Least energy solutions for a model of liquid crystals.

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We study the model of a molecule in a flux of nematic liquid crystals. The position and the velocity are determined by the following two functions

$$u : \mathbb{R}^+ \times \mathbb{R}^3 \to \mathbb{R}^3, \quad Q : \mathbb{R}^+ \times \mathbb{R}^3 \to S_0(3, \mathbb{R})$$

Here and below with $S_0(3, \mathbb{R})$ we denote the space of 3×3 symmetric matrices with zero trace. We start following the model treaten by

Dai M., Feireisl E., Rocca E., Schimperna G., Schonbek M.E., On Asymptotic Isotropy for a Hydrodyinamic Model of Liquid Crystals, Asymptotic Analysis, 2016

We consider the model

$$\begin{cases} \partial_t Q + (u \cdot \nabla) Q - (\omega(u) Q - Q\omega(u)) = \Delta_x Q - L[\partial F(Q)] \\ \partial_t u - \text{div}_x (u \otimes u) + \nabla_x p = \\ \Delta_x u + \text{div}_x \left(-Q \Delta_x Q + \Delta_x Q Q - \nabla_x Q \odot \nabla_x Q\right) \\ div_x u = 0 \end{cases}$$

Where $Q = (q_{ij})_{i,j=1,2,3}$ and

$$\omega(u) := \frac{1}{2}\left(\nabla_x u - \nabla_x^t u\right), \quad L[A] := A - \frac{1}{3}\operatorname{tr}(A)Id \quad \forall A \in M(3,\mathbb{R})$$

$$(\nabla_x Q \odot \nabla_x Q)_{ij} := \sum_{\alpha,\beta} \partial_{x_i} q_{\alpha\beta} \partial_{x_j} q_{\alpha\beta}$$

$$\Delta Q = (\Delta q_{ij})_{i,j} \quad \forall i,j = 1,2,3$$

Here and below $p : \mathbb{R}^3 \to \mathbb{R}$ is the pressure, while $F : M(3,\mathbb{R}) \to \mathbb{R}$ is given by:

$$F(Q) = \frac{a}{2}|Q|^2 + \frac{b}{3}\operatorname{tr}\left(Q^3\right) + \frac{c}{4}|Q|^4$$

We are looking for a stationary solution, when the velocity is zero. Our system becomes

$$\begin{cases} \Delta Q = L[\partial F(Q)] = \partial F(Q) - \frac{1}{3}\operatorname{tr}(\partial F(Q)) Id \\ \operatorname{tr}(Q) = 0 \\ Q \in H^1\left(\mathbb{R}^3; S(3,\mathbb{R})\right) \end{cases}$$

Now we use the following parametrization for the matrices of $S_0(3,\mathbb{R})$:

$$Q(q(x)) = \begin{pmatrix} q_1(x) & q_3(x) & q_4(x) \\ q_3(x) & q_2(x) & q_5(x) \\ q_4(x) & q_5(x) & -q_1(x) - q_2(x) \end{pmatrix}$$

$$q = (q_1, q_2, q_3, q_4, q_5).$$

With this parametrization, it can be proved that the critical points q of the following functional

$$J(q) = \int |\nabla_x q|^2 + \nabla_x q_1 \cdot \nabla_x q_2 dx +$$

$$+ \int a\left(|q|^2 + q_1 q_2\right) + \frac{b}{3} tr(Q(q)^3) + c\left(|q|^2 + q_1 q_2\right)^2 dx$$

Give a matrix $Q(q)$ which resolves the previous system.
We studied the case $a > 0$ and $c < 0$ and we proved the existence of a Least Energy Solution:

Definition

Set q the solution of the system

$$\begin{cases} -2\Delta q - \alpha\left(\Delta q_1 e_2 + \Delta q_2 e_1\right) = \nabla_q G(q)\mathbb{1}_{\{q\neq 0\}} \\ q \in H^1(\mathbb{R}^d;\mathbb{R}^n) \end{cases} \tag{1.1}$$

Where $\alpha \in [0,1]$, $n \geq 2$ ed e_1, e_2 are the following vectors of $\mathbb{R}^n$:

$$e_1 = (1, 0, \dots, 0)^T, \quad e_2 = (0, 1, 0, \dots, 0)^T$$

Then we say that q is a **Least Energy Solution** if it resolves

$$J(q) = \inf\{J(v) \mid v \in H^1(\mathbb{R}^d;\mathbb{R}^n) \setminus \{0\},\ \ v \text{ solution of } (1.1)\}$$

Where

$$J(q) = \int |\nabla q|^2 + \nabla q_1 \nabla q_2 - G(q)dx.$$

Following

Brezis H., Lieb E., Minimum Action Solution of Some Vector Field Equations, Commun. Math. Phys., 96 – 113 (1984)

We consider the function $G \in C^1(\mathbb{R}^n \setminus \{0\})$ which satisfies the following properties:

- $G(0) = 0$;
- $\limsup_{|q|\to+\infty} |q|^{-p} G(q) \leq 0$;
- $\limsup_{|q|\to 0} |u|^{-p} G(q) \leq 0$;
- It exists $\xi_0 \in \mathbb{R}^n$ such that $G(\xi_0) > 0$;
- For all $\gamma > 0$ it exists C_γ such that

$$|G(q+w) - G(q)| \leq \gamma[|G(q)| + |q|^p] + C_\gamma[|G(w)| + |w|^p + 1] \tag{2.1}$$

  for all $q, w \in \mathbb{R}^n$;
- There exists a constant $C > 0$ such that

$$g(q) \leq C + C|q|^{p-1} \quad \forall q \in \mathbb{R}^n$$

Then we have the following result, that is a small generalization of the result of Brezis and Lieb (which treats only the case $\alpha = 0$)

Theorem

Let $d \geq 3$ *and* $n \geq 2$*, If* $p = \frac{2d}{d-2}$ *and* $g(q) = \nabla_q G(q) \mathbb{1}_{\{q \neq 0\}}$*, then there exists a least energy solution* $q \colon \mathbb{R}^d \to \mathbb{R}^n$ *for the system (1.1).*

It's not difficult to prove the following lemma:

Lemma

If $d \geq 3$, $G : \mathbb{R}^n \to \mathbb{R}$ is continuous in $\mathbb{R}^n$ and

$$\limsup_{|q| \to +\infty} |q|^{-p} |G(q)| = 0$$

Then G satisfies the condition (2.1).

In our case

$$G(q) - a(|q|^2 + q_1 q_2) - \frac{b}{3} tr(Q(q))^3 - c(|q|^2 + q_1 q_2)^2$$

So we're in the hypothesis of the theorem.

The proof starts with the existence of the minimum for

$$T = \inf\left\{\int |\nabla q|^2 + \alpha \nabla q_1 \nabla q_2 dx \,\middle|\, q \in \mathscr{C}, \int G(q)dx \geq 1\right\}$$

Where

$$\mathscr{C} = \left\{q \in L^p(\mathbb{R}^d) \mid \nabla q \in L^2(\mathbb{R}^d), G(q) \in L^1(\mathbb{R}^d)\right\}$$

Let $\{q^j\}$ a minimizing sequence for T then, less then subsequences and translations, it can be proved that

$$q^j \xrightarrow{L^p} q, \quad \nabla q^j \xrightarrow{L^2} \nabla q$$

With $q \neq 0$ and $q \in \mathscr{C}$.

Theorem

Let $q \in \mathscr{C}$ *the limit function of the minimizing sequence, then* $\int G(q) = 1$ *and*

$$\int |\nabla q|^2 + \alpha \nabla q_1 \nabla q_2 dx = T.$$

Proof.

Let $v \in \mathscr{C}$ with $\int G(v) > 0$. It's easy to see by scaling that

$$\int |\nabla v|^2 + \alpha \nabla v_1 \nabla v_2 dx \geq T \left[\int G(v) dx \right]^{\frac{d-2}{d}} \qquad (3.1)$$

With the estimate (2.1) and taking $v = q^j$ in the previous one, it can be prove the following fact: if $\phi \in L^p$ with compact support and $G(\phi) \in L^1$ then, for $j \to +\infty$, we have that

$$\int G(q^j + \phi) dx \geq 1 + \int G(q + \phi) dx - \int G(q) dx + o(1)$$

If we take $v = q^j + \phi$ in (3.1) with an appropriate choice of $\phi \in H^1$ and then we pass to the limit for $j \to +\infty$ we get

$$T + (\lambda^{2-d} - 1) \int |\nabla q|^2 + \alpha \nabla q_1 \nabla q_2 + \geq T \left[1 + (\lambda^{-d} - 1) \int G(q) \right]^{\frac{d-2}{d}}$$

If we choose $\lambda = 1 \pm \varepsilon$ and expand with Taylor series, we get

$$T \int G(q)dx = \int |\nabla q|^2 + \alpha \nabla q_1 \nabla q_2 dx \qquad (3.2)$$

Since $q \neq 0$, then $\int G(q) > 0$.

Thanks to the previous remark we can choose $v = q$ in (3.1), so we get:

$$T \int G(q)dx = \int |\nabla q|^2 + \alpha \nabla q_1 \nabla q_2 dx \geq T \left[\int G(q)dx \right]^{\frac{d-2}{d}}$$

So we deduce that $\int G(q)dx \geq 1$ ($T \neq 0$ by identity (1.5)) and

$$\int |\nabla q|^2 + \alpha \nabla q_1 \nabla q_2 dx \geq T$$

For weak inferior semicontinuity of the left hand side we conclude.

The functional which we minimized is an equivalent norm of L^2 of the vector ∇q, for this we get

Corollary

$\nabla q^j \to \nabla q$ in L^2 e $q^j \to q$ in L^p.

Theorem

Let q the minimizing function of T, then $\exists \theta > 0$ such that, if we called $\overline{q}(x) = q(\theta x)$, the function $\overline{q}$ resolves weakly the equation

$$-\Delta\overline{q} - \alpha\left(\Delta\overline{q}_1 e_2 + \Delta\overline{q}_2 e_1\right) = g(\overline{q}) = \nabla G(\overline{q})$$

Proof.

Let $\phi \in C_0^\infty(\mathbb{R}^d)$ and $t \in \mathbb{R}$, then

$$\int_{\mathbb{R}^d} G(q + t\phi) - G(q)dx = t \int_{\mathbb{R}^d} \int_0^1 g(q + st\phi) \cdot \phi dsdx$$

By the hypothesis on g, we get that

$$\begin{cases} \int_{\mathbb{R}^d} (G(q + t\phi) - G(q))\mathbb{1}_{\{q \neq 0\}} dx = t \int_{\mathbb{R}^d} g(q) \cdot \phi dx + o(t) \\ \int_{\mathbb{R}^d} |G(q + t\phi) - G(q)| \mathbb{1}_{\{q = 0\}} dx \lesssim |t| \int_{\mathbb{R}^d} |\phi| \mathbb{1}_{\{q = 0\}} \end{cases}$$

If we combined these estimates with the one given by (1.3) with $v = q + t\phi$ and $t \ll 1$ we get

$$\int \left(|\nabla(q + t\phi)|^2 + \alpha \nabla(q + t\phi)_1 \nabla(q + t\phi)_2 \right) dx =$$

$$= T + t \int \left[2\nabla q \cdot \nabla \phi + \alpha \left(\nabla q_1 \cdot \nabla \phi_2 + \nabla q_2 \cdot \nabla \phi_1 \right) \right] dx$$

If we distinguish the cases $t > 0$ and $t < 0$, it can be proved that

$$\left| \int \left[2\nabla q \cdot \nabla \phi + \alpha \left(\nabla q_1 \cdot \nabla \phi_2 + \nabla q_2 \cdot \nabla \phi_1 \right) \right] dx + \right.$$

$$\left. - T \left(\frac{d-2}{d} \right) \int g(q) \cdot \phi dx \right| \leq C \int |\phi| \mathbb{1}_{\{q=0\}} dx.$$

If we call $A(\phi)$ the left hand side of the previous estimate extended to L^1 by density, then it exists $h \in L^\infty(\mathbb{R}^d)$ such that

$$A(\phi) = \int h \cdot \phi \quad \forall \phi \in L^1(\mathbb{R}^d)$$

Thanks to the previous estimate, it's not difficult to proved that $h\mathbb{1}_{\{q \neq 0\}} = 0$. By elliptic regularity theory $q \in W^{2,\frac{p}{p-1}}_{loc}$. This implies that $(-2\Delta q - \alpha\Delta q_1 e_2 - \alpha\Delta q_2 e_1)\mathbb{1}_{\{q=0\}} = 0$ and therefore

$$-2\Delta q - \alpha\left(\Delta q_1 e_2 + \Delta q_2 e_1\right) = T\left(\frac{d-2}{d}\right) g(q)$$

So, choosing $\theta^2 = \frac{d}{T(d-2)}$, we get the solution of our system.

Lemma

Let $G \in C^1(\mathbb{R}^n \setminus \{0\})$ and $q \in L^\infty_{loc} \cap \mathscr{C}$ a solution for the system (1.1), then

$$\int |\nabla q|^2 + \alpha \nabla q_1 \nabla q_2 dx = \frac{d}{d-2} \int G(q) dx$$

Theorem

If we defined

$$S(q) = \int |\nabla q|^2 + \alpha \nabla q_1 \nabla q_2 dx - \int G(q) dx$$

then

$$0 < S(\overline{q}) \leq S(v)$$

For all $v \in L^\infty_{loc} \cap \mathscr{C}$ not zero which resolves (1.1).

Proof.

Let $v \in L^{\infty}_{loc} \cap \mathscr{C}$ another competitor, then we know by the previous lemma that

$$\begin{cases} \int |\nabla \overline{q}|^2 + \alpha \nabla \overline{q}_1 \nabla \overline{q}_2 dx = \frac{d}{d-2} \int G(\overline{q}) dx \\ \int |\nabla v|^2 + \alpha \nabla v_1 \nabla v_2 dx = \frac{d}{d-2} \int G(v) dx \end{cases}$$

Moreover

$$\begin{cases} \int |\nabla v|^2 + \alpha \nabla v_1 \nabla v_2 dx \geq T \left[\int G(v) dx \right]^{\frac{d}{d-2}} \\ \left[\int G(\overline{q}(x)) dx \right]^{\frac{d-2}{d}} = \frac{1}{|\theta|^{d-2}} \end{cases}$$

Then we get

$$\int |\nabla \overline{q}|^2 + \alpha \nabla \overline{q}_1 \nabla \overline{q}_2 dx = \frac{T}{|\theta|^{d-2}} = T \left[\int G(\overline{q}(x)) dx \right]^{\frac{d-2}{d}}$$

So $\overline{q}$ satisfies (1.3) with an equality.

$$\left[\int G(\overline{q}) dx \right]^{1-\frac{d-2}{d}} \leq \left[\int G(v) dx \right]^{1-\frac{d-2}{d}} \Rightarrow \int G(\overline{q}) dx \leq \int G(v) dx$$

Then we're ready to conclude:

$$S(\overline{q}) = \int |\nabla \overline{q}|^2 + \alpha \nabla \overline{q}_1 \nabla \overline{q}_2 dx - \int G(\overline{q}) dx =$$

$$= \left(\frac{2}{d-2} \right) \int G(\overline{q}) dx \leq \frac{2}{d-2} \int G(v) dx = S(v)$$

It can be proved also regularity results for the solutions of (1.1):

Theorem

Let $q \in \mathscr{C}$ with $g(q) \in L^1_{loc}$ be a distributional solution of (1.1). Then we have the properties

- $q \in W^{2,t}_{loc}$ *for all* $t < \infty$ *(therefore* $q \in C^{1,\alpha}_{loc}$ *for* $\alpha < 1$*);*
- $q \in L^{\infty}$*;*
- q *goes to 0 when* $|x| \to +\infty$*.*