

# Assembly of confined nanoparticles in nematic phases

by

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# Abstract

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The study of nematic phases covers diverse branches of academics. From a purely academical standpoint, the morphologies exhibited by this material are the most direct and tangible way of demonstrating algebraic topology. From experimental work, this material is the perfect messenger of molecular events since any occurrence on the surface of the system modifies the molecular orientation and the effects of this change is felt over macroscopic distances thus emitting a different optical signal. From the theoretical point of view, the behavior of nematic phases is found in a wide variety of materials, specially in biological materials, thus any model that represents different phases in an accurate matter serves for the prediction of equilibrium states that later can be harnessed in technological applications. In this thesis we focus on the study of confined nematics from the theoretical point of view using a free energy functional in the continuum scale. The free energy minimization is done with two methods: a relaxation that stems from the Euler–Lagrange equations, and a novel theoretically informed Monte Carlo method. The results presented here consist on a numerical analysis of meshfree interpolation schemes in 3D, and a formulation of a new methodology that allows the calculation of gradients with high accuracy and efficiency. The second part of this document is dedicated to the analysis of confined chiral nematics, specially focused on the effect curvature has on the formation of blue phases. The third part consists on the study of nematic colloids, more specifically nanoparticles adsorbed in bipolar droplets in order to determine self-assembled structures.

**Keywords:** Nematic liquid crystals, Blue phases, Nematic colloids, Confined complex fluids, Free energy functional, Meshfree interpolation methods, Theoretically informed Monte Carlo.

# Resumen

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El estudio de fases nemáticas se ha realizado desde diversas ramas de la academia. Desde un punto de vista exclusivamente teórico, las morfologías que se encuentran en este tipo de material son la evidencia más directa y tangible de la topología algebraica. Desde el trabajo experimental, este material traduce eventos moleculares a señales ópticas perceptibles a simple vista, gracias a que eventos que ocurren en la superficie del sistema modifica las orientaciones moleculares y estas se amplifican hasta distancias macroscópicas. Desde la teoría, el comportamiento de las fases nemáticas ha sido observado en diferentes materiales, especialmente biológicos, y un modelo que represente estas fases sirve como herramienta para predecir estructuras estables que pueden ser aprovechados en aplicaciones tecnológicas. Esta tesis está enfocada al estudio teórico en la escala continua de nemáticos confinados. La minimización de la energía libre se hace por dos métodos: una relajación que proviene de las ecuaciones de Euler–Lagrange, y un método novedoso que emplea la información del funcional de energía libre para la minimización por medio de un método Monte Carlo. Los resultados contenidos en este documento constan del análisis numérico de esquemas de interpolación en 3D y una nueva metodología que permite el cálculo de gradientes con gran eficiencia y precisión. La segunda parte contiene el estudio de nemáticos quirales confinados, especialmente el efecto de la curvatura sobre la formación de fases azules. La tercera parte consiste en el estudio de coloides nemáticos, específicamente en nanopartículas adsorbidas en la superficie de gotas bipolares con el fin de determinar estructuras ensambladas espontáneamente.

**Palabras clave:** Cristales líquidos nemáticos, fases azules, coloides nemáticos, fluidos complejos confinados, funcional de energía libre, métodos de interpolación libres de malla, Monte Carlo informado por la teoría.

# Contents

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<b>Resumen</b>	<b>ii</b>
<b>1. Introduction</b>	<b>1</b>
1.1 Overview . . . . .	3
1.2 Dissemination of results . . . . .	4
<b>2. Modeling of Liquid Crystals</b>	<b>6</b>
2.1 Physics of nematic phases . . . . .	8
2.1.1 Order description . . . . .	8
2.1.2 Free energy description . . . . .	10
2.1.2.1 Landau–de Gennes free energy . . . . .	10
2.1.2.2 Elastic energy: Frank–Oseen theory . . . . .	13
2.1.2.3 Surface free energy . . . . .	15
2.1.3 Topological defects . . . . .	16
2.2 Numerical methods . . . . .	18
2.2.1 Radial Basis Functions . . . . .	18
2.2.2 Gaussian quadrature with Finite Element Method . . . . .	19
2.3 Free energy minimization . . . . .	19
2.3.1 Ginzburg–Landau relaxation . . . . .	19
2.3.2 Theoretically informed Monte Carlo . . . . .	20
<b>3. Educated local meshfree interpolation</b>	<b>22</b>
3.1 Radial Basis Functions . . . . .	23

## CONTENTS

3.2	Shape parameter optimization . . . . .	26
3.3	Results . . . . .	27
3.3.1	Analytical Functions . . . . .	28
<b>4.</b>	<b>Chiral nematics confined in spheroids</b>	<b>37</b>
4.1	Results . . . . .	39
4.1.1	Free energy analysis . . . . .	40
4.1.2	Phase diagram: Droplet . . . . .	43
4.1.3	Phase diagram: Prolate . . . . .	45
4.1.4	Phase diagram: Oblate . . . . .	48
4.1.5	Additional details on chiral tactoids . . . . .	48
<b>5.</b>	<b>Adsorbed nanoparticles on bipolar droplets</b>	<b>53</b>
5.1	Description of the MC method . . . . .	57
5.2	Results . . . . .	59
5.2.1	Homeotropic particles . . . . .	60
5.2.2	Planar particles . . . . .	61
5.2.3	Segregation of particles . . . . .	63
<b>6.</b>	<b>Conclusions</b>	<b>66</b>
<b>7.</b>	<b>Future projects</b>	<b>69</b>

# List of Figures

---

2.1	Representation of a rod-like molecule of 5CB and a disk-like molecule of triphenylene.	6
2.2	Different phases for thermotropic uniaxial liquid crystals as temperature decreases.	7
2.3	Molecular orientation for (a) uniaxial and (b) biaxial molecules. . . . .	9
2.4	Free energy density of the 5CB as a function of the uniaxial order parameter $S$ at three different temperatures. . . . .	11
2.5	Elastic deformation moduli . . . . .	13
2.6	Schematic representation of different anchoring conditions for a confined liquid crystal. . . . .	16
2.7	Director field configurations for different phases induced by the anchoring conditions in a droplet of nematic liquid crystals. . . . .	17
2.8	Schematic representation of three different cholesteric defects. . . . .	17
2.9	. . . . .	18
3.1	CPU time for global and local RBF schemes in a 3D sphere with random nodes. .	29
3.2	Interpolation errors from global RBF schemes. . . . .	30
3.3	Optimal shape parameter for random meshes in a cubic domain. . . . .	31
3.4	Interpolation errors from a LRBF using a MQ basis as the node density varies. . . .	32
3.5	Interpolation errors from a LRBF using a MQ basis as the stencil size varies. . . . .	33
3.6	LC free energy as a function of the anchoring strength for homeotropic and planar droplets with $R = 500$ nm. . . . .	35
3.7	Liquid crystalline phases within homeotropic and planar droplets of size $R = 500$ nm.	36
4.1	Schematic of the types of geometries: oblate spheroid, sphere, and prolate spheroid.	39



LIST OF FIGURES

4.2	Total free energy in function of the aspect ratio $\varphi$ for strong anchoring $W = 1 \times 10^{-3} J/m^2$ and $U = 2.9$ . . . . .	40
4.3	Landau–de Gennes free energy and (Bottom) surface free energy in function of the aspect ratio, $\varphi$ , for strong anchoring $W = 1 \times 10^{-3} J/m^2$ and $U = 2.9$ . . . . .	41
4.4	Elastic free energy in function of the aspect ratio, $\varphi$ , for strong anchoring $W = 1 \times 10^{-3} J/m^2$ and $U = 2.9$ . . . . .	42
4.5	Phase diagram $\tau$ vs. $N$ of a prolate ( $\varphi > 1$ ) with strong ( $W = 1 \times 10^{-3} J/m^2$ ) and moderate ( $W = 1 \times 10^{-4} J/m^2$ ) planar degenerate anchoring, and representative configurations. . . . .	44
4.6	Phase diagram $\tau$ vs. $N$ of a prolate ( $\varphi > 1$ ) with strong ( $W = 1 \times 10^{-3} J/m^2$ ) and moderate ( $W = 1 \times 10^{-4} J/m^2$ ) planar degenerate anchoring, and representative configurations. . . . .	47
4.7	Phase diagram $\tau$ vs. $N$ of an oblate ( $\varphi < 1$ ) with strong ( $W = 1 \times 10^{-3} J/m^2$ ) and moderate ( $W = 1 \times 10^{-4} J/m^2$ ) planar degenerate anchoring, and representative configurations. . . . .	49
4.8	Twist cylinder structure in a droplate and a prolate. . . . .	50
4.9	Rotated TC on a prolate-shaped geometry. . . . .	51
4.10	Unfolding of blue phases as $\varphi$ increases for high temperature and moderate anchoring conditions. . . . .	52
5.1	Schematic of planar (blue) and homeotropic (purple) particles with radius $r_P$ half-submerged in a planar droplet with radius $R$ . Strong anchoring conditions induce a bipolar configuration in the droplet, when no particles are present, characterized by two boojums (green) in opposite poles. . . . .	54
5.2	Schematic of displacement attempt for nanoparticles on the droplet surface. . . . .	58
5.3	Free energy difference for homeotropic particles with infinite anchoring in a planar droplet as a function of the number of particles $N$ , taking as reference the minimum free energy for each $N$ pictured in the insert. Small round markers indicate metastable configurations (not shown), while big markers represent configurations with the maximum and minimum free energy density. Labels (a)-(k) correspond to the inserts and show the specific assembly of nanoparticles. . . . .	61

LIST OF FIGURES

5.4 Free energy difference for planar particles with anchoring strength  $W = 1 \times 10^{-3} \text{ J/m}^2$ , with the minimum free energy for each  $N$  as the reference shown in the insert. Small round markers indicate metastable configurations (not shown), while big markers represent configurations with the maximum and minimum free energy density. The inserts show the defect structure exhibited by nanoparticles positioned on (a) the boojum of the bipolar droplet, and (b) the equator. (c) Bridge defect between two nanoparticles near the boojum location. . . . . 62

5.5 Free energy difference for planar particles with anchoring strength  $W = 1 \times 10^{-4} \text{ J/m}^2$ , taking the minimum free energy for each  $N$  as reference and shown in the insert. Small round markers indicate metastable configurations (not shown), while big markers represent configurations with the maximum and minimum free energy density. Labels (a)-(e) are assigned to the most characteristic assembly of nanoparticles pictured in the inserts. . . . . 63

5.6 Free energy difference as a function of the angle between two nanoparticles on the surface of a bipolar droplet. Void and filled markers correspond to the case of homeotropic and planar particles respectively. . . . . 64

# List of Symbols and Abbreviations

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## Greek Letters

Symbol	Description
$\alpha$	Coefficients for the linear combination of radial basis functions
$\delta_{ij}$	Kronecker delta
$\delta$	Identity matrix, $3 \times 3$
$\epsilon_{ijk}$	Levi-Civita tensor
$\epsilon$	Shape parameter
$\gamma$	Rotational viscosity, in $Pa \cdot s$
$\eta$	Biaxiality
$\kappa$	Condition number
$\lambda^m$	Cholesteric disclinations with a topological charge $m$
$\phi$	Radial Basis Function
$\varphi$	Aspect ratio
$\psi$	Probability distribution function of molecular orientation
$\Pi_Q$	Projector tensor
$\tau$	Inverse temperature

## Latin Letters

Symbol	Description
$A_i$	Phenomenological coefficients of the Landau free energy in the Doi notation
$F$	Free energy functional
$k_{ii}$	Elastic constants in the director representation
$k_B$	Boltzmann constant
$L_i$	Elastic constants in the tensor representation
$\mathbf{n}, \mathbf{n}'$	Director field
$N$	Number of turns of the cholesteric pitch in a distance
$p_0$	Pitch of the chiral liquid crystal, in $nm$
$\mathbf{Q}$	Tensor order parameter
$q_0$	Chirality or inverse pitch, in $\mu m^{-1}$
$R$	Radius of the droplet
$S$	Scalar order parameter
$T$	Temperature
$\text{tr}(\mathbf{M})$	Trace of the matrix $\mathbf{M}$
$\mathbf{u}$	Molecular orientation
$U$	Adimensional parameter related to temperature in the Landau free energy with the Doi notation
$W$	Anchoring strength, in $J/m^2$

## Abbreviations

Abbreviation	Description
5CB	4-cyano-4'-pentylbiphenyl
B	Bipolar
BCC	Body Centered Cubic

LIST OF SYMBOLS AND ABBREVIATIONS

<b>Abbreviation</b>	<b>Description</b>
BPI,II	Blue Phase I and II
CPU	Central Processing Unit
dBP	Derived Blue Phase
GL	Ginzburg–Landau
GMQ	Generalized Multiquadratics
hBP	Hybrid Blue Phase
LC	Liquid Crystal
LRBF	Localized Radial Basis Functions
LU	Lower Upper decomposition
MC	Monte Carlo
MQ	Multiquadratics
NI	Nematic–Isotropic
PDE	Partial Differential Equation
RBF	Radial Basis Function
RSS	Radial Spherical Structure
SC	Simple Cubic
$\tau$ -Ch	$\tau$ -Cholesteric
TC	Twist cylinder
TPS	Thin–plate Spline
TwBs	Twisted Bipolar structure
U	Uniaxial