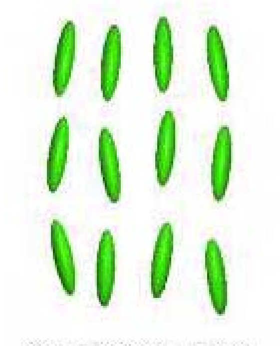
Models and PDEs from Liquid Crystal Theory

Dan Phillips
Purdue University
August 3, 2009

Liquid Crystal-substance with a degree of crystalline order that remains in a liquid state

- Simple picture- long thin molecules



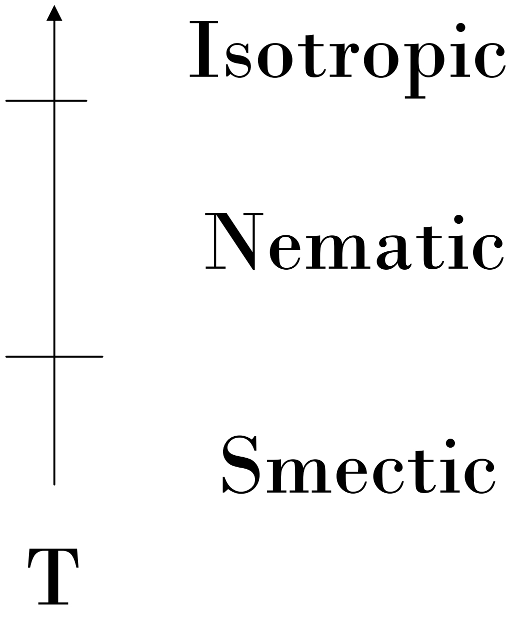
Liquid Crystal

Energy to describe static stable configurations

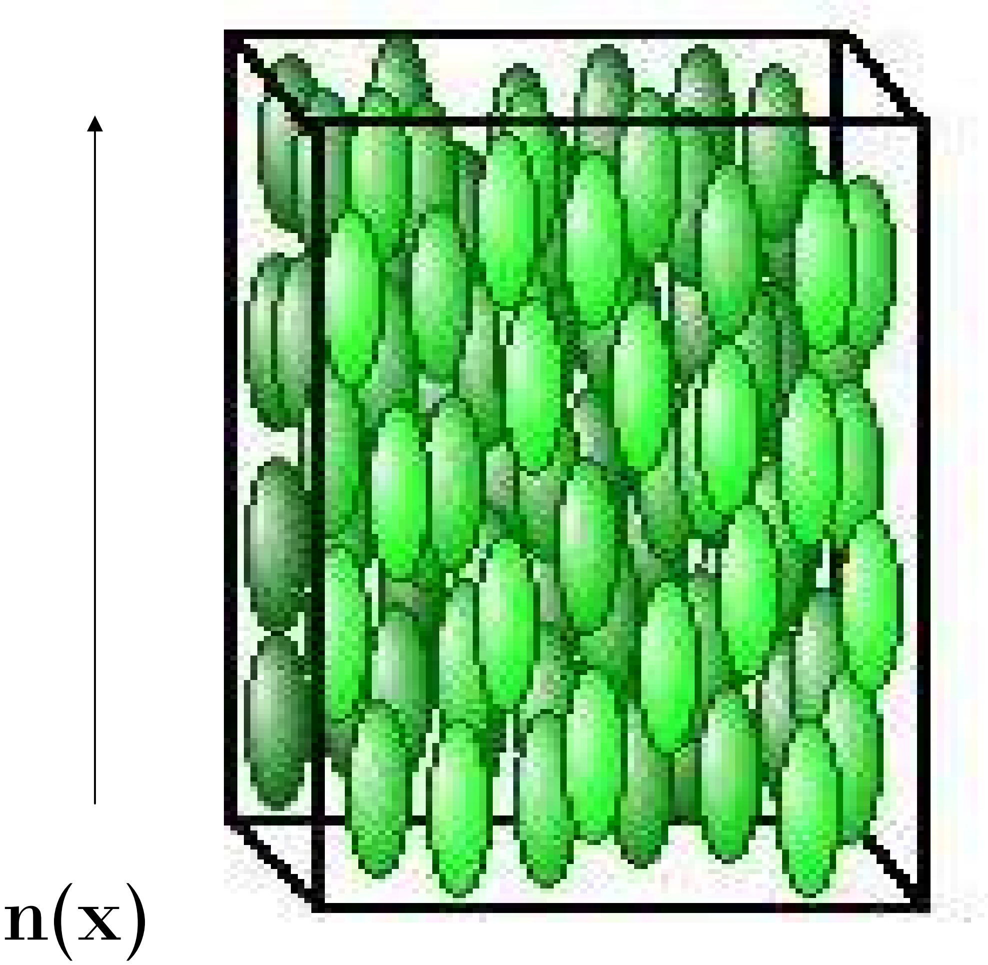
Made up of competing energies

- Molecular packing (molecular alignment)
- Thermal effects (randomize alignment)
- External stresses (mechanical, electrical..)

Temperature dependent-different terms become dominant at different temperatures



- Nematic phase-energy seeks local alignment of long axes.
- n(x) is the “local average”of long axes.
- |n(x)|=1



n (x) is a unit vector field

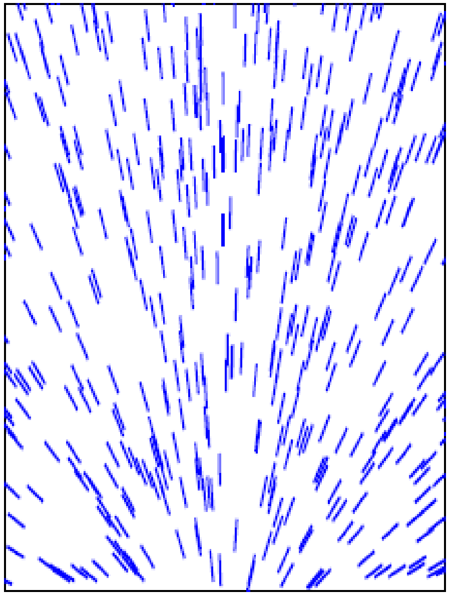
- Molecules do not have a head and tail as n(x) does.
- In problems where this does not lead to inconsistencies n(x) is the simplest way to describe a nematic liquid crystal.
- n (x)-director field , n (x)$\in$ S^2
- In cases where there are we use {n (x), -n (x)}$\in$ RP^2

Oseen Frank Energy

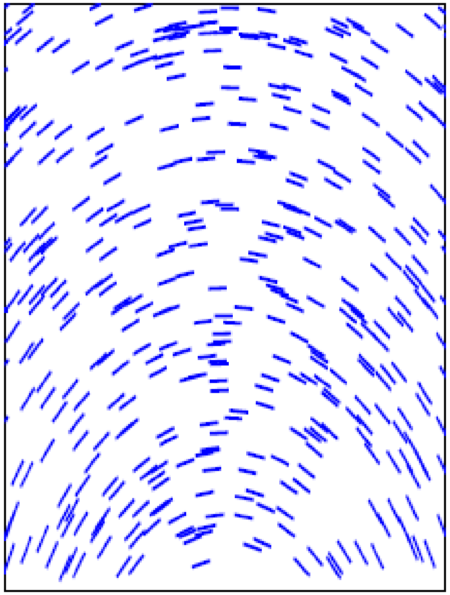
- Energy records the cost of distortions away from n(x)=const.
- Written in terms of pure splay, twist, and bend. These have K_1 ,K_2, K_3 as coefficients respectively

$$
\begin{aligned}
F_F(\mathbf{n}) = {} & K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_3|\mathbf{n} \times (\nabla \times \mathbf{n})|^2 \\
& +(K_2 + K_4)(tr(\nabla\mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2)
\end{aligned}
$$

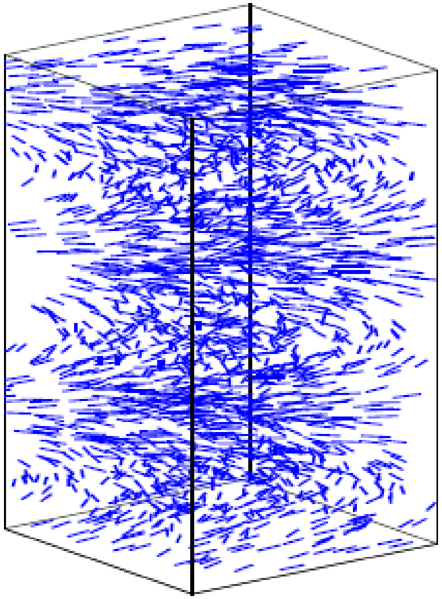
Pure Distortions



Splay



Bend



Twist

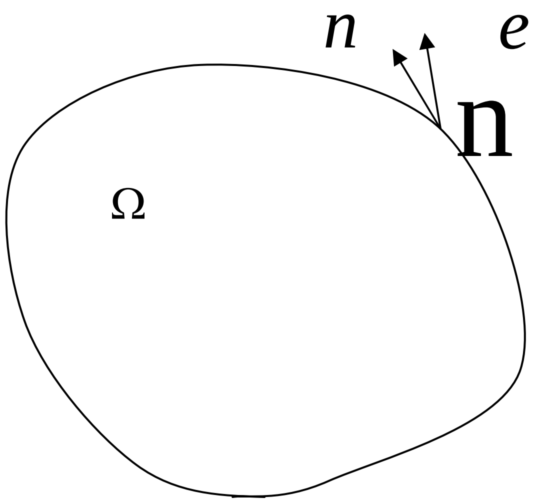
Special case, $K_1 = K_2 = K_3 = K$, $\mathrm{K}_4 = 0$, one constant approximation

vector identity

$$\mathrm{tr}(\nabla \mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2 = |\nabla \mathbf{n}|^2 - |\nabla \times \mathbf{n}|^2 - (\nabla \cdot \mathbf{n})^2,$$

$$\Rightarrow \quad F_F(n) = \int_\Omega K |\nabla \mathbf{n}|^2 \, d\mathbf{x},$$

Boundary Conditions



1) $n = n_0$ on $\partial\Omega$ $, |n_0| = 1$

2) $F_b = c\int_{\partial\Omega} (n \cdot e(x))^2$

1) Strong anchoring problem

$F = F_F + F_b$ weak anchoring

If $c<0$ then n(x) tends to be parallel to e(x). e(x) is the easy axis.

If n_0 (x) or e(x) are parallel to the boundary normal

we are promoting “homeotropic” boundary values.

If c>0 then n(x) tends to be $\perp$ e(x) on the boundary. If e(x) is parallel to the boundary normal then n(x) tends towards tangential boundary values.

$$
\begin{aligned}
F_F(\mathbf{n}) = K_1(\nabla\cdot\mathbf{n})^2 + K_2(\mathbf{n}\cdot\nabla\times\mathbf{n})^2 + K_3|\mathbf{n}\times(\nabla\times\mathbf{n})|^2 \\
+(K_2+K_4)(tr(\nabla\mathbf{n})^2-(\nabla\cdot\mathbf{n})^2)
\end{aligned}
$$

Thm (Hardt - Kinderlehrer - Lin)

Assume $\partial\Omega$ is a smooth surface, n_0 is smooth, K_1 ,K_2, K_3 >0 and that

$$A=\{u\,|\,u:\Omega\rightarrow S^2, u=n_0\,|_{\partial\Omega}, \int_\Omega|\nabla u|^2<\infty\}$$

is nonempty. Then there is a minimizer for F(n) in A.

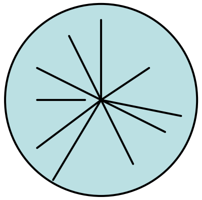
n(x) may have singularities, “defects”

- ex . n(x)=x/|x|

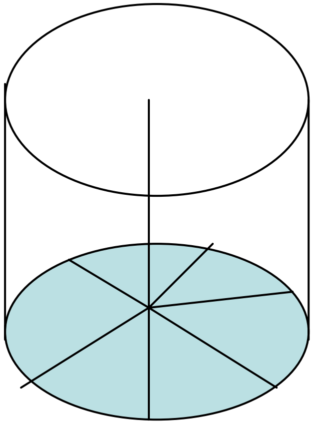
“Hedgehog”. n(x) has homeotropic b.v. and a defect at one point. Minimizers from the theorem can not be singular on a curve. Line singularities in liquid crystals do exist, “disclination lines”.

Try n(r, θ,z)=e_r and get

$$\int |\nabla n|^2 = \infty$$

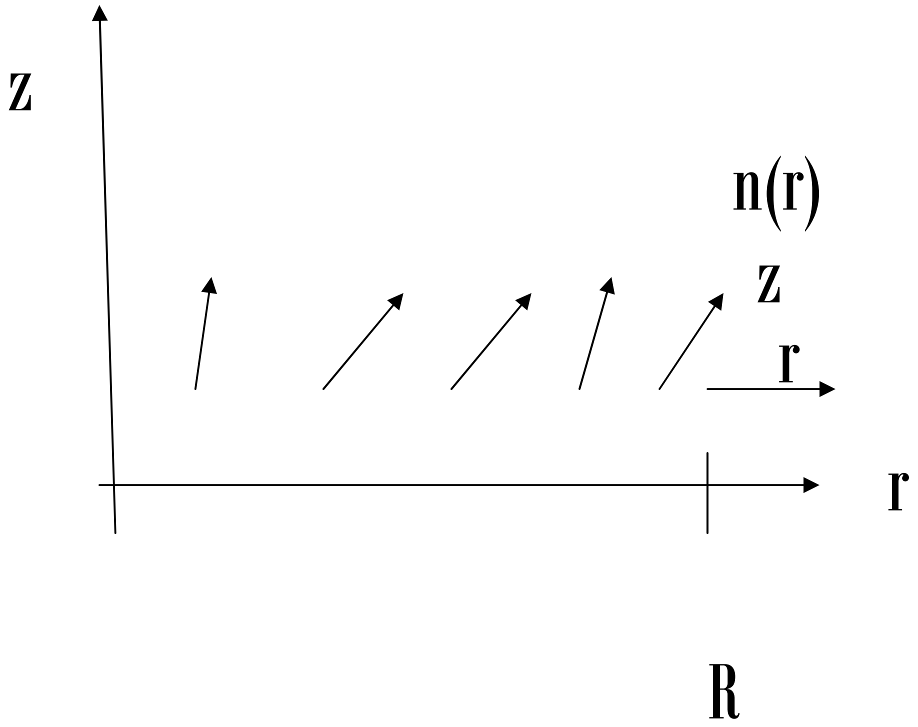


$$\Omega = B_R$$



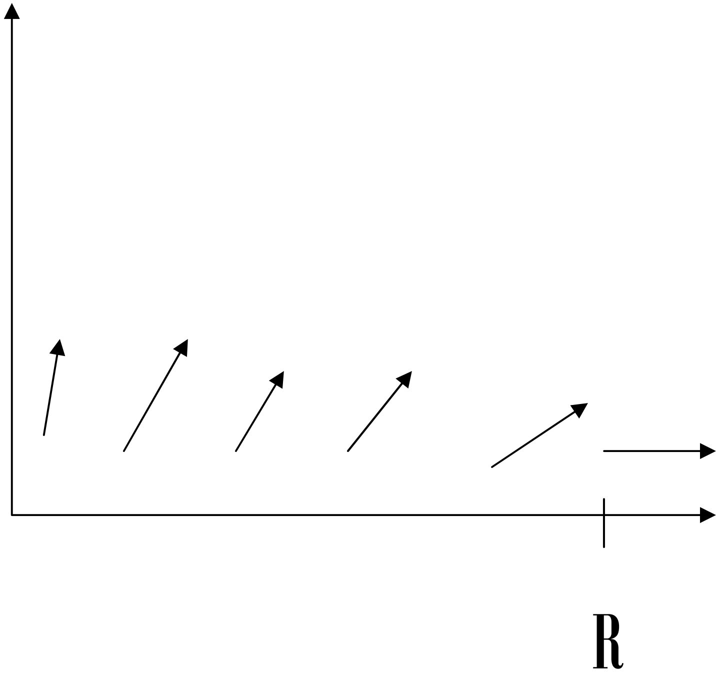
Cladis and Kleman consider :

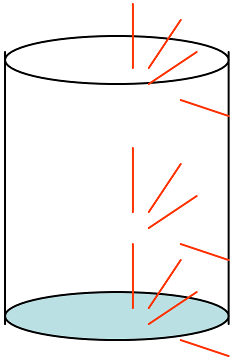
$n(r) = \cos\varphi(r) e_r + \sin\varphi(r) e_z$ with $\varphi(R) = 0$



$$F = \int_{B_R} |\nabla n|^2 \, dxdy = 2\pi \int_0^R \left((\varphi')^2 + \frac{\cos^2 \varphi}{r^2}\right) r\,dr$$

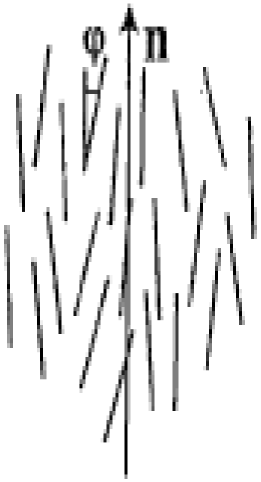
They prove the minimizer is $\varphi(r) = \frac{\pi}{2} - 2\tan^{-1}\left(\frac{r}{R}\right)$





Solution is not singular. It escapes to the third dimension.

Introduce an order parameter that allows n to “melt’ near r=0



$f(\varphi)$ probability density that the director of molecules near x are within an angle φ

Of n(x).

$f_0(\varphi) = \frac{1}{4\pi}$

s(x) is the the isotropic order parameter .

Measures how concentrated f is near φ =0.

$$s(x) = \frac{3}{2} \oiint_{S^2} \cos^2(\varphi)(f - f_0)$$

s=1 strongly nematic, s=0 isotropic

Ericksen considers a nematic described by the pair $(s, \mathbf{n})$

$$\int (k\,|\nabla s|^2 + \; s^2 \cdot |\nabla n|^2)dx$$

$If \quad k \le 1$

Mizel, Roccato, and Virga prove that this has a minimizer

$(\tilde{s}, \tilde{n})$ in the family

$$\{s(r), \cos\varphi(r)e_r + \sin\varphi(r)e_z, \varphi(R) = 0, s(R) = s_0 > 0\}$$

of the form $\tilde{\varphi} \equiv 0, \tilde{s}(r) > 0,\ for\_r > 0, \tilde{s}(0) = 0$

The solution is allowed to melt into the isotropic phase at r=0,

has finite energy, and has a disclination line along the z axis.

$If \quad k > 1 \ \ then \quad the \quad solution \quad has \ \ \tilde{s}(0) > 0 \ \ and \ \ \tilde{\varphi}(0) = \frac{\pi}{2}.$

Defect Core Structure in Nematic Liquid Crystals

N. Schopohl and T. J. Sluckin(a)

$$F_{\text{bulk}} = A\,\text{tr}\mathbf{Q}^2 + \tfrac{2}{3}B\,\text{Tr}\mathbf{Q}^3 + \tfrac{1}{2}C\,\text{Tr}\mathbf{Q}^4,$$

$$F_{\text{kin}} = L_1 \frac{\partial Q_{ij}}{\partial x_k}\frac{\partial Q_{ij}}{\partial x_k} + L_2 \frac{\partial Q_{ij}}{\partial x_j}\frac{\partial Q_{ik}}{\partial x_k} + L_3 \frac{\partial Q_{ij}}{\partial x_k}\frac{\partial Q_{ik}}{\partial x_j},$$

$$Q_{ij} = Q_{ji} \text{ and } \text{tr}\mathbf{Q} = 0$$

The full free-energy functional

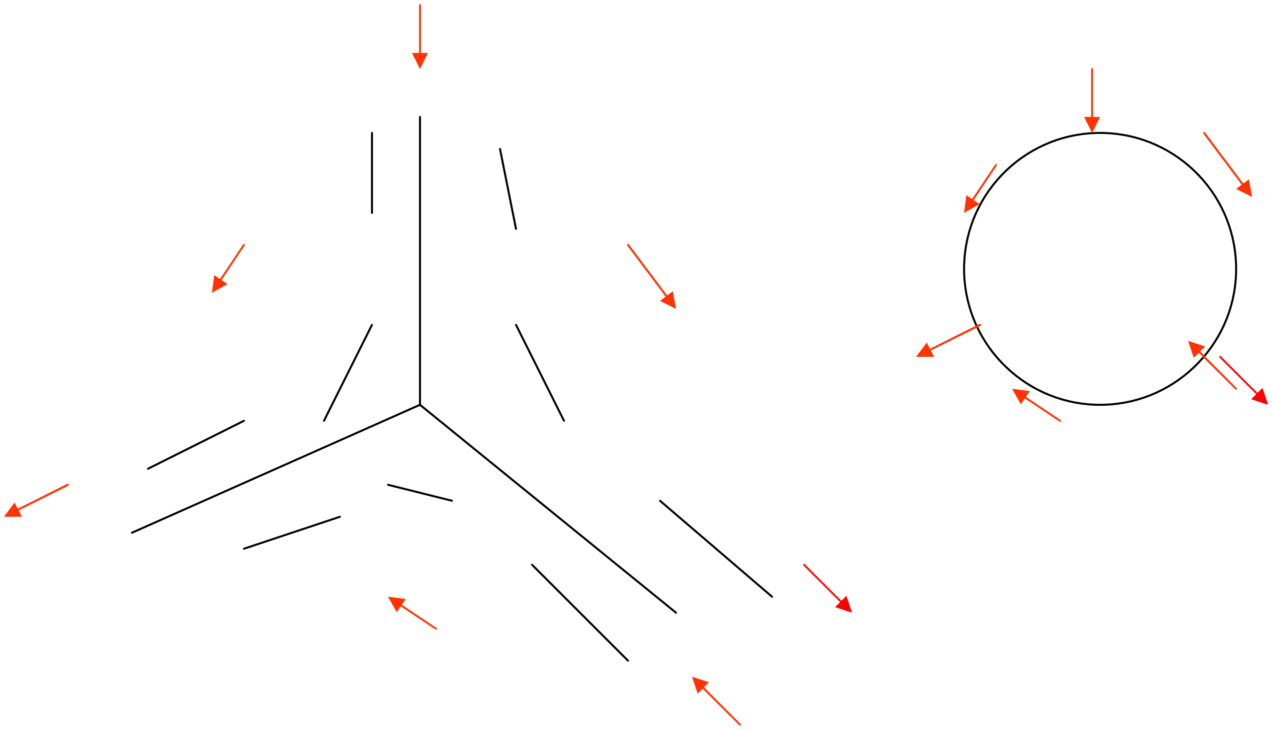
$$F(\mathbf{Q},\mathbf{\Lambda}) = F_{\text{bulk}} + 2\,\text{tr}(\mathbf{\Lambda}\mathbf{Q}) + F_{\text{kin}}$$

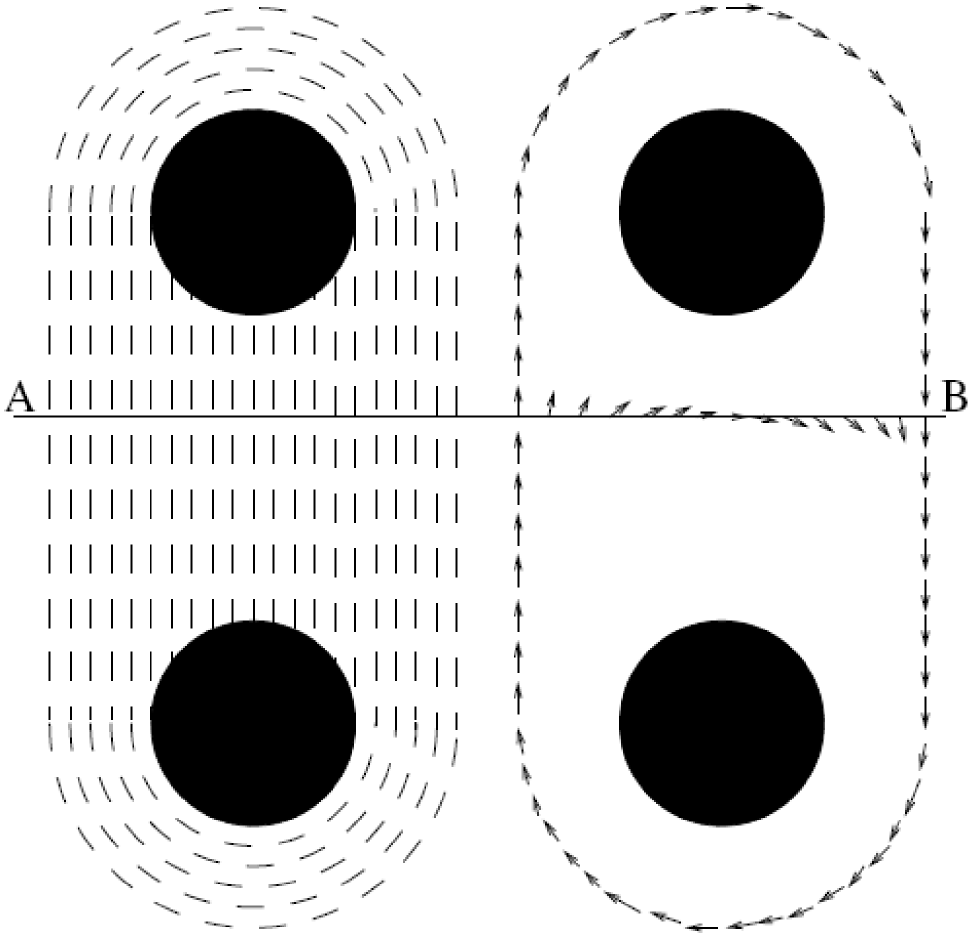
uniaxial

$$\mathbf{Q} = s(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I})$$

biaxial

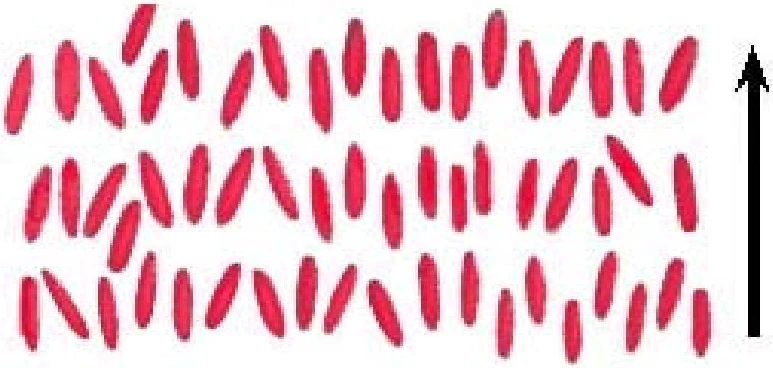
$$\mathbf{Q} = -(s_1 \mathbf{n} \otimes \mathbf{n} + s_2 \mathbf{m} \otimes \mathbf{m}) + \frac{1}{3}(s_1 + s_2)\mathbf{I},$$





John M. Ball and **Arghir Zarnescu**

Smectics



Picture of the smectic A phase

Photo courtesy of
Dr. Mary Neubert LCI-KSU

Photo of the smectic A phase
(using polarizing microscope)

Picture of the smectic C phase

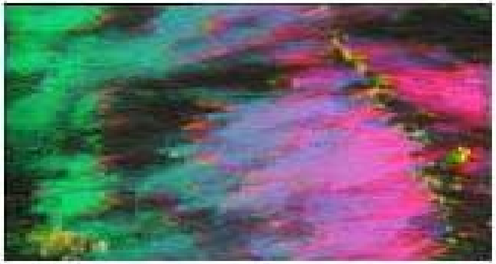
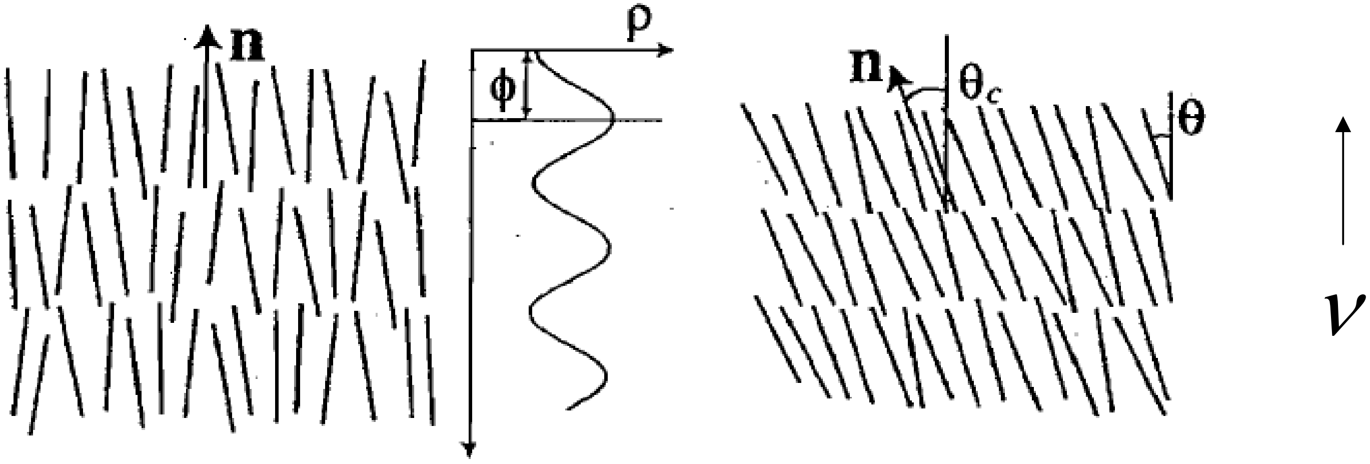


Photo courtesy Dr. Mary Neubert LCI-KSU

Photo of the smectic C phase
(using polarizing microscope)

Molecules locally align and in addition form layers



- Layer normal ν
- Density modulation $\rho(x) = \rho_0 + \rho_1 \cos(\underbrace{\frac{2\pi}{d}\nu \cdot x)}_{\varphi}$
- $q = \frac{2\pi}{d}$, d = layer thickness
- If $\rho_1 > 0$ then layers exist - smectic phase
- If $\rho_1 = 0$ then no layers - nematic phase

- If $\nu \parallel n$ - smectic A
- If not - smectic C
- Complex order parameter

$$\psi = \rho_1(x) e^{i\varphi(x)} \qquad 2\rho_1 \cos\varphi = \psi + \psi^*$$

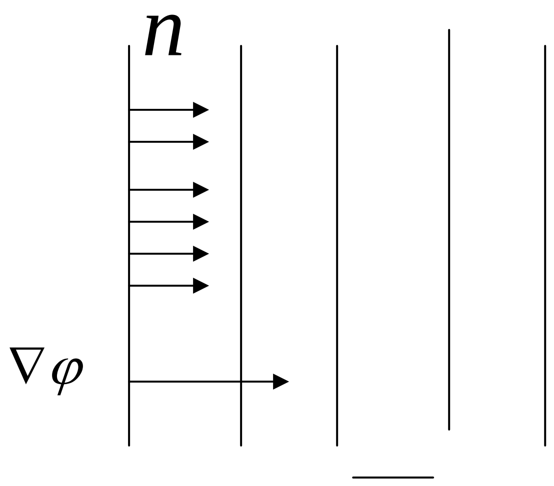
- $\psi = 0$ nematic, $\psi \neq 0$ smectic

Smectic A energy.

$$
\begin{aligned}
F_A &= |\nabla\psi - iq\mathbf{n}\psi|^2 + \mu^2(1-|\psi|^2)^2 \\
&= |\nabla\rho_1|^2 + \rho_1^2|\nabla\varphi - q\mathbf{n}|^2 + \mu^2(1-\rho_1^2)^2
\end{aligned}
$$

III II I

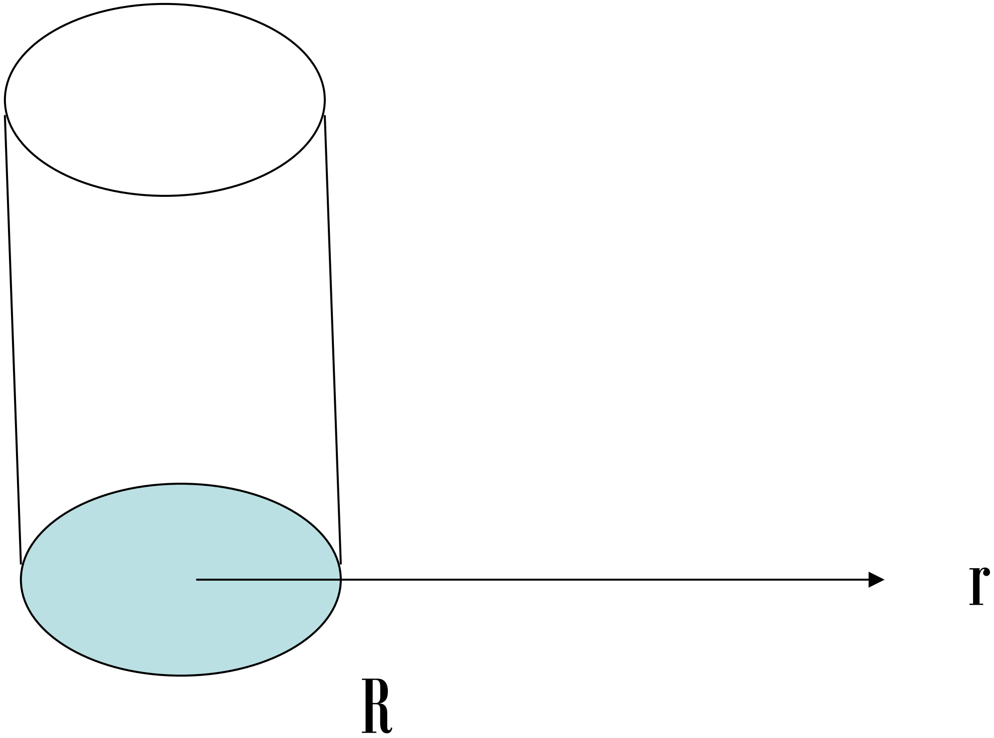
- I $\rho_1 = 1$ prefers smectic phase
- II locally the level sets of φ are the layers, $\nabla\varphi \parallel n, \quad |\nabla\varphi| \approx q$
- III penalizes phase transitions



$$d = \frac{2\pi}{q}$$

Smectic-*A* structures in submicrometer cylindrical cavities

S. Kralj[1,2] and S. Žumer[2] Phys Rev E (2) 54, 1996



$$f = f_n^{\mathrm{loc}} + f_n^{\mathrm{non}} + f_s^{\mathrm{loc}} + f_s^{\mathrm{non}}$$

$$f_n^{\mathrm{loc}} = A(T - T^*)S^2 - BS^3 + CS^4.$$

$$f_n^{\mathrm{non}} = \frac{K_{11}(\mathrm{div}\vec{n})^2}{2} + \frac{K_{22}(\vec{n}\cdot\mathrm{curl}\vec{n})^2}{2} + \frac{K_{33}(\vec{n}\times\mathrm{curl}\vec{n})^2}{2}$$

$$+ L(\mathrm{grad}S)^2,$$

$$f_s^{\mathrm{loc}} = a(T - T_{NA})|\tilde{\psi}|^2 + \frac{b|\tilde{\psi}|^4}{2},$$

$$f_s^{\mathrm{non}} = C_{\parallel}|(\vec{n}\cdot\mathrm{grad} - iq_0)\tilde{\psi}|^2 + C_{\perp}|(\vec{n}\times\mathrm{grad})\tilde{\psi}|^2,$$

$$f_{\mathrm{surf}} = -\frac{S}{2}(\vec{n}\cdot\vec{e}_{\mathrm{easy}})^2$$

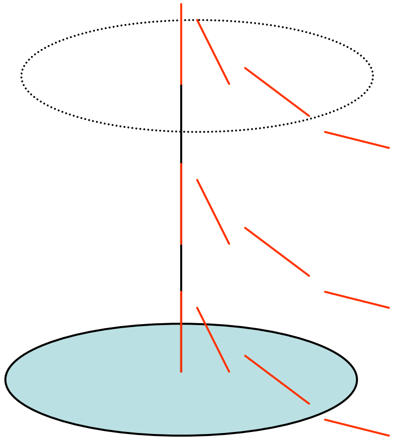
$$\int_0^R frdr + f_{surf}R$$

$$K_{ii} = S^2 k_{ii},$$

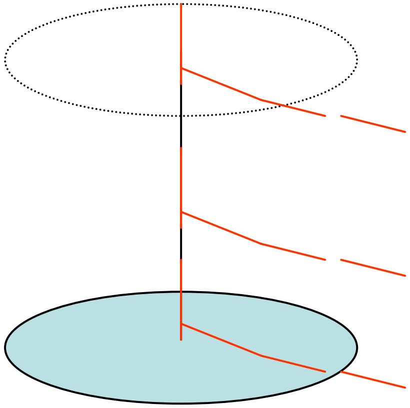
$$e_{easy} = e_r$$

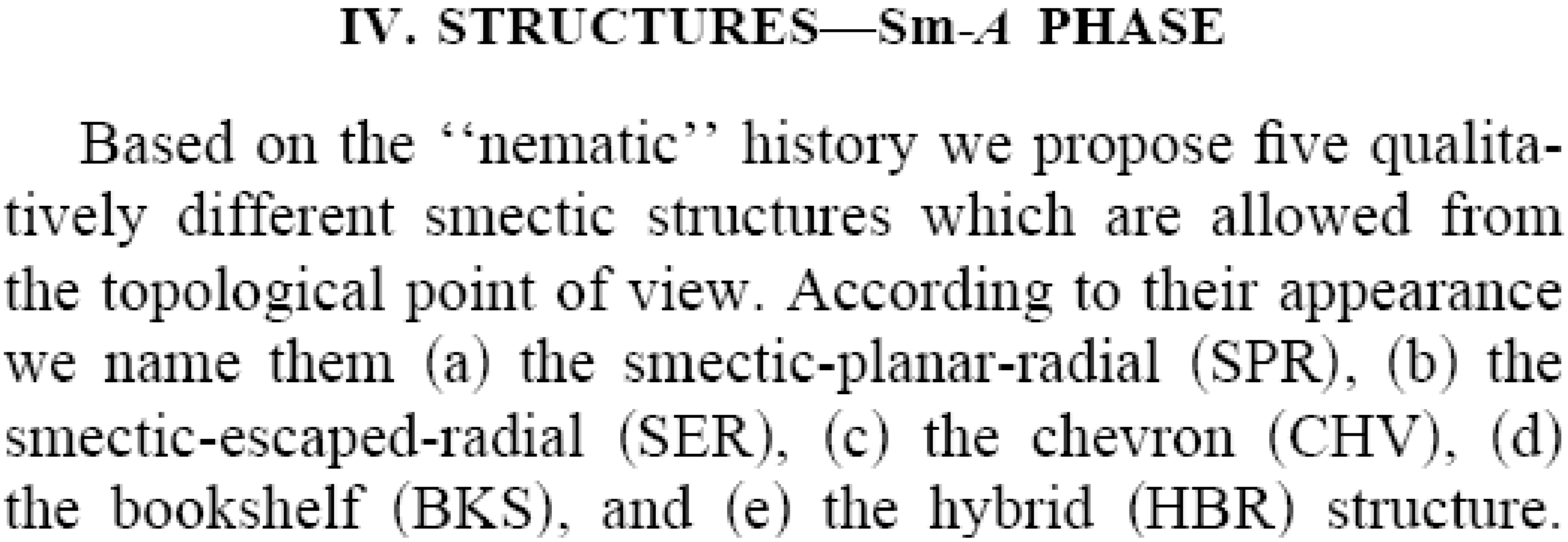
First consider the nematic case.

- T decreases though T_{NA}
- K_1/K_2 and K_1/K_3 increase
- This retards the director **n** escaping to e_z



$T_1 > T_2$





IV. STRUCTURES—Sm-A PHASE

Based on the “nematic” history we propose five qualitatively different smectic structures which are allowed from the topological point of view. According to their appearance we name them (a) the smectic-planar-radial (SPR), (b) the smectic-escaped-radial (SER), (c) the chevron (CHV), (d) the bookshelf (BKS), and (e) the hybrid (HBR) structure.

All of these are possible metastable states.

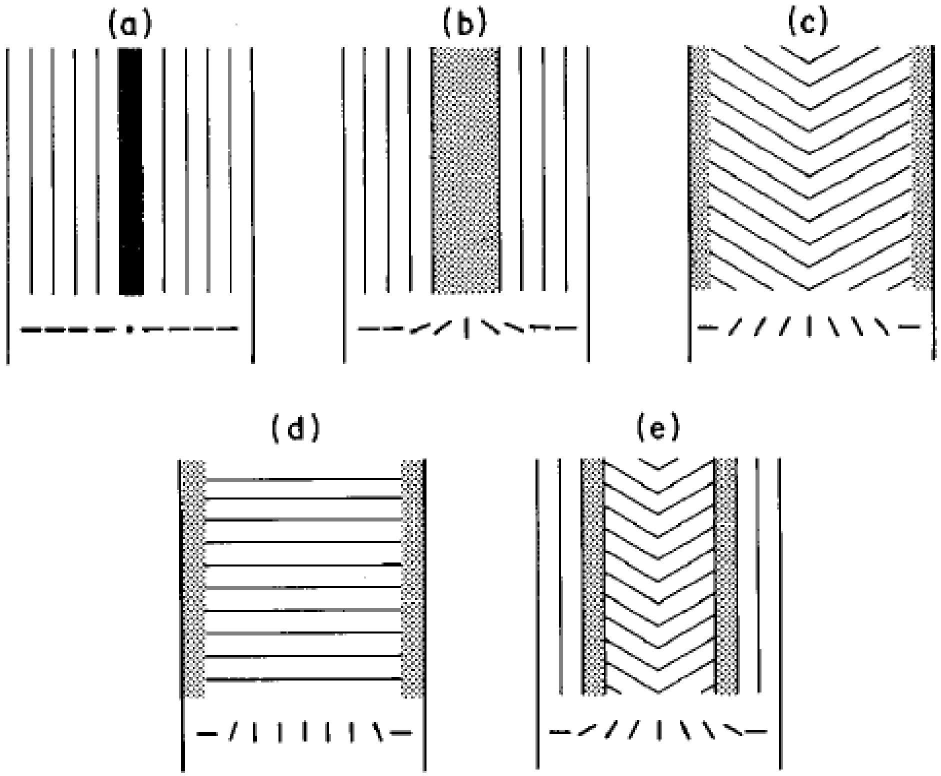


FIG. 1. Schematic presentation of different Sm-A structures for the case of strong homeotropic anchoring and smooth surface: (a) SPR, (b) SER, (c) CHV, (d) BKS, and (e) HBR structure. The smectic layers are drawn with the full line. The nematic director field spatial variation is indicated at the bottom part of each structure. The dotted regions describe places where nematic (a) or smectic (a)–(e) ordering melts.

The End