FRANK ENERGY FOR NEMATIC ELASTOMERS: A NONLINEAR MODEL

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Abstract. We discuss the well-posedness of a new nonlinear model for nematic elastomers. The main novelty in our work is that the Frank energy penalizes spatial variations of the nematic director in the *deformed*, rather than in the reference configuration, as it is natural in the case of large deformations.

In this paper we discuss a new nonlinear model for nematic elastomers, which contains a Frank energy term penalizing spatial variations of the nematic director n in the deformed configuration. Our main result is a theorem on the existence of energy minimizers, which identifies a class of energy densities for which the model is mathematically well-posed.

In recent years, considerable attention has been devoted to fully nonlinear mechanical models describing the coupling between elasticity and nematic order (see [16, 1, 2, 6, 7, 10] and references therein). The Frank term, however, has been typically evaluated in the reference configuration while, when large deformations are in order, it is more natural to consider spatial variations in the deformed configuration. Our main result is precisely that of establishing (under reasonable assumptions) existence of minimal energy states when the Frank term is written in the deformed configuration.

From the mathematical point of view, the difficulty we face is that our energy functional has two terms, the Frank one defined on the deformed configuration, and the mechanical one defined on the reference configuration. Therefore, we need to push-forward the second one in order to work on the same domain. For this task, it becomes necessary to work with the inverse of the deformation mapping and establishing sufficient regularity properties of this inverse map using only the natural energy bounds is problematic.

Let $\mathcal{M} := \{F \in \mathbb{R}^{3 \times 3} : \det F = 1\}$ and let $W : \mathcal{M} \to [0, \infty)$ be a function such that $\widetilde{W}(F) := W(FF^T)$ is polyconvex and W(F) = 0 if and only if F = I. We follow [1, 10] and we consider an energy density $W_{\text{mec}} : \mathcal{M} \times \mathbb{S}^2 \to [0, \infty)$ defined by

$$W_{\mathrm{mec}}(F, \boldsymbol{n}) := W(V_{\boldsymbol{n}}^{-1}F),$$

where $V_{\boldsymbol{n}}$ is the stretch in the direction $\boldsymbol{n} \in \mathbb{S}^2$ of a fixed amplitude $\alpha > 0$:

$$V_{\boldsymbol{n}} := \alpha \boldsymbol{n} \otimes \boldsymbol{n} + (I - \boldsymbol{n} \otimes \boldsymbol{n}) / \sqrt{\alpha}.$$

Observe that $W_{\text{mec}}(F, \mathbf{n}) = 0$ implies $V_{\mathbf{n}}^{-1}F(V_{\mathbf{n}}^{-1}F)^T = I$ and so, since $V_{\mathbf{n}}^{-1}$ is symmetric, $FF^T = V_{\mathbf{n}}^2$. In particular, since det F = 1, by polar decomposition it follows that $F = V_{\mathbf{n}}R$ for some $R \in SO(3)$. This last equality summarizes in one formula the main features of

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the coupling between deformation F and nematic order n envisaged in [16], showing that every pair $(V_n R, n)$ is a 'natural' (or 'stress-free') state of the material.

We propose the following type of energy to describe nematic elastomers:

$$\mathcal{I}(u,\boldsymbol{n}) := \int_{u(\Omega)} |\nabla \boldsymbol{n}(y)|^2 dy + \int_{\Omega} W_{\text{mec}} \big(\nabla u(x), \boldsymbol{n}(u(x)) \big) dx, \tag{1}$$

where $u : \Omega \to \mathbb{R}^3$ is a deformation of a body whose reference configuration is Ω (a bounded, connected, open subset of \mathbb{R}^3) and $\boldsymbol{n} : u(\Omega) \to \mathbb{S}^2$ is the director field describing the nematic order in the elastomer. Note that the gradient operator in the first integral is meant with respect to the current spatial variable y, while the gradient in the second term is with respect to the material coordinate x. In what follows, $\mathcal{I}_{\text{nem}}(u, \boldsymbol{n}) = \int_{u(\Omega)} |\nabla \boldsymbol{n}|^2 dy$ and $\mathcal{I}_{\text{mec}}(u, \boldsymbol{n}) = \int_{\Omega} W_{\text{mec}}(\nabla u, \boldsymbol{n} \circ u) dx$ will denote the nematic (or Frank) and the mechanical term of our energy, respectively. As already highlighted, the main feature (and novelty) of our model is that it is formulated in the deformed configuration rather than in the reference one.

Let us introduce the ambient space of our problem, namely, the class of competitors we allow when minimizing energy (1). We assume that the deformations belong to

$$\mathcal{W}(\Omega, \mathbb{R}^3) := \left\{ u \in W^{1,3}(\Omega, \mathbb{R}^3) : \det \nabla u = 1 \text{ a.e. in } \Omega \right\}.$$

A function $u \in \mathcal{W}(\Omega, \mathbb{R}^3)$ has nice properties (see [12]): firstly, it is continuous and differentiable a.e. in Ω . Moreover, it satisfies the N property (|u(D)| = 0 whenever $D \subset \Omega$ is a measurable set such that |D| = 0), and the N^{-1} property $(|u^{-1}(D)| = 0$ whenever $D \subset \mathbb{R}^3$ is a measurable set such that |D| = 0).

Let $\Omega_u := \{x \in \Omega : u \text{ is differentiable in } x\}$. By [11, Theorem 3.1], u is almost locally invertible in Ω_u : for every $x_0 \in \Omega_u$ there are $r = r(x_0) > 0$, an open neighborhood $O \subset \Omega$ of x_0 , and a function $w \in W^{1,1}(B_r(y_0), \mathbb{R}^3)$ (with $y_0 = u(x_0)$) such that

$$u(O) = B_r(y_0)$$
 and $w \circ u(x) = x$ a.e. $x \in O$;
 $w(B_r(y_0)) = O$ a.e. and $u \circ w(y) = y$ for all $y \in B_r(y_0)$;
 $\nabla w(y) = (\nabla u)^{-1}(w(y))$ a.e. $y \in B_r(y_0)$.

Note that, if $[u(\Omega)]$ denotes the interior of $u(\Omega)$, then $u(\Omega_u) \subset [u(\Omega)]$ and therefore, by the N property, $|u(\Omega) \setminus [u(\Omega)]| = 0$.

Remark. In general a map $u \in \mathcal{W}(\Omega, \mathbb{R}^3)$ could be not open, as shown in [5, Example 1] by considering the cylinder $\Omega := \{x \in \mathbb{R}^3 : 0 \le R < 1, |x_3| < 1\}$, with $R := (x_1^2 + x_2^2)^{1/2}$, and the deformation $u(x) := 2^{1/3}(R^{-1/2}x_1, R^{-1/2}x_2, Rx_3)$. Since u maps the axis of the cylinder into the origin, $u(\Omega)$ is not open.

Regarding the director field \boldsymbol{n} , we assume that, given a deformation u, it belongs to $H^1([u(\Omega)], \mathbb{S}^2)$. Note that, since \boldsymbol{n} is measurable and u is continuous, the composition $\boldsymbol{n} \circ u$ is measurable. Moreover, since u has the N^{-1} property, this composition does not depend on the particular representative of \boldsymbol{n} . Therefore, the mechanical part of our energy is well defined.

Let us make some comments about our ambient space. The stored energy density we have in mind is the standard one describing incompressible Ogden materials [10, 1]:

$$\widetilde{W}(F) := \sum_{i} a_1 \left(v_1^{\alpha_i} + v_2^{\alpha_i} + v_3^{\alpha_i} - 3 \right) + \sum_{j} b_1 \left((v_1 v_2)^{\beta_j} + (v_1 v_3)^{\beta_j} + (v_2 v_3)^{\beta_j} - 3 \right),$$

where $v_k = v_k(F)$ are the singular values of F, $a_i > 0$, $\alpha_i \ge 1$, $b_j > 0$, $\beta_j \ge 1$, and the normalizing constant 3 = trI is added so that \widetilde{W} vanishes when $FF^T = I$. By [8, Theorem 4.9-2], we know that on \mathcal{M} such energy is polyconvex and satisfies a coerciveness inequality of the form

$$W(F) \ge a|F|^{\alpha} + b|\mathrm{cof}\,F|^{\beta} - c,$$

for suitable a, b, c > 0 and with $\alpha = \max_{i} \{\alpha_i\}, \beta = \max_{j} \{\beta_j\}$. At the moment our existence result is limited to the case $\alpha = 3$, so that the right ambient space is $\mathcal{W}(\Omega, \mathbb{R}^3)$. Indeed we need a certain regularity not only on the deformation u, but also on its "inverse" u^{-1} . Of course it should be desirable to extend the result to weaker coercivity assumptions already considered in nonlinear elasticity, such as $\alpha = 2$ and $\beta = 3/2$ (see [4, 15]), but this goal seems hard to achieve. It would also be interesting to formulate our model in the setting introduced in [13, 14], namely, a variational model that allows for cavitation, through a functional that measures in the deformed configuration the surface area of the cavities opened by the deformation.

In order to prove the existence of minimizers in our model, we need a couple of ingredients. The first one is a stability result about invertibility in the space $\mathcal{W}(\Omega, \mathbb{R}^3)$.

Lemma 1. Let $u, u_k \in \mathcal{W}(\Omega, \mathbb{R}^3)$ be such that $u_k \rightharpoonup u$ in $W^{1,3}$ and let Ω' be an open set compactly included in Ω . Then there exists a subsequence of $\{u_k\}$ (not relabeled) such that u_k converges to u uniformly in $\overline{\Omega}'$. Moreover, for any $x_0 \in \Omega'_u$ there exist open neighborhoods $O, O_k \subset \Omega'$ of $x_0, k_0 \in \mathbb{N}$, $r = r(x_0) > 0$, and $w, w_k : B_r(y_0) \to \mathbb{R}^3$ with $y_0 = u(x_0)$ such that for $k \ge k_0$

- $u(O) = B_r(y_0)$ and $w \circ u(x) = x$ a.e. $x \in O$;
- $u_k(O_k) = B_r(y_0)$ and $w_k \circ u_k(x) = x$ a.e. $x \in O_k$;
- $u \circ w(y) = y$ and $\nabla w(y) = (\nabla u)^{-1}(w(y))$ a.e. $y \in B_r(y_0);$
- $u_k \circ w_k(y) = y$ and $\nabla w_k(y) = (\nabla u_k)^{-1}(w_k(y))$ a.e. $y \in B_r(y_0);$
- $\inf\{\operatorname{diam}(w(B_s(y_0))) : s \le r\} = 0;$
- $\chi_{O_k} \rightarrow \chi_O$ pointwise a.e.;
- $w, w_k \in W^{1,\frac{3}{2}}(B_r(y_0), \mathbb{R}^3)$ and $w_k \rightharpoonup w$ in $W^{1,\frac{3}{2}}$; $\operatorname{cof} \nabla w, \operatorname{cof} \nabla w_k \in L^3(B_r(y_0), \mathbb{R}^{3 \times 3})$ and $\operatorname{cof} \nabla w_k \rightharpoonup \operatorname{cof} \nabla w$ in L^3 .

Proof. With the exception of the last point, this lemma can be obtained from [11, Lemmata 4.3 and 4.5]. Remember that if $F \in \mathcal{M}$, then $\operatorname{cof} F^T = F^{-1}$. By a change of variables (see [11, Lemmata 2.4 and 3.5]) we have

$$\int_{B_r(y_0)} |\cos \nabla w_k|^3 dy = \int_{B_r(y_0)} |(\nabla w_k)^{-1}|^3 dy = \int_{O_k} |\nabla u_k|^3 dx,$$

so that $\{cof \nabla w_k\}$ is bounded in L^3 . Similar arguments show that $cof \nabla w$ belongs to L^3 . In order to prove weak convergence, we still make use of a change of variables. Indeed, because of the low integrability of ∇w_k , we cannot appeal to the usual continuity of the cofactor ([9, Theorem 8.20]). Let $\phi \in C_0^{\infty}(B_r(y_0))$. Note that $\chi_{O_k}\phi \circ u_k$ converges to $\chi_O\phi \circ u$ pointwise a.e. and therefore in L^p for any p finite (by Vitali convergence theorem, being bounded in L^{∞}). We have

$$\lim_{k} \int_{B_{r}(y_{0})} \phi(y) \operatorname{cof} \nabla w_{k}(y) dy = \lim_{k} \int_{O_{k}} \phi(u_{k}(x)) (\nabla u_{k}(x))^{T} dx$$
$$= \int_{O} \phi(u(x)) (\nabla u(x))^{T} dx = \int_{B_{r}(y_{0})} \phi(y) \operatorname{cof} \nabla w(y) dy.$$

The second ingredient is the continuity of the cofactor of the "perturbed" gradient $\nabla w V_n$ with respect to weak convergence.

Lemma 2. Let B be a bounded open subset of \mathbb{R}^3 , and let $\{w_k\} \subset W^{1,\frac{3}{2}}(B,\mathbb{R}^3)$ and $\{n_k\} \subset L^{\infty}(B,\mathbb{S}^2)$ be two sequences such that $w_k \to w$ weakly in $W^{1,\frac{3}{2}}$, $\operatorname{cof} \nabla w_k \to \operatorname{cof} \nabla w$ weakly in L^3 , and $n_k \to n$ pointwise a.e.. Then $\nabla w_k V_{n_k} \to \nabla w V_n$ weakly in $L^{\frac{3}{2}}$ and $\operatorname{cof}(\nabla w_k V_{n_k}) \to \operatorname{cof}(\nabla w V_n)$ weakly in L^3 .

Proof. First of all, note that $\mathbf{n} \in L^{\infty}(B, \mathbb{S}^2)$. Moreover $V_{\mathbf{n}_k} \to V_{\mathbf{n}}$ and $V_{\mathbf{n}_k}^{-1} \to V_{\mathbf{n}}^{-1}$ pointwise a.e.. On the other hand, since $\{V_{\mathbf{n}_k}\}$ and $\{V_{\mathbf{n}_k}^{-1}\}$ are both bonded in L^{∞} , Vitali convergence theorem leads to $V_{\mathbf{n}_k} \to V_{\mathbf{n}}$ and $V_{\mathbf{n}_k}^{-1} \to V_{\mathbf{n}}^{-1}$ strongly in any L^p , p finite. This directly implies that $\nabla w_k V_{\mathbf{n}_k} \to \nabla w V_{\mathbf{n}}$ weakly in L^1 , and then in $L^{\frac{3}{2}}$ because there $\{\nabla w_k V_{\mathbf{n}_k}\}$ is bounded. Similarly

$$\operatorname{cof}(\nabla w_k V_{\boldsymbol{n}_k}) = (V_{\boldsymbol{n}_k})^{-1}(\operatorname{cof} \nabla w_k) \rightharpoonup (V_{\boldsymbol{n}})^{-1}(\operatorname{cof} \nabla w) = \operatorname{cof}(\nabla w V_{\boldsymbol{n}}) \text{ weakly in } L^3.$$

We are now ready to prove our main result.

Theorem. Assume that \widetilde{W} satisfies the following coercivity condition:

$$\widetilde{W}(F) \ge c_1 |F|^3 - c_2 \quad \forall F \in \mathcal{M}$$
 (2)

for some constants $c_1, c_2 > 0$. Assume also that Ω has smooth boundary and let $\Gamma \neq \emptyset$ be an open (in the relative topology) subset of $\partial\Omega$. Given $(u_0, \mathbf{n}_0) \in \mathcal{W}(\Omega, \mathbb{R}^3) \times H^1([u_0(\Omega)], \mathbb{S}^2)$ such that $\mathcal{I}(u_0, \mathbf{n}_0)$ is finite, define $\mathcal{W}_{\Gamma, u_0}(\Omega, \mathbb{R}^3) := \{u \in \mathcal{W}(\Omega, \mathbb{R}^3) : u = u_0 \text{ on } \Gamma\}$ (the equality is intended in the sense of traces). Then, there exists $(u, \mathbf{n}) \in \mathcal{W}_{\Gamma, u_0}(\Omega, \mathbb{R}^3) \times H^1([u(\Omega)], \mathbb{S}^2)$ minimizing \mathcal{I} .

Proof. We are going to use the direct method of the calculus of variations. Let $\{(u_k, n_k)\} \subset W_{\Gamma, u_0}(\Omega, \mathbb{R}^3) \times H^1([u_k(\Omega)], \mathbb{S}^2)$ be a minimizing sequence. Since $F(u_k, n_k) \leq F(u_0, n_0)$, and $\{(V_{n_k})^{-1}\}$ is bounded in L^{∞} , assumption (2) implies that $\{\nabla u_k\}$ is bounded in L^3 . Moreover, thanks to the boundary condition and the Poincaré inequality, $\{u_k\}$ is bounded in L^3 . Therefore, by refining the sequence if necessary, we have that u_k converges weakly in $W^{1,3}$ to a certain u. The continuity of the determinant (see [9, Theorem 8.20]) ensures that det $\nabla u_k \to \det \nabla u$ in distribution and then that det $\nabla u = 1$ a.e. in Ω . Since the boundary condition is preserved in the limit, we conclude that u belongs to $W_{\Gamma, u_0}(\Omega, \mathbb{R}^3)$.

We now extend by zero n_k and ∇n_k to the whole \mathbb{R}^3 . Since the sequence $\{n_k\}$ is bounded in L^{∞} and the sequence $\{\nabla n_k\}$ is bounded in L^2 , by refining if necessary, we can assume that for certain l, l'

$$\lim_{k} \boldsymbol{n}_{k} = l \text{ weakly* in } L^{\infty} \text{ and } \lim_{k} \nabla \boldsymbol{n}_{k} = l' \text{ weakly in } L^{2}.$$

We have to prove that there exists $\boldsymbol{n} \in H^1([u(\Omega)], \mathbb{S}^2)$ such that $l = \boldsymbol{n}$ and $l' = \nabla \boldsymbol{n}$ on $[u(\Omega)]$. By locality, it is sufficient to prove this in an open neighborhood of each point of $[u(\Omega)]$. Given $\Omega' \subset \Omega$, let $x_0 \in \Omega'_u$ and O, O_k, r, y_0 as in Lemma 1. Since $B_r(y_0) = u_k(O_k) \subset [u_k(\Omega)]$, we have $\{\boldsymbol{n}_k|_{B_r(y_0)}\} \subset H^1(B_r(y_0), \mathbb{R}^3)$. Therefore $\boldsymbol{n} := l|_{B_r(y_0)}$ belongs to $H^1(B_r(y_0), \mathbb{R}^3)$ and $\nabla \boldsymbol{n} = l'|_{B_r(y_0)}$. By the compact embedding of H^1 in L^2 , we can also assume that $\boldsymbol{n}_k \to \boldsymbol{n}$ pointwise a.e. in $B_r(y_0)$. In particular $\boldsymbol{n} \in \mathbb{S}^2$ a.e.

By lower semicontinuity of convex functionals with respect to weak convergence, we have

$$\liminf_k \mathcal{I}_{\rm nem}(u_k, \boldsymbol{n}_k) = \liminf_k \int_{\mathbb{R}^3} |\nabla \boldsymbol{n}_k|^2 dy \ge \int_{\mathbb{R}^3} |l'|^2 dy \ge \mathcal{I}_{\rm nem}(u, \boldsymbol{n})$$

It remains to show that $\liminf_k \mathcal{I}_{\text{mec}}(u_k, n_k) \geq \mathcal{I}_{\text{mec}}(u, n)$. Refining the sequence $\{(u_k, n_k)\}$ we can assume that the limit is actually a limit: in this way, if necessary, we can further refine the sequence keeping the estimates. In order to avoid the difficulty related to the convergence of the composition $n_k \circ u_k$, we operate a change of variables and work on the deformed configuration.

We start with a localization argument. Using the same notation of Lemma 1, given $\Omega' \subset \Omega$, $x_0 \in \Omega'_u$ and $s \leq r$, we set $U := w(B_s(y_0))$ and $U_k := w_k(B_s(y_0))$. For $k \geq k_0$ we have

$$\int_{U_k} W_{\text{mec}} \left(\nabla u_k(x), \boldsymbol{n}_k(u_k(x)) \right) dx = \int_{U_k} \widetilde{W} \left(V_{\boldsymbol{n}_k}^{-1}(u_k(x)) \nabla u_k(x) \right) dx$$
$$= \int_{B_s(y_0)} \widetilde{W} \left(V_{\boldsymbol{n}_k}^{-1}(y) (\nabla w_k)^{-1}(y) \right) dy = \int_{B_s(y_0)} \widetilde{W} \left((\nabla w_k V_{\boldsymbol{n}_k})^{-1}(y) \right) dy$$

and similarly

$$\int_{U} W_{\text{mec}} \big(\nabla u(x), \boldsymbol{n}(u(x)) \big) dx = \int_{B_s(y_0)} \widetilde{W} \big((\nabla w V_{\boldsymbol{n}})^{-1}(y) \big) dy.$$

Since $(\nabla w_k V_{\boldsymbol{n}_k})^{-1} = \operatorname{cof}(\nabla w_k V_{\boldsymbol{n}_k})^T$ and $\operatorname{cof}(\nabla w_k V_{\boldsymbol{n}_k})^{-1} = (\nabla w_k V_{\boldsymbol{n}_k})^T$, by using Lemma 2, the polyconvexity of \widetilde{W} , and the semicontinuity of convex functionals, we obtain

$$\liminf_{k} \int_{U_{k}} W_{\text{mec}} \big(\nabla u_{k}(x), \boldsymbol{n}_{k}(u_{k}(x)) \big) dx \ge \int_{U} W_{\text{mec}} \big(\nabla u(x), \boldsymbol{n}(u(x)) \big) dx.$$

We then use a covering argument. For any $x \in \Omega'_u$, let w^x , $w^x_k : B_{r(x)}(u(x)) \to \mathbb{R}^3$ be the inverse functions of u, u_k in a neighborhood of u(x) given by Lemma 1. Since

$$\{w^x(B_s(u(x))): x \in \Omega'_u \text{ and } s \le r(x)\}$$

is a covering of Ω'_u and $\inf\{\operatorname{diam}(w^x(B_s(u(x)))) : s \leq r(x)\} = 0$, by Vitali covering theorem (see [3, Theorem 2.2.2]), there exists $\{(x_j, s_j)\}_{j \in \mathbb{N}}$ such that, setting $U^j := w^{x_j}(B_{s_j}(u(x_j)))$, the family $\{U^j\}_{j \in \mathbb{N}}$ is a covering of Ω' (up to a set of zero measure) and $\overline{U}^j \cap \overline{U}^i = \emptyset$ if $j \neq i$. For $\varepsilon \in (0, r(x_j) - s_j)$, let $U^{j,\varepsilon} := w^{x_j}(B_{s_j+\varepsilon}(u(x_j)))$. For fixed $h \in \mathbb{N}, i, j \in \{1, \ldots, h\}$, and choosing ε small enough we have $U^{j,\varepsilon} \cap U^{i,\varepsilon} = \emptyset$ if $j \neq i$. Observe now that, since u_k converges to u uniformly in Ω' , for k large enough (depending on ε) one has $U_k^j := w_k^{x_j}(B_{s_j}(u(x_j))) \subset U^{j,\varepsilon}$ so that $U_k^j \cap U_k^i = \emptyset$ if $j \neq i$. Indeed, if $z \in U_k^j$, then

$$|u(z) - u(x_j)| \le |u(z) - u_k(z)| + |u_k(z) - u(x_j)| < s_j + \varepsilon$$

as soon as $||u - u_k||_{\infty} \leq \varepsilon$. By the previous localization argument, we have

$$\begin{split} \lim_{k} \mathcal{I}_{\mathrm{mec}}(u_{k}, \boldsymbol{n}_{k}) &\geq \liminf_{k} \int_{\bigcup_{j=1}^{h} U_{k}^{j}} W_{\mathrm{mec}}\big(\nabla u_{k}(x), \boldsymbol{n}_{k}(u_{k}(x))\big) dx \\ &\geq \int_{\bigcup_{j=1}^{h} U^{j}} W_{\mathrm{mec}}\big(\nabla u(x), \boldsymbol{n}(u(x))\big) dx. \end{split}$$

By letting h go to infinity and by invading Ω with Ω' we conclude the proof.

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