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On the Disclination Lines of Nematic Liquid Crystals

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Abstract. Defects in liquid crystals are of great practical importance and theoretical interest. Despite tremendous efforts, predicting the location and transition of defects under various topological constraint and external field remains to be a challenge. We investigate defect patterns of nematic liquid crystals confined in three-dimensional spherical droplet and two-dimensional disk under different boundary conditions, within the Landau-de Gennes model. We implement a spectral method that numerically solves the Landau-de Gennes model with high accuracy, which allows us to study the detailed static structure of defects. We observe five types of defect structures. Among them the 1/2-disclination lines are the most stable structure at low temperature. Inspired by numerical results, we obtain the profile of disclination lines analytically. Moreover, the connection and difference between defect patterns under the Landau-de Gennes model and the Oseen-Frank model are discussed. Finally, three conjectures are made to summarize some important characteristics of defects in the Landau-de Gennes theory. This work is a continuing effort to deepen our understanding on defect patterns in nematic liquid crystals.

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1 Introduction

Nematic liquid crystals (LCs) are composed of rigid rod-like molecules. When subject to topological constraints, discontinuity in the alignment direction of LCs can form, which is known as *defects*. Defects are commonly found to exist as isolated point or disclination

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line in experiments [8]. When conditions such as temperature and boundary constraint vary, the location and topology of defects may change drastically [15]. Predicting defect pattern is the key to design self-assembly biomolecule and colloidal suspensions, and is thus of particular practical interest but remains to be a difficult problem [12, 19, 20, 24].

Three commonly used continuum theories to describe nematic LCs at equilibrium are the Oseen-Frank model, Ericksen's model and the Landau-de Gennes model [19]. In the Oseen-Frank model the state of nematic LCs is described by a unit-vector field, $\boldsymbol{n}\in W^{1,2}(\Omega;\mathbb{S}^2)$, where $\Omega\in\mathbb{R}^d$, $d=2,3$ is the region occupied by the LCs material. In its simplest form, the Oseen-Frank free-energy functional can be written as

$$F_{OF}[\boldsymbol{n}]=\int_\Omega |\nabla \boldsymbol{n}|^2 d\boldsymbol{x}.$$

The vector filed $\boldsymbol{n}$ that minimizes F_{OF} is a $\mathbb{S}^2$-valued harmonic map [19, 32].

There are two deficiencies in the Oseen-Frank model in describing nematic LCs. First, $\boldsymbol{n}$ and $-\boldsymbol{n}$ are treated as discontinuity in the model while physically they are equivalent. As a result, the *head-to-tail* symmetry is not preserved [3]. Secondly, the model can only predict point defects but not the more complex disclination lines observed in experiments [18].

The Ericksen's model can admit solutions that contain disclination lines [13, 19]. In this model the state of LCs is described by $(s,\boldsymbol{n})\in W^{1,2}(\Omega;\mathbb{R}\otimes\mathbb{S}^2)$. Compared with the Oseen-Frank model, it contains an extra order parameter $s\in\mathbb{R}$ which measures the degree of orientational order along $\boldsymbol{n}$. The free-energy functional is given by

$$F_E[s,\boldsymbol{n}]=\int_\Omega s^2|\nabla \boldsymbol{n}|^2+k|\nabla s|^2+\omega_0(s)d\boldsymbol{x},$$

where ω_0 is a bulk energy term and k is a constant. Singularity of $\boldsymbol{n}$ in $\mathbb{S}^2$ in the Oseen-Frank model at the defect can be removed by allowing $s=0$ in $\mathbb{R}\otimes\mathbb{S}^2$ in the Ericksen's model. In this sense the Ericksen's model can be considered as a regularization of the Oseen-Frank model.

In the physically more realistic Landau-de Gennes (LdG) model the state of LCs is described by a matrix-valued tensor field, $\mathsf{Q}\in W^{1,2}(\Omega;\mathscr{S}_0)$. The set $\mathscr{S}_0:=\{\mathsf{Q}\in\mathbb{R}^{3\times 3}:\mathsf{Q}=\mathsf{Q}^T,\mathrm{tr}(\mathsf{Q})=0\}$ contains all the three-by-three symmetric traceless matrix. A tensor $\mathsf{Q}\in\mathscr{S}_0$ has five degree-of-freedom and can be written as

$$\mathsf{Q}=s\left(\boldsymbol{nn}-\frac{\mathsf{I}}{3}\right)+r\left(\boldsymbol{mm}-\frac{\mathsf{I}}{3}\right),\quad s,r\in\mathbb{R},\quad \boldsymbol{n},\boldsymbol{m}\in\mathbb{S}^2, \tag{1.1}$$

where I is the three-by-three identity matrix. When $s=r=0$, $\mathsf{Q}=0$ and is called *isotropic*. When $s\neq 0$ and $r=0$, $\mathsf{Q}=s\left(\boldsymbol{nn}-\frac{\mathsf{I}}{3}\right)$ is called *uniaxial*. It corresponds to the physical configuration that the orientation of the LC molecules are rotational symmetric with respect to $\boldsymbol{n}$. A uniaxial Q has two identical eigenvalues. The set of uniaxial and isotropic Q,

$$\mathscr{U}:=\left\{\mathsf{Q}=s\left(\boldsymbol{nn}-\frac{\mathsf{I}}{3}\right):s\in\mathbb{R},\boldsymbol{n}\in\mathbb{S}^2\right\}, \tag{1.2}$$