Exotic Applications of Liquid Crystals

Epifanio G. Virga
University of Pavia, Italy

Summary

Preliminaries
Variational Theory
Surface Nematic Bistability
Surface Nematic Dynamics
Lipid Adhesion Dynamics

Slide 1

Preliminaries

Liquid crystals are ***mesophases***, that is, intermediate states of matter, which flow like incompressible viscous fluids, and yet retain several features of crystals, especially the ***optical*** ones.

Friedel's ***classification***

nematics, chiral nematics (cholesterics), and smectics.

Nematic comes from the Greek ***νῆμα*** which means ***thread***.

Nematic ***molecules*** resemble ***rods***, with typical dimensions 5Å × 20Å. They further enjoy the ***head–tail*** symmetry, at least on average.

Slide 2

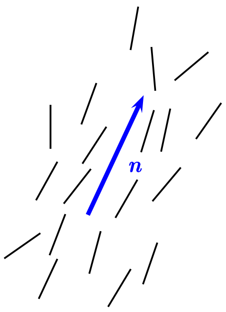
Partial orientational order

The nematic phase manifests itself when the interaction between neighbouring molecules tends to make them ***parallel*** to one another.

No positional order is present in nematics.

Nematic director

$\boldsymbol{n}$ represents the ***average*** of the local molecular orientation.



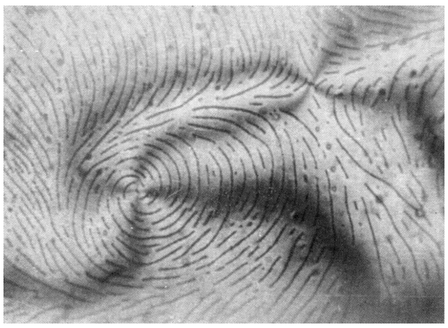
Slide 3

Optical properties

We interpret $\boldsymbol{n}$ at a point as the ***optic axis*** at that point.

Most liquid crystals are optically uniaxial: their Fresnel ellipsoid is round about $\boldsymbol{n}$, and its orientation may change in space.

Liquid crystals, like any optically anisotropic medium, can appear transparent when observed between crossed polarizers.



Slide 4

Variational Theory

Oseen-Frank *energy*

The most general elastic free-energy density W both quadratic in $\nabla\boldsymbol{n}$ and invariant under rotations in space and reflections of $\boldsymbol{n}$ is

$$2W(\boldsymbol{n},\nabla\boldsymbol{n}) = K_1(\operatorname{div}\boldsymbol{n})^2 + K_2(\boldsymbol{n}\cdot\operatorname{curl}\boldsymbol{n})^2$$
$$+K_3|\boldsymbol{n}\wedge\operatorname{curl}\boldsymbol{n}|^2 + (K_2+K_4)\left(\operatorname{tr}(\nabla\boldsymbol{n})^2 - (\operatorname{div}\boldsymbol{n})^2\right)$$

$$\boldsymbol{n}:\mathcal{B}\to S^2$$

$\mathcal{B}$ ***region*** in space occupied by the liquid crystal

S^2 ***unit sphere*** in 3-space

$K_1,\dots,K_4$ Frank's ***constants***

one-constant approximation

$$K_1 = K_2 = K_3 = K \qquad K_4 = 0$$

$$W = \tfrac{1}{2}K|\nabla\boldsymbol{n}|^2$$

Slide 5

Twisted nematic display

Electric energy density

$$W_e = -\frac{1}{8\pi}\boldsymbol{D}\cdot\boldsymbol{E} = -\frac{1}{8\pi}\left(\varepsilon_\perp E^2 + \varepsilon_a(\boldsymbol{E}\cdot\boldsymbol{n})^2\right)$$

in c.g.s. electromagnetic units

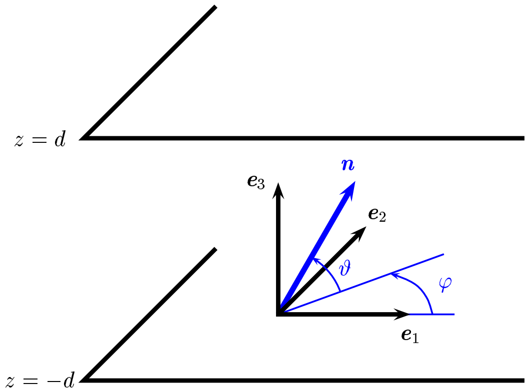
dielectric constants $\varepsilon_\parallel \quad \varepsilon_\perp$

dielectric anisotropy $\varepsilon_a := \varepsilon_\parallel - \varepsilon_\perp$

$\boldsymbol{E}$ *electric field* $\qquad$ $\boldsymbol{D}$ *electric displacement*

For liquid crystals, ε_a may be either positive or negative. When $\varepsilon_a > 0$, $\boldsymbol{n}$ is oriented by $\boldsymbol{E}$.

Slide 6



$$\boldsymbol{n} = \cos\vartheta\cos\varphi\,\boldsymbol{e}_1 + \cos\vartheta\sin\varphi\,\boldsymbol{e}_2 + \sin\vartheta\,\boldsymbol{e}_3$$

$$\vartheta = \vartheta(z) \qquad \varphi = \varphi(z)$$

$$-d \le z \le d$$

Slide 7

strong anchoring

$$\vartheta(-d) = \vartheta(d) = 0 \qquad \varphi(-d) = -\frac{\pi}{4} \qquad \varphi(d) = \frac{\pi}{4}$$

applied transverse field $\quad \boldsymbol{E} = E\boldsymbol{e}_3 \quad E = \frac{V}{2d}$

free-energy functional

$$F[\vartheta,\varphi] = \int_{-d}^{d}\left\{f(\vartheta)\vartheta'^2 + g(\vartheta)\varphi'^2 - \frac{1}{8\pi}\varepsilon_a E^2\sin^2\vartheta\right\}\mathrm{d}z$$

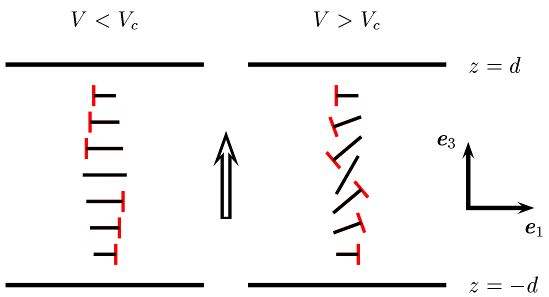
$$2f(\vartheta) := K_1\cos^2\vartheta + K_3\sin^2\vartheta$$

$$2g(\vartheta) := \cos^2\vartheta\left(K_2\cos^2\vartheta + K_3\sin^2\vartheta\right)$$

uniform twist $\quad \vartheta = 0 \quad \varphi = \frac{\pi}{4d}z$

Slide 8

Bulk bifurcation



$$\boldsymbol{E} = \frac{V}{2d}\,\boldsymbol{e}_3$$

The uniform twist is always a solution to the EULER-LAGRANGE equation for F. It becomes unstable as soon as

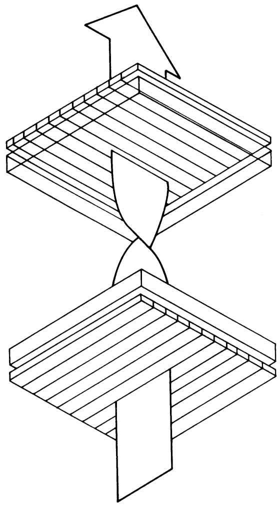
$$V > V_c := \pi\sqrt{\frac{\pi}{\varepsilon_a}}\sqrt{4K_1 + K_3 - 2K_2},$$

$$K_3 - 2K_2 \geq 0$$

Slide 9

Adiabatic approximation

When the wavelength of the incoming light is small compared with the pitch of the uniform twist, then the polarization is ***guided*** inside the cell by the optic axis.



Slide 10

Transition

When $V > V_c$, the uniform twist is destroyed in the cell, as $\boldsymbol{n}$ acquires a component in the direction orthogonal to the plates.

For voltages sufficiently higher than V_c, $\boldsymbol{n}$ is parallel to the applied field in most of the cell, which then acts as an ***optical switch***.

typical values (PEBAB):

- $2d = 10\mu$m
- $V_c = 3$V
- operating voltage 6V

Monostable display

Writing the untwisted texture requires the application of a persistent voltage: the untwisted texture is ***erased*** by only switching off the field.

Slide 11

SURFACE NEMATIC BISTABILITY

Bistable devices exhibit two distinct director textures, both stable in the absence of an external field, but electrically switchable.

Several passive ***bulk*** devices with intrinsic bistability have recently been proposed, but they are all too slow (in the ms range) for ***video*** applications (μs).

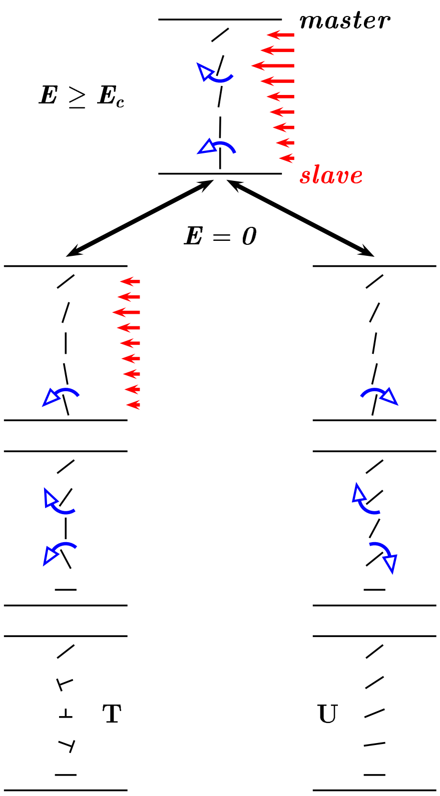
Surface controlled bistable switching with the desired rate has been realized by use of smectic C* liquid crystals. They, are however, too sensitive to mechanical shocks, which may produce irreversible stress damage.

Slide 12

Surface anchoring breaking

A new ***nematic*** bistable device has just been proposed with switching time in the μs range and a large self-healing capability after mechanical shocks.

Slide 13



Slide 14

The nematic anchoring is ***strong*** on one plate of the device (the ***master*** plate), and ***weak*** on the other (the ***slave*** plate).

Two different couplings are exhibited by the plates: one is ***quasi-static*** and the other ***dynamic***.

The dynamic coupling always writes the twisted texture **T** at the end of a sharp electric pulse, while the quasi-static coupling writes the uniform texture **U** after a slower pulse. Both textures are ***erased*** by an electric field so strong to ***break*** the anchoring on the slave plate.

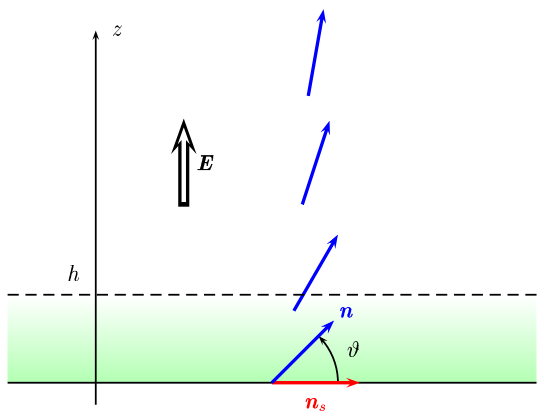
The rapid inhomogeneous rotation of the director near the master plate, after the sudden removal of the field, generates a ***backflow*** in the fluid, which exerts a hydrodynamic torque on the slave plate, thus determining the switching of the director.

Surface nematic dynamics

A detailed analysis of the nematic surface dynamics near the slave plate is needed to model this new promising device.

This has not been achieved by describing surface effects through surface energies: the surface torques acting on $\boldsymbol{n}$ need to be ***diluted*** in a thin boundary layer.

Slide 15



$\boldsymbol{n}_s$ ***surface preferred orientation***

Slide 16

diluted surface energy

$$\mathcal{F}_s = \frac{A}{2h}\int_0^\infty d(z) f_s(\vartheta(z))\mathrm{d}z$$

$$0 \leq f_s \leq 1$$

$$\int_0^\infty d(z)\mathrm{d}z = h$$

surface coherence length

$$\xi_s := \sqrt{\frac{Kh}{A}}$$

K ***elastic constant***

extrapolation length

$$L := \frac{K}{A} \qquad \xi_s^2 = Lh$$

weak anchoring $\quad h \ll \xi_s \ll L$

Slide 17

diluted surface energy

$$\mathcal{F}_s = \frac{1}{2}\int_0^\infty D(z) W_s(\boldsymbol{n}(z)\cdot\boldsymbol{n}_s)\mathrm{d}z$$

$$0 \leq W_s \leq 1$$

$$f_s(\vartheta) := W_s(\cos\vartheta)$$

total anchoring strength

$$A := \int_0^\infty D(z)\mathrm{d}z$$

dilution length

$$h := \frac{\int_0^\infty zD(z)\mathrm{d}z}{\int_0^\infty D(z)\mathrm{d}z}$$

dimensionless dilution function

$$d(z) := \frac{h}{A}D(z)$$

evolution equation

$$\tau_s(\vartheta)\vartheta_t = \xi_s^2\vartheta_{zz} - d(z)\sin\vartheta\cos\vartheta$$

Rapini-Papoular ***energy***

$$f_s = \sin^2\vartheta$$

boundary condition

$$\vartheta_z(0,t) = 0 \qquad \text{for all} \quad t \geq 0$$

That is, ***no*** localized torque is transmitted at the boundary.

surface relaxation time

$$\tau_s(\vartheta) := \frac{\gamma_s(\vartheta)}{A} = \frac{\gamma_\mathrm{e}(\vartheta)}{K}\xi_s^2$$

effective surface viscosity $\quad \gamma_s(\vartheta) := \gamma_\mathrm{e}(\vartheta)h$

Slide 18

effective viscosity

$$\gamma_e(\vartheta) := \gamma_1 - \frac{2(\alpha_2 \cos^2\vartheta - \alpha_3 \sin^2\vartheta)^2}{f(\vartheta)}$$

$$\begin{aligned} f(\vartheta) :&= 2\alpha_1 \sin^2\vartheta \cos^2\vartheta + \alpha_4 \\ &+ (\alpha_5 - \alpha_2)\cos^2\vartheta + (\alpha_6 + \alpha_3)\sin^2\vartheta \end{aligned}$$

$\gamma_1 := \alpha_3 - \alpha_2$ ***rotational viscosity***

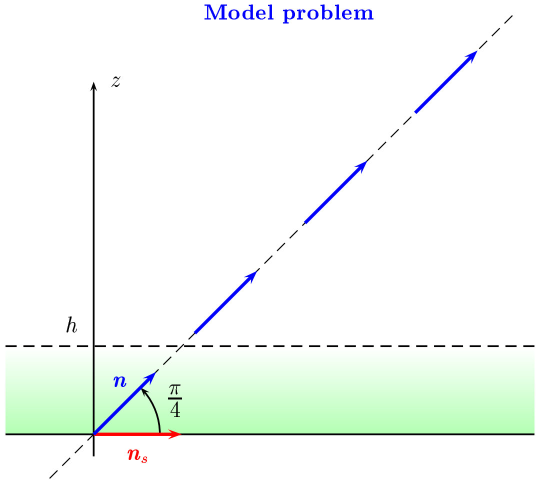
α_i LESLIE ***viscosities***

By the dissipation inequality,

$$0 < \gamma_e \leq \gamma_1$$

Slide 19

Model problem



initial condition

$$\vartheta(z,0) = \frac{\pi}{4} \qquad \text{for all} \quad z \geq 0$$

shortest surface time

$$\tau_h = \frac{h^2}{\xi_s^2}\tau_s(\frac{\pi}{4})$$

Slide 20

Special choice

$$\xi_s = 5h \qquad L = 25h$$

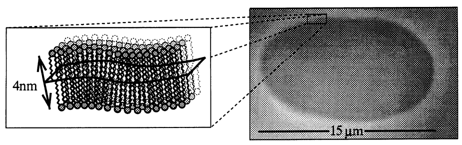
Slide 21

LIPID ADHESION DYNAMICS

Lipid membranes consist of amphiphilic molecules. They are ubiquitous constituents of living organisms.

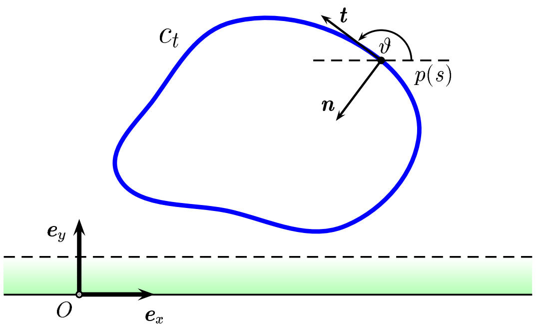
Each lipid molecule has a ***hydrophilic*** (polar) head and a ***hydrophobic*** tail (aliphatic chain).

When dispersed in an aqueous environment, the tails hide themselves from the surrounding medium.



Slide 22

Two-dimensional model



elastic energy

$$\mathcal{F}_e[c_t] = \frac{1}{2}\int_0^L k\sigma^2 \mathrm{d}s$$

c_t ***curve*** at time t

$k > 0$ ***bending rigidity***

σ ***curvature*** of c_t

kinematic constraint: c_t ***is inextensible***

Slide 23

adhesion energy

$$\mathcal{F}_a[c_t] := w\int_0^L f(y(s))\mathrm{d}s$$

$w > 0$ ***adhesion potential***

f ***diluted surface adhesion***

The function f describes how the adhesive effect of the wall is diluted in space.

normalization

$$f(y) \geq f(0) = -1 \qquad \text{for all} \quad y \geq 0$$

$$\lim_{y\to\infty} f(y) = 0$$

Slide 24

dissipated energy

We apply the Rouse model to describe the viscous dissipation in the environment: The flow induced by the motion of the membrane is disregarded.

$$\mathcal{D}[c_t] := \int_0^L \gamma_n v_n^2 \mathrm{d}s$$

v_n ***normal velocity***

$\gamma_n > 0$ ***normal viscosity coefficient***

dissipation principle

Neglecting the membrane's inertia, we write the dynamical principle as

$$\dot{\mathcal{F}} + \mathcal{D} = 0$$

$$\mathcal{F} := \mathcal{F}_e + \mathcal{F}_a$$

Slide 25

non-local shape evolution

$$k\sigma'' + w\cos\vartheta\frac{\mathrm{d}f}{\mathrm{d}y} - \sigma\left(wf - \frac{1}{2}k\sigma^2 + \alpha_0\right) = -\gamma_n v_n$$

$$\alpha_0 = \frac{\int_0^L \sigma\left\{k\sigma'' + w\cos\vartheta\frac{\mathrm{d}f}{\mathrm{d}y} - \sigma\left(wf - \frac{1}{2}k\sigma^2\right)\right\}\mathrm{d}s}{\int_0^L \sigma^2 \mathrm{d}s}$$

$$(\cdot)' := \frac{\mathrm{d}}{\mathrm{d}s}(\cdot)$$

The scalar α_0 represents the ***tension*** arising from the inextensibility constraint:

$$\int_0^L \sigma v_n = 0$$

Slide 26

Animations

Units

time $\tau = \dfrac{\gamma L^4}{k}$

length L

tension $\dfrac{k}{L^2}$

gravity $\dfrac{k}{L^3}$

Slide 27

Essential bibliography

E.G. Virga, *Variational Theories for Liquid Crystals*, Chapman & Hall, London, 1994.

I. Dozov, M. Nobili & G. Durand, Fast bistable nematic display using monostable surface switching, *Appl. Phys. Lett.*, **70**(1997), 1179-1181.

I. Dozov & G. Durand, Surface controlled nematic bistability, *Liquid Crystals Today*, **8**(2) (1998), 1-7.

G. Durand & E.G. Virga, Hydrodynamic model for surface nematic viscosity, *Phys. Rev. E*, **59**(1999), 4137-4142.

U. Seifert, Configurations of fluid membranes and vesicles, *Adv. Phys.*, **46**(1997), 13-137.

R. Rosso & E.G. Virga, Adhesion by curvature of lipid tubules, *Continuum Mech. Thermodyn.*, **10** (1998), 359-367.

Slide 28

More information

Minisymposium ***MSP-025***, 16.00-18.00, WRB-9

Soft Matter Mathematical Modelling Group
Department of Mathematics, University of Pavia, Italy

`http://smmm.unipv.it`

Slide 29

Thanks to

People

M. Carme Calderer
Ivan Dozov
Georges Durand
E. Chuck Gartland
Frank M. Leslie
Riccardo Rosso
André M. Sonnet

Institutions

IAN, CNR
Istituto di Analisi Numerica del CNR, Pavia

INFM
Istituto Nazionale di Fisica della Materia

MURST
Ministero per l'Università e la Ricerca Scientifica e Tecnologica

Slide 30