Numerical Simulation and Tensor Representation of Liquid Crystal Director Configuration

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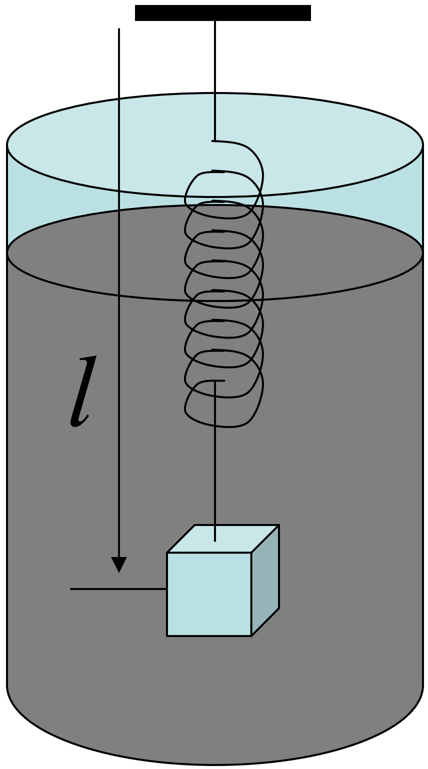
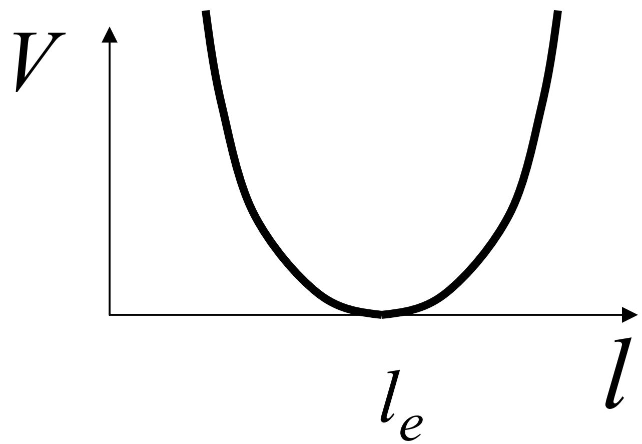
Equilibrium State



Potential

$$V = \frac{1}{2}K(l - l_o)^2 - mgl$$

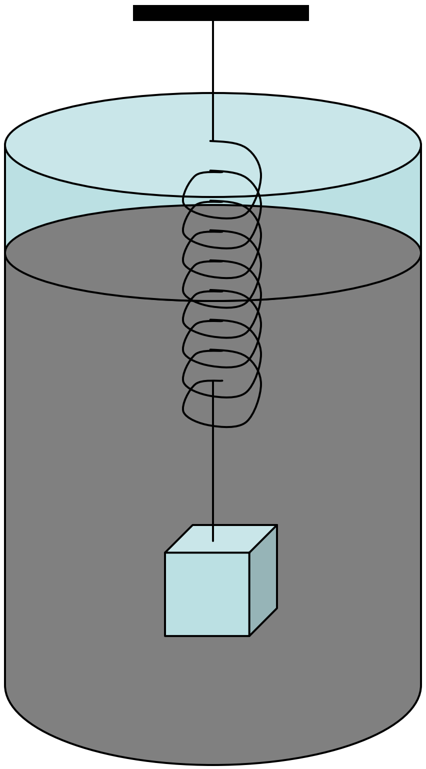


$$\frac{\partial V}{\partial l} = K(l - l_o) - mg = 0$$

$$l = l_e = l_o + \frac{mg}{K}$$

Potential energy is minimized in the equilibrium state

Equilibrium State



Force

Elastic force $-\frac{\partial V}{\partial l} = -K(l - l_o) + mg$

Viscosity $-\gamma \frac{\partial l}{\partial t}$

Dynamic Equation $m\frac{\partial^2 l}{\partial t^2} = -K(l - l_o) + mg - \gamma \frac{\partial l}{\partial t}$

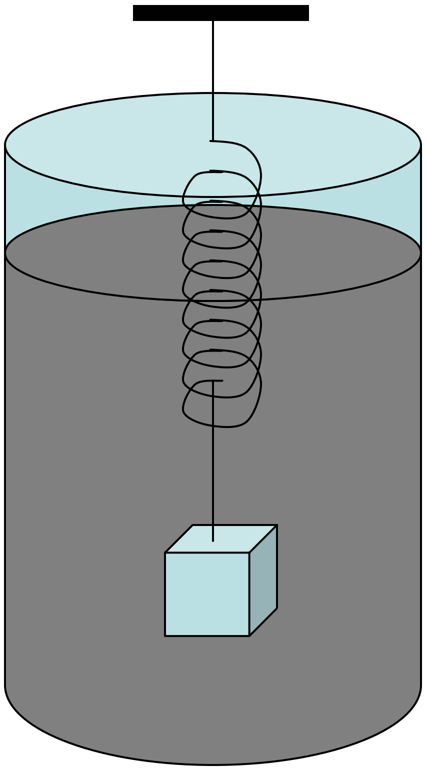
Over-damped $m\frac{\partial^2 l}{\partial t^2} = -K(l - l_o) + mg - \gamma \frac{\partial l}{\partial t} = 0$

$$\gamma \frac{\partial l}{\partial t} = -\frac{\partial V}{\partial l} = -K(l - l_o) + mg$$

In the equilibrium state $\gamma \frac{\partial l}{\partial t} = -\frac{\partial V}{\partial l} = -K(l - l_o) + mg = 0$

The force is 0 and potential energy is minimized

Equilibrium State



Numerical calculation: relaxation method

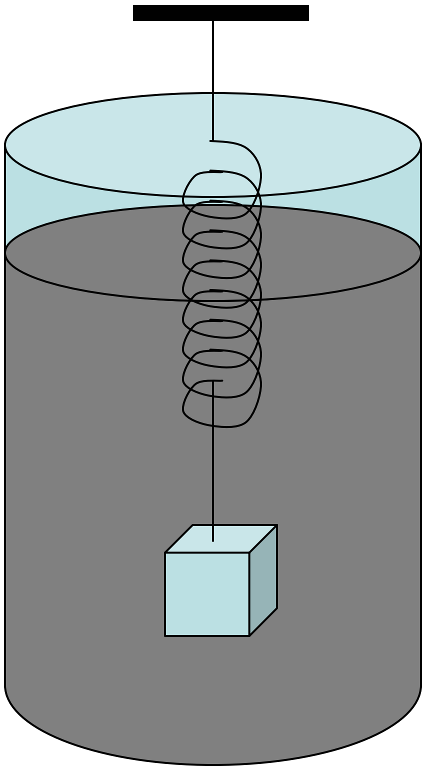
$$l_{t+\Delta t} = l_t + \left(\frac{\partial l}{\partial t}\right)_t \Delta t = l_t + \frac{\Delta t}{\gamma}\left(-\frac{\partial V}{\partial l}\right)_t$$

$$l^{\tau+1} = l^{\tau} + \frac{\Delta t}{\gamma}\left(-\frac{\partial V}{\partial l}\right)^{\tau} = l^{\tau} + \alpha\left(-\frac{\partial V}{\partial l}\right)^{\tau}$$

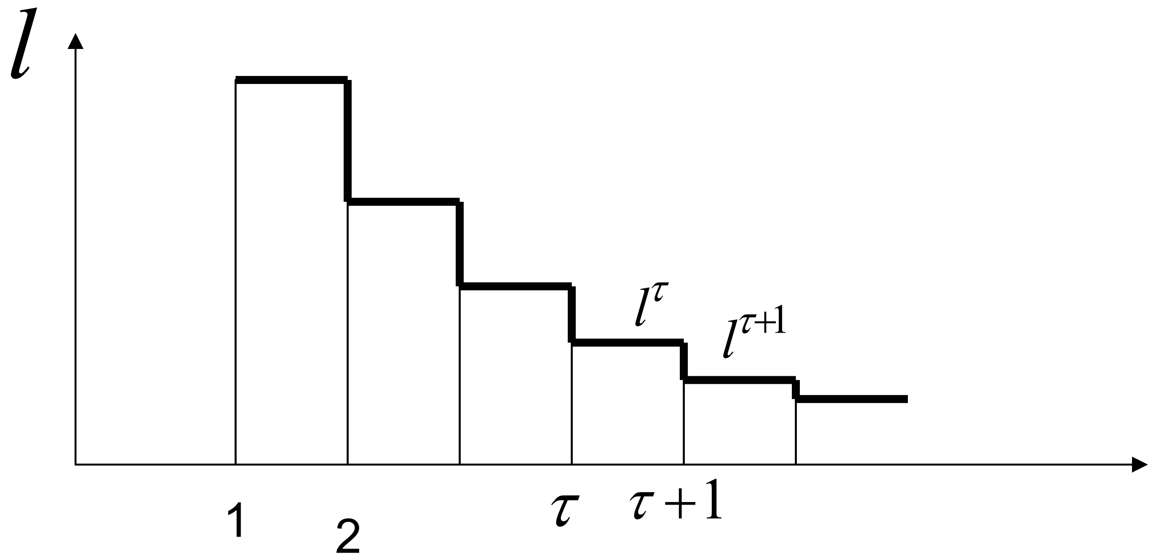
$$\Delta l^{\tau} = \alpha\left(-\frac{\partial V}{\partial l}\right)^{\tau}$$

Relaxation constant: α Iteration order: τ

Equilibrium State



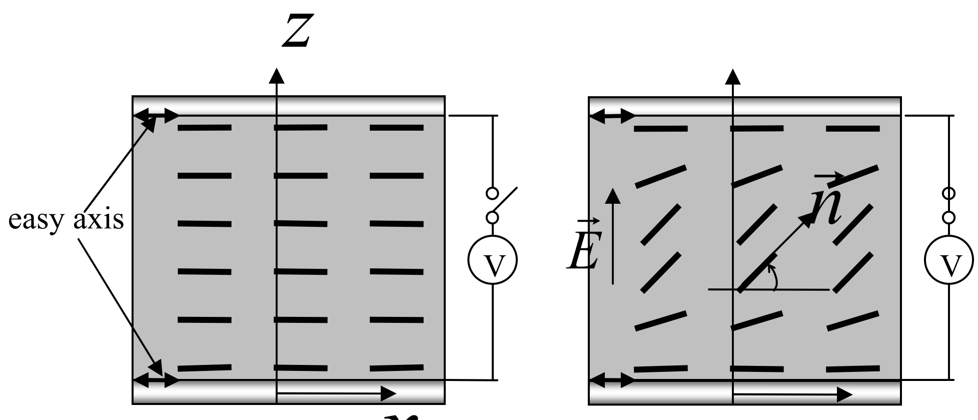
Numerical calculation



Stop the iteration when $\Delta l^{\tau} << 1$

That means $-\frac{\partial V}{\partial l} = 0$ So equilibrium state is reached

Liquid Crystal Director Configuration



LC director configuration: $\vec{n} = \vec{n}(z)$

Free energy

$$f = \frac{1}{2}K_{11}(\nabla\cdot\vec{n})^2 + \frac{1}{2}K_{22}(\vec{n}\cdot\nabla\times\vec{n} + q_o)^2 + \frac{1}{2}K_{33}(\vec{n}\times\nabla\times\vec{n})^2 - \frac{1}{2}\varepsilon_o\Delta\varepsilon(\vec{E}\cdot\vec{n}) = f(\vec{n},\vec{n}',z)$$

In the equilibrium state, the free energy is minimized

$$\frac{\delta f}{\delta\vec{n}} = \frac{\partial f}{\partial\vec{n}} - \frac{d}{dz}\left(\frac{\partial f}{\partial\vec{n}'}\right) = 0$$

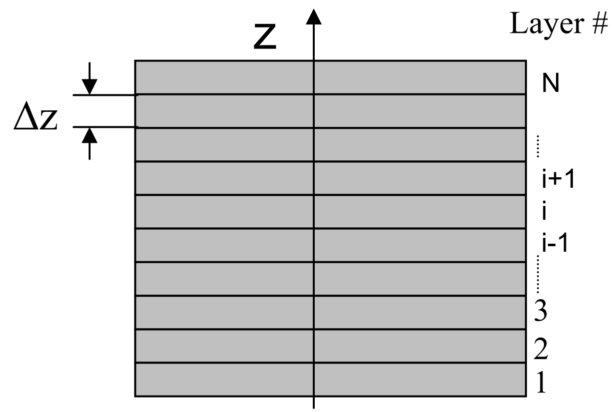
Liquid Crystal Director Configuration

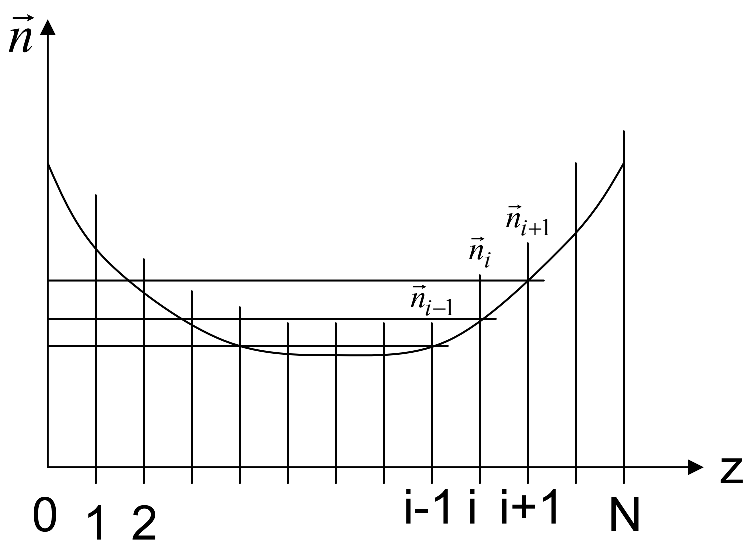
Numerical simulation

$$n_i(z)^{\tau+1} = n_i(z)^{\tau} + \Delta n_i(z)^{\tau} = n_i(z)^{\tau} + \alpha\left(-\frac{\delta f}{\delta n_i}\right)^{\tau}$$

!-D case

Divide the LC cell into N layers





Liquid Crystal Director Configuration

Derivatives

$$\frac{\partial \vec{n}}{\partial z}(i) = \frac{\vec{n}(i+1) - \vec{n}(i-1)}{2\Delta z}$$

$$\frac{\partial^2 \vec{n}}{\partial z^2}(i) = \frac{\vec{n}'(i+1) - \vec{n}'(i)}{\Delta z} = \frac{[\vec{n}(i+1) - \vec{n}(i)]/\Delta z - [\vec{n}(i) - \vec{n}(i-1)]/\Delta z}{\Delta z} = \frac{\vec{n}(i+1) + \vec{n}(i-1) - 2\vec{n}(i)}{(\Delta z)^2}$$

Change

$$\Delta \vec{n}^{\tau}(i) = \alpha (\Delta z)^2 \left(-\frac{\delta f}{\delta \vec{n}} \right)^{\tau} (i)$$

Renormalization

Because $|\vec{n}| = 1$

$$\vec{n}^{\tau+1}(i) = \frac{\vec{n}^{\tau}(i) + \Delta \vec{n}^{\tau}(i)}{\left| \vec{n}^{\tau}(i) + \Delta \vec{n}^{\tau}(i) \right|}$$

Liquid Crystal Director Configuration

Updating

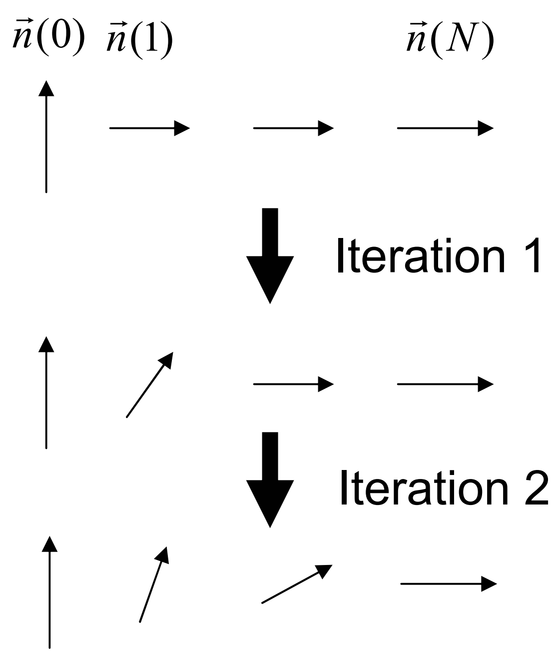
Relaxation method

Loop for calculate change

```
For i=0 to N
    calculate the derivative
    calculate Δn⃗
End loop
```

Loop for update

```
For i=0 to N
    update n⃗
End loop
```



- Slow relaxation
- Longer computation time
- correct dynamics

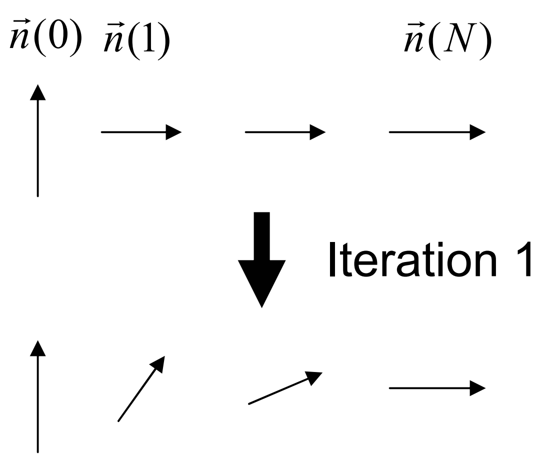
Liquid Crystal Director Configuration

Updating

Over relaxation method

Loop for calculate change and update

For i=0 to N
calculate the derivative
calculate $\Delta\vec{n}$
update $\vec{n}$
End loop



- Fast relaxation
- shorter computation time
- wrong dynamics

Vector Representation

LC director

$$\vec{n} = n_i \hat{x}_i$$

$$\hat{x}_1 = \hat{x},\ \hat{x}_2 = \hat{y},\ \hat{x}_3 = \hat{z}$$

Divergence $\nabla \cdot \vec{n} = \dfrac{\partial n_i}{\partial x_i}$ $\qquad (\nabla \cdot \vec{n})^2 = \dfrac{\partial n_i}{\partial x_i} \cdot \dfrac{\partial n_j}{\partial x_j}$

convention of summing over repeating indices

Example $n_i n_i = n_1 n_1 + n_2 n_2 + n_3 n_3 = \vec{n}^2 = 1$

Vector Representation

Curl $\nabla \times \vec{n} = e_{ijk} \frac{\partial n_k}{\partial x_j} \hat{x}_i$

e_{ijk} is the Levi-Civita symbol $e_{xyz} = e_{yzx} = e_{zxy} = -e_{xzy} = -e_{zyx} = -e_{yxz} = 1$

and all other $e_{ijk} = 0$

$$\vec{n} \cdot \nabla \times \vec{n} = e_{ijk} n_i \frac{\partial n_k}{\partial x_j}$$

$$(\nabla \times \vec{n})^2 = \left(e_{ijk} \frac{\partial n_k}{\partial x_j} \right)\left(e_{iuv} \frac{\partial n_v}{\partial x_u} \right) = (\delta_{ju}\delta_{kv} - \delta_{jv}\delta_{ku})\left(\frac{\partial n_k}{\partial x_j} \right)\left(\frac{\partial n_v}{\partial x_u} \right) = \frac{\partial n_k}{\partial x_j}\frac{\partial n_k}{\partial x_j} - \frac{\partial n_k}{\partial x_j}\frac{\partial n_j}{\partial x_k}$$

$$\vec{n} \times \nabla \times \vec{n} = e_{lmi} (\vec{n})_m (\nabla \times \vec{n})_i \hat{x}_l = e_{lmi} (n_m) \left(e_{ijk} \frac{\partial n_k}{\partial x_j} \right) \hat{x}_l = (\delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}) \left(n_m \frac{\partial n_k}{\partial x_j} \right) \hat{x}_l$$

$$= \left(n_k \frac{\partial n_k}{\partial x_l} - n_j \frac{\partial n_l}{\partial x_j} \right) \hat{x}_l = 0 - n_j \frac{\partial n_l}{\partial x_j} \hat{x}_l$$

$$(\vec{n} \times \nabla \times \vec{n})^2 = \left(-n_k \frac{\partial n_l}{\partial x_k} \right)\left(-n_j \frac{\partial n_l}{\partial x_j} \right) = n_k n_j \frac{\partial n_l}{\partial x_k}\frac{\partial n_l}{\partial x_j}$$

$$(\vec{n} \cdot \nabla \times \vec{n})^2 = (\nabla \times \vec{n})^2 - (\vec{n} \times \nabla \times \vec{n})^2 = \left(\frac{\partial n_k}{\partial x_j}\frac{\partial n_k}{\partial x_j} - \frac{\partial n_k}{\partial x_j}\frac{\partial n_j}{\partial x_k} \right) - n_k n_j \frac{\partial n_l}{\partial x_k}\frac{\partial n_l}{\partial x_j}$$

Vector Representation

Electric energy

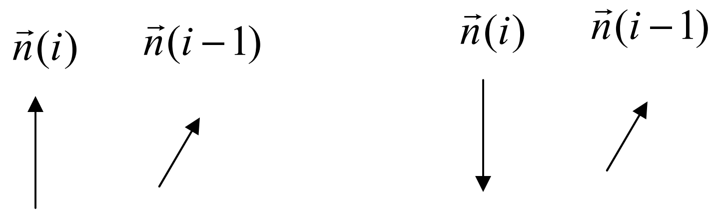
$$-\frac{1}{2}\vec{E}\cdot\vec{D}=-\frac{1}{2}\vec{E}\cdot(\vec{\varepsilon}\cdot\vec{E})=-\frac{1}{2}\vec{E}\cdot[\varepsilon_o\varepsilon_\perp\vec{E}+\varepsilon_o\Delta\varepsilon(\vec{E}\cdot\vec{n})\vec{n}]=-\frac{1}{2}\varepsilon_o\varepsilon_\perp E^2-\frac{1}{2}\varepsilon_o\Delta\varepsilon E_i E_j n_i n_j$$

Free energy

$$f=\frac{1}{2}K_{11}\frac{\partial n_i}{\partial x_i}\cdot\frac{\partial n_j}{\partial x_j}+\frac{1}{2}K_{22}\left(\frac{\partial n_j}{\partial x_i}\frac{\partial n_j}{\partial x_i}-\frac{\partial n_i}{\partial x_j}\frac{\partial n_j}{\partial x_i}\right)+\frac{1}{2}(K_{33}-K_{22})n_i n_j\frac{\partial n_k}{\partial x_i}\frac{\partial n_k}{\partial x_j}+q_o K_{22}e_{ijk}n_i\frac{\partial n_k}{\partial x_j}-\frac{1}{2}\varepsilon_o\Delta\varepsilon E_i E_j n_i n_j$$

Liquid Crystal Director Configuration

Problem with vector representation



Physically Same

Derivatives different

Tensor Representation

$$\overleftrightarrow{Q} = \vec{n}\vec{n} - \frac{1}{3}\overleftrightarrow{I} \tag{1}$$

In component $$Q_{ij} = n_i n_j - \frac{1}{3}\delta_{ij} \tag{2}$$

where δ_{ij} is the Kronecker delta

Express the free energy in terms of the tensor and its derivatives

convention of summing over repeating indices

$$n_i n_i = n_1 n_1 + n_2 n_2 + n_3 n_3 = \vec{n}^2 = 1$$

Index contraction

$$G_1 = Q_{jk,l} Q_{jk,l} = \frac{\partial Q_{jk}}{\partial x_l}\frac{\partial Q_{jk}}{\partial x_l}$$ Scalar

Derivative

$$
\begin{aligned}
G_1 = Q_{jk,l}Q_{jk,l} &= \frac{\partial Q_{jk}}{\partial x_l}\frac{\partial Q_{jk}}{\partial x_l} = \frac{\partial (n_j n_k)}{\partial x_l}\frac{\partial (n_j n_k)}{\partial x_l} \\
&= \left(n_k \frac{\partial n_j}{\partial x_l} + n_l \frac{\partial n_k}{\partial x_l} \right)\left(n_k \frac{\partial n_j}{\partial x_l} + n_l \frac{\partial n_k}{\partial x_l} \right) \\
&= n_k n_k \frac{\partial n_j}{\partial x_l}\frac{\partial n_j}{\partial x_l} + n_j n_k \frac{\partial n_k}{\partial x_l}\frac{\partial n_j}{\partial x_l} + n_k n_j \frac{\partial n_j}{\partial x_l}\frac{\partial n_k}{\partial x_l} + n_j n_j \frac{\partial n_k}{\partial x_l}\frac{\partial n_k}{\partial x_l} \\
&= 1 \cdot \frac{\partial n_j}{\partial x_l}\frac{\partial n_j}{\partial x_l} + \frac{1}{4}\frac{\partial n_k^2}{\partial x_l}\frac{\partial n_j^2}{\partial x_l} + \frac{1}{4}\frac{\partial n_j^2}{\partial x_l}\frac{\partial n_k^2}{\partial x_l} + 1 \cdot \frac{\partial n_k}{\partial x_l}\frac{\partial n_k}{\partial x_l} \\
&= 1 \cdot \frac{\partial n_j}{\partial x_l}\frac{\partial n_j}{\partial x_l} + \frac{1}{4}\cdot 0 + \frac{1}{4}\cdot 0 + 1 \cdot \frac{\partial n_k}{\partial x_l}\frac{\partial n_k}{\partial x_l} \\
&= 2\frac{\partial n_j}{\partial x_l}\frac{\partial n_j}{\partial x_l} \qquad (3)
\end{aligned}
$$

$$
G_1 = 2[(\nabla \cdot \vec{n})^2 + (\nabla \times \vec{n})^2 - \nabla \cdot (\vec{n}\nabla \cdot \vec{n} + \vec{n} \times \nabla \times \vec{n})] =
$$

$$
= 2[(\nabla \cdot \vec{n})^2 + (\vec{n} \cdot \nabla \times \vec{n})^2 + (\vec{n} \times \nabla \times \vec{n})^2 - \nabla \cdot (\vec{n}\nabla \cdot \vec{n} + \vec{n} \times \nabla \times \vec{n})]
$$

Derivative

$$
\begin{aligned}
G_2 &= Q_{jk,k} Q_{jl,l} = \frac{\partial Q_{jk}}{\partial x_k}\frac{\partial Q_{jl}}{\partial x_l} = \frac{\partial (n_j n_k)}{\partial x_k}\frac{\partial (n_j n_l)}{\partial x_l} \\
&= \left(n_j \frac{\partial n_k}{\partial x_k} + n_k \frac{\partial n_j}{\partial x_k} \right)\left(n_j \frac{\partial n_l}{\partial x_l} + n_l \frac{\partial n_j}{\partial x_l} \right) \\
&= n_j n_j \frac{\partial n_k}{\partial x_k}\frac{\partial n_l}{\partial x_l} + n_j n_l \frac{\partial n_k}{\partial x_k}\frac{\partial n_j}{\partial x_l} + n_k n_j \frac{\partial n_j}{\partial x_k}\frac{\partial n_l}{\partial x_l} + n_k n_l \frac{\partial n_j}{\partial x_k}\frac{\partial n_j}{\partial x_l} \\
&= 1 \cdot \frac{\partial n_k}{\partial x_k}\frac{\partial n_l}{\partial x_l} + \frac{1}{2} n_l \frac{\partial n_k}{\partial x_k}\frac{\partial n_j^2}{\partial x_k} + \frac{1}{2} n_k \frac{\partial n_j^2}{\partial x_k}\frac{\partial n_l}{\partial x_l} + n_k n_l \frac{\partial n_j}{\partial x_k}\frac{\partial n_j}{\partial x_l} \\
&= 1 \cdot \frac{\partial n_k}{\partial x_k}\frac{\partial n_l}{\partial x_l} + \frac{1}{2} n_l \frac{\partial n_k}{\partial x_k} \cdot 0 + \frac{1}{2} n_k \, 0 \cdot \frac{\partial n_l}{\partial x_l} + n_k n_l \frac{\partial n_j}{\partial x_k}\frac{\partial n_j}{\partial x_l} \\
&= \frac{\partial n_k}{\partial x_k}\frac{\partial n_l}{\partial x_l} + n_k n_l \frac{\partial n_j}{\partial x_k}\frac{\partial n_j}{\partial x_l} \\
&= (\nabla \cdot \vec{n})^2 + (\vec{n} \times \nabla \times \vec{n})^2
\end{aligned}
\tag{3}
$$

Derivative

$$
\begin{aligned}
G_4 &= e_{jkl} Q_{jm} Q_{km,l} = e_{jkl} Q_{jm} \frac{\partial Q_{km}}{\partial x_l} = e_{jkl} (n_j n_m - \frac{1}{3}\delta_{jm}) \frac{\partial (n_k n_m)}{\partial x_l} \\
&= e_{jkl} \left(n_j n_m n_k \frac{\partial n_m}{\partial x_l} + n_j n_m n_m \frac{\partial n_k}{\partial x_l} \right) - \frac{1}{3} e_{jkl} \frac{\partial (n_k n_j)}{\partial x_l} \\
&= e_{jkl} \left(\frac{1}{2} n_j n_k \frac{\partial n_m^2}{\partial x_l} + n_j \cdot 1 \cdot \frac{\partial n_k}{\partial x_l} \right) - \frac{1}{3} e_{jkl} \frac{1}{2} \left[\frac{\partial (n_k n_j)}{\partial x_l} + \frac{\partial (n_j n_k)}{\partial x_l} \right] \\
&= e_{jkl} n_j \frac{\partial n_k}{\partial x_l} - \frac{1}{6} e_{jkl} \frac{\partial (n_k n_j)}{\partial x_l} - \frac{1}{6} e_{jkl} \frac{\partial (n_j n_k)}{\partial x_l} \\
&= e_{jkl} n_j \frac{\partial n_k}{\partial x_l} - \frac{1}{6} e_{jkl} \frac{\partial (n_k n_j)}{\partial x_l} + \frac{1}{6} e_{kjl} \frac{\partial (n_j n_k)}{\partial x_l} \qquad (3) \\
&= e_{jkl} n_j \frac{\partial n_k}{\partial x_l} \\
&= -\vec{n} \cdot \nabla \times \vec{n}
\end{aligned}
$$

Derivative

$$
\begin{aligned}
G_6 &= Q_{jk}Q_{lm,j}Q_{lm,k} = Q_{jk}\frac{\partial Q_{lm}}{\partial x_j}\frac{\partial Q_{lm}}{\partial x_k} = (n_j n_k - \frac{1}{3}\delta_{jk})\frac{\partial(n_l n_m)}{\partial x_j}\frac{\partial(n_l n_m)}{\partial x_k} = \\
&= n_j n_k \frac{\partial(n_l n_m)}{\partial x_j}\frac{\partial(n_l n_m)}{\partial x_k} - \frac{1}{3}\frac{\partial(n_l n_m)}{\partial x_j}\frac{\partial(n_l n_m)}{\partial x_j} \\
&= n_j n_k \left(n_m \frac{\partial n_l}{\partial x_j} + n_l \frac{\partial n_m}{\partial x_j} \right)\left(n_m \frac{\partial n_l}{\partial x_k} + n_l \frac{\partial n_m}{\partial x_k} \right) - \frac{1}{3}G_1 \\
&= n_j n_k \left(n_m^2 \frac{\partial n_l}{\partial x_j}\frac{\partial n_l}{\partial x_k} + n_l n_m \frac{\partial n_m}{\partial x_j}\frac{\partial n_l}{\partial x_k} + n_m n_l \frac{\partial n_l}{\partial x_j}\frac{\partial n_m}{\partial x_k} + n_l^2 \frac{\partial n_m}{\partial x_j}\frac{\partial n_m}{\partial x_k} \right) - \frac{1}{3}G_1 \\
&= n_j n_k \left(1 \cdot \frac{\partial n_l}{\partial x_j}\frac{\partial n_l}{\partial x_k} + 0 + 0 + 1 \cdot \frac{\partial n_m}{\partial x_j}\frac{\partial n_m}{\partial x_k} \right) - \frac{1}{3}G_1 \\
&= 2 n_j n_k \frac{\partial n_m}{\partial x_j}\frac{\partial n_m}{\partial x_k} - \frac{1}{3}G_1 \\
&= 2(\vec{n} \times \nabla \times \vec{n})^2 - \frac{1}{3}G_1
\end{aligned}
\qquad (3)
$$

Free energy

$$f = \frac{1}{12}(-K_{11} + 3K_{22} + K_{33})G_1 + \frac{1}{2}(K_{11} - K_{22})G_2 + \frac{1}{4}(-K_{11} + K_{33})G_6 - q_o K_{22} G_4 + \frac{1}{2} K_{22} \nabla \cdot (\vec{n}\nabla \cdot \vec{n} + \vec{n} \times \nabla \times \vec{n})$$
$$- \frac{1}{2}\varepsilon_o \Delta\varepsilon E_i E_j n_i n_j$$

Variation of free energy with respect to n_i

$$\frac{\delta f}{\delta n_i} = \frac{\delta f}{\delta Q_{jk}} \frac{\partial Q_{jk}}{\partial n_i} = \frac{\delta f}{\delta Q_{jk}} \frac{\partial (n_j n_k)}{\partial n_i} = \frac{\delta f}{\delta Q_{jk}} (n_j \delta_{ik} + n_k \delta_{ij}) = 2n_j \frac{\delta f}{\delta Q_{ji}}$$

Variation of Free energy

$$H_{1i} = \frac{\delta G_1}{\delta n_i} = 2n_j \left[\frac{\partial G_1}{\partial Q_{ji}} - \frac{\partial}{\partial x_l}\left(\frac{\partial G_1}{\partial Q_{ji,l}} \right) \right] = -2n_j \frac{\partial}{\partial x_l}\left[\frac{\partial (Q_{uv,w} Q_{uv,w}}{\partial Q_{ji,l}} \right] = -2n_j \frac{\partial (2Q_{uv,w}\delta_{ju}\delta_{iv}\delta_{lw})}{\partial x_l} = -4n_j \frac{\partial^2 Q_{ji}}{\partial x_l \partial x_l}$$

$$H_{2i} = \frac{\delta G_2}{\delta n_i} = -2n_j \left(\frac{\partial^2 Q_{jl}}{\partial x_i \partial x_l} + \frac{\partial^2 Q_{il}}{\partial x_j \partial x_l} \right)$$

$$H_{4i} = \frac{\delta G_4}{\delta n_i} = -2n_j \left(e_{jkl} \frac{\partial Q_{li}}{\partial x_k} + e_{ikl} \frac{\partial Q_{lj}}{\partial x_k} \right)$$

$$H_{6i} = \frac{\delta G_6}{\delta n_i} = -2n_j \left(2 \frac{\partial Q_{kl}}{\partial x_k} \frac{\partial Q_{ji}}{\partial x_l} + 2Q_{kl} \frac{\partial^2 Q_{ji}}{\partial x_l \partial x_k} - \frac{\partial Q_{kl}}{\partial x_i} \frac{\partial Q_{kl}}{\partial x_j} \right)$$

$$\Delta n_i^{\tau+1} = \alpha (\Delta x)^2 [-\frac{1}{12}(-K_{11} + 3K_{22} + K_{33}) H_{1i}^{\tau} - \frac{1}{2}(K_{11} - K_{22}) H_{2i}^{\tau}$$
$$-\frac{1}{4}(-K_{11} + K_{33}) H_{6i}^{\tau} + K_{22} q_o H_{4i}^{\tau} + \Delta\varepsilon\varepsilon_o (E_i E_j n_j)]$$

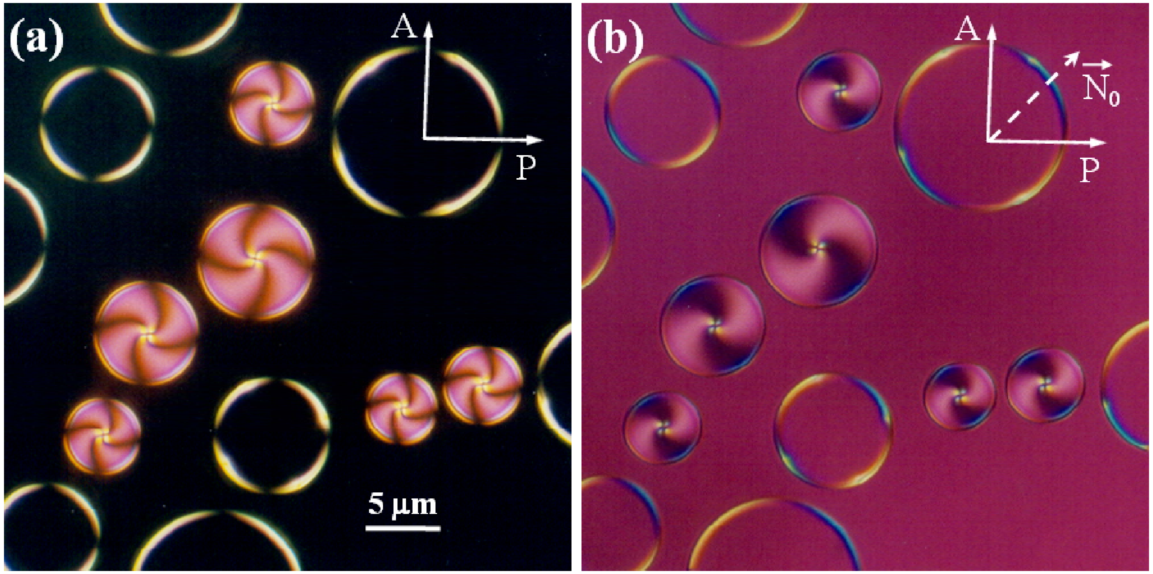
How to calculate derivatives numerically

$$\frac{\partial Q}{\partial x}(i,j,k) = \frac{Q(i+1,j,k) - Q(i-1,j,k)}{2\Delta x}$$

$$\frac{\partial^2 Q}{\partial x^2}(i,j,k) = \frac{Q_x^{'}(i+1,j,k) - Q_x^{'}(i,j,k)}{\Delta x} = \frac{Q(i+1,j,k) + Q(i-1,j,k) - 2Q(i,j,k)}{(\Delta x)^2}$$

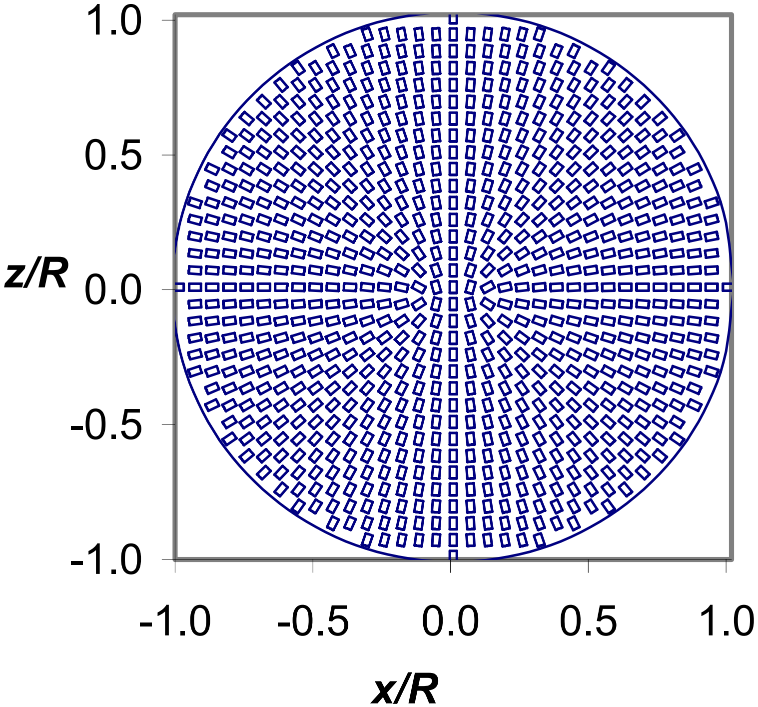
$$\frac{\partial^2 Q}{\partial x \partial z}(i,j,k) = \frac{Q_x^{'}(i,j,k+1) - Q_x^{'}(i,j,k-1)}{2\Delta z} = \frac{Q(i+1,j,k+1) + Q(i-1,j,k-1) - Q(i+1,j,k-1) - Q(i-1,j,k+1)}{4\Delta x \Delta z}$$

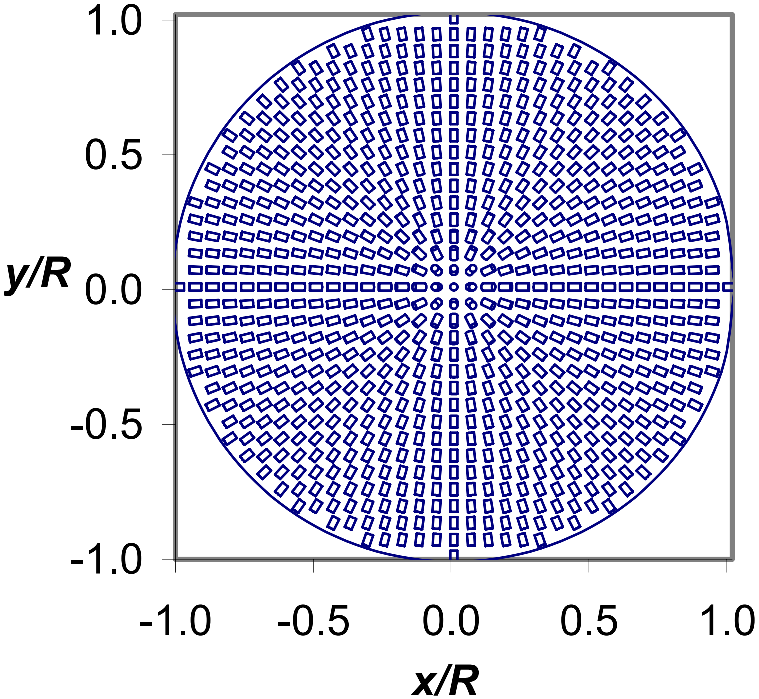
Liquid Crystal Droplet



Liquid Crystal Droplet

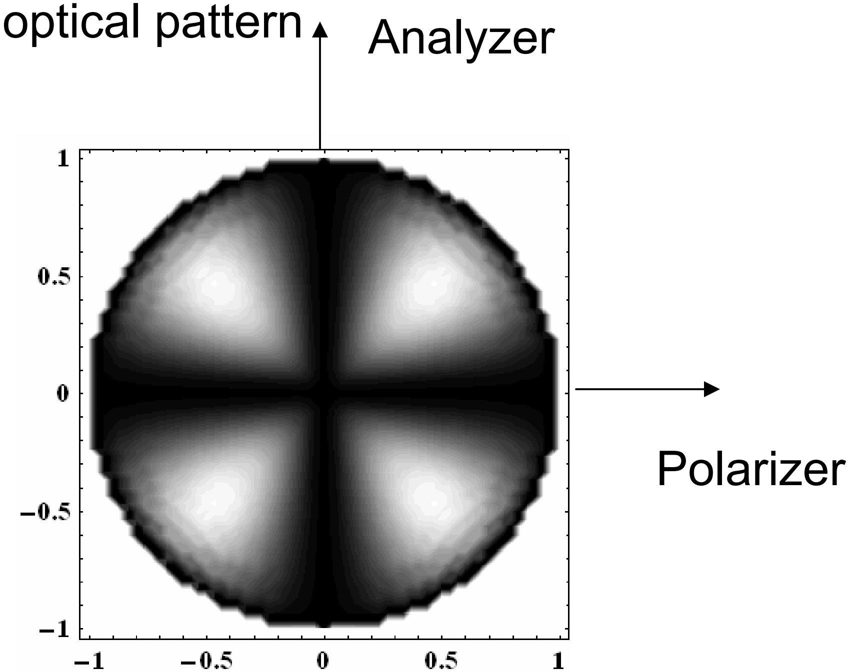
Radial droplet, LC director





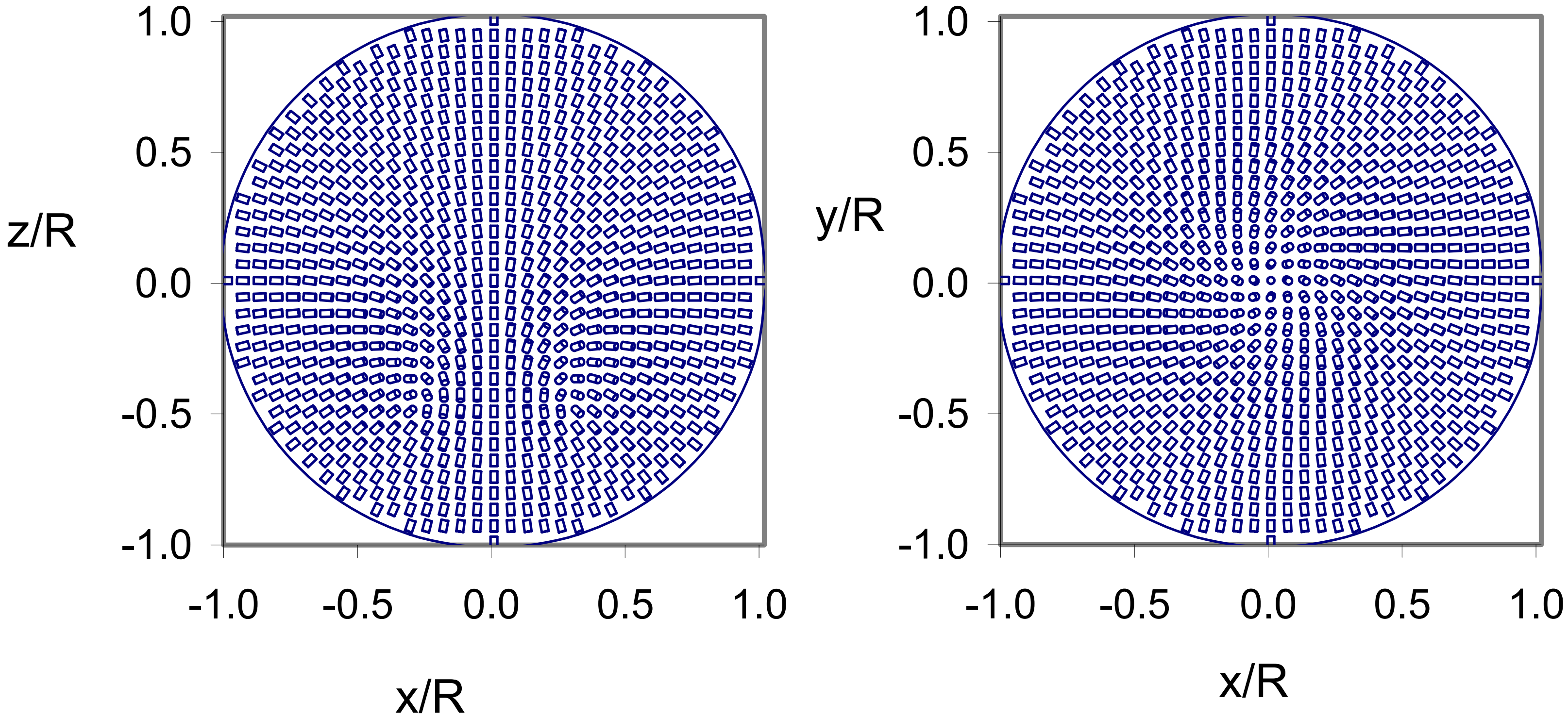
Liquid Crystal Droplet

Radial droplet, optical pattern



Liquid Crystal Droplet

Propeller droplet, LC director



Liquid Crystal Droplet

Propeller droplet, optical pattern