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Transition of Defect Patterns from 2D to 3D in Liquid Crystals

Yang Qu, Ying Wei and Pingwen Zhang*

School of Mathematical Sciences, Peking University, Beijing 100871, P.R. China.

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Abstract. Defects arise when nematic liquid crystals are under topological constraints at the boundary. Recently the study of defects has drawn a lot of attention because of the growing theoretical and practical significance. In this paper, we investigate the relationship between two-dimensional defects and three-dimensional defects within nematic liquid crystals confined in a shell. A highly accurate spectral method is used to solve the Landau-de Gennes model to get the detailed static structures of defects. Interestingly, the solution is radial-invariant when the thickness of the shell is sufficiently small. As the shell thickness increases, the solution undergoes symmetry break to reconfigure the disclination lines. We study this three-dimensional reconfiguration of disclination lines in detail under different boundary conditions. In particular, we find that the temperature plays an important role in deciding whether the transition between two-dimensional defects and three-dimensional defects is continuous or discontinuous for the shell with planar anchoring condition on both inner and outer surfaces. We also discuss the characterization of defects in two- and three-dimensional spaces within the tensor model.

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Key words: Transition of defects, liquid crystal, Landau-de Gennes model, spectral method.

1 Introduction

Nematic liquid crystals (LCs) are composed of rigid rod-like molecules which tend to parallel align with each other due to inter-molecular interaction. When the alignment of LC molecules is under topological constraints at the boundary, discontinuity in the alignment direction of LCs can form, which is known as defect. Typically, there are point defects and disclination lines [18]. The prediction of defect patterns is of great theoretical and practical interests, and remains to be a difficult problem. Because defect patterns are

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*Corresponding author. *Email addresses:* `quyang@pku.edu.cn` (Y. Qu), `wyheyhey@163.com` (Y. Wei), `pzhang@pku.edu.cn` (P. Zhang)

not only affected by the temperature and the constraints, but also affected by the shape of the geometric regions bounding them.

In the past decade, many systematic work has been done on nematic LCs confined on the spherical droplets and the regions outside solid balls. Mkaddem and Gartland [16] investigated the defect patterns of nematic LCs confined in spherical droplet under radial anchoring condition. They obtained the radial hedgehog, ring disclination and split-core solutions by assuming rotational symmetry around the z-axis. Hu et al. [1] obtained three configurations (single-core, double-core and split-core) in the spherical droplet under planar anchoring condition. When spherical colloids are dispersed in nematic LCs with radial anchoring condition on the surface, two configurations (Saturn-ring and dipole) are obtained in the article of Ravnik and Zumer [11]. After enforcing planar anchoring condition on the surface, three stable configurations of boojum cores (single-core, double-core and split-core) are obtained [7].

In this paper, we investigate the defect patterns of nematic LCs confined in spherical shells, which is a recent interesting topic of researches. Such as Vitelli et al. [30] experimentally investigated the defect structures of nematic LCs shells; [10] studied the defect texture of nematic LCs shells by a vector model; [28] and [29] exploited the experiments and computer simulations simultaneously to study the defect in nematic LCs shells; Bates et al. [14] utilized the Monte Carlo simulation to study the nematic ordering confined in shells; and Seyednejad et al. [27] used a finite element method to minimize the free energy functional of nematic LCs shells. Although many experiments and simulation methods were designed to investigate the defect patterns in nematic shells, but they didn't give the local structure of the defect patterns clearly. Due to the complexities of the defect patterns, we need high-fidelity simulations with advanced numerical methods for the nematic LCs shells. In this article, we use the spectral method based on Zernike polynomial expansion [23] and BFGS algorithm [24] to solve the Landau-de Gennes model of nematic LCs shells. By these methods, the relationships between defect patterns and the thickness of the shell, the temperature, and the boundary conditions are investigated systematically. We show that when the shell thickness is small, the defect patterns tend to be radial-invariant, which means that the configuration of every layer is same up to a scaling constant in the shell. We call this kind of structures as two-dimensional (2D) structure. When the shell becomes thicker, defects may undergo dramatic reconfigurations and do not hold the radial-invariant property. We call these defect patterns as three-dimensional (3D) structure. The reconfiguration of the defect patterns between 2D and 3D structures is the emphasis of our study.

It is generally known that defects can be classified by their topological invariants. Lavrentovich [4] elaborated the topological charge by homotopy group theory, which is also called winding number in 2D space [6]. In the case of 2D space, winding number is an appropriate metric, and easy to be understood. But in the case of 3D space, winding number and topological charge are different. We use the winding number on the normal plane of defect points to measure the disclination line in this paper, and discuss the distinctions between the winding number and the topological charge of disclination