Defects on Nematic Shells

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Summary

Nematic Shells

A ***thin*** film of nematic liquid crystal deposited on a ***colloidal*** particle is a ***nematic shell***, which is treated here as a ***two-dimensional*** order texture.

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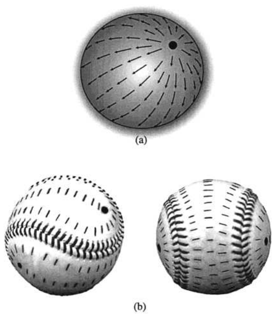
Defects in the order texture are potential ***hot spots*** where ligands may adhere bridging one particle to another in a ***metamaterial*** structure. Nelson (2002)

tetravalent tennis balls



Mathematical Model

Molecules are envisaged as ***ribbons*** lying flat on a closed surface $\mathscr{S}$ and freely gliding on it.

planar degenerate anchoring

This picture is perhaps too naive: a degenerate planar anchoring ***diluted*** in a thin layer is a more realistic microscopic picture.

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$\boldsymbol{\ell}$ molecular director
$\mathscr{S}$ closed orientable surface
$\boldsymbol{\nu}$ outer unit normal

$$\boldsymbol{\ell}\cdot\boldsymbol{\nu}\equiv 0$$

order tensor

$$\mathbf{Q} := \left\langle \boldsymbol{\ell}\otimes\boldsymbol{\ell} - \tfrac{1}{2}\mathbf{P}\right\rangle$$
$$\mathbf{P} := \mathbf{I} - \boldsymbol{\nu}\otimes\boldsymbol{\nu}$$

$\langle\cdot\rangle$ ensemble average

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$\mathbf{Q}$ is a fully biaxial tensor

$$\mathbf{Q} = \lambda(\boldsymbol{n}\otimes\boldsymbol{n} - \boldsymbol{n}_\perp\otimes\boldsymbol{n}_\perp) \qquad \boldsymbol{n}_\perp := \boldsymbol{\nu}\times\boldsymbol{n}$$

Defects occur whenever $\lambda = 0$ and so $\mathbf{Q} = \mathbf{0}$

order bounds

$$0 \leq \lambda \leq \tfrac{1}{2}$$

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q-representation

$$\mathbf{Q} = q_1(\boldsymbol{e}\otimes\boldsymbol{e} - \boldsymbol{e}_\perp\otimes\boldsymbol{e}_\perp) + q_2(\boldsymbol{e}\otimes\boldsymbol{e}_\perp + \boldsymbol{e}_\perp\otimes\boldsymbol{e})$$

$\boldsymbol{e}$, $\boldsymbol{e}_\perp$ tangent unit vector fields

$$\boldsymbol{e}_\perp := \boldsymbol{\nu}\times\boldsymbol{e} \qquad \boldsymbol{e}\cdot\boldsymbol{\nu}\equiv 0$$

$$\boldsymbol{n} = \cos\varphi\boldsymbol{e} + \sin\varphi\boldsymbol{e}_\perp$$

$$\boldsymbol{n}_\perp = -\sin\varphi\boldsymbol{e} + \cos\varphi\boldsymbol{e}_\perp$$

$$\cos 2\varphi = \frac{q_1}{\sqrt{q_1^2+q_2^2}} \qquad \sin 2\varphi = \frac{q_2}{\sqrt{q_1^2+q_2^2}}$$

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Levi-Civita Parallel Transport

For ***planar*** director fields, the ***topological charge*** of a defect is directly related to the ***winding number***.

For ***non-flat*** fields, an intrinsic distortion is due to the curvature of the underling surface.

Along a curve $\mathscr{C}$ on $\mathscr{S}$

$$\boldsymbol{\nu}' = \boldsymbol{\Omega}_\parallel \times \boldsymbol{\nu}$$

$$\boldsymbol{\Omega}_\parallel = \boldsymbol{\nu}\times(\nabla_s\boldsymbol{\nu})\boldsymbol{t}$$

$'$ arc-length derivative

$\nabla_s\boldsymbol{\nu}$ surface gradient of $\boldsymbol{\nu}$

$\boldsymbol{t}$ unit tangent to $\mathscr{C}$

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principal curvatures

$$\nabla_s\boldsymbol{\nu} = \sigma_1\boldsymbol{e}_1\otimes\boldsymbol{e}_1 + \sigma_2\boldsymbol{e}_2\otimes\boldsymbol{e}_2$$

$H := \frac{1}{2}(\sigma_1+\sigma_2)$ mean curvature

$K := \sigma_1\sigma_2$ Gaussian curvature

intrinsic distortion

Transporting a tangent unit vector $\boldsymbol{u}$

$$\boldsymbol{u}' = \boldsymbol{\Omega}_\parallel\times\boldsymbol{u}$$

$$\Delta\vartheta_{\mathscr{C}} = \int_{\mathscr{S}_{\mathscr{C}}} K da$$

$\mathscr{S}_{\mathscr{C}}$ surface on $\mathscr{S}$ enclosed by $\mathscr{C}$

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topological charge

$$\boldsymbol{n}' = \boldsymbol{\Omega}\times\boldsymbol{n}$$

$$\boldsymbol{\Omega} = \Omega_\nu\boldsymbol{\nu} + \boldsymbol{\Omega}_\parallel$$

$$\Omega_\nu := \boldsymbol{n}'\cdot\boldsymbol{n}_\perp \qquad \boldsymbol{n}_\perp := \boldsymbol{\nu}\times\boldsymbol{n}$$

For the field $\boldsymbol{n}$

$$2\pi m_{\boldsymbol{n}} = \oint_{\mathscr{C}} \boldsymbol{n}'\cdot\boldsymbol{n}_\perp ds + \int_{\mathscr{S}_{\mathscr{C}}} K da \qquad \forall\mathscr{C}$$

$2m_{\boldsymbol{n}}\in\mathbb{Z}$ $\quad$ $\boldsymbol{n}$ and $-\boldsymbol{n}$ give the same $\mathbf{Q}$

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$$2\pi m_{\boldsymbol{n}} = \oint_{\mathscr{C}} \boldsymbol{n}' \cdot \boldsymbol{n}_\perp ds + \int_{\mathscr{S}_{\mathscr{C}}} K da$$

For another tangent unit vector field $\boldsymbol{e}$

$$2\pi m_{\boldsymbol{e}} = \oint_{\mathscr{C}} \boldsymbol{e}' \cdot \boldsymbol{e}_\perp ds + \int_{\mathscr{S}_{\mathscr{C}}} K da$$

In the q-representation

$$\mathbf{Q} = q_1(\boldsymbol{e} \otimes \boldsymbol{e} - \boldsymbol{e}_\perp \otimes \boldsymbol{e}_\perp) + q_2(\boldsymbol{e} \otimes \boldsymbol{e}_\perp + \boldsymbol{e}_\perp \otimes \boldsymbol{e})$$

$$m_{\boldsymbol{n}} = m_{\boldsymbol{e}} + \frac{1}{4\pi} \oint_{\mathscr{C}} \frac{q_1 q_2' - q_1' q_2}{q_1^2 + q_2^2} ds$$

$$m_{\boldsymbol{n}} = m_{\boldsymbol{e}} + \frac{1}{2\pi} \oint_{\mathscr{C}} \varphi' ds$$

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It is easily shown that the topological charge is ***additive*** in the contour enclosure.

total charge

If $\mathscr{S}$ splits into the union of N patches, each containing a defect of $\boldsymbol{n}$

$$2\pi m_i = \oint_{\mathscr{C}_i} \boldsymbol{n}' \cdot \boldsymbol{n}_\perp ds + \int_{\mathscr{S}_i} K da \qquad \mathscr{S} = \bigcup_{i=1}^{N} \mathscr{S}_i$$

$$2\pi \sum_{i=1}^{N} m_i = \int_{\mathscr{S}} K da$$

Euler characteristics

$$\int_{\mathscr{S}} K da = 2\pi\chi(\mathscr{S}) = 2(1 - g(\mathscr{S}))$$

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$$\chi(\mathscr{S}) = F - E + V$$

F number of faces

E number of edges — of ***any*** tessellation of $\mathscr{S}$

V number of vertices

$g(\mathscr{S})$ number of ***handles***

$\mathscr{S}$	g	χ
sphere	0	2
torus	1	0

Poincaré Theorem $\sum_{i=1}^{N} m_i = \chi(\mathscr{S})$

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Surface Nematic Elasticity

The measure of surface ***order distortion*** is $\nabla_s \mathbf{Q}$

$$\iota_i := Q_{ij;k} Q_{ij;k} = |\nabla_s \mathbf{Q}|^2$$

$$\iota_2 := Q_{ij;k} Q_{ik;j}$$

$$\iota_3 := Q_{ij;j} Q_{ik;k} = (\operatorname{div}_s \mathbf{Q})^2$$

$;$ surface derivative

null-Langrangian ?

$$\int_{\mathscr{S}} (\iota_2 - \iota_3) da = -\int_{\mathscr{S}} K (\operatorname{tr} \mathbf{Q}^2) da$$

elastic free-energy density

$$f_e := c_1\iota_1 + c_2\iota_2 + c_{24}(\iota_2 - \iota_3)$$
$$= \frac{1}{2}(k_1 + k_3)Q_{ij;k}Q_{ij;k} + \frac{1}{2}(k_1 - k_3)Q_{ij;k}Q_{ik;j} - \frac{1}{2}k_{24}K\,\mathrm{tr}\,\mathbf{Q}^2$$
$$k_1 = c_1 + c_2 \qquad k_3 = c_1 - c_2 \qquad k_{24} = c_{24}$$

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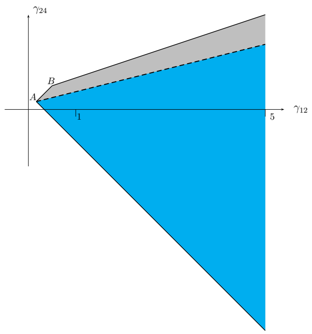
Ericksen's inequalities

f_e is ***positive definite*** in the admissible region



$$\gamma_{12} = \frac{2c_1 + c_2}{2c_1 - c_2 - c_{24}}$$
$$\gamma_{24} = \frac{c_{24}}{2c_1 - c_2 - c_{24}}$$

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one-constant approximation

$$k_1 = k_3 = \tfrac{1}{2}k$$

$$f_e = \frac{1}{2}\left(k|\nabla_{\mathrm{s}}\mathbf{Q}|^2 - k_{24}K(\mathrm{tr}\,\mathbf{Q}^2)\right)$$
$$-1 \le \frac{k_{24}}{k} \le 1$$

internal potential

$$f_p(\mathbf{Q}) = \frac{A}{2}\,\mathrm{tr}\,\mathbf{Q}^2 + \frac{C}{4}(\mathrm{tr}\,\mathbf{Q}^2)^2$$
$$A = A_0\frac{T - T_{\mathrm{c}}}{T_{\mathrm{c}}} \qquad A_0 > 0$$

T temperature

T_{c} critical temperature

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condensation order

$$\lambda_c = \sqrt{\frac{A_0}{2C}\left(\frac{T_{\mathrm{c}} - T}{T_{\mathrm{c}}}\right)} \qquad T < T_{\mathrm{c}}$$

nematic coherence length

$$\xi_0 := \sqrt{\frac{k}{A_0}}$$

reduced temperature

$$t := \frac{T - T_{\mathrm{c}}}{T_{\mathrm{c}}}$$

free-energy functional

$$\mathscr{F} := \frac{1}{2}\int_{\mathscr{S}}\left\{k|\nabla_{\mathrm{s}}\mathbf{Q}|^2 + (A - k_{24}K)(\mathrm{tr}\,\mathbf{Q}^2) + \frac{C}{2}(\mathrm{tr}\,\mathbf{Q}^2)^2\right\}da$$

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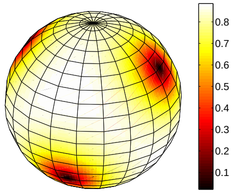
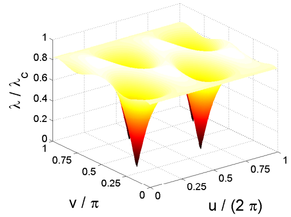
Valence Control

Both k_{24} and K appear capable of controlling both number and location of defects

sphere





$R = 20\xi_0 \qquad k_{24} = 0 \qquad t = -0.03$

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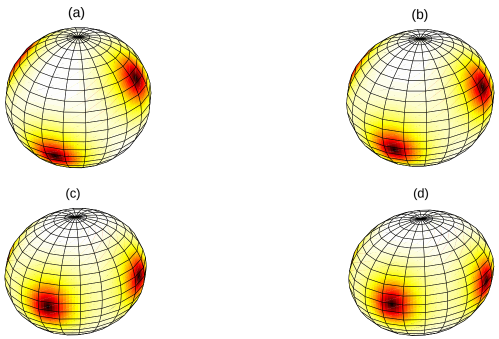
oblate ellipsoids



$R = 20\xi_0 \qquad k_{24} = 0 \qquad t = -0.03$

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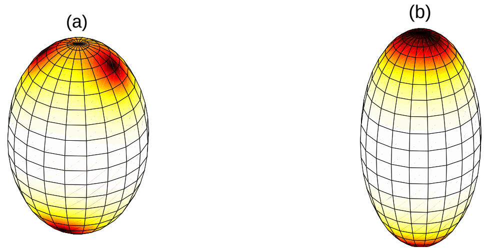
prolate ellipsoids



$R = 40\xi_0 \qquad k_{24} = 0 \qquad t = -0.03$

Defects migrate towards the region the largest K, to the point of possibly ***merging***.

This confirms simulations of Bates, Skačej & Zannoni (2010), which however did not show defect merging.

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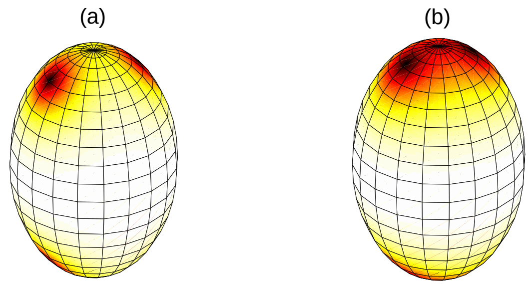
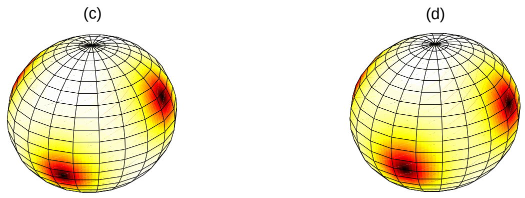
role of k_{24}



$k_{24} = k \qquad k_{24} = -k$

$R = 20\xi_0 \qquad t = -0.03$



$k_{24} = k$ $\qquad$ $k_{24} = -k$

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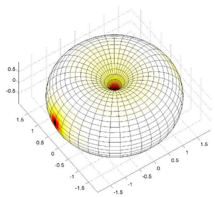
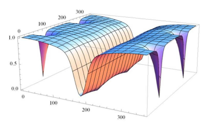
$R = 20\xi_0 \qquad t = -0.03$

For $K > 0$ a ***negative*** k_{24} enhances the migration of defects towards the regions with the largest K.





torus

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Credits

Co-workers

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Discussion

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More information

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