

# Design of nematic liquid crystals through colloidal homogenisation

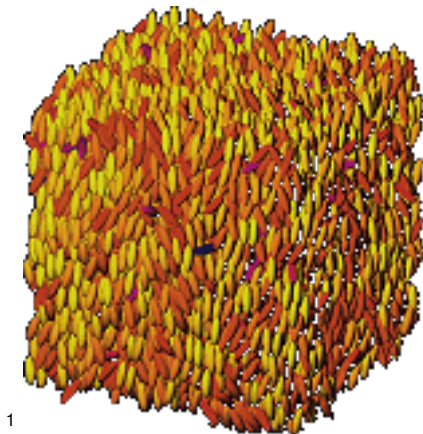
Arghir Dani Zarnescu

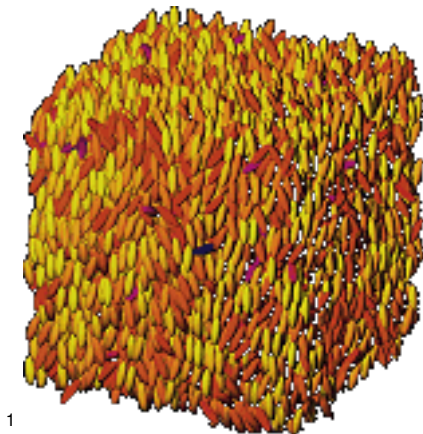
Basque Center for Applied Mathematics, Spain  
and  
“Simion Stoilow” Institute of Mathematics of the Romanian Academy

joint work with Giacomo Canevari (Università di Verona)

**Analysis of Nematic Liquid Crystal Flows Workshop  
CIRM-Luminy, April 2022**

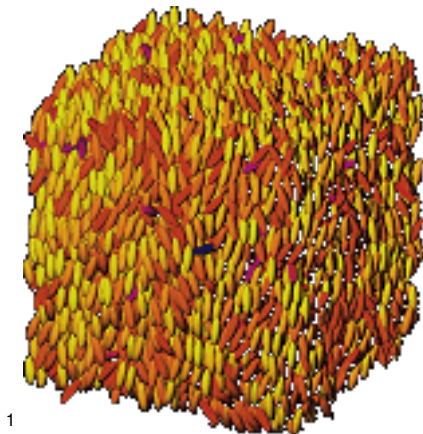
# Liquid crystals modelling: physics





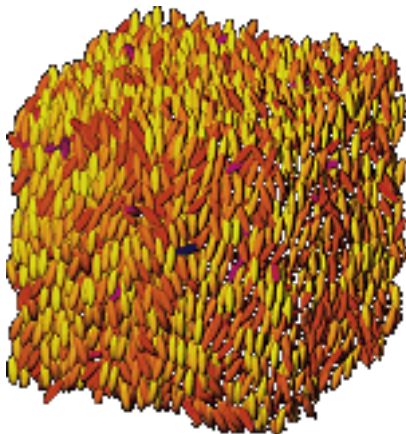
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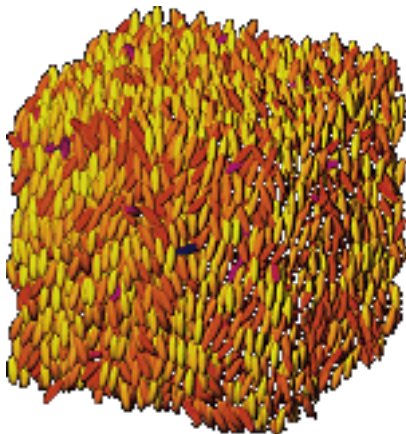
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# Landau-de Gennes Q-tensor and other simpler theories

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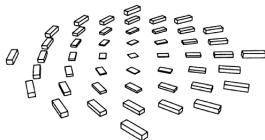
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- **Oseen-Frank theory (1958)** take  $s$  in the uniaxial representation to be a fixed constant  $s_+$

# Q-tensors: visualisation

- One can visualise a Q-tensor as either a:
  - ▶ *parallelepiped* whose axis are parallel with the eigenvectors of Q and whose lengths are proportional to the eigenvalues of Q or an
  - ▶ *ellipsoid* whose axis are parallel with the eigenvectors of Q and whose radii are proportional to the eigenvalues of Q
- Some Q-tensor fields in the two representations:

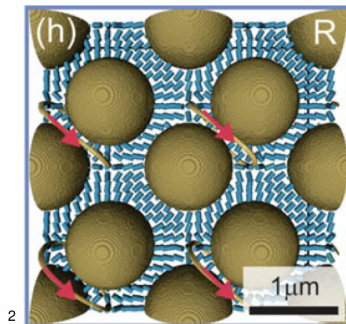


Index 1/2 defect (parallelepipeds)  
(ellipsoids)



Index 1/2 defect

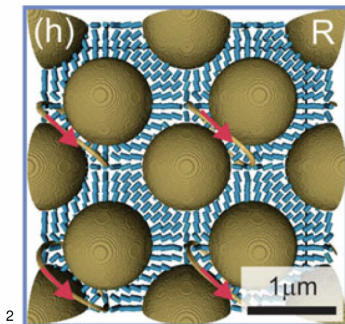
# Nematic colloids



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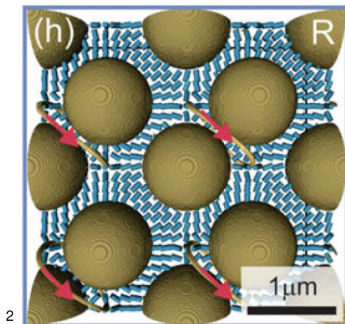
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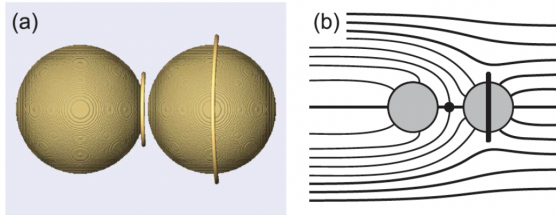
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# Nematic colloids in recent literature: between defects and homogenisation



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Physical literature:

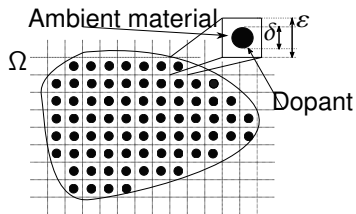
- Wang, Zhang, Chen, Phys Rev E '96
- Ravnik, Žumer, Liq. Crys.'09
- Lavrentovich, Lev, Trokhymchuk, Condens. Matter Phys. '10
- Smalyuk, Ann.Rev. Condens Matter Phys. '18

Mathematical literature:

- (defects) Alama, Bronsard, Lamy, ARMA '16, Alama, Bronsard, Lamy, J.Non.Sci'18
- (homogenization) Berlyand, Cioranescu, Golovaty, J. Math. Pure et App. '05
- (homogenization) Calderer, De Simone, Golovaty, Panchenko, SIAM J. Appl. Math '14

<sup>3</sup>Figure from *Ravnik and Žumer Liquid Crystals*, 36:10-11, 1201-1214

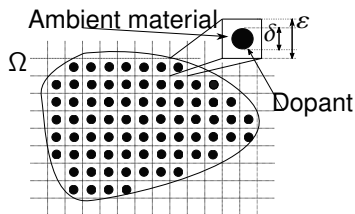
# Homogenisation: the physical modelling



- A mixture of two materials: one outside the holes and another one, a dopant, inside the holes

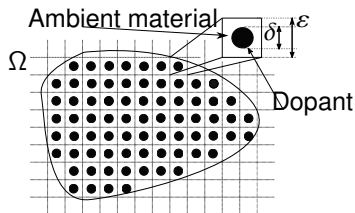


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- A mixture of two materials: one outside the holes and another one, a dopant, inside the holes
- Periodically distributed (at least as a start!) holes with the dopant material
- Size of the holes  $\delta$  is smaller than the periodicity  $\epsilon$ . Number of cells of the order  $\epsilon^{-d}$  where  $d$  is dimension of the ambient space ( $d = 3$  in most physical cases)

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- As  $\delta, \epsilon \rightarrow 0$  the holes are vanishing but their effect can persist producing a homogenized material

# Homogenisation: the setting

We take

- $\Omega_\varepsilon := \Omega \setminus \mathcal{P}_\varepsilon$  i.e. the ambient material  $\Omega$  minus the dopant

$$\mathcal{P}_\varepsilon := \bigcup_{i=1}^{N_\varepsilon} \mathcal{P}_\varepsilon^i \quad \text{and} \quad \mathcal{P}_\varepsilon^i := x_\varepsilon^i + \mathcal{P},$$

where the  $x_\varepsilon^i$ 's are centers of the spheres  $\mathcal{P}_\varepsilon^i$  in  $\Omega$ ,  $\delta > 0$  is their common radius.

- $H_{g,\varepsilon}^1$  is a space of functions where the boundary conditions on the ambient material  $\partial\Omega$  and the dopant  $\partial\mathcal{P}_\varepsilon$  are suitably fixed
- Number of the holes  $N_\varepsilon \sim \frac{|\Omega|}{\varepsilon^3}$  with total volume  $\frac{\delta^3}{\varepsilon^3} \rightarrow 0$  for  $\delta \ll \varepsilon$  (the dilute regime!).

# The Landau-de Gennes (LDG) model of colloidal nematics

We denote

$$\mathcal{S}_0 := \{Q \in \mathbb{R}^{3 \times 3}, Q = Q^T, \text{tr}(Q) = 0\}$$

and refer to its elements as **Q-tensors**.

The material is described through functions  $Q : \Omega_\varepsilon \rightarrow \mathcal{S}_0$  that minimise the following (non-dimensionalized) Landau-de Gennes free energy functional:

$$\mathcal{F}_\varepsilon[Q] := \int_{\Omega_\varepsilon} (f_e(\nabla Q) + f_b(Q)) \, dx + \varepsilon^{3-2\alpha} \int_{\partial\mathcal{P}_\varepsilon} f_s(Q, \nu) \, d\sigma.$$

(where  $\nu(x)$  denotes as usually the exterior normal at the point  $x$  on the boundary).

We take:

- $\delta = \varepsilon^\alpha, \alpha > 1$  i.e.  $\delta = \varepsilon^\alpha \ll \varepsilon$  as  $\varepsilon \rightarrow 0$  i.e. a dilute regime
- $\alpha < \frac{3}{2}$  i.e.  $\varepsilon^{3-2\alpha} \rightarrow 0$  as  $\varepsilon \rightarrow 0$  i.e. weak influence of the surface energy

# The liquid crystal terms in the LDG functional

- The term  $f_e(\nabla Q)$  models *the spatial variations* of the material. Physical invariances require the symmetry  $f_e(D) = f_e(D^*)$  where we denote the third order tensor  $D_{ijk} := \frac{\partial Q_{ij}}{\partial x_k}$  and we have  $D_{ijk}^* = R_{il}R_{jm}R_{kp}D_{lmp}$ . Some terms satisfying these invariances are (where we denote  $Q_{ij,k} := \frac{\partial Q_{ij}}{\partial x_k}$  and assume summation over repeated indices):

$$f_e^1 := Q_{ij,k} Q_{ij,k}, \quad f_e^2 := Q_{ij,k} Q_{ik,j}, \quad f_e^3 = Q_{ij,j} Q_{ik,k}$$

The most commonly used one is the first one above, that provides a reasonably good approximation in many cases of interest.

- the **bulk potential**  $f_b(Q)$  that models *the phase transition* from the liquid phase to the nematic phase. Physical invariances require the symmetry assumption  $f_b(Q) = f_b(RQR^T)$  for any  $Q \in \mathcal{S}_0$  and  $R \in O(3)$ , and the most commonly used form is the Landau-de Gennes potential, up to fourth order, given as:

$$f_b^{LDG}(Q) := a \operatorname{tr}(Q^2) - b \operatorname{tr}(Q^3) + c (\operatorname{tr}(Q^2))^2 \quad (1)$$

Here  $a, b, c \in \mathbb{R}$  are material constants, with **a being proportional with the temperature**.

# The surface energy on the particles

The effects induced by the particles are modeled through the surface energy term that encodes the effect produced by the interaction between the boundary of the colloidal particles and the ambient fluid. The physical invariances require the following

$$f_s(RQR^T, Ru) = f_s(Q, u) \quad \text{for any } (Q, u) \in S_0 \times \mathbb{R}^3, R \in O(3). \quad (2)$$

The most commonly used surface energy is the so-called **Rapini-Papoular type energy, of the form:**

$$f_s(Q, \nu) = W \operatorname{tr} \left( Q - s_+ \left( \nu \otimes \nu - \frac{1}{3} I \right) \right)^2 \quad (3)$$

with  $W > 0$  a coefficient measuring the strength of the anchoring and the overall term measuring the deviation from the homeotropic (perpendicular) anchoring on the boundary.

# Heuristics on the behaviour of the surface energy

Take  $f_s(Q, \nu) = Q^2 \nu \cdot \nu$ ,  $\mathcal{P} = B_1$ . Then we have, where we denote  $\mathcal{P}_\varepsilon = \cup_{i=1}^{N_\varepsilon} B(x_i, \varepsilon^\alpha)$ :

$$\begin{aligned} \varepsilon^{3-2\alpha} \int_{\partial \mathcal{P}_\varepsilon} Q^2 \nu \cdot \nu \, d\sigma &= \varepsilon^{3-2\alpha} \sum_{i=1}^{N_\varepsilon} \int_{\partial B(x_i, \varepsilon^\alpha)} Q^2(x) \nu \cdot \nu \, d\sigma \\ &\sim \varepsilon^{3-2\alpha} \sum_{i=1}^{N_\varepsilon} Q^2(x_\varepsilon + \mathbf{e}_1 \cdot \varepsilon^\alpha) : \int_{\partial B(x_i, \varepsilon^\alpha)} \nu \otimes \nu \, d\sigma \end{aligned}$$

Change of variables:  $B(x_i, \varepsilon^\alpha) \rightarrow B(0, 1)$ :

$$\begin{aligned} \varepsilon^{3-2\alpha} \sum_{i=1}^{N_\varepsilon} Q^2(x_\varepsilon + \mathbf{e}_1 \cdot \varepsilon^\alpha) : \int_{\partial B(x_i, \varepsilon^\alpha)} \nu \cdot \nu \, d\sigma &\sim \varepsilon^3 \sum_{i=1}^{N_\varepsilon} Q^2(x_\varepsilon + \mathbf{e}_1 \cdot \varepsilon^\alpha) : \int_{\partial B(0,1)} \nu \otimes \nu \, d\sigma \\ &\sim \frac{4\pi\varepsilon^3}{3} \sum_{i=1}^{N_\varepsilon} \text{tr}(Q^2(x_\varepsilon + \mathbf{e}_1 \cdot \varepsilon^\alpha)) \\ &\sim \frac{4\pi}{3} \int_{\Omega} \text{tr}(Q^2(x)) \, dx \end{aligned}$$

# The homogenized limit and the design problem

The homogenized material is described by the energy functional:

$$\mathcal{F}_{hom}[Q] := \int_{\Omega} (f_e(\nabla Q) + f_b(Q)) \, dx + f_{hom}(Q(x)) \, dx$$

where the  $f_{hom}(Q)$  can be **explicitly** calculated in terms of the surface energy and the geometry of the colloidal particles.



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Question: The design (inverse!) problem: given  $f_{hom}(Q)$  satisfying physical invariances, can we design suitable surface energies and shape of the colloidal particle in order to obtain the given  $f_{hom}$ ?

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Answer: For arbitrary  $f_{hom}(Q)$  this is not clear....but for the polynomial ones yes!

# Physical symmetries of the surface energy

## Proposition

Let  $f: \mathcal{S}_0 \times \mathbb{R}^3 \rightarrow \mathbb{R}$  be a function that satisfies

$$f(UQU^T, Uu) = f(Q, u) \quad \text{for any } (Q, u) \in \mathcal{S}_0 \times \mathbb{R}^3, U \in O(3). \quad (4)$$

Then, there exists a function  $\tilde{f}: \mathbb{R}^5 \rightarrow \mathbb{R}$  such that

$$f(Q, u) = \tilde{f}(\text{tr}(Q^2), \text{tr}(Q^3), |u|^2, u \cdot Qu, u \cdot Q^2u)$$

for all  $(Q, u) \in \mathcal{S}_0 \times \mathbb{R}^3$ .

# The design of the standard quartic potential

## Theorem

Consider the energy functional:

$$\mathcal{F}_\varepsilon[Q] := \int_{\Omega_\varepsilon} \left( f_\varepsilon(\nabla Q) + a \operatorname{tr}(Q^2) - b \operatorname{tr}(Q^3) + c \left( \operatorname{tr}(Q^2) \right)^2 \right) dx + \varepsilon^{3-2\alpha} \int_{\partial \mathcal{P}_\varepsilon} f_s(Q, \nu) d\sigma.$$

Then, under suitable technical assumptions, we have:

- 1 For any two sets of parameters  $(a, b, c)$  and  $(a', b', c')$  there exists an explicitly given surface energy (depending on  $a, b, c, a', b', c'$ ) and particle shapes such the homogenized energy functional is:

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- 2 If  $b = b', c = c'$  then the surface energy can be chosen of the standard Rapini-Papoular type  $W \operatorname{tr} \left( Q - s_+ \left( \nu \otimes \nu - \frac{1}{3} I \right) \right)^2$ .

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Note: the second part say that we can modify  $a$ , related to the phase transition temperature, just by using the most standard Rapini-Papoular type surface energy

# Some technical aspects: boundedness from below and lower semi-continuity

- ①  $\mathcal{F}_\varepsilon$  might not be bounded from below for fixed  $\varepsilon$ ! E.g. take surface energy  $f_s(Q, \nu) = -(\operatorname{tr}(Q^2))^2$ . Then  $\inf_{\mathcal{A}_\varepsilon} \mathcal{F}_\varepsilon = -\infty$ .
- ②  $\mathcal{F}_\varepsilon$  might not be lower semi-continuous for fixed  $\varepsilon$ ! Take for instance a simplified functional:

$$\mathcal{G}_\varepsilon[Q] := \int_{\Omega_\varepsilon} |\nabla Q|^2 + |Q|^4 - \varepsilon^{3-2\alpha} \int_{\partial\mathcal{P}_\varepsilon} |Q|^4 d\sigma$$

and  $\mathcal{P}_\varepsilon = \cup_k (x_k + [-\varepsilon^\alpha, \varepsilon^\alpha])$ . There are sequences  $Q_j \rightharpoonup 0$  weakly in  $H^1$  but

$$0 > \liminf_{j \rightarrow \infty} \mathcal{G}[Q_j]$$

(This is because the Sobolev embedding  $H^{\frac{1}{2}}(\partial\Omega) \hookrightarrow L^4(\partial\Omega)$  is not compact so the surface energy is not a lower order term)

# An analytical tool: traces and extensions

## Lemma

Let  $\mathcal{P} \subseteq \mathbb{R}^3$  be a compact, convex set whose interior contains the origin. Let  $p \in [2, 4]$ . Then, there exists  $C = C(\mathcal{P}, \phi, p) > 0$  such that, for any  $a > 0$ ,  $b \geq 2a$  and any  $u \in H^1(b\mathcal{P} \setminus a\mathcal{P})$ , there holds

$$\int_{\partial(a\mathcal{P})} |u|^p \, d\sigma \leq C \int_{b\mathcal{P} \setminus a\mathcal{P}} (|\nabla u|^2 + |u|^{2p-2}) \, dx + \frac{Ca^2}{b^3} \int_{b\mathcal{P} \setminus a\mathcal{P}} |u|^p \, dx.$$

## Lemma

For any  $Q \in H^1(\Omega_\varepsilon, \mathcal{S}_0)$  and any  $p \in [2, 4]$ , there holds

$$\varepsilon^{3-2\alpha} \int_{\partial\mathcal{P}_\varepsilon} |Q|^p \, d\sigma \lesssim \varepsilon^{3-2\alpha} \int_{\Omega_\varepsilon} (|\nabla Q|^2 + |Q|^{2p-2}) \, dx + \int_{\Omega_\varepsilon} |Q|^p \, dx.$$

# Solving the technical aspects: lower semicontinuity for small $\varepsilon$

## Proposition

For any  $M > 0$  there exists a  $\varepsilon_0(M) > 0$  such that for any  $\varepsilon \in (0, \varepsilon_0(M))$  we have for any sequence  $(Q_j)_{j \in \mathbb{N}} \subset H^1$  with

$$\int_{\Omega_\varepsilon} |\nabla Q_j|^2 \leq M$$

and

$$Q_j \rightharpoonup Q \text{ weakly in } H^1$$

there holds

$$\mathcal{F}_\varepsilon[Q] \leq \liminf_{j \rightarrow \infty} \mathcal{F}_\varepsilon[Q_j]$$



# Isolated local minimizers and convergence

## Theorem

*Under suitable assumptions on  $f_{\text{bulk}}$  and  $f_e$  let us suppose, moreover, that  $Q_0 \in H_g^1(\Omega, S_0)$  is an isolated  $H^1$ -local minimiser for  $\mathcal{F}_0$  — that is, there exists  $\delta_0 > 0$  such that*

$$\mathcal{F}_0[Q_0] < \mathcal{F}_0[Q]$$

*for any  $Q \in H_g^1(\Omega, S_0)$  such that  $Q \neq Q_0$  and  $\|Q - Q_0\|_{H^1(\Omega)} \leq \delta_0$ . Then, for any  $\varepsilon$  small enough, there exists an  $H^1$ -local minimiser  $Q_\varepsilon$  for  $\mathcal{F}_\varepsilon$  such that  $E_\varepsilon Q_\varepsilon \rightarrow Q_0$  strongly in  $H^1(\Omega)$  as  $\varepsilon \rightarrow 0$ .*

The theorem applies, in particular, to any critical point  $Q_0$  of  $\mathcal{F}_0$  that is locally (strictly) stable, that is, satisfies

$$\frac{d^2}{dt^2} \Big|_{t=0} \mathcal{F}_0[Q_0 + tP] > 0$$

for any  $P \in H_0^1(\Omega, S_0)$  with  $P \neq 0$ .

# Global minimizers for higher order potential

## Theorem

*Under suitable assumptions on  $f_{\text{bulk}}$  and  $f_e$  let us suppose, moreover, that there exist positive constants  $\mu$  and  $C$  such that*

$$f_b(Q) \geq \mu|Q|^6 - C \quad \text{for any } Q \in S_0.$$

*Then, for  $\varepsilon$  small enough, there exists a global minimiser  $Q_\varepsilon$  for  $\mathcal{F}_\varepsilon$  in  $H_g^1(\Omega_\varepsilon, S_0)$ . Moreover, up to a (non-relabelled) subsequence,  $E_\varepsilon Q_\varepsilon$  converges strongly in  $H^1(\Omega)$  to a global minimiser for  $\mathcal{F}_0$  in  $H_g^1(\Omega, S_0)$ .*

The bulk potential should satisfy the symmetry requirement  $f_b(Q) = f_b(RQR^T)$  for any  $Q \in S_0$  and  $R \in O(3)$  and as such it can be shown that it is a function of  $\text{tr}(Q^2)$  and  $\text{tr}(Q^3)$ .

The Theorem does not apply to the standard fourth order potential but it does applies to the sextic Landau-de Gennes potential that can be relevant for the so-called biaxial minimizers (i.e. all eigenvalues are distinct)

$$\begin{aligned} f_b(Q) = & a_2 \text{tr}(Q^2) - a_3 \text{tr}(Q^3) + a_4 \left( \text{tr}(Q^2) \right)^2 \\ & + a_5 \text{tr}(Q^2) \text{tr}(Q^3) + a_6 \left( \text{tr}(Q^2) \right)^3 + a'_6 \left( \text{tr}(Q^3) \right)^2, \end{aligned}$$

so long as  $a_6 > 0$  and  $6a_6 + a'_6 > 0$ .

## A specific example: changing the transition temperature in MBBA colloids with Rapini-Papoular surface energy

For MBBA (values taken from [Priestley, Wotjowicz, Sheng, '75]):

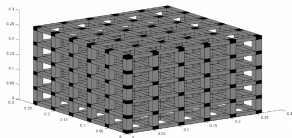
- Material coefficient  $a=0.42 \text{ Jm}^{-3}\text{K}^{-1}$
- Surface anchoring strength  $W \sim 10^{-3} \text{ Jm}^{-2}$
- Distance between inclusions  $d \sim 10^{-5} \text{ m}$

gives an effective (homogenized) phase transition temperature:

$$T^* - T_{eff}^* \sim \frac{2\pi W}{ad} \sim 1 \text{ K}$$

# Work of Razvan Ceuca ESAIM: COCV 27 (2021) 95: cubic microlattices homogenisation

Consider the colloidal "cage" to be placed in a nematic liquid crystal environment:



**Figure:** Example of a cubic microlattice.

# Work of Razvan Ceuca ESAIM: COCV 27 (2021) 95: cubic microlattices homogenisation

## Theorem

Let  $(a, b, c)$  and  $(a', b', c')$  be two set of parameters with  $c > 0$  and  $c' > 0$ . Under suitable assumption for  $\varepsilon > 0$  sufficiently small enough and for any isolated  $H^1$ -local minimiser  $Q_0$  of the functional:

$$\begin{aligned}\mathcal{F}_0^{\text{asym}}[Q] := & \int_{\Omega} \left( f_e(\nabla Q) + a' \operatorname{tr}(Q^2) - b' \operatorname{tr}(Q^3) + c' (\operatorname{tr}(Q^2))^2 \right) dx + \\ & + \frac{1}{\omega} \int_{\Omega} \left( (a' - a) \operatorname{tr}(A \cdot Q^2(x)) - (b' - b) \operatorname{tr}(A \cdot Q^3(x)) + (c' - c) \operatorname{tr}(A \cdot Q^4(x)) \right) dx\end{aligned}$$

there exists a sequence of local minimisers  $Q_\varepsilon$  of the functionals  $\mathcal{F}_\varepsilon^{\text{asym}}$  such that  $E_\varepsilon Q_\varepsilon \rightarrow Q_0$  strongly in  $H_g^1(\Omega, S_0)$ .

# Conclusions

- A dilute solution of nematic colloids can produce a mixture that behaves as a nematic material but with enhanced properties
- Given an apriorily desired homogenised material one can choose appropriately the surface energy on the colloids to obtain that material
- In particular, using just the standard Rapini-Papoular surface energy one can increase or decrease the isotropic-nematic transition temperature depending on whether one favours tangential or normal (homeotropic) anchoring

**THANK YOU!**