Assembly of confined nanoparticles in nematic phases

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Abstract

The study of nematic phases covers diverse branches of academics. Form 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

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 nuérico 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 nemÃ¡ticos, fluidos complejos confinados, funcional de energía libre, métodos de interpolación libres de malla, Monte Carlo informado por la teoría.

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List of Symbols and Abbreviations

Greek Letters

Symbol	Description
α	Coefficients for the linear combination of radial basis functions
δ_{ij}	Kronecker delta
$\boldsymbol{\delta}$	Identity matrix, 3×3
ϵ_{ijk}	Levi–Civita tensor
ε	Shape parameter
γ	Rotational viscosity, in $Pa \cdot s$
η	Biaxiality
κ	Condition number
λ^m	Cholesteric disclinations with a topological charge m
ϕ	Radial Basis Function
φ	Aspect ratio
ψ	Probability distribution function of molecular orientation
$\Pi_{\mathbf{Q}}$	Projector tensor
τ	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 μm^{-1}
R	Radius of the droplet
S	Scalar order parameter
T	Temperature
$\mathrm{tr}(\mathbf{M})$	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

Abbreviation	**Description**
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
τ–Ch	τ–Cholesteric
TC	Twist cylinder
TPS	Thin–plate Spline
TwBs	Twisted Bipolar structure
U	Uniaxial