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2nd Lecture

2.0 EQUILIBRIUM DIRECTOR PROFILE WITH APPLIED FIELDS

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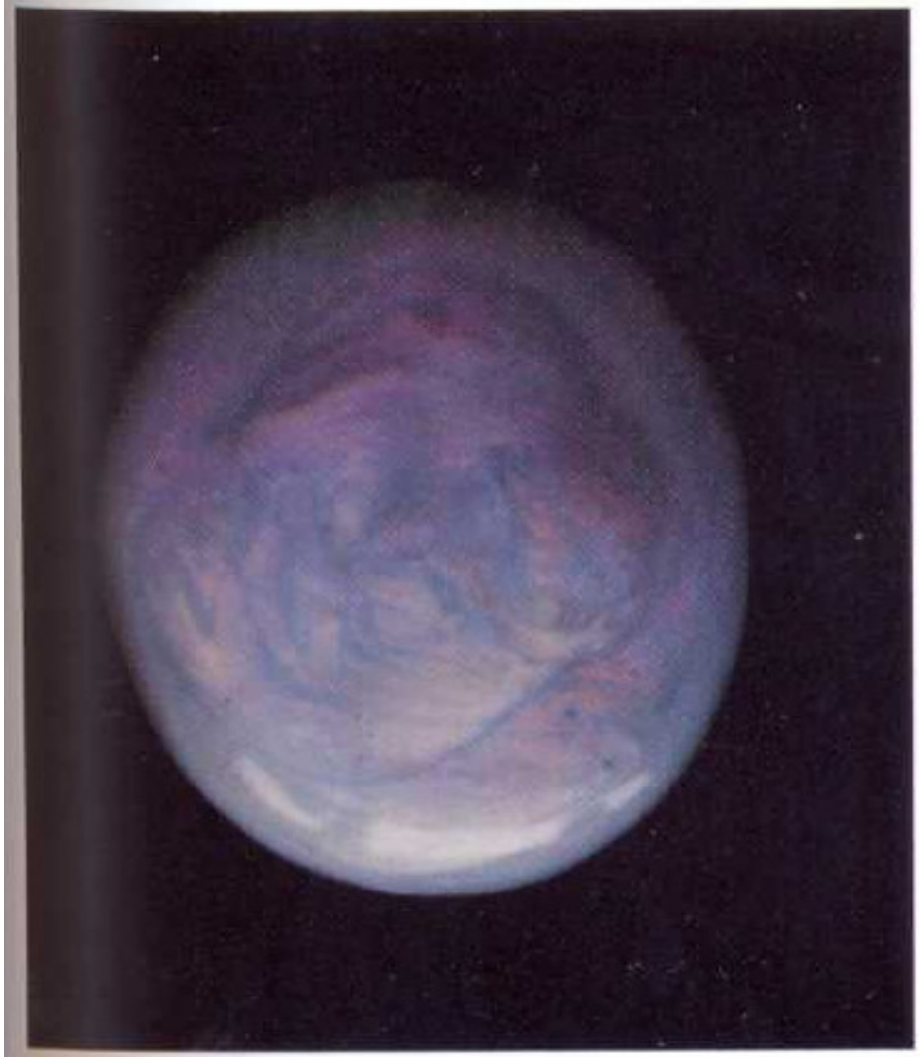
MEPhI, Moscow, 17 September 2014

How to find the director profile in a sample of LC ?



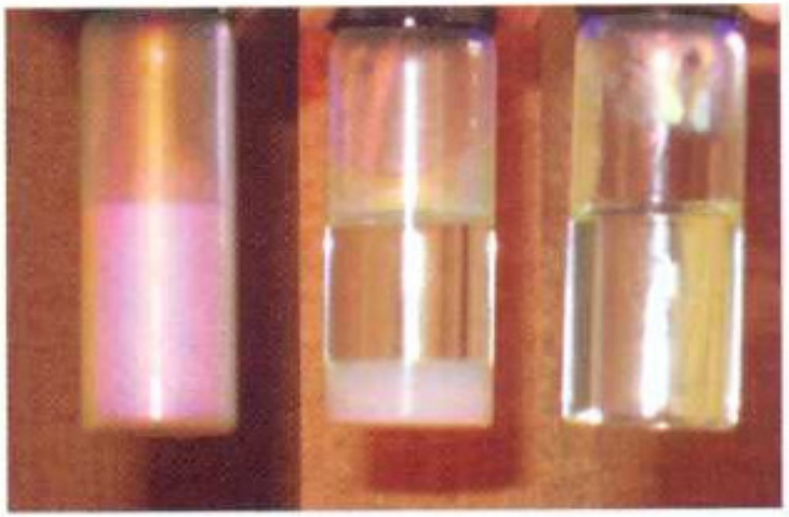
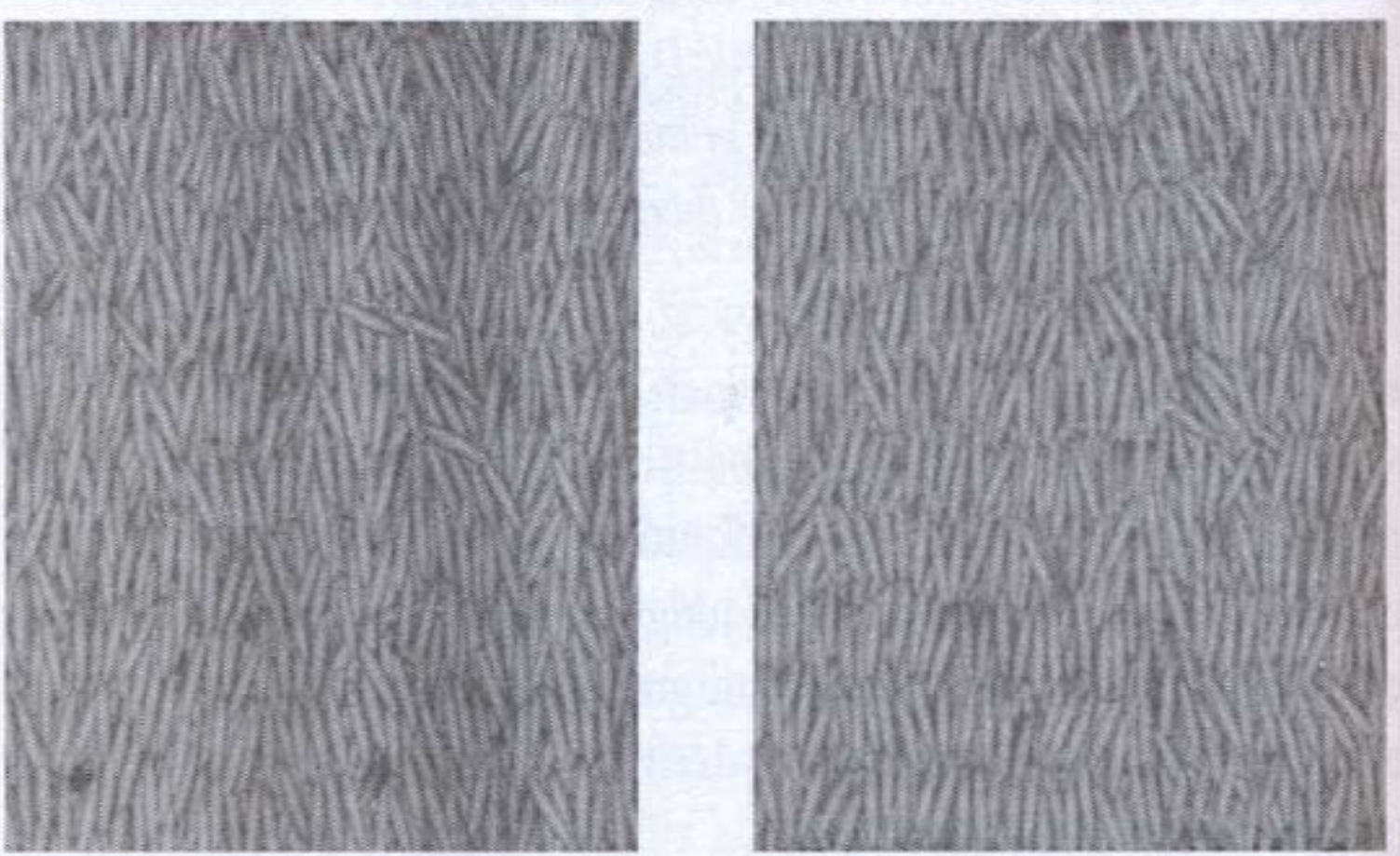


Plate 1 A droplet of cholesteric liquid crystal exhibiting the hues of a changeable silk. (See Figure 1.1, p.3)

Plate 2 Liquid crystal sample in a test-tube, warmed from room temperature. Samples go left to right. The sample starts cloudy, develops a region in which it is clear, with the interface between the two regions advancing until the whole sample is clear. On cooling, the process is reversed. (See Figure 2.2, p.19)

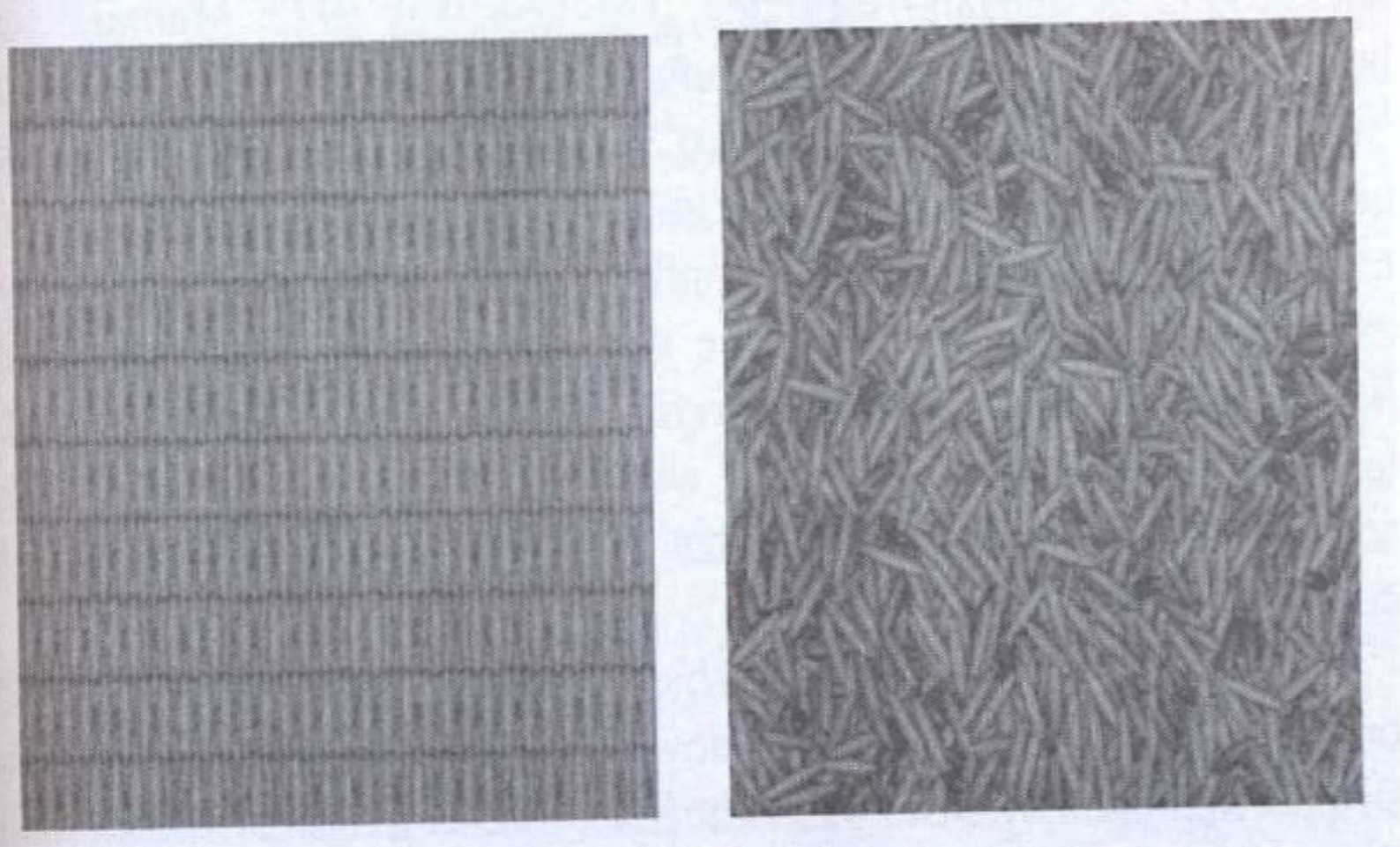
This is just a computer model



The images are generated by assuming that liquid crystal molecules can be represented by ellipsoids, and then allowing them to interact with intermolecular forces that model the interactions we now believe to be responsible for the formation of liquid crystals. Above left is the computer-calculated image of a

NLC- and right of a S_ALC structure

And this is a model too

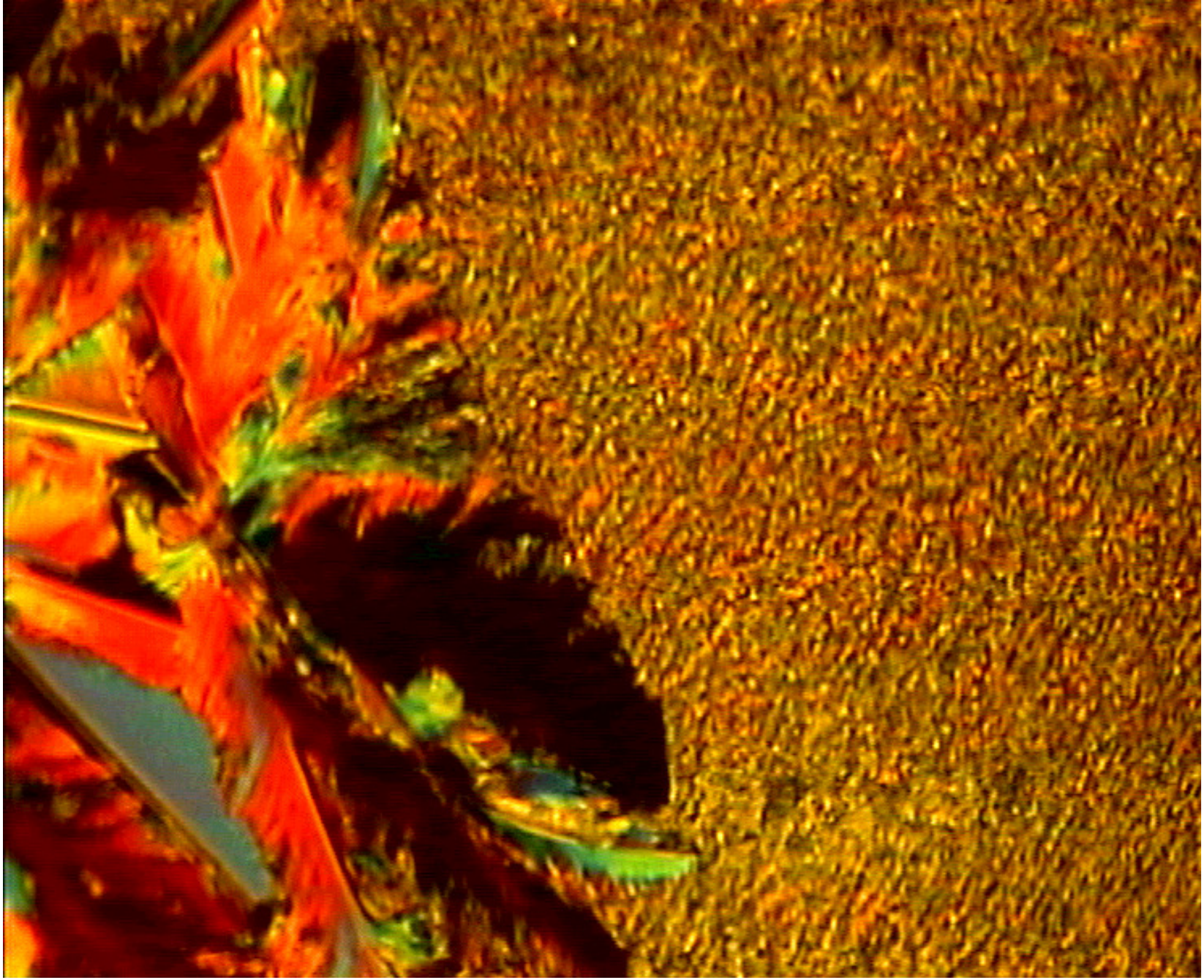


The images above are, of course, not of real molecules.

However, using a modern technique known as scanning tunnelling microscopy, it is possible to generate images of real molecules. Friedel, and indeed Lehmann and Vorländer, would have been amazed to see a picture of liquid crystal molecules organizing in a parallel fashion, just as expected in a liquid crystal phase.

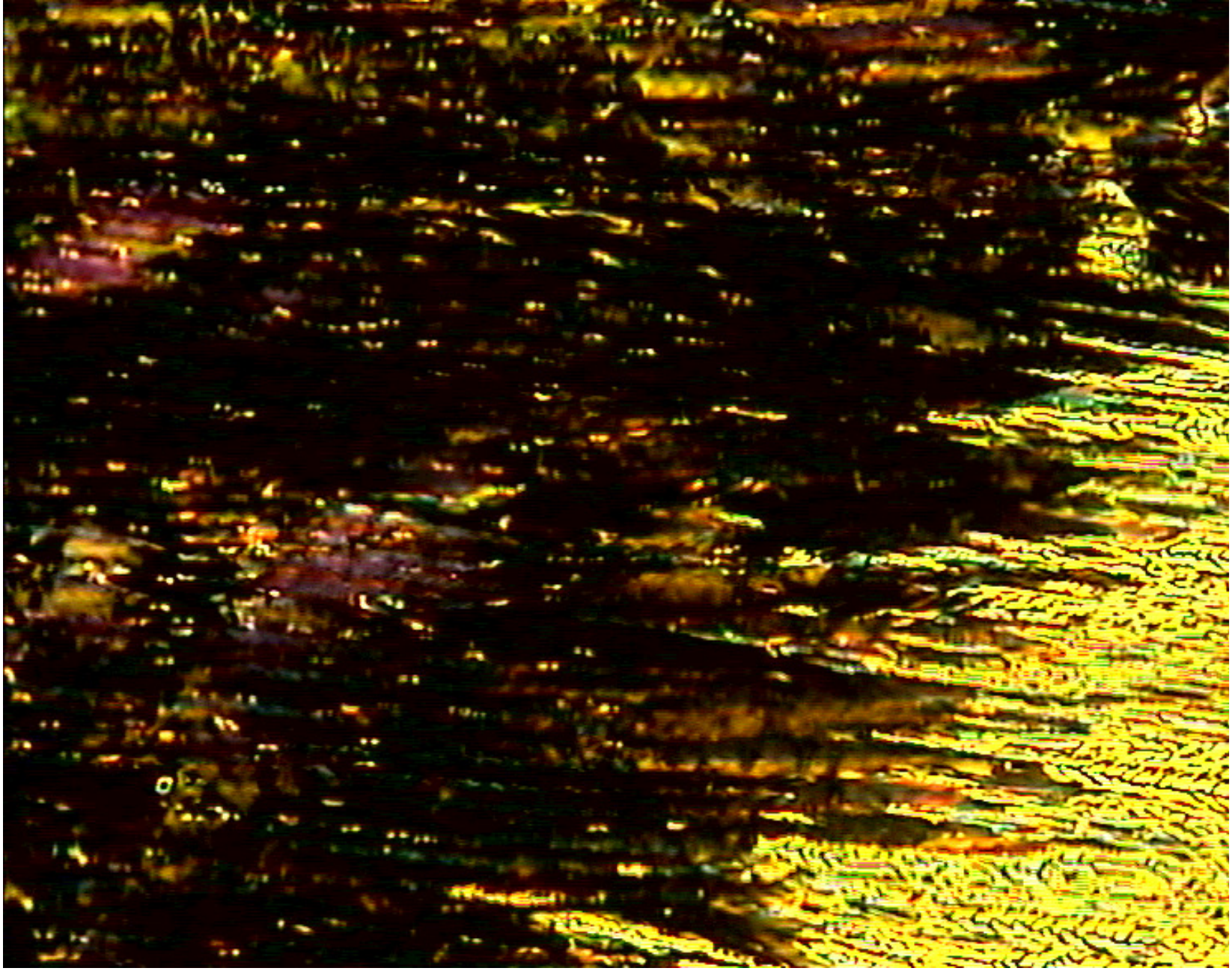
Left a Crystal, right an isotropic L structure

And we have to be sure to be above the melting point



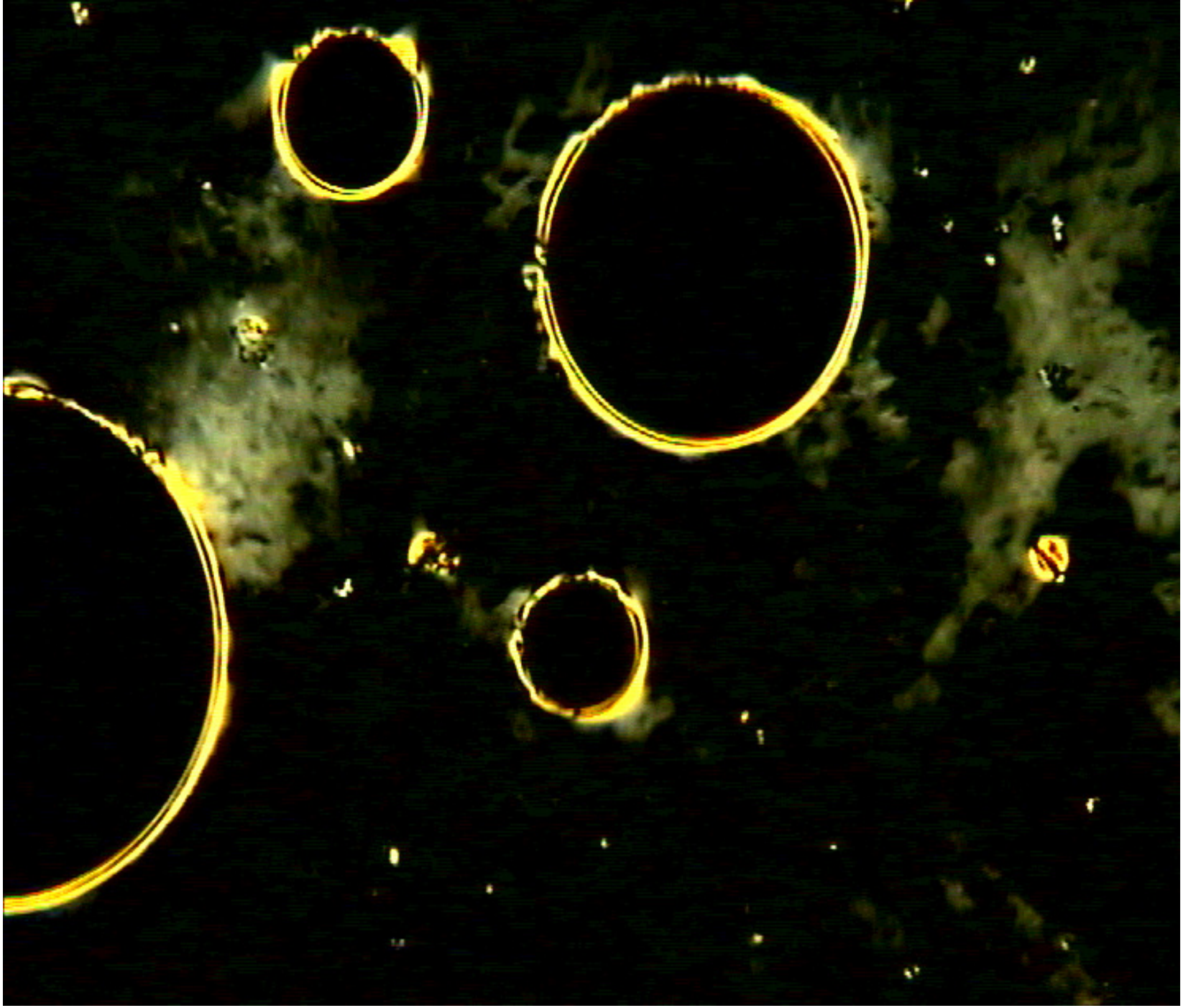
Crystallization (left) at the temperature 51.4 °C during cooling of eth-3 (S. Torgova, LC Lab Poli TO)

And far from any transition, even from an alignment transition (here from smectic A not homeotropic to a homeotropic one



Transition at temperature 75.0 °C during heating of eth-3 (S. Torgova, LC Lab, Poli TO)

If we have to deal with a NLC, we want to know its director profile. Here the black field between crossed polarizers ensures us that the orientation is…



NLC (homeotropic) at temperatuire 77.5°C during heating of eth-5 (S. Torgova, LC Lab, Poli TO)

But pay attention: the **homeotropic** alignment in the previous picture is only *outside of the circles*!

Inside there is nothing, the sample is empty

To predict the equilibrium director profile in certain given circumstances, it is necessary to introduce the concept of **Free energy**, and **Free energy density**

And to work on them, without been afraid by *Mathematics*

2.1. Free energy density and stationary state

2.1.1. Free energy

Definition

$$F \equiv U - TS \qquad (1)$$

where

U is the total potential energy of fields acting on the system,

T is the thermodinamic temperature of system,

S is the system entropy

In International Measurement System SI we have [*F*]=[*U*]= J , [*T*] = K , [*S*] = J/K

Only if the system is homogeneous **the free energy density** is constant in every point of the system

$$f \equiv \frac{\mathrm{d}F}{\mathrm{d}V} \tag{2}$$

where V is the system volume.

In SI it is $[f] = \mathrm{J/m^3}$.

During a thermodynamic elemental reversible transform

$$\mathrm{d}F = \mathrm{d}U - S\mathrm{d}T - T\mathrm{d}S \tag{3}$$

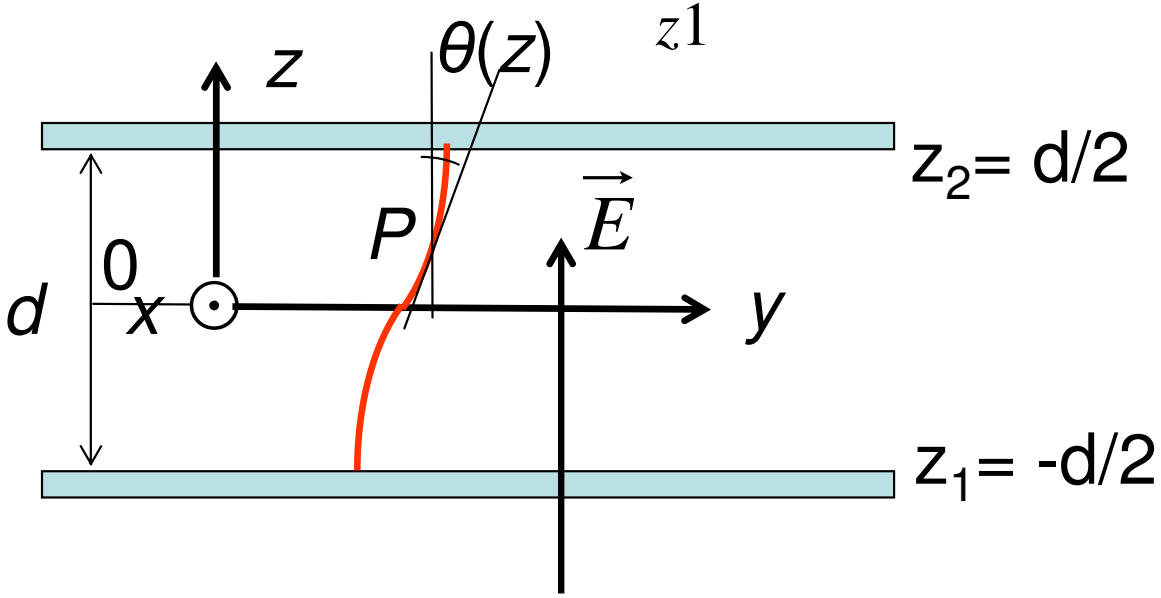
If the transform is isothermal and can be considered isentropic, then the only contribution to free energy is given by potential energy of the interacting fields:

$$\mathrm{d}F = \mathrm{d}U \tag{4}$$

2.1.2. Functionals with fixed border

Let *F* be the NLC cell free energy, and *f* the free energy density. It is esplicit continuous function of *z*, and the director tilt angle *θ* as well, with its 1° derivative.

$$F(\theta,\theta') = \int_{z1}^{z2} f(z,\theta(z),\theta'(z))\mathrm{d}z \qquad (5)$$



Here an electric field is shown as source of distortion.

The red line is the distorted director profile

*The free energy $F(\theta,\theta')$, regarded as function of $\theta(z)$ and $\theta'(z)$, is called a **functional** in the Dominion z_1-z_2 :*

The free energy density $f(z,\theta,\theta')$ must be posed

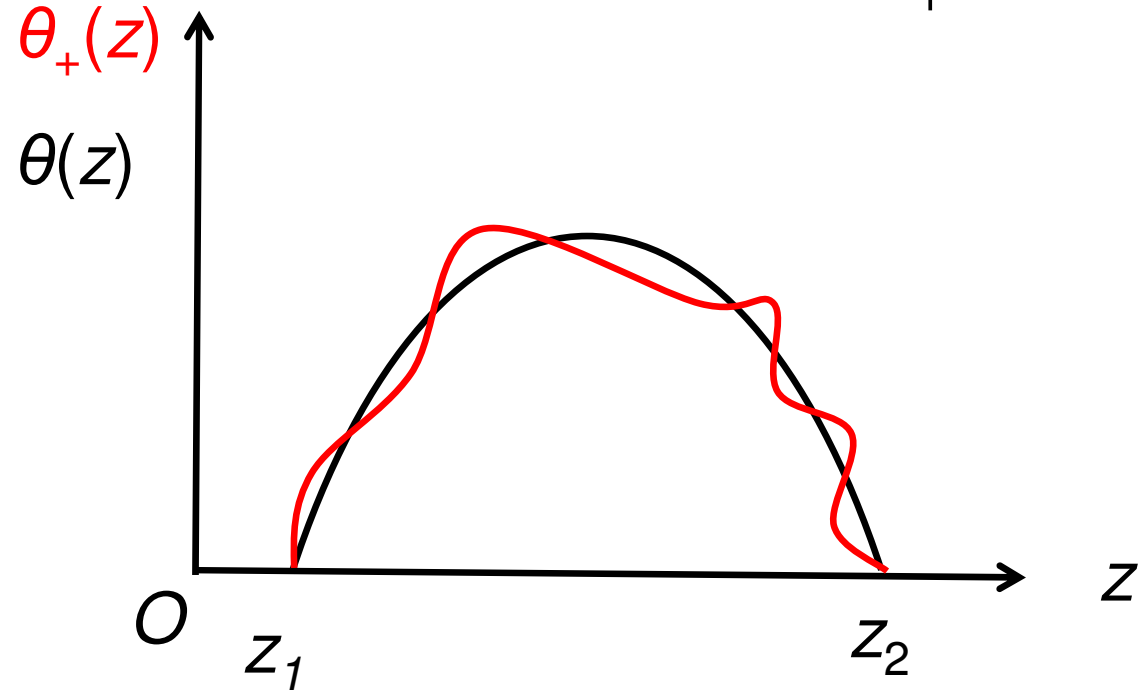
θ(z)** (and consequently θ'(z)) **is unknown, and has to be found.

Mark that in SI it is $[z]$ = m, $[\theta]$ = rad .

The idea is to look for actual profile in the ensemble of the virtual director lines $\theta_+(z)$ having tangent lines $\theta_+'(z)$ among which the actual profile $\theta(z)$ characterized by the actual $\theta'(z)$ arises, providing the functional F to be **extremal**.

Now, $\theta_+(z)$ are curves ε-close of 0-order to $\theta(z)$ such as $\left|\theta_+(z)-\theta(z)\right|<\varepsilon$, $\theta'_+(z)$ are ε-close of 1st order such as

$$\left|\theta_+'(z)-\theta'(z)\right|<\varepsilon$$



Let us suppose that the **<u>boundary conditions</u>** at the estreme of the Dominion *have fixed values* $\theta(z_1)= \theta_1$, $\theta(z_2)= \theta_2$.

A functional *F has a* ***relative extremal*** *if on the curve θ(z) it has a value either always greater (MAX) or always smaller (min) than*

on every curve $\theta_+(z)$ ε-close to $\theta(z)$

This is the recipe for calculating θ(z)

2.1.3. Euler-Lagrange (E-L) eq. with fixed boundary conditions.

Let us define a continuous finite function *η(z) going to zero at the dominion extremes,* such as

$$\theta_+(z) = \theta(z) + \alpha\eta(z) \tag{6}$$

where α<<1 is a small real number. Then

$$\theta_+(z_{1,2}) = \theta(z_{1,2}) \tag{7}$$

at the boundary.

Then the free energy by substituting (6) into def.(5) is a function of α:

$$F(\alpha)=\int_{z1}^{z2} f[z,\underbrace{\theta(z)+\alpha\eta(z)}_{\theta_+(z)},\underbrace{\theta'(z)+\alpha\eta'(z)}_{\theta'_+(z)}]\mathrm{d}z \qquad (8)$$

being extremal for α=0. Hence $F'(\alpha)\big|_{\alpha=0}=0$ (9)

Deriving *F* with respect to *α*, we get

$$F'(\alpha)\big|_{\alpha=0}=0=\int_{z1}^{z2}[f_{\theta+}\eta(z)+f_{\theta'+}\eta'(z)]\mathrm{d}z \qquad (10)$$

Mark that $f_{\theta+}\equiv\dfrac{\mathrm{d}f}{\mathrm{d}\theta_+}$

Re-writing the 1° integral and integrating per part the 2° integral with differental factor $\eta'(z)\mathrm{d}z$, we obtain:

$$0 = \int_{z1}^{z2} f_\theta \eta(z)\mathrm{d}z + f_{\theta'}\eta(z)\Big|_{z1}^{z2} - \int_{z1}^{z2} \eta(z)\frac{\mathrm{d}}{\mathrm{d}z} f_{\theta'}\mathrm{d}z \qquad (11)$$

The 2° term is identically zero, then

$$\int_{z1}^{z2} \eta(z)\left\{ f_\theta - \frac{\mathrm{d}}{\mathrm{d}z} f_{\theta'} \right\}\mathrm{d}z = 0 \qquad (12)$$

and thus the 1-dimension **Euler-Lagrange** eq. is obtained:

$$f_\theta - \frac{\mathrm{d}}{\mathrm{d}z} f_{\theta'} = 0 \qquad (13)$$

with **<u>boundary conditions</u>**

$$\begin{cases} \theta(z_1) = \theta_1 \\ \theta(z_2) = \theta_2 \end{cases} \qquad (14)$$

2.1.4. Mechanism of interaction between NLC cell and applied fields

2.1.4.1. Basic principles

The free energy of a liquid crystal system can be treated via the **classical procedure of *extremalization***, with the aim of obtaining the equilibrium configuration of the director in the whole volume, provided the fields acting, the elasticity of the material and the **boundary conditions** are known.

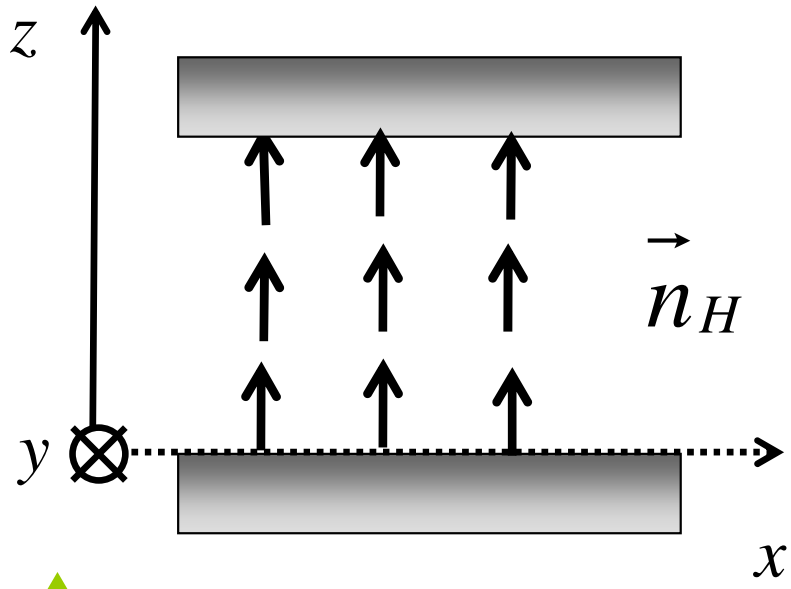
NLC molecules do **not** possess **permanent electric dipoles,** then an electric field creates **induced dipoles**, and acts on them modifying the molecular (mlc) orientation.

The parallel (ıı) and normal ($\perp$) components of the induced dipole depend on the mlc structure. Accordingly, some NLC have mlc with induced electric dipole essentially ıı with respect to the mlc long axis (***positive*** *dielectric anisotropy* ε_a), other NLC have induced dipoles essentially $\perp$ (***negative*** ε_a).

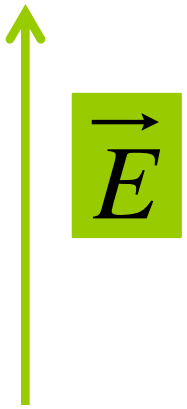
Moreover, NLC exhibit **induced magnetic dipoles** too, usually ıı with respect to the mlc long axes (but they can be $\perp$ as well). Thus, NLC are characterized by a magnetic susceptibility anisotropy χ_{ma} (either positive or negative), and a magnetic field can orient the mlc via such induced dipoles.

1.4.2. Homeotropic NLC cell

Let us consider a NLC cell with HOMEOTROPIC alignment



If the permittivity anisotropy $\varepsilon_a > 0$,



an electric field normal to the cell plates stabilizes the homeotropic orientation of the NLC director

On the contrary, if $\varepsilon_a < 0$

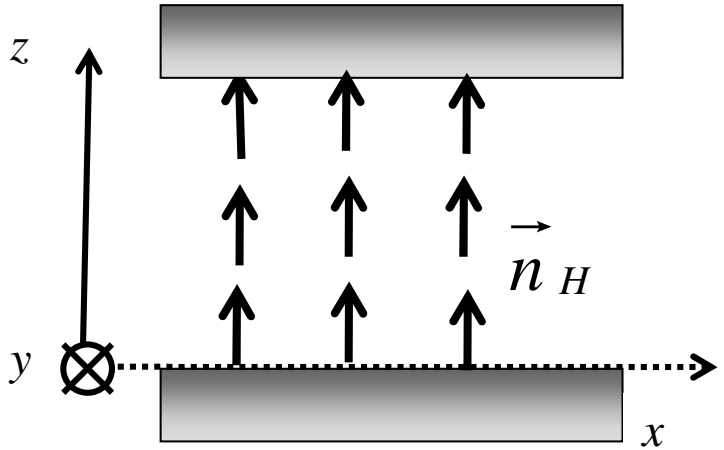
The same field $\vec{E}$ destabilizes the homeotropic alignment

And we have already told that it is a threshold phenomenon (Frederiks transition)

In the following, we will demonstrate this behaviour

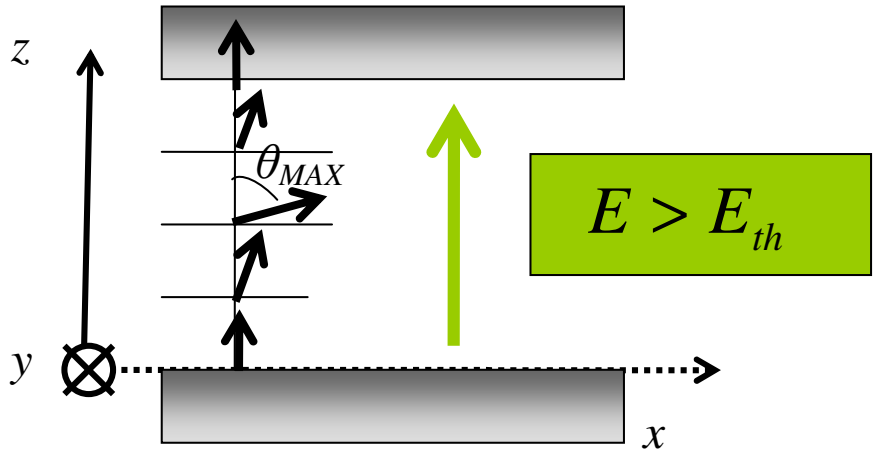
Interaction of homeotropic **NEMATICS** with electric field

Frederiks transition: NLC with $\varepsilon_a<0$, NLC-cell with homeotropic alignment and **strong anchoring:** *elastic distortion above a threshold*.



$$0 \le E < E_{th}$$

$$E_{th} = \frac{\pi}{d}\sqrt{\frac{K_{33}}{\varepsilon_o|\varepsilon_a|}}$$

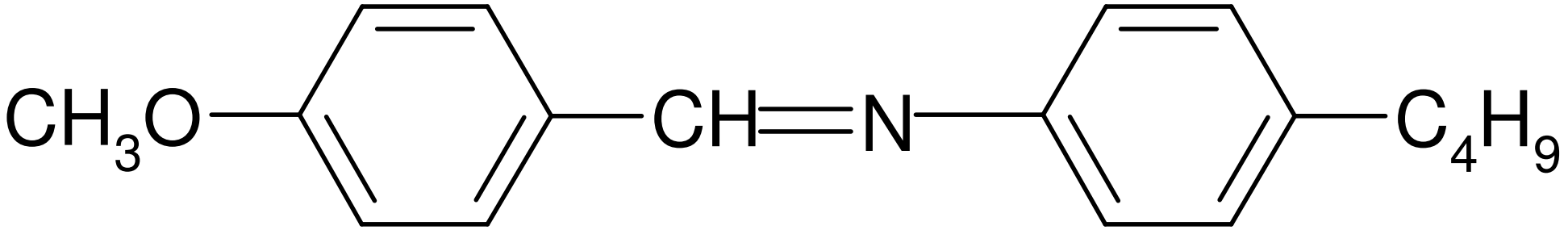


Strong anchoring implies homeotropic alignment at the surfaces also in the presence of field

1

The compound

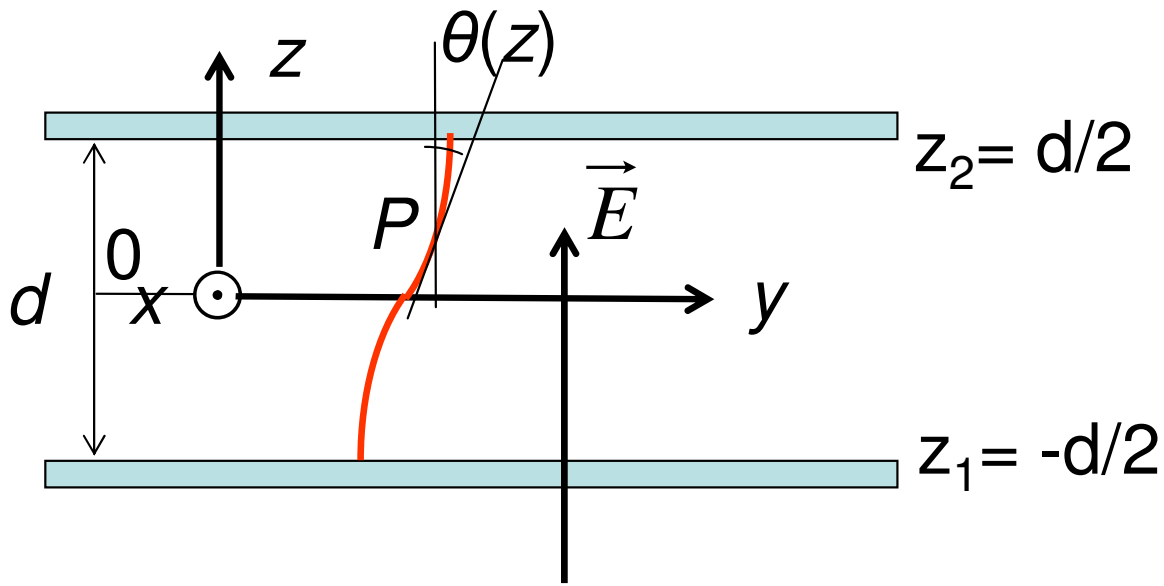
***N*-(4-Methoxybenzylidene)-4-butylaniline** (**MBBA**) ,
achieved 1969 by Hans Kelker (Hoescht)



presents nematic phase **at room temperature**, and exhibits $\boldsymbol{\varepsilon_a < 0}$

2.1.5. Demonstrating the splay-bend elastic free energy density

Let us consider a Nematic Liquid Crystal (NLC) with negative dielectric anisotropy ε_a, in a **homeotropic** cell.
If E>Eth, a distortion arises dependent only on one co-ordinate, z = the direction normal to the cell plates



The director profile (picted in red) due to the presence of an electric field $\vec{E} \parallel z-\text{axis}$ has to be calculated

Data:

1. NLC: **MBBA**, **negative** dielectric anisotropy $\varepsilon_a \equiv \varepsilon_{\parallel} - \varepsilon_{\perp} < 0$
, three bulk elastic constants (K_{11}, K_{22}, K_{33});

Mark that in SI the elastic constants are measured in Newton, $[K_{ii}]$ = N .

Constant electric field *E* normal to the cell plate, i.e. ıı *z-axis; E* can be preselected and adjusted during the experiment;

Cell thickness *d*=10μm ;

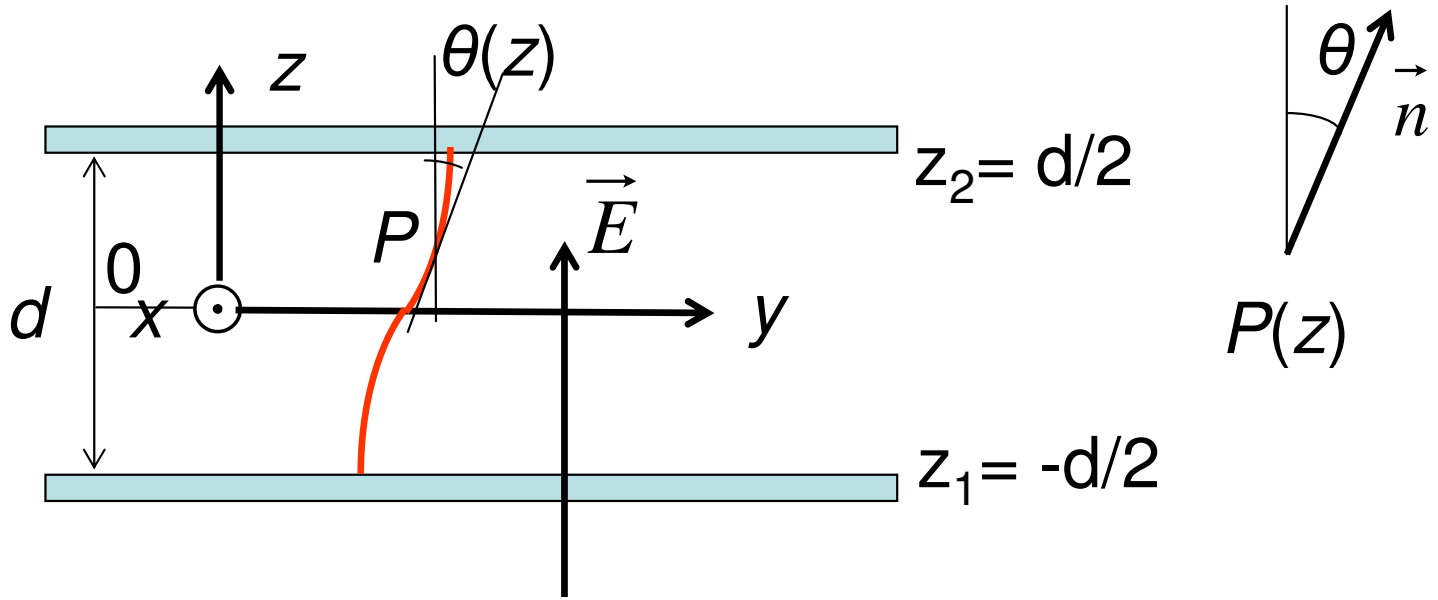
Initial alignment homeotropic, i.e. *θ(z)=0* everywhere $\forall z$;

Surface treatment for having distortion only in [yz]-plane;

Strong **boundary condition**: θ_1=0, θ_2=0.

Let us derive the **free energy density**. for the material in the cell.

The red line represents the director profile, which tangent is locally parallel to the director $\vec{n}$



In the absence of $\vec{E}$, the director profile is uniform and normal to the cell plates

$\vec{E}$ can induce a distortion in the [*y,z*] plane, then

$$\vec{n} = \vec{j}\sin\theta + \vec{k}\cos\theta \qquad (14)$$

The free energy density of **splay** is

$$f_s \equiv \frac{1}{2} K_{11} (\mathrm{div}\vec{n})^2 = \frac{1}{2} K_{11} (-\sin\theta \cdot \theta')^2 = \frac{1}{2} K_{11} \sin^2\theta \cdot \theta'^2 \quad (15)$$

For twist, it is zero, since:

$$f_t \equiv \frac{1}{2} K_{22} (\vec{n} \cdot \mathrm{rot}\vec{n})^2 \quad (16)$$

and

$$\mathrm{rot}\vec{n} = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ 0 & 0 & \dfrac{\partial}{\partial z} \\ 0 & \sin\theta & \cos\theta \end{vmatrix} = -\vec{i}\cos\theta \cdot \theta' \quad (17)$$

being normal to $\vec{n}$

The free energy density for **bend** is

$$f_B \equiv \frac{1}{2} K_{33} (\vec{n} \times \mathrm{rot}\vec{n})^2 = \frac{1}{2} K_{33} \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ 0 & \sin\theta & \cos\theta \\ -\cos\theta \cdot \theta' & 0 & 0 \end{vmatrix}^2 =$$

$$= \frac{1}{2} K_{33} \theta'^2 \cos^2\theta (\cos^2\theta + \sin^2\theta) = \frac{1}{2} K_{33} \theta'^2 \cos^2\theta \qquad (18)$$

We will show that the free energy density due to electric interaction, if NLC is an insulator and the field $\vec{E}$ is applied by an external power supply is given by

$$f_E = -\frac{1}{2} \varepsilon_o \varepsilon_a (\vec{E} \cdot \vec{n})^2 = \frac{1}{2} \varepsilon_o |\varepsilon_a| E^2 \cos^2\theta \qquad (19)$$

where the dielectric anisotropy ε_a for MBBA is **negative**.

Mark that in SI ε_o is the vacuum permittivity and it is $[\varepsilon_o]$= F/m , [E] = V/m.

Hence the total free energy density is given by

$$f = \frac{1}{2}\left[\theta'^2 (K_{11}\sin^2\theta + K_{33}\cos^2\theta) + \varepsilon_o|\varepsilon_a|E^2\cos^2\theta\right] \quad (20)$$

and the functional, which extremalization process has to be performed to find the actual profile $\theta(z)$

is the total free energy

$$F = \int_{-d/2}^{d/2} f[\theta(z), \theta'(z)]\mathrm{d}z \quad (21)$$

Mark that in SI (21) gives $[F]$= J/m^2.

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2.2. Homeotropic cell with ε_a<0-NLC under Electric field normal to the cell plates

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MEPhI, Moscow, 17 September 2014

2.2.1. Demonstrating the free energy density of the interaction NLC- $\vec{E}$

Let us demonstrate now why the interaction NLC- $\vec{E}$ can be written as in (19) – *in the frame of International Measurement System* SI :

$$f_E = -\frac{1}{2}\varepsilon_o \varepsilon_a (\vec{E}\cdot\vec{n})^2 \qquad (19)$$

where ε_o= 8.85·10^{-12} F/m (=Faraday/meter) is the vacuum permittivity, and the permittivity anisotropy=electric susceptibility anisotropy is

$$\varepsilon_a \equiv \varepsilon_{\parallel} - \varepsilon_{\perp} = \chi_{e\parallel} - \chi_{e\perp} \equiv \chi_{ea} \qquad (19\text{-})$$

Mark that *E* in SI is measured in Volt/meter: [*E*] =V/m, whereas $\varepsilon_{II,\perp}$ and $\chi_{eII,\perp}$ are pure numbers. Then in (19) [f_E] = J/m^3.

If NLC is a perfect insulator the applied $\vec{E}$ induces only an electric polarization (electric dipole moment per unit volume):

$$\vec{P} = \varepsilon_o \overline{\overline{\chi}}_e \vec{E} \qquad (20\text{-})$$

Mark that in SI the polarization *P* is measured in Coulomb/square meter, i.e. [*P*] = C/m^2=A·s/m^2

$\vec{P}$ can be also not ıı with respect to $\vec{E}$, being the electric susceptibility $\overline{\overline{\chi}}_e$ a 3x3 matrix, which elements are pure numbers :

that is diagonal due to symmetry

$$\overline{\overline{\chi}}_e \equiv \begin{pmatrix} \chi_{e\perp} & 0 & 0 \\ 0 & \chi_{e\perp} & 0 \\ 0 & 0 & \chi_{e\parallel} \end{pmatrix} \qquad (21\text{-})$$

The electric displacement is then

$$\vec{D} = \varepsilon_o \vec{E} + \vec{P} = \varepsilon_o \overline{\overline{\varepsilon}} \vec{E} \qquad (22\text{-})$$

Mark that in SI the displacement D is measured in C/m^2, like the polarization P as well: $[D]$ = C/m^2.

Note that in (22-) due to (20-) the relative permittivity matrix is given by

$$\overline{\overline{\varepsilon}} \equiv \overline{\overline{I}} + \overline{\overline{\chi}}_e \qquad (23\text{-})$$

being $\overline{\overline{I}}$ the unit matrix.

This means that the relative permittivity matrix writes

$$\overline{\overline{\varepsilon}} = \begin{pmatrix} \varepsilon_\perp & 0 & 0 \\ 0 & \varepsilon_\perp & 0 \\ 0 & 0 & \varepsilon_\parallel \end{pmatrix} \quad , \quad \varepsilon_{\parallel,\perp} = 1 + \chi_{e\parallel,\perp} \qquad (24\text{-})$$

Writing more conveniently, in order to put in evidence the dielectric anisotropy dependence of the electric displacement

we choose a local reference frame $[x_o,y_o,z_o]$ such as the mlc director reads $\vec{n}_o \equiv \vec{k}_o$. Hence, from

$$\begin{cases} D_{xo} = \varepsilon_o \varepsilon_\perp E_{xo} \\ D_{yo} = \varepsilon_o \varepsilon_\perp E_{yo} \\ D_{zo} = \varepsilon_o \varepsilon_\parallel E_{zo} \end{cases} \qquad (25\text{-})$$

the electric displacement eventually writes:

$$\vec{D} = \varepsilon_o \left[\varepsilon_\perp E_{xo} \vec{i}_o + \varepsilon_\perp E_{yo} \vec{j}_o + \varepsilon_\parallel E_{zo} \vec{n}_o - \varepsilon_\perp E_{zo} \vec{n}_o + \varepsilon_\perp E_{zo} \vec{n}_o \right] =$$

$$= \varepsilon_o \left[\varepsilon_\perp \vec{E} + \varepsilon_a \left(\vec{E} \cdot \vec{n}_o \right) \vec{n}_o \right] \qquad (26\text{-})$$

Which means, for every director orientation:

$$\vec{D} = \varepsilon_o \left[\varepsilon_\perp \vec{E} + \varepsilon_a \left(\vec{E} \cdot \vec{n} \right) \vec{n} \right] \qquad (27\text{-})$$

It's evident that the displacement is in general not ıı to the field: the polarizing back-effect on the imposed field is important, due to the NLC properties.

Calculating the electric free energy density

$$f_E = -\int_0^E \vec{D} \cdot \mathrm{d}\vec{E} \qquad (28\text{-})$$

and finally

$$f_E = -\frac{1}{2}\vec{D}\cdot\vec{E} = -\frac{1}{2}\varepsilon_o\varepsilon_\perp E^2 - \frac{1}{2}\varepsilon_o\varepsilon_a(\vec{E}\cdot\vec{n})^2 \qquad (29\text{-})$$

It is possible to neglect the term which is independent of the director alignment, then

$$f_E = -\frac{1}{2}\varepsilon_o\varepsilon_a(\vec{E}\cdot\vec{n})^2 = -\frac{1}{2}\varepsilon_o\chi_{ea}(\vec{E}\cdot\vec{n})^2 \qquad (30\text{-})$$

I.Let us remark that Maxwell eq.s without charge carriers have to be satisfied, i.e.

$$\begin{cases} \mathrm{div}\,\vec{D} = 0 \\ \mathrm{rot}\,\vec{E} = 0 \end{cases} \qquad (31\text{-})$$

II. Remember that in Gaussian System (GS) eq. (20-, 22- and 30-) write DIFFERENTLY:

$$\vec{P} = \overline{\overline{\chi}}_e \vec{E} \qquad (20\text{-G})$$

$$\vec{D} = \vec{E} + 4\pi\vec{P} = \overline{\overline{\varepsilon}}\vec{E} \qquad (22\text{-G})$$

$$f_E = -\frac{1}{8\pi}\varepsilon_a(\vec{E}\cdot\vec{n})^2 \qquad \text{(30-G)}$$

Since in GS the vacuum permittivity is set as a pure number, ε_o=1, then *E*, *P*, *D*, in GS have the same dimensions

[*E*] = [*P*] = [*D*] = statV/cm, even if people prefer for the polarization to indicate [*P*] = statC/cm^2, which is the same.

III. As a consequence, ε_a *surprisingly* has the same numerical value in both GS and SI.

But not χ_{ea} , since eq. (22-G)

$$\vec{D} = \vec{E} + 4\pi\vec{P} = \overline{\overline{\varepsilon}}\vec{E} \qquad (22\text{-G})$$

implies

$$\boxed{\overline{\overline{\varepsilon}} = 1 + 4\pi\overline{\overline{\chi}}} \qquad (23\text{-G})$$

Hence $$\chi_{ea}^{\ SI} = 4\pi\chi_{ea}^{GS} \qquad (23\text{--})$$

The electric susceptibility anisotropy χ_{ea}

DOES NOT HAVE the same numerical value

in both GS and SI : *this is a source of mistakes made*

by some valuable scientists!

IV. For nematic MBBA at 25°C it is $\varepsilon_a = -0.7 < 0$

V. For nematic 5CB at 24 ÷ 34°C it is $\varepsilon_a = 8 \div 11 > 0$

We have seen in 2.1 that the total free energy density (elastic and electric) is given by

$$f = \frac{1}{2}\left[\theta'^{2}\left(K_{11}\sin^{2}\theta + K_{33}\cos^{2}\theta\right) + \varepsilon_{o}\left|\varepsilon_{a}\right|E^{2}\cos^{2}\theta\right] \quad (20)$$

and the functional which the actual profile $\theta(z)$ renders extremal is the total free energy

$$F = \int_{-d/2}^{d/2} f[\theta(z), \theta'(z)]\mathrm{d}z \quad (21)$$

2.2.2. E-L eq. with fixed boundary condition for this homeotropic cell

$$f_\theta - \frac{\mathrm{d}}{\mathrm{d}z} f_{\theta'} = 0 \qquad (13)$$

From E-L eq. (13) , calculating the derivatives f_θ and $\mathrm{d}f_{\theta'}/\mathrm{d}z$ we get

$$f_\theta = \frac{1}{2}\left[\theta'^2 (2K_{11}\sin\theta\cos\theta - 2K_{33}\cos\theta\sin\theta) - \varepsilon_o|\varepsilon_a|E^2 2\cos\theta\sin\theta\right] =$$

$$= \frac{1}{2}\left[\theta'^2 (K_{11} - K_{33}) - \varepsilon_o|\varepsilon_a|E^2\right]\sin 2\theta \qquad (22)$$

and

$$\frac{\mathrm{d}}{\mathrm{d}z} f_{\theta'} = \theta''(K_{11}\sin^2\theta + K_{33}\cos^2\theta) \qquad (23)$$

Combining (22), (23) we get

$$\theta''(K_{11}\sin^2\theta + K_{33}\cos^2\theta) +$$

$$+\frac{1}{2}\left[-\theta'^2(K_{11} - K_{33}) + \varepsilon_o|\varepsilon_a|E^2\right]\sin 2\theta = 0 \qquad (24)$$

Eq. (24) shows the presence of a threshold. In fact, if $\theta \to 0$ also $\theta' \to 0$, then (24) reads:

$$\theta'' K_{33} + \varepsilon_o|\varepsilon_a|E^2\theta = 0 \qquad (25)$$

2.2.3. Threshold for bend electric Frederiks transition with strong anchoring.

Eq. (25) becomes the pendulum canonic eq.:

$$\theta'' + k_H{}^2 \theta = 0 \tag{26}$$

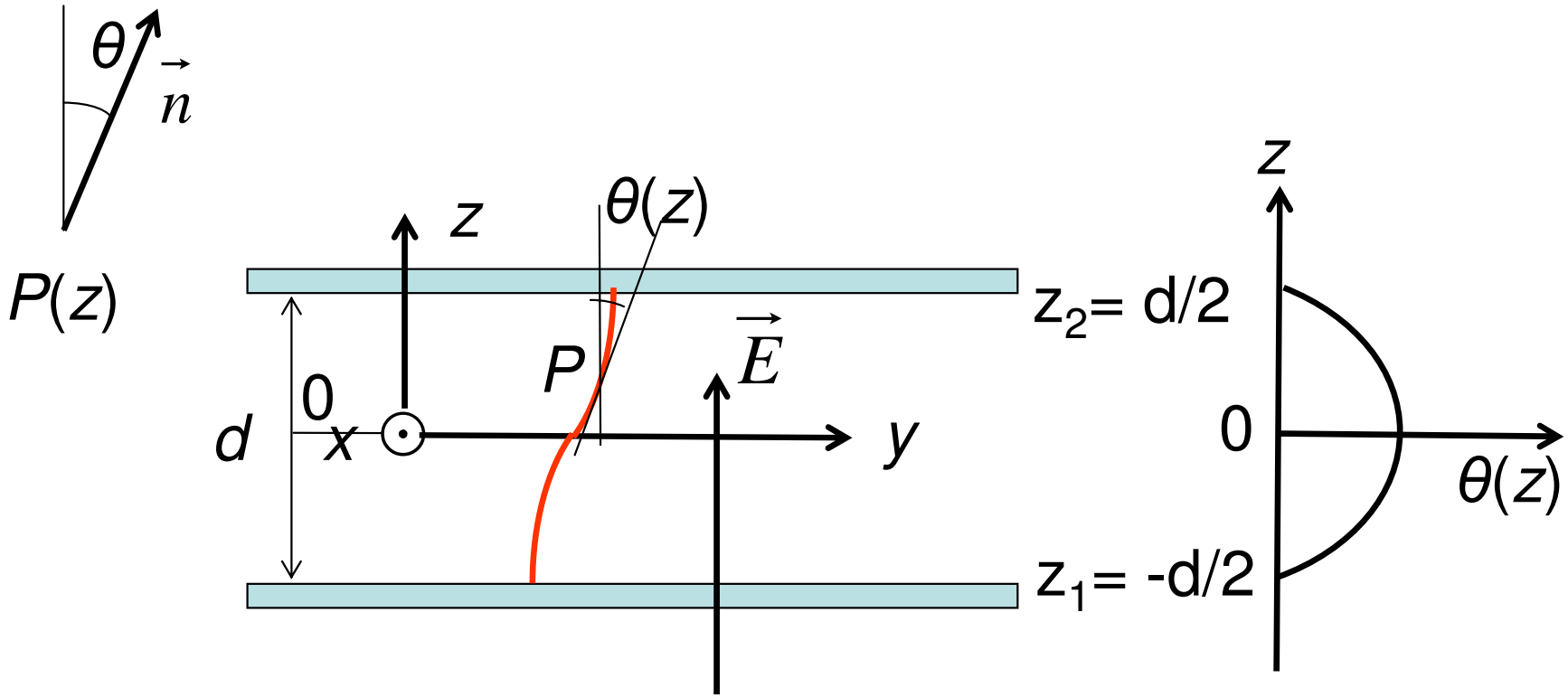
where

$$k_H \equiv \sqrt{\frac{\varepsilon_o |\varepsilon_a|}{K_{33}}} E \tag{27}$$

Then the arising distortion is harmonic, and the boundary conditions (**strong anchoring**) imply

$$\theta = \theta_o \cos k_H z \tag{28}$$

being the cell thickness $d = \lambda/2$.



Then

$$k_H d = \pi \tag{29}$$

gives the critical field for the arising of the **bend** electric Frederiks transition in homeotropic NLC cells with $\varepsilon_a<0$

$$E_{crit} = \frac{\pi}{\mathrm{d}}\sqrt{\frac{K_{33}}{\varepsilon_o|\varepsilon_a|}} \tag{30}$$

We note that the threshold has been found inversely proportional to the cell thickness (Fredericks, late 1920ths). Then it is possible to introduce *the critical voltage* applied to the cell

$$V_{crit} = \pi \sqrt{\frac{K_{33}}{\varepsilon_o |\varepsilon_a|}} \qquad (30')$$

The relevant MBBA data are $K_{33} = 7.5*10^{-12}$N, $\varepsilon_a = -0.7$. The vacuum permittivity is $\varepsilon_o = 8.85*10^{-12}$. Let be the cell thickness $d = 10$ μm.

We obtain $V_{crit} = 3.46$ V and $E_{crit} = 3.46*10^5$ V/m= 0.346 V/μm

2.2.4. Pay attention to Gaussian System!

Should we appreciate GS, as many physicists do (if they are theoreticians), we would have found instead of (30') the result

$$V_{crit} = \pi \sqrt{\frac{4\pi K_{33}}{|\varepsilon_a|}} \qquad \text{(30"-G)}$$

where to put K_{33}=7.5*10^{-7} dyn , ε_a = -0.7 (the same value as in SI), obtaining

$$V_{crit} = 1.1523*10^{-2} \text{ statV}$$

and, since 1 statV = 10^{-6}|c| V, being |c| = 2.998*10^{8} the value in SI of the light speed in vacuum, eventually getting

$$V_{crit} = 3.46 \text{ V}$$

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2.3. Unidirectional planar cell with $\chi_{ma}>0$-NLC under Magnetic field normal to the cell plates

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2.3.1. Demonstrating the free energy density of the interaction NLC- Magnetic field $\vec{H}$

Let us look now for **the form** of the free energy density relevant to the interaction NLC-magnetic field – *in the frame of SI of measurement,* :

Usually NLC are diamagnetic, then the applied magnetic field $\vec{H}$, due to the mlc anisotropy providing ıı and ⊥ susceptibilities $\chi_{\text{ıı}}$ and $\chi_{\perp}$

induces into the NLC material only a weak magnetization (magnetic dipole moment per unit volume):

$$\vec{M} = \overline{\overline{\chi}}_m \vec{H} \qquad (20+)$$

Comparing with (20-), mark that here the measuring unit of *M* and *H* are the same. In SI, it is [*M*]=[*H*]=A/m.

In (20+), as in the case of electric field polarization, the magnetic susceptibility is a 3x3 matrix, and then the magnetization $\vec{M}$ can be not $\shortparallel$ with respect to the magnetizing field $\vec{H}$

In any case due to symmetry $\overline{\overline{\chi}}_m$ writes

$$\overline{\overline{\chi}}_m \equiv \begin{pmatrix} \chi_{m\perp} & 0 & 0 \\ 0 & \chi_{m\perp} & 0 \\ 0 & 0 & \chi_{m\shortparallel} \end{pmatrix} \qquad (21+)$$

and its elements are pure numbers

As a result, NLC is affected by the magnetic induction field given by

$$\vec{B} = \mu_o(\vec{H} + \vec{M}) = \mu_o \overline{\overline{\mu}}\vec{H} \qquad (22+)$$

Mark that *B* in SI is measured in Tesla: [*B*] = T.

In (22+) the constant μ_o= 4π*10^{-7} H/m (= Henry/meter) is the vacuum permeability, and the permeability matrix $\overline{\overline{\mu}}$ is stated as:

$$\overline{\overline{\mu}} \equiv \overline{\overline{I}} + \overline{\overline{\chi}}_m \qquad (23+)$$

being $\overline{\overline{I}}$ the unit matrix.

As a conclusion, we get

$$\overline{\overline{\mu}} = \begin{pmatrix} \mu_{\perp} & 0 & 0 \\ 0 & \mu_{\perp} & 0 \\ 0 & 0 & \mu_{\parallel} \end{pmatrix} \quad , \quad \mu_{\parallel,\perp} = 1 + \chi_{m\parallel,\perp} \qquad (24+)$$

and the permeability anisotropy=magnetic susceptibility anisotropy is reported as

$$\mu_a \equiv \mu_{\parallel} - \mu_{\perp} = \chi_{m\parallel} - \chi_{m\perp} \equiv \chi_{ma} \qquad (19+)$$

Discussing in the same way as in the case of NLC-electric interaction, we will put in evidence the permeability anisotropy dependence of the induction field $\vec{B}$

We choose a local reference frame [x_o,y_o,z_o] such as the mlc director reads $\vec{n}_o \equiv \vec{k}_o$. Hence, from

$$\begin{cases} B_{xo} = \mu_o \mu_\perp H_{xo} \\ B_{yo} = \mu_o \mu_\perp H_{yo} \\ B_{zo} = \mu_o \mu_\parallel H_{zo} \end{cases} \qquad (25+)$$

the magnetic induction field eventually writes:

$$\vec{B} = \mu_o \left[\mu_\perp H_{xo} \vec{i}_o + \mu_\perp H_{yo} \vec{j}_o + \mu_\parallel H_{zo} \vec{n}_o - \mu_\perp H_{zo} \vec{n}_o + \mu_\perp H_{zo} \vec{n}_o \right] =$$

$$= \mu_o \left[\mu_\perp \vec{H} + \mu_a \left(\vec{H} \cdot \vec{n}_o \right) \vec{n}_o \right] \qquad (26+)$$

which means, for every director orientation:

$$\vec{B} = \mu_o \left[\mu_\perp \vec{H} + \mu_a \left(\vec{H} \cdot \vec{n} \right) \vec{n} \right] \qquad (27+)$$

It's evident that the magnetic induction $\vec{B}$ is in general not ıı to the field $\vec{H}$

Calculating the magnetic free energy density

$$f_H = -\int_0^H \vec{B} \cdot \mathrm{d}\vec{H} \qquad (28+)$$

we get

$$f_H = -\frac{1}{2}\vec{B} \cdot \vec{H} = -\frac{1}{2}\mu_o \mu_\perp H^2 - \frac{1}{2}\mu_o \mu_a (\vec{H} \cdot \vec{n})^2 \qquad (29+)$$

It is possible to neglect the term which is independent of the director alignment, then

$$\boxed{f_H = -\frac{1}{2}\mu_o \mu_a (\vec{H} \cdot \vec{n})^2} \qquad (30+)$$

Mark that f_H in SI is measured in J/m^3

Comparing (30+) with (30-), we realize that the magnetic free energy density corresponds in SI to the electric one just substituting

$$"\varepsilon_o\varepsilon_a = \varepsilon_o\chi_{ea} \text{ with } \mu_o\mu_a = \mu_o\chi_{ma} \quad \text{and } E \text{ with } H" \qquad (31)$$

I.Let us remark that Maxwell eq.s have to be satisfied, i.e.

$$\begin{cases} \mathrm{div}\vec{B} = 0 \\ \mathrm{rot}\vec{H} = 0 \end{cases} \qquad (31+)$$

II. Remember that in Gaussian System (GS) eq. (30+) writes

$$f_H = -\frac{1}{2}\chi_{ma}(\vec{H}\cdot\vec{n})^2 \qquad (30\text{-}G)$$

since in GS the vacuum permeability is set μ_o=1. Moreover, [H] = Oe (=Oersted) and [f_H] = erg/cm^3

III. As a consequence of point II., the magnetic susceptibility anisotropy χ_{ma} **DOES NOT HAVE** the same numerical value in both GS and SI : *this is a source of mistakes made by many valuable scientists!*

$$\chi_{ma}^{SI} = 4\pi\chi_{ma}^{GS} \qquad (31\text{-}G)$$

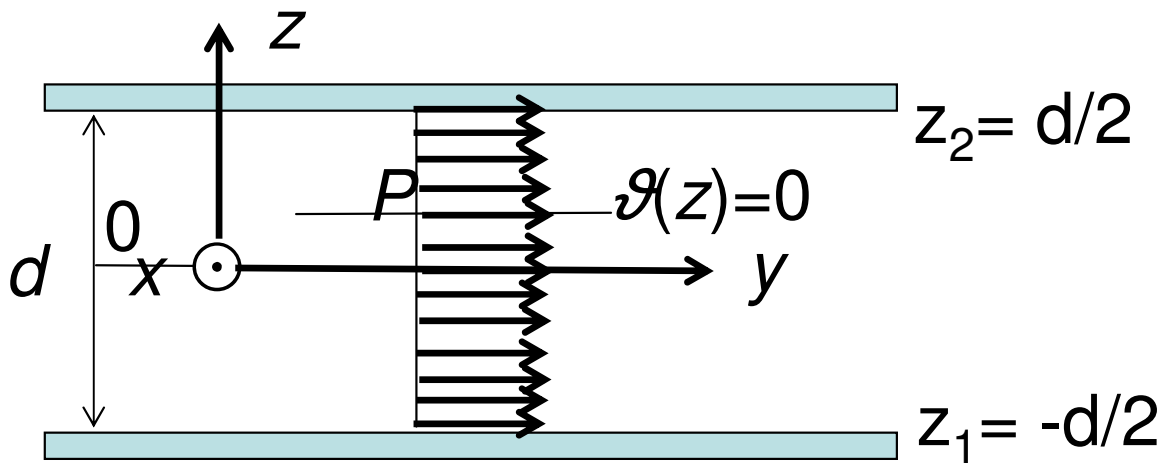
Recommended Recipe: ***Always use*** **SI** ***!***

IV. For nematic MBBA at 19℃ it is $\chi_a = 1.55 \cdot 10^{-6}$ in SI
but $\chi_a = 1.23 \cdot 10^{-7}$ in GS

V. For nematic 5CB at 26℃ it is $\chi_a = 1.43 \cdot 10^{-6}$ in SI
but $\chi_a = 1.14 \cdot 10^{-7}$ in GS

2.3.2. E-L eq. with fixed boundary condition for a unidirectional planar cell

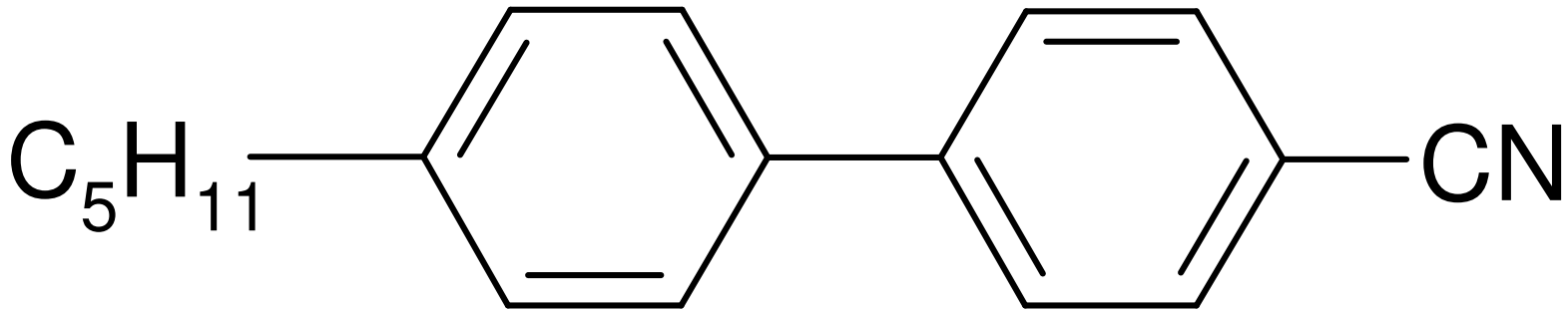
Let us consider the NLC **5CB**, having positive dielectric anisotropy, filling a cell with initial alignment unidirectional planar along *y*-axis



and strong anchoring: $\vartheta_1 = \vartheta(z_1)=0$, $\vartheta_2 = \vartheta(z_2)=0$, ϑ *being the angle between the director and y-axis.*

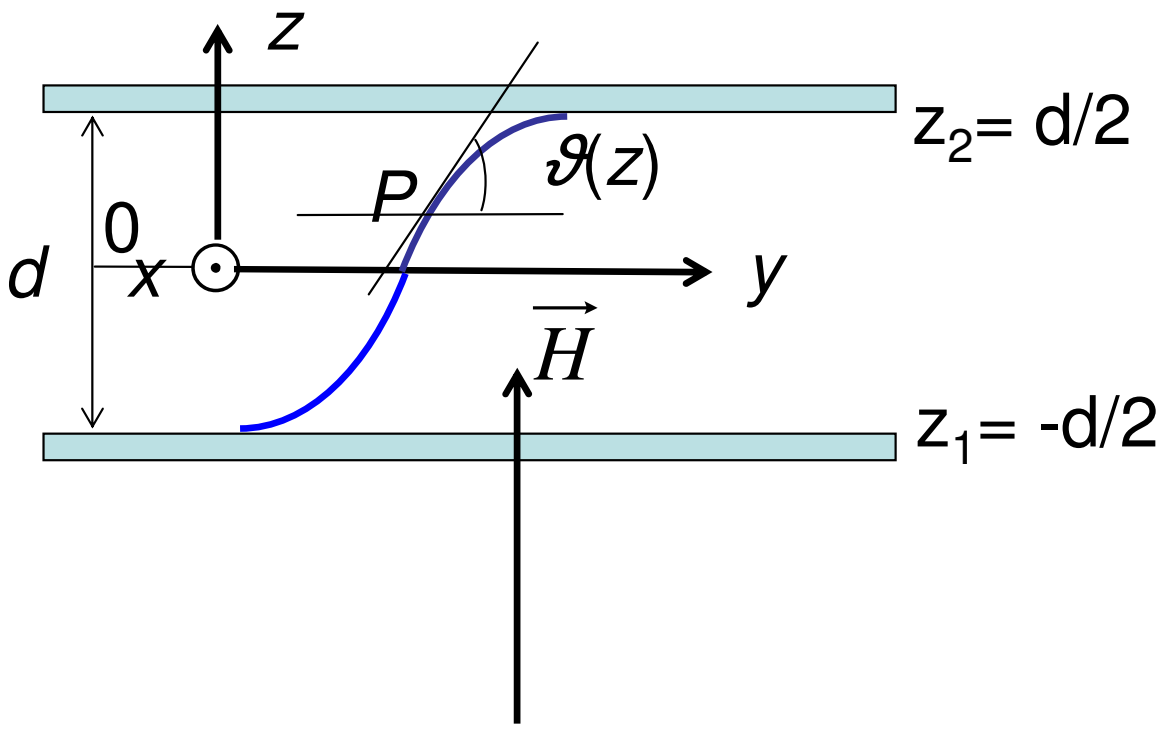
The compound

5CB: **4'amylcyanobiphenyl**, achieved 1972 by George Gray**,** Univ of Hull



presents nematic phase **at room temperature**, and exhibits $\boldsymbol{\varepsilon_a > 0}$

By applying a magnetic field $\vec{H}$ normal to the cell plates



the director is, as already stated:

$$\vec{n} = \vec{j}\cos\vartheta + \vec{k}\sin\vartheta \qquad (14')$$

The interaction free energy density between magnetic field and director reads

$$f_H = -\frac{1}{2}\mu_o \chi_{ma} (\vec{H} \cdot \vec{n})^2 = -\frac{1}{2}\mu_o \chi_{ma} H^2 \sin^2 \vartheta \qquad (20^*)$$

Comparing (20*) with (20'), we remember here that the magnetic free energy density corresponds to the electric one just substituting

$$"\varepsilon_o \varepsilon_a = \varepsilon_o \chi_{\mathrm{ea}} \text{ with } \mu_o \mu_a = \mu_o \chi_{ma} \quad \text{and } E \text{ with } H" \qquad (31)$$

the same geometry providing the same ϑ-trigonometric function,

whereas the elastic contribution remains unchanged.

This means that the total free energy density is

$$f = \frac{1}{2}\left[\vartheta'^2 (K_{11}\cos^2\vartheta + K_{33}\sin^2\vartheta) + \mu_o \chi_{ma} H^2 \sin^2\vartheta\right] \qquad (20^{**})$$

and consequently the E-L eq. is

$$-\theta''(K_{11}\cos^2\vartheta + K_{33}\sin^2\vartheta) +$$
$$+\frac{1}{2}\left[-\vartheta'^2(-K_{11}+K_{33}) - \mu_o\chi_{ma}H^2\right]\sin 2\theta = 0 \qquad (24^{*})$$

with strong anchoring unidirectional planar boundary conditions.

2.3.3. Threshold for splay magnetic Frederiks transition with strong anchoring

Linearizing close to the threshold, when $\vartheta \to 0$ also $\vartheta' \to 0$, then (24') reads:

$$\vartheta'' K_{11} + \mu_o \chi_{ma} H^2 \vartheta = 0 \qquad (25^*)$$

becoming the canonic pendulum eq.:

$$\vartheta'' + h_P{}^2 \vartheta = 0 \qquad (26^*)$$

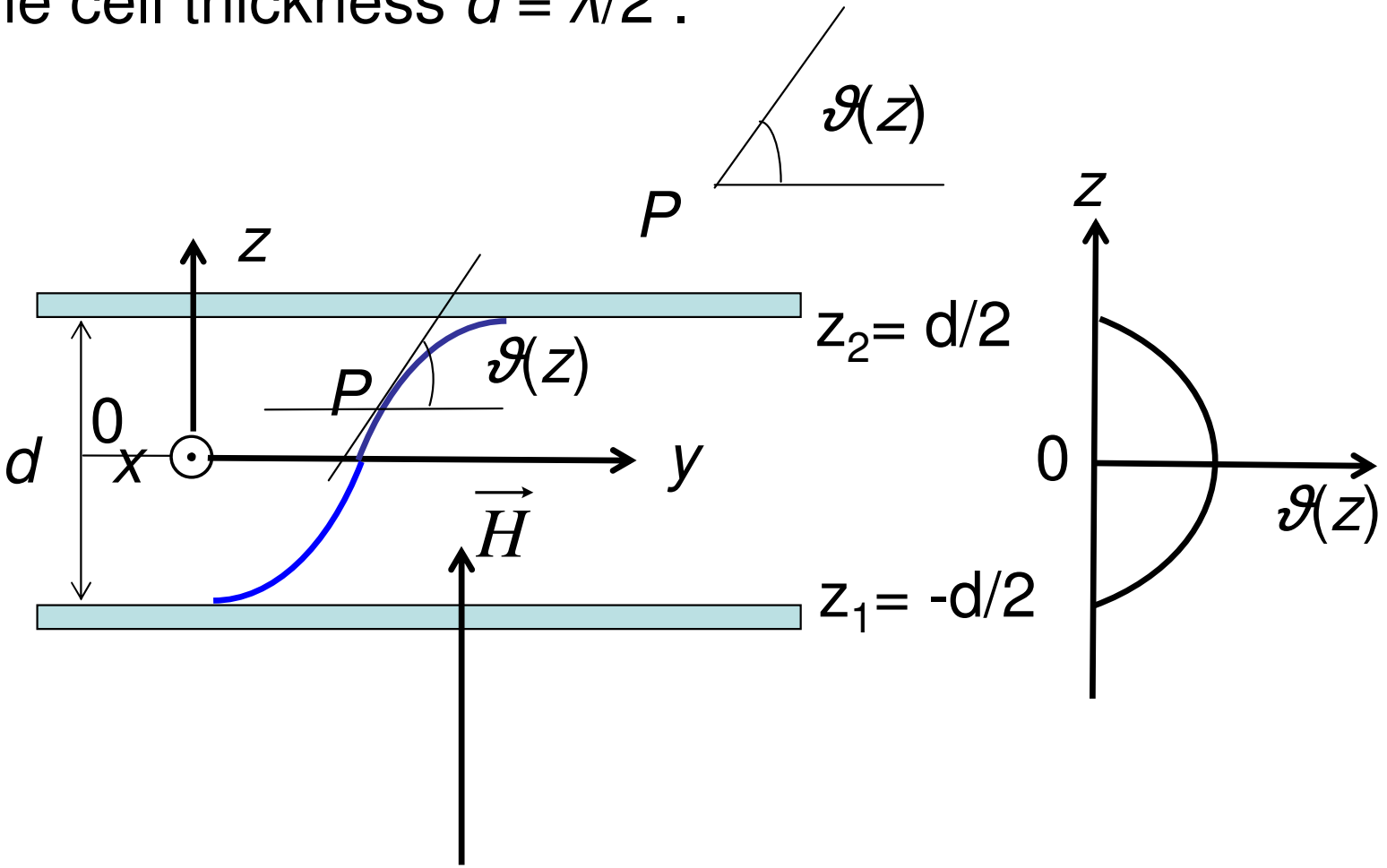
where

$$h_P \equiv \sqrt{\frac{\mu_o \chi_{ma}}{K_{11}}} H \qquad (27^*)$$

Then the arising distortion is as usual harmonic, and the boundary conditions (**strong anchoring**) imply

$$\vartheta = \vartheta_o \cos\ h_P z \qquad (28^*)$$

being the cell thickness $d = \lambda/2$.



Finally,

$$h_P d = \pi \qquad (29^*)$$

gives the critical field for the arising of the magnetic Frederiks transition (1st one discovered, 1927) in unidirectional planar NLC cells

$$H_{crit} = \frac{\pi}{\mathrm{d}} \sqrt{\frac{K_{11}}{\mu_o \chi_{ma}}} \qquad (30^*)$$

We note that, as for electric field, the magnetic threshold has been found inversely proportional to the cell thickness

$$H_{crit} = \frac{\pi}{d}\sqrt{\frac{K_{11}}{\mu_o \chi_{ma}}} \qquad (30^{*\prime})$$

The relevant 5CB data are $K_{11} = 6.2*10^{-12}$N, $\chi_{ma} = 1.43*10^{-6}$.
The vacuum permeability is $\mu_o = 4\pi*10^{-7}$.

Let be the cell thickness $d = 10$ μm.

We obtain $H_{crit} = 5.835*10^5$ A/m = 0.5835 A/μm

2.3.4. Always pay attention to Gaussian System!

What about GS ? Dealing with it, we would have found instead of (30*) the result

$$H_{crit} = \frac{\pi}{d}\sqrt{\frac{K_{11}}{\chi_{ma}}} \qquad (30^{*\prime})$$

where to put K_{11}= 6.2*10^{-7} dyn , χ_{ma} = 1.14*10^{-7} (**NOT** the same value as in SI, but that one shared by 4π), with the same cell thickness, obtaining

$$H_{crit} = 3.25*10^{-3}\ \text{Oe}$$

and, since $1\ \text{Oe} = \frac{1}{4\pi}10^{3}\frac{\text{A}}{\text{m}}$, eventually getting the same result as found before in SI

(*provided you didn't do some mistake*!):

$$H_{crit} = 0.5830\ \text{A/μm}$$

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2.1. Conclusions

- The extremal of a LC-cell free energy determines the Euler-Lagrange eq.
- Solving E-L eq. it gets the director profile
- The elastic free energy density of a homeotropic NLC cell with in-plane distortion involves splay and bend

2.2. Conclusions

- A homeotropic NLC cell undergoes an electric Frederik transition with field normal to the cell plates only if the NLC has permittivity anisotropy $\varepsilon_a < 0$
- The interaction NLC-electric field involves a free energy density **quadratic** with the field
- The threshold of Frederiks transition in a homeotropic NLC cell is determined by the **bend** elastic constant
- Always use the International System of measurement (SI)

2.3. Conclusions

•A unidirectional planar NLC cell undergoes a magnetic Frederik transition with field normal to the cell plates only if the NLC has permeability anisotropy $\mu_a > 0$

•The interaction NLC-magnetic field involves a free energy density **quadratic** with the field (like the interaction with electric field as well)

•Mark the logic symmetry between magnetic and electric field: $"\varepsilon_o \varepsilon_a = \varepsilon_o \chi_{ea}$ with $\mu_o \mu_a = \mu_o \chi_{ma}$ and E with $H"$

•The threshold of Frederiks transition in a unidirectional planar NLC cell is determined by the **splay** elastic constant

•Forget using the **G**aussian **S**ystem of measurement (GS), especially when dealing with magnetism !

2. References

1. Vladimir I. Smirnov, Автор популярного «Курса высшей математики» (т. 1—5, 1947), "*A Course in Higher Mathematics"*, vol. IV, 1969, MIR, Moscow

2. Ian W. Stewart, "*The Static and Dynamic Continuum Theory of Liquid Crystals - A mathematical introduction*", 2004, Taylor and Francis, London

3. Pierre-Gilles de Gennes, Jacques Prost, "*The Physics of Liquid Crystals*",1995, Clarendon Press, Oxford