Numer. Math. Theor. Meth. Appl.
doi: 10.4208/nmtma.2017.s01

Vol. **10**, No. 2, pp. 205-221
May 2017

Defects Around a Spherical Particle in Cholesteric Liquid Crystals

Yu Tong, Yiwei Wang and Pingwen Zhang*

Laboratory of Mathematics and Applied Mathematics, School of Mathematical Sciences, Peking University, Beijing 100871, China

Received 2 November 2016; Accepted (in revised version) 5 January 2017

Dedicated to Professor Zhenhuan Teng on the occasion of his 80th birthday

Abstract. We investigate the defect structures around a spherical colloidal particle in a cholesteric liquid crystal using spectral method, which is specially devised to cope with the inhomogeneity of the cholesteric at infinity. We pay particular attention to the cholesteric counterparts of nematic metastable configurations. When the spherical colloidal particle imposes strong homeotropic anchoring on its surface, besides the well-known twisted Saturn ring, we find another metastable defect configuration, which corresponds to the dipole in a nematic, without outside confinement. This configuration is energetically preferable to the twisted Saturn ring when the particle size is large compared to the nematic coherence length and small compared to the cholesteric pitch. When the colloidal particle imposes strong planar anchoring, we find the cholesteric twist can result in a split of the defect core on the particle surface similar to that found in a nematic liquid crystal by lowering temperature or increasing particle size.

AMS subject classifications: 65N35, 76A15

Key words: Cholesteric liquid crystal, defects, Landau-de Gennes theory, spectral method.

1. Introduction

Dispersing colloidal particles in liquid crystals usually disrupts the orientation order and leads to formation of topological defects around each particle. These topological defects play a important role in the long-range interaction between particles, which determines the self-assembled structures of the colloids-liquid crystals composite materials [6, 24]. Therefore much attention has been paid to the defect configurations around colloidal particles.

*Corresponding author. *Email addresses:* tong_yu@pku.edu.cn (Y. Tong), yiweiwang@pku.edu.cn (Y. W. Wang), pzhang@pku.edu.cn (P. W. Zhang)

The defect configurations around one spherical particle in a nematic liquid crystal are extensively studied by both experiments and simulations [9,19,28,29]. For a spherical particle with strong homeotropic anchoring, two types of metastable configurations are found, known as dipole and Saturn ring. And for strong planar anchoring, three types of boojums will arise, known as single-, double- and split-cores [32]. For the cholesteric case, relatively little work has been done even for the one spherical particle case.

The theories that widely used to describe the liquid crystals can be classified into three levels [12]: the molecular theory, the Q-tensor theory and the vector theory. The vector theory, such as the Oseen-Frank theory [26] and the Ericksen's theory [5], uses unit-vectors $\mathbf{n}(\mathbf{x})$ as an order parameter, called "director", to describe the average orientation of molecules in the vicinity of each point $\mathbf{x}$. The vector theory gives a simple description of liquid crystals. However, it fails to preserve the head-to-tail symmetry of liquid crystals [1] and cannot be used to study the detailed structures of defects. The molecular theory [25], which uses an orientational distribution function $f(\mathbf{x},\mathbf{n})$ as an order parameter, gives the precise description of liquid crystals, but simulations based on it involve large computational cost. The the Q-tensor theory, such as the Landau-de Gennes theory [4], uses a 3×3 symmetric traceless tensor $\mathsf{Q}(\mathbf{x})$ as an order parameter. The Q-tensor theory enjoys the benefit that Q is continuous around defects and it gives a physically realistic description of liquid crystals.

There are some simulation studies devoted to investigate the defect structures around a spherical particle in a cholesteric liquid crystal within Landau-de Gennes theory. By using lattice Boltzmann method (LBM), a twisted Saturn ring configuration is reported with strong homeotropic anchoring on the particle surface [16]. A pair of defect patches or helical disclination lines that link the point defects on particle surface are reported for strong planar anchoring [17]. Besides, the Monte Carlo simulations have also been used to study these problems [22].

It is easy to understand the twisted Saturn ring found in a cholesteric, which can be regarded as the nematic Saturn ring undergoing a twist. Then a natural question is, what will dipole become in a cholesteric? Recently, a dipole-like profile around colloidal particle in a cholesteric liquid crystal has been reported in the confinement-unwound homeotropic cells, found through experiments and numerical simulations with finite difference method [27]. However, the structure they studies is in a bounded domain between two glass plates, and the perpendicular anchoring on glass plates here plays a dominant role, forcing a uniform director field far away from the particle, which is in contrast with the layer structure in the cholesteric.

Also, the helical disclination lines can be realized by moving the two point defects of a split-core away from each other and wrapping the disclination line around the particle. But will the nematic single- and double-cores lead to the same configuration after applying cholesteric twist?

The questions mentioned above motivate us to study these problems within the Landau-de Gennes theory using spectral method. One of the difficulties of solving these problems numerically is that the size of the defect core may be much smaller than the