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Motion of Singularities in the Heat Flow of Harmonic Maps into a Sphere

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Abstract. Numerical experiments are used to determine the motion of singularities in the heat flow of harmonic maps into a unit sphere. These singularities are closely related to point defects in a nematic liquid crystals. The motion of singularities is affected by initial positions and interaction between singularities and boundary conditions. In particular, it is shown that the motion of singularities is the same as the motion of point defects in nematic liquid crystals under Neumann boundary conditions. For Dirichlet boundary conditions, the results do not properly reflect the crystal defect motion due to the shortcoming of the model.

AMS subject classifications: 65M99, 65S05

Key words: Heat flow of harmonic maps, singularity, boundary effect, interaction.

1. Introduction

The properties of liquid crystals have been widely studied by physicists, chemists, material scientists, mathematicians and so on. The results of these investigations are successfully applied in technology, including the display development and manufacturing. A simplified version of the general Ericksen-Leslie system [12, 18] for modeling the hydrodynamic flow of nematic liquid crystal materials has the form

$$\begin{aligned}
&\mathbf{u}_t + \mathbf{u}\cdot\nabla\mathbf{u} - \mu\Delta\mathbf{u} + \nabla P = -\lambda\nabla\cdot\Big(\nabla\mathbf{d}\odot\nabla\mathbf{d} - \frac{1}{2}|\nabla\mathbf{d}|^2\mathbb{I}_n\Big),\\
&\nabla\cdot\mathbf{u} = 0,\\
&\mathbf{d}_t + \mathbf{u}\cdot\nabla\mathbf{d} = \gamma\Big(\Delta\mathbf{d} + |\nabla\mathbf{d}|^2\mathbf{d}\Big),
\end{aligned} \tag{1.1}$$

where $\mathbf{u} : \Omega\times(0,T)\to\mathbb{R}^n$ is the velocity field of the underlying incompressible fluid, $P : \Omega\times(0,T)\to\mathbb{R}$ the pressure function, $\mathbf{d} : \Omega\times(0,T)\to S^2 := \{v\in\mathbb{R}^3 : |v| = 1\}$

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the averaged orientation of the nematic liquid crystal molecules. The positive constants μ, λ and γ denote fluid viscosity, competition between kinetic energy and potential energy, and macroscopic elastic relaxation time for the molecular orientation field, respectively. From the viewpoint of mathematics, the Ericksen-Leslie equations are coupled by Navier-Stokes and harmonic heat flow equations. Such coupled systems have been studied in Refs. [4, 19, 28–30] by a penalty function method. Besides, the Doi-Onsager model, which simplifies the states of liquid crystal particles was considered in [20, 21]. If $\mathbf{u} = 0$ and $\gamma = 1$, the third equation in (1.1) reduces to the heat flow of harmonic maps into a sphere — viz.

$$\begin{aligned} &\mathbf{d}_t = \Delta \mathbf{d} + |\nabla \mathbf{d}|^2 \mathbf{d}, \\ &|\mathbf{d}| = 1. \end{aligned} \tag{1.2}$$

If $\mathbf{u} = 0$, the Eq. (1.2) represents the orientation field of nematic liquid crystal molecules and geometrical methods have been successfully used to study this situation. Weinan and Wang [11] considered an implicit unconditionally stable first-order projection scheme. For two-dimensional equations, Struwe [25] and Chang [2] proved the existence of unique global weak solutions with at most finitely many singular points. Chang *et al.* [3] and Huang *et al.* [15] constructed examples of finite-time singularities for two- and three-dimensional equations, respectively. Other examples of finite-time singularities for three-dimensional equations have been presented by Coron and Ghidaglia [9] and also by Chen and Ding [5]. The existence of global partially regular weak solutions in higher dimensions is shown by Chen and Struwe [6] and by Chen and Lin [7].

In mathematical sense, defects in nematic liquid crystals can be considered as singularities. They attracted a substantial attention in the recent years. Here, we assume the validity of the continuum theory — i.e. the direction of liquid crystals is supposed to be continuous with respect to the spatial variables. Nevertheless, black filaments are often found in liquid crystal displays. It was noted by Friedel [13] in the beginning of twenties of the last century that this phenomenon is caused by discontinuities in the arrangement of liquid crystal molecules so that there is no well-defined direction. Such a state is called dislocation. We note that there are only two types of stable defects in crystals — viz. disclination lines and point defects. The dislocation can be characterised by the strength S represented either by half-integer or integer value and $S \in \mathbb{Z}$ for point defects [17].

Repnik *et al.* [24] studied the interaction between defects and the annihilation of point defects in nematic liquid crystals. Svetec and Slavinec [26] considered the annihilation of hedgehog-antihedgehog defects in confined nematic liquid crystals and demonstrated the collision and merging of defects. Bogi *et al.* [1] studied the anchoring influence of two parallel $+1/2$ and $-1/2$ disclination lines on the annihilation dynamics in nematic liquid crystals. Dierking *et al.* [10] discovered that a backflow effect induced by elastic constants and anisotropy leads to the defect overlap and velocity asymmetry in the annihilation of umbilic defects of strength $S = \pm 1$. This is confined to Hele-Shaw cells with homeotropic boundary conditions. Besides, Tóth *et al.* [27] demonstrated that backflow, which is the coupling between the order parameter and the velocity fields, has a significant effect on the motion of defects in nematic liquid crystals. Moreover, the topological strength of defects