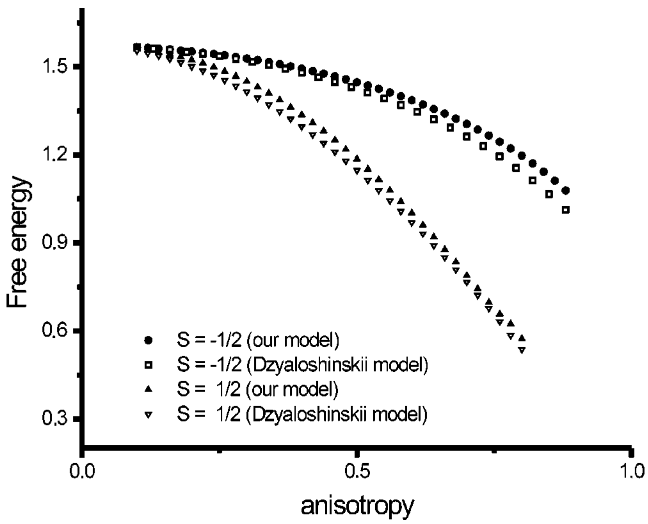

FIG. 3. Total free energy computed along a line at a fixed distance r from the origin. The solid symbols correspond to the results obtained from our model, and the open symbols correspond to the results obtained with the Dzyaloshinskii solution. Observe that the anisotropy $a=(K_{33}-K_{11})/(K_{33}+K_{11})$ of the elastic constants produces different values for free energy of the disclinations $S=-1/2$ and $S=1/2$ [10]. Arbitrary unities were used for the density of energy.

At this point Dzyaloshinskii introduced the radial symmetry of the disclinations and, on this equation, imposed the condition $\partial_r\psi=0$. So, the first and last terms are zero. Furthermore, as the variable ψ depends no more on r, but depends only on χ, the term linear in $\partial_\chi\psi$, that comes from $(\partial_\chi\psi+1)^2$, becomes a total differential and may be subtracted from the free energy. So, the Dzyaloshinskii free energy density becomes

$$\mathcal{F}_D=\frac{1}{r^2}(1-a\cos 2\psi)((\partial_\chi\psi)^2+1), \qquad (7)$$

which gives the following equation for the polar disclination:

$$(1-a\cos 2\psi)(\partial_\chi^2\psi)+a[(\partial_\chi\psi)^2-1]\sin 2\psi=0. \qquad (8)$$

When the term $\partial_r\psi$ is disregarded in Eq. (6), all radial contributions become fixed and their consequences cannot be computed. Here, another approach will be considered. First we will deduce the differential equation giving the director configuration and, only then, we will regard the radial symmetry, by imposing the limit $\partial_r\psi\to 0$. When this is done it is observed that the first term of Eq. (6) becomes null, as happened in the Dzyaloshinskii approach. However, the contribution coming from $2a/r\sin 2\psi(\partial_\chi\psi+1)(\partial_r\psi)$ does not have the same destination, and does not disappear when the limit $\partial_r\psi\to 0$ is taken. In this case, the resulting equation for the disclinations becomes

$$(1-a\cos 2\psi)(\partial_\chi^2\psi)+a[(\partial_\chi\psi)^2-1]\sin 2\psi$$
$$-a(\partial_\chi\psi+1)\sin 2\psi=0, \qquad (9)$$

that differs from the Dzyaloshinskii equation in the last term.

III. COMPARISON BETWEEN THE SOLUTIONS

Our first remark concerns the trivial solutions that, like $\psi=0$, satisfy the differential equations given by Eqs. (8) and (9). As Dzyaloshinskii, we have found that $\psi=0$ $(S=1)$ and $\partial_\chi\psi+1=0$ $(S=0)$ are equivalent to the isotropic solutions described by Eq. (1). Due to that we will call these solutions as isotropiclike solutions. But, while the Dzyaloshinskii equation predicts that $\partial_\chi\psi-1=0$ $(S=2)$ would be an isotropic-like solution, our approach does not predict that. In fact, our approach predicts that $\partial_\chi\psi-2=0$ $(S=3)$ would be an isotropiclike solution.

Of course, the majority of the solutions of these differential equations are not isotropiclike solutions. We will call the anisotropic solution ψ, corresponding to the disclination S and anisotropy a, as $\psi_S^a(\chi)$. Hence, $\psi_S^a(\chi)$ satisfies the same boundary conditions of the similar isotropic disclination. For example, for $S=1/2$ we have $\psi_{1/2}^a(0)=0$ and $\psi_{1/2}^a(2\pi)=-\pi$. In Figs. 2(a) to 2(h) graphic representations of the numeric solutions of some functions related with ψ_S^a, for fixed r, are displayed. Two distinct values of the anisotropy a and two distinct values disclination index S are exhibited ($\psi_{-1/2}^{0.33}$, $\psi_{-1/2}^{0.66}$, $\psi_{1/2}^{0.33}$, and $\psi_{1/2}^{0.66}$). The anisotropy $a=0.33$ corresponds to $K_{33}=2K_{11}$, and the anisotropy $a=0.66$ corresponds to $K_{33}=4K_{11}$.

Figure 2 also compares the distribution of the free energy, for fixed r, between our approach and the one by Dzyaloshinskii. The distribution of energy is strongly different between these two configurations; in our approach the maxima and the minima are more accentuated. Nevertheless, the corresponding difference in total energy is not dramatic. In the Fig. 3 the configurations $\psi_{-1/2}^a$ and $\psi_{1/2}^a$ show this difference, as function of the anisotropy a. The free energy, according our configurations, is always around 5% greater than the configuration previously known.

IV. FINAL REMARKS AND CONCLUSION

In this paper we have shown that the shape of the radial disclinations depends on the manner by which we deal with the radial symmetry of these structures. The condition $\partial_r\psi=0$ is a constraint (a nonholonomic one), and as a constraint it must be handled. So, when it is imposed directly on the free energy a strong limitation in the nature of the admissible configurations is being done and, surely, the character of the problem under consideration is also being changed. A constraint can never be imposed directly on the functional. As a rule [11], it must be imposed on the configuration giving the extreme of a functional.

Finally, it must be observed that an absolutely perfect radial configuration would require a so restrictive set of experimental conditions, that in practice, the radial symmetry would be only an approximation. Therefore, as happens to any approximation, it must be maintained until the last equations, where its influence may be computed.

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