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Topological defects in nematic shells: a discrete-to-continuum approach

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Banff International Research Station

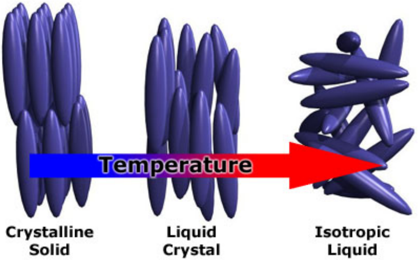
Workshop on Phase Transitions Models

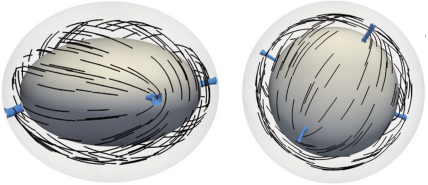
Oxford Centre for Nonlinear P∂E

Nematic shells

Nematic liquid crystals:
intermediate phase of matter

- ▷ Rod-shaped molecules
- ▷ Directional order, but no positional order

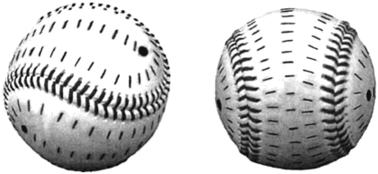


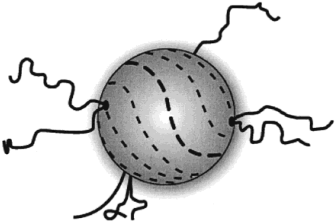


Nematic shell: small particle coated with a thin nematic film

[Figure: Bates, Skačej, Zannoni, ’10]

Defects in nematic shells





The alignment of the molecules is not perfect, as **defects** arise.

[Figures: Nelson, ’02; . . .]

ARTICLES
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nature materials

Topological defects in liquid crystals as templates for molecular self-assembly

Xiaoguang Wang[1], Daniel S. Miller[1], Emre Bukusoglu[1], Juan J. de Pablo[2] and Nicholas L. Abbott[1*]

Continuum variational models

- Smooth, compact surface $M \subseteq \mathbb{R}^3$ without boundary, with smooth unit normal $\gamma \colon M \to \mathbb{R}^3$.

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- Smooth, compact surface $M \subseteq \mathbb{R}^3$ without boundary, with smooth unit normal $\gamma \colon M \to \mathbb{R}^3$.

- **Oseen-Franck** energy (in its simplest form):

$$E(\mathbf{v}) := \frac{\kappa}{2} \int_M |\nabla \mathbf{v}|^2 \, \mathrm{d}S$$

on a space of unit-norm, tangent fields:

$$\mathscr{A}_0 := \left\{ \mathbf{v} \in W^{1,2}(M, \mathbb{R}^3) \colon \ |\mathbf{v}| = 1, \ \mathbf{v} \cdot \gamma = 0 \ \text{ a.e.} \right\}$$

$\nabla = \mathbb{R}^3$-gradient, restricted to tangent directions

[Napoli, Vergori, '10–'12;
Segatti, Snarski, Veneroni, '14-'15. . .]

Is the space $\mathscr{A}_0$ non-empty?

The Poincaré-Hopf Theorem

For any unit-norm, tangent field **v** on M that is smooth except at the points $x_1, x_2, \ldots x_p$, there holds

$$\sum_{i=1}^{p} \mathrm{ind}(\mathbf{v}, x_i) = \chi(M)$$

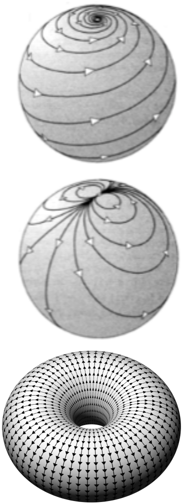
where $\chi(M)$ is the Euler characteristic, $\chi(M) = 2 - 2g$.

In particular,

$$\mathscr{A}_0 \neq \emptyset \quad \Leftrightarrow \quad M \simeq \mathbb{T}^2$$

Extension to Sobolev setting

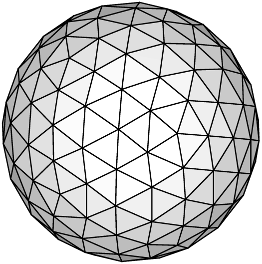
[Bethuel, '91; Brezis, Nirenberg, '95–'96; C., Segatti, Veneroni, '15]



The XY-model

- Introduced by **Heisenberg** as a model for **spins**.
- Defects-mediated phase transition (ferromagnetism, superconductors. . .) **[Kosterlitz, Thouless, ’73]**
- Lattices in $\mathbb{R}^n$
  - Discrete-to-continuum limit (equilibrium configurations) **[Alicandro, Cicalese, ’09; Alicandro, Cicalese, Ponsiglione, ’14; Alicandro, De Luca, Garroni, Ponsiglione, ’16. . .]**
  - Dynamics **[Alicandro, De Luca, Garroni, Ponsiglione, ’16. . .]**

XY-model on a surface



- $\mathcal{T}_\varepsilon$ triangulation on M, $\widehat{M}_\varepsilon := \cup_{T \in \mathcal{T}_\varepsilon} T$
- $\mathcal{T}_\varepsilon^0 := \{\text{vertices of } \mathcal{T}_\varepsilon\} \subseteq M$
- Discrete vector fields:

$$\mathscr{A}_\varepsilon := \Big\{ \mathbf{v} \colon \mathcal{T}_\varepsilon^0 \to \mathbb{R}^3, \ |\mathbf{v}(i)| = 1, \ \mathbf{v}(i) \cdot \boldsymbol{\gamma}(i) = 0 \\ \text{for any } i \in \mathcal{T}_\varepsilon^0 \Big\}$$

- $\widehat{\mathbf{v}} \colon \widehat{M}_\varepsilon \to \mathbb{R}^3$ piecewise-affine interpolant

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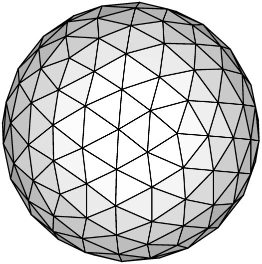

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- **Discrete energy:** for $\mathbf{v} \in \mathscr{A}_\varepsilon$,

$$XY_\varepsilon(\mathbf{v}) := \frac{1}{2}\int_{\widehat{M}_\varepsilon} |\nabla\widehat{\mathbf{v}}|^2 \,\mathrm{d}S = \frac{1}{2}\sum_{i,j\in\mathcal{T}_\varepsilon^0} \kappa_\varepsilon^{i,j}\,|\mathbf{v}(i)-\mathbf{v}(j)|^2$$

Assumptions on $\mathcal{T}_\varepsilon$

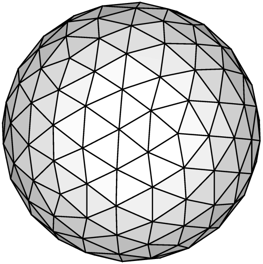
(H$_1$) $\mathcal{T}_\varepsilon$ is **quasi-uniform** of size ε: for any $T \in \mathcal{T}_\varepsilon$,

$$C^{-1}\varepsilon \leq \mathrm{diameter}(T) \leq C\varepsilon, \qquad \alpha_{\min}(T) \geq C^{-1}$$

(H$_2$) $\mathcal{T}_\varepsilon$ is **weakly acute**: for any $i, j \in \mathcal{T}_\varepsilon^0$ with $i \neq j$,

$$\kappa_\varepsilon^{i,j} := -\int_{\widehat{M}_\varepsilon} \nabla\widehat{\varphi}_\varepsilon^i \cdot \nabla\widehat{\varphi}_\varepsilon^j \, \mathrm{d}S \geq 0$$

(H$_3$) The projection $P\colon \widehat{M}_\varepsilon \to M$ is well-defined and a bijection.



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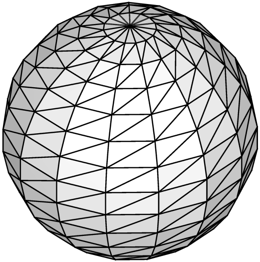
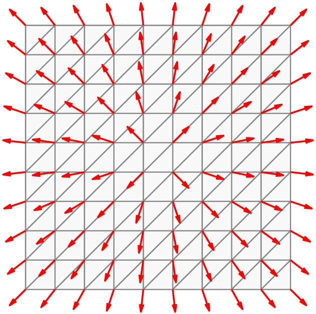


Not allowed



- Due to Poincaré-Hopf Theorem,

$$\inf_{\mathscr{A}_\varepsilon} XY_\varepsilon \to +\infty \qquad \text{as } \varepsilon \to 0$$

unless $M \simeq \mathbb{T}^2$.

- In fact, by comparison we have

$$\inf_{\mathscr{A}_\varepsilon} XY_\varepsilon \simeq C\,|\log \varepsilon|$$

(discretisation of $x \mapsto x/|x|$).

- Compare with the analysis of **Ginzburg-Landau** functional **[Bethuel, Brezis, Hélein, '94; Sandier, Serfaty, '07. . .]**; **[Ignat, Jerrard, '16]** for the analysis on a surface.

How to detect the topological information in the discrete setting?

Jacobians of vector fields

Identify $\mathbb{R}^2 \simeq \mathbb{R}^2 \times \{0\} \subseteq \mathbb{R}^3$. For $\mathbf{u} \in C^2(\mathbb{R}^2, \mathbb{R}^2)$, we define the "pre-jacobian"

$$\jmath^{\#}(\mathbf{u}) := \left(\mathbf{e}_3 \cdot (\mathbf{u} \times \partial_1 \mathbf{u}),\ \mathbf{e}_3 \cdot (\mathbf{u} \times \partial_2 \mathbf{u})\right), \qquad \boxed{\operatorname{curl} \jmath^{\#}(\mathbf{u}) = 2 \det \nabla \mathbf{u}}$$

We will work in the language of differential forms:

$$\jmath(\mathbf{u}) \colon \mathbf{w} \in \mathbb{R}^2 \mapsto \jmath^{\#}(\mathbf{u}) \cdot \mathbf{w} = \mathbf{e}_3 \cdot (\mathbf{u} \times \nabla_{\mathbf{w}} \mathbf{u}),$$

in short $\jmath(\mathbf{u}) = \mathbf{e}_3 \cdot (\mathbf{u} \wedge \mathrm{d}\mathbf{u})$.

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in short $\jmath(\mathbf{u}) = \mathbf{e}_3 \cdot (\mathbf{u} \wedge \mathrm{d}\mathbf{u})$.

For $\mathbf{u} \in (W^{1,1} \cap L^\infty)(M, \mathbb{R}^3)$, define

$$\jmath(\mathbf{u}) := \boldsymbol{\gamma} \cdot (\mathbf{u} \wedge \mathrm{d}\mathbf{u})$$

If $\mathbf{u}$ is a unit-norm, tangent field, locally we can write

$$\mathbf{u} = \cos\alpha \, \mathbf{e}_1 + \sin\alpha \, \mathbf{e}_2, \qquad \jmath(\mathbf{u}) = \mathrm{d}\alpha - \mathbf{A}$$

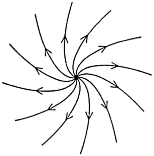
where $\mathbf{A}$ is a smooth form that only depends on $(\mathbf{e}_1, \mathbf{e}_2)$. (Also **[Ignat, Jerrard, '16]**)

Properties of the Jacobian

Lemma

Let $\mathbf{u} \in W^{1,1}(M, \mathbb{R}^3)$ *be s.t.* $|\mathbf{u}| = 1$, $\mathbf{u} \cdot \boldsymbol{\gamma} = 0$ *a.e. Suppose that* $\mathbf{u} \in C^2(M \setminus \{x_1, \ldots, x_K\})$*. Then*

$$\star \mathrm{d}\jmath(\mathbf{u}) = 2\pi \sum_{i=1}^{K} \mathrm{ind}(\mathbf{u}, x_i)\delta_{x_i} - G\,\mathrm{d}S \qquad \text{in } \mathscr{D}'(M).$$



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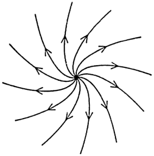
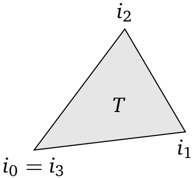


- **Discrete vorticity measure**:

$$\mathbf{v} \in \mathscr{A}_\varepsilon \quad \rightsquigarrow \quad \widehat{\mathbf{v}} \colon \widehat{M}_\varepsilon \to \mathbb{R}^3 \quad \rightsquigarrow \quad \widehat{\jmath}_\varepsilon(\mathbf{v}) := \widehat{\boldsymbol{\gamma}}_\varepsilon \cdot (\widehat{\mathbf{v}}_\varepsilon \wedge \mathrm{d}\widehat{\mathbf{v}}_\varepsilon)$$

$$\widehat{\mu}_\varepsilon(\mathbf{v}) := \sum_{T \in \mathcal{T}_\varepsilon} \left(\int_T \mathrm{d}\widehat{\jmath}_\varepsilon(\mathbf{v}) \right) \delta_{x(T)}$$

$$\widehat{\mu}_\varepsilon(v)[T] = \sum_{k=0}^{2} \frac{\boldsymbol{\gamma}(i_k) + \boldsymbol{\gamma}(i_{k+1})}{2} \cdot \mathbf{v}(i_k) \times \mathbf{v}(i_{k+1})$$



Energetics: Leading order terms

Theorem (C., Segatti, '17)

Let $\mathbf{v}_\varepsilon \in \mathscr{A}_\varepsilon$ *be such that* $XY_\varepsilon(\mathbf{v}_\varepsilon) \leq C\,|\log\varepsilon|$.

(i) Up to subsequences, $\widehat{\mu}_\varepsilon(\mathbf{v}_\varepsilon) \xrightarrow{\text{flat}} \mu$ *where*

$$\mu = 2\pi \sum_{i=1}^{K} d_i \delta_{x_i} - G\,\mathrm{d}S, \qquad x_i \in M, \quad d_i \in \mathbb{Z}, \quad \sum_{i=1}^{K} d_i = \chi(M). \qquad (\star)$$

(ii) If $\widehat{\mu}_\varepsilon(\mathbf{v}_\varepsilon) \xrightarrow{\text{flat}} \mu$ *as in* $(\star)$*, then*

$$\pi \sum_{i=1}^{K} |d_i| \leq \liminf_{\varepsilon\to 0} \frac{XY_\varepsilon(\mathbf{v}_\varepsilon)}{|\log\varepsilon|}.$$

(iii) For any μ *of the form* $(\star)$*, there exist* $\mathbf{v}_\varepsilon \in \mathscr{A}_\varepsilon$ *such that* $\widehat{\mu}_\varepsilon(\mathbf{v}_\varepsilon) \xrightarrow{\text{flat}} \mu$ *and*

$$\pi \sum_{i=1}^{K} |d_i| = \lim_{\varepsilon\to 0} \frac{XY_\varepsilon(\mathbf{v}_\varepsilon)}{|\log\varepsilon|}.$$

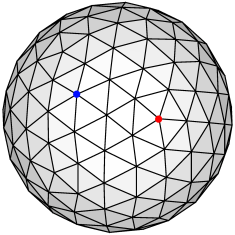
Here, flat = dual of C^1.

- **Warning:** in general, the sequence of fields $\mathbf{v}_\varepsilon$ is **not** strongly precompact!
  - ▷ Role of the Jacobian — **compensated compactness**

- **Warning:** in general, the sequence of fields $\mathbf{v}_\varepsilon$ is **not** strongly precompact!
  - ▷ Role of the Jacobian — **compensated compactness**
- However, if $\mathbf{v}_\varepsilon^*$ is a minimiser of XY_ε, then
  - ▷ $\mathbf{v}_\varepsilon^* \to \mathbf{v}^*$ in $W^{1,2}_{\mathrm{loc}}(M \setminus \{x_1, \ldots, x_K\}, \mathbb{R}^3)$, where $K = |\chi(M)|$
  - ▷ $\mathrm{ind}(\mathbf{v}^*, x_i) = \mathrm{sign}(\chi(M))$

  so we control the number and local degree of defects.

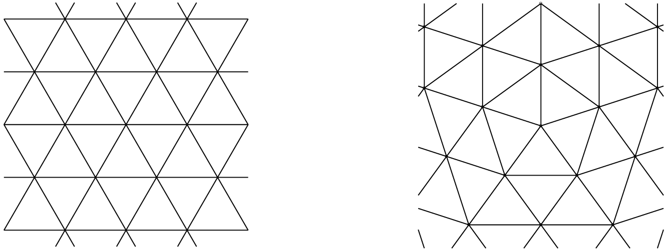
Can one characterize the position of defects?



We need an additional assumption on the sequence of triangulations, namely, for any $x \in M$ and small $\delta > 0$, there is a triangulation $\mathcal{S}(x)$ on $\mathbb{R}^2$ such that

$$\varphi_* \left(\mathcal{T}_{\varepsilon\,|B_\delta(x)}\right) \approx \varepsilon\,\mathcal{S}(x) \qquad \text{as } \varepsilon \to 0,$$

where $\varphi\colon M \to \mathrm{T}_x M \simeq \mathbb{R}^2$ are geodesic coordinates at x.



$\mathcal{S}(x)$ $\mathcal{S}(y)$

Energetics: Second-to-leading order terms

Theorem (C., Segatti, '17)

Let $K := |\chi(M)|$ and $\mathbf{v}_\varepsilon \in \mathscr{A}_\varepsilon$ be such that $XY_\varepsilon(\mathbf{v}_\varepsilon) \leq \pi K |\log \varepsilon| + C$. Then, up to subsequences, $\mathbf{v}_\varepsilon \to \mathbf{v}$ in $W^{1,2}_{\mathrm{loc}}(M \setminus \{x_1, \dots, x_K\})$ and

$$XY_\varepsilon(\mathbf{v}_\varepsilon) = \pi K |\log \varepsilon| + \mathbb{W}(\mathbf{v}) + \sum_{i=1}^{K} \gamma(x_i) + \mathrm{o}_{\varepsilon \to 0}(1).$$

- $\mathbb{W}(\mathbf{v})$ = **Renormalised Energy**,

$$\mathbb{W}(\mathbf{v}) := \lim_{\delta \to 0} \left(\frac{1}{2} \int_{M_\delta} |\nabla \mathbf{v}|^2 \, \mathrm{d}S - \pi K |\log \delta| \right)$$

  where $M_\delta := M \setminus \cup_i B_\delta(x_i)$ **[Bethuel, Brezis, Hélein, '94]**

- $\gamma(x_i)$ = **core energy**, localised in a ball of radius $C\varepsilon$ around the defect. Depends on the triangulation

- The local properties of the triangulation may trigger the position of the defects!
  $\neq$ continuous case, uniform grid on $\mathbb{R}^2$

- **Question.** For $\mu = 2\pi \sum_i d_i \delta_{x_i} - G\mathrm{d}S$, can we characterise

$$\mathbb{W}(\mu) := \inf_{\mathbf{v}\colon \star\mathrm{d}\jmath(\mathbf{v})=\mu} \mathbb{W}(\mathbf{v})?$$

- The local properties of the triangulation may trigger the position of the defects! $\neq$ continuous case, uniform grid on $\mathbb{R}^2$
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$$\mathbb{W}(\mu) := \inf_{\mathbf{v}:\ \star \mathrm{d}\jmath(\mathbf{v}) = \mu} \mathbb{W}(\mathbf{v})?$$

If ∇ is replaced by covariant derivative D, we have

$$\mathbb{W}_{\mathrm{intr}}(\mu) = 4\pi^2 \sum_{i \neq j} d_i d_j \Gamma(x_i, x_j) + 2\pi \sum_i \left(\pi d_i^2 H(x_i) - d_i V(x_i)\right) + \mathrm{const}$$

where

$$\begin{cases} -\Delta_M \Gamma(\cdot, x_0) = \delta_{x_0} - |M|^{-1} \\ \int_M \Gamma(\cdot, x_0)\, \mathrm{d}S = 0, \end{cases} \qquad \begin{cases} -\Delta_M V = G - 2\pi\chi(M)\, |M|^{-1} \\ \int_M V\, \mathrm{d}S = 0, \end{cases}$$

$$H(x_0) := \lim_{x \to x_0} \Gamma(x, x_0) + \frac{1}{2\pi} \log \mathrm{dist}(x, x_0).$$

[Vitelli, Nelson, '04; Ignat, Jerrard, '16].

Conclusions

- Use of Jacobian: compactness + topological information
- Energetics of defects: Renormalised Energy + sensitivity to the mesh
- More physically realistic models (non-oriented models. . .) ?
- Numerics?