Lecture 8

Defects in liquid crystals

In equilibrium, depending on boundaries $\vec{n}$ can vary in space. Sometimes there are singularities in $\vec{n}(r)$

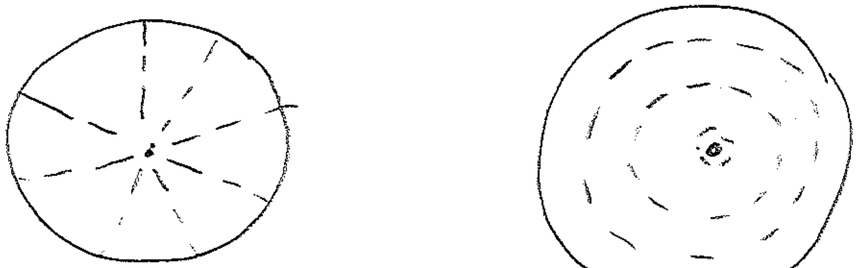


Fig 1.

normal boundary condition — tangential boundary condition

<u>disclinations</u> (from the Greek "kline" - slope (Frank)

Consider line disclinations then $n = n(\varphi)$

n doesn't depend on r, because there is no other length scale in the problem and n - dimensionless

$\psi = \vartheta - \varphi$, $n_r = \cos\psi$, $n_\varphi = \sin\psi$

Since when we go around $\vec{n}$ is unchanged ($\vec{n} = -\vec{n}$)

then $\vartheta(\varphi + 2\pi) = \vartheta(\varphi) + 2\pi n$ (n = integer or half integer)

Frank index

$$\psi(\varphi + 2\pi) = 2\pi(n-1) + \psi(\varphi)$$

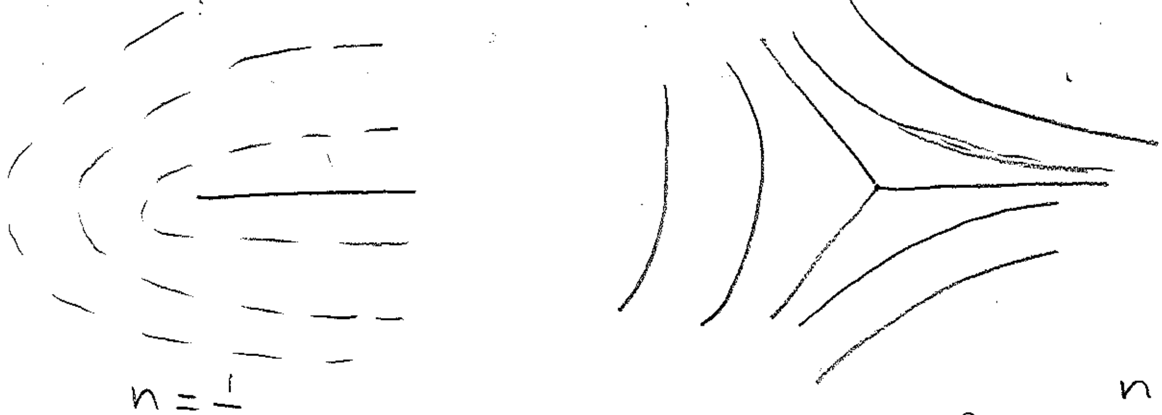


Fig. 2

$n = \frac{1}{2}$ $n = -\frac{1}{2}$

Energy of disclination $\sim K n^2 \ln \frac{R}{a}$

Fig. 4.4. Bubble decoration technique displaying the arrangement of the molecules at a free surface (courtesy P. Pieranski) [4]. In the present example we see two singular points of strength $(+1)$ and (-1) between crossed polarizers.

Deformation around disclination

$$F = \frac{1}{2}\left(K_1 (\operatorname{div}\vec{n})^2 + K_2 (\vec{n}\cdot\operatorname{rot}\vec{n})^2 + K_3 [\vec{n}\times\operatorname{rot}\vec{n}]^2\right)$$

$$\operatorname{div}\vec{n} = \frac{1}{r}\frac{dn_\varphi}{d\varphi} + \frac{n_r}{r} = \frac{1}{r}\cos\psi\,(1+\psi')$$

$$\operatorname{rot}_z n = -\frac{1}{r}\frac{dn_r}{d\varphi} + \frac{n_\varphi}{r} = \frac{1}{r}\sin\psi\,(1+\psi')$$

$n\cdot\operatorname{rot} n = 0 \Rightarrow$

$$\int F\, r\,dr\,d\varphi = \frac{K_1+K_3}{4}\int (1-\alpha\cos 2\psi)(1+\psi'^2)\,d\varphi\,\frac{dr}{r} \qquad (1)$$

where $\alpha = \dfrac{K_3-K_1}{K_3+K_1}$ (mixed term $(1-\alpha\cos 2\psi)2\psi'$ - total derivative)

1. $F_d = \int \frac{dr}{r}\int \_\_\, d\varphi \sim \underline{\ln\frac{R}{a}}$

2. varying (1) $\Rightarrow (1-\alpha\cos 2\psi)\psi'' = \alpha\sin 2\psi\,(1-\psi'^2)$

two trivial solutions $\psi = 0$, $\psi = \frac{\pi}{2}$ $\Rightarrow n=1 \Rightarrow$ Fig. 1

3. simplification if $\alpha = 0$, $K_1 = K_3 \Rightarrow$ $F \sim \int \psi'^2 dV \Rightarrow$

$\Rightarrow \psi = (n-1)\varphi$; $\vartheta = n\varphi$

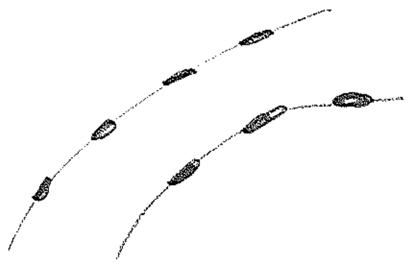
General case see Landau Lifshitz

<u>Problem 1</u>, show that the disclination has C_m symmetry (rotation by $\frac{2\pi}{m}$) with $m = 2|n-1|$

check fig. 1, 2.

Problem 2, draw disclination with $n=-1$

"Streamlines" of director are defined as lines that are tangential to $\vec{n}$ at any point



Their length element $\vec{dl}$: $dl_r = dr$, $dl_\varphi = r\,d\varphi$

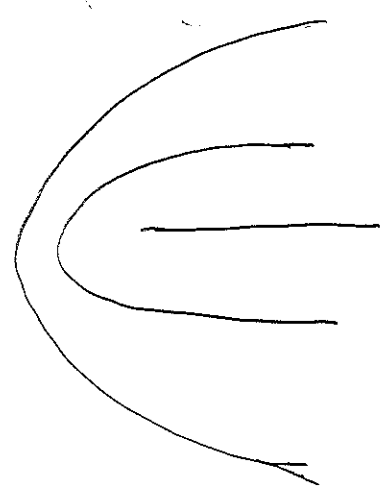
Condition $\vec{dl} \parallel \vec{n}$ =>

$$\frac{dl_\varphi}{dl_r} = \frac{n_\varphi}{n_r} \quad => \quad \frac{r\,d\varphi}{dr} = \frac{d\varphi}{d\ln r} = \operatorname{tg}\psi$$

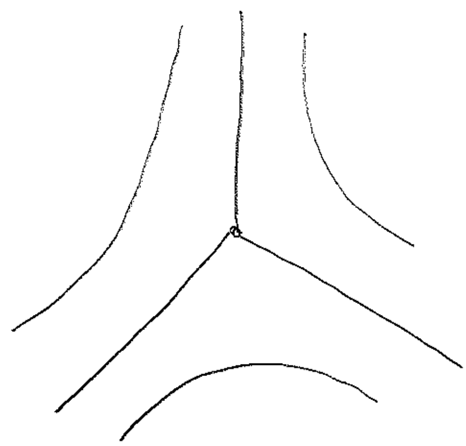
Thus there are straight streamlines where $\psi = p\pi$ (p - integer)

These are $2(n-1)$ radial rays

$n = \frac{3}{2}$

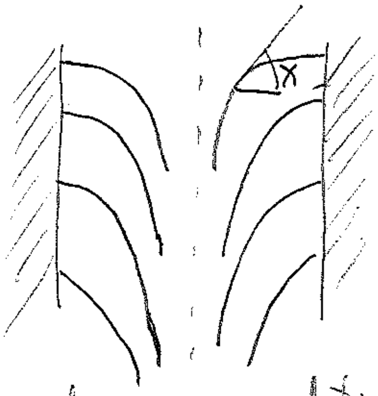


$n = \frac{1}{2}$



$n = -\frac{1}{2}$

Escape to the third dimension



disclination with $n=1$ (Cladis, Kléman 1972)

– nonsingular solution

$$n_r = \cos\chi(r),\quad n_\varphi = 0,\quad n_z = \sin\chi(r)$$

Boundary conditions $\chi = 0\ ,\ r = R$
$\chi = \frac{\pi}{2}\ ,\ r = 0$

$$\mathrm{rot}_\varphi n = -\frac{dn_z}{dr} = -\cos\chi\,\frac{d\chi}{dr}\ ,\quad \mathrm{div}\, n = \frac{1}{r}\frac{d(r n_r)}{dr} = -\sin\chi\frac{d\chi}{dr} + \frac{\cos\chi}{r}$$

In the simple case $K_1 = K_3 = K$ we have

$$\int_0^R F\, 2\pi r\, dr = \pi K \int_{-\infty}^{0} d\xi\, \left(\chi'^2 + \cos^2\chi - \chi' \cdot \sin 2\chi\right)$$

where $\xi = \ln\frac{r}{R}$ $\left(\chi' = \frac{d\chi}{d\xi}\right)$ $\Rightarrow \chi'^2 - \cos^2\chi = \mathrm{const} = 0 \Rightarrow$
(at $r=0$, $r\frac{d\chi}{dr} = \cos\frac{\pi}{2} = 0$)

$$\Rightarrow \chi = \frac{\pi}{2} - 2\,\mathrm{arctg}\,\frac{r}{R}$$

Energy is finite $\sim K$ thus this nonsingular solution is energetically more favorable than the disclination with $E \sim K \ln\frac{R}{a}$

A Disclination with $n=1$ can be <u>continuously</u> transformed to a nonsingular texture!

Topological classification of defects

Order parameter space M : For xy model $M = S_1$ 

for the Heisenberg model $M = S_2$ 

For 2d nematics P_1

3d nematics P_2

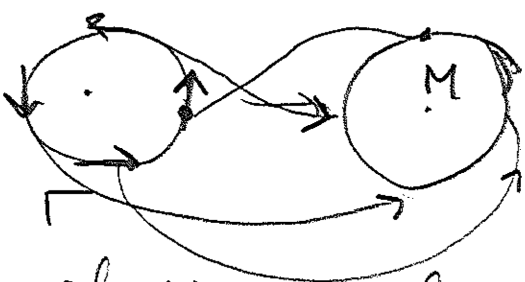
$P_n = S_n$ with $n = -n$

Any order parameter configuration in some real space domain $\mathcal{D}$ defines a mapping $\mathcal{D} \to M$

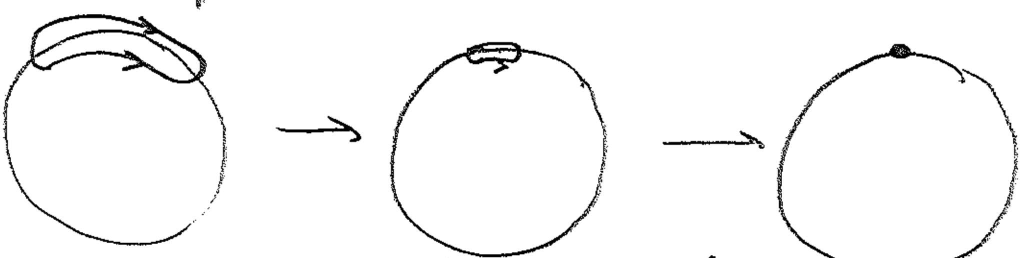
Consider closed loop Γ around the linear defect in 3d or around the point defect in 2d.

For example for XY model

mapping to one point



Two mappings f_1, f_2 are <u>homotopic</u> if they can be continuously deformed to each other $h_{t=0} = f_1,\ h_{t=1} = f_2$



non encircling paths can be deformed to points

Homotopy <u>classes</u>. Defects are in the same class if mappings can be continuously transformed to each other.

Homotopy <u>group</u>

Group associated with mapping of loops ≡ fundamental group or first homotopy group $\equiv \pi_1(M)$

Group with spheres $S_n = \pi_n(M)$

for $M = S_1$ (XY model) $\pi_1(S_1) = Z$ (integer numbers) → vortices with winding number N

But $\pi_1(S_2) = 0 = \pi_n(S_m)$ $m > N$

thus there are no defects in Heisenberg model

All contours can be transformed into a point.

For nematics in 2d ⇒ $\pi_1(P_1)$ = group of half integer numbers – disclinations

For nematics in 3d $\pi_1(P_2) = Z_2$

all closed loops → to a point  but

 contour connecting $\vec{n}$ and $-\vec{n}$ cannot be transformed to a point. Thus all disclinations with integer number can be removed and all halfinteger are topologically equivalent.

Point defects $\pi_2(P_2)$ – hedgehog $= Z$