NULL LAGRANGIANS FOR NEMATIC ELASTOMERS

GIUSEPPE SACCOMANDI AND RAFFAELE VITOLO

Abstract. In this paper we compute all possible null Lagrangians (null energies) for the mechanics of a distinguished class of continua, the nematic elastomers. The computation is done in order to help to relate different physically equivalent theories of nematic elastomers. We discuss both local and global (hence topological) aspects of the problem.

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1. Introduction

A rubber-like solid that has been formed by the cross-linking of a polymeric fluid and that includes liquid crystals in molecules as elements of its main-chain is called an *optical* or *nematic elastomer* [22]. A continuum theory for the mechanical behaviour of nematical elastomers has been recently developed by Anderson, Carlson and Fried [2]. This theory has been developed following closely the pioneering approach by Ericksen [5] and Leslie [11]. In some sense, nematic elastomers is a field theory generalising both nonlinear elasticity and classical liquid crystal theory. Indeed, for a nematic elastomer the free energy ψ is a function of the deformation gradient $\boldsymbol{F}$ of the elastomer, the orientation of the nematic molecule $\boldsymbol{n}$ and the orientation gradient $\boldsymbol{G} = \operatorname{Grad} \boldsymbol{n}$. Specifically, the deformation assigns to each point $\boldsymbol{X}$ of the body in a reference state $\mathcal{R}_0$ a point $\boldsymbol{x} = \boldsymbol{x}(\boldsymbol{X})$ in the deformed region $\mathcal{R}_1$ ($\mathcal{R}_0$ and $\mathcal{R}_1$ are regular regions of the 3-dimensional Euclidean space). Therefore, considering only smooth invertible deformations, $\boldsymbol{F}(\boldsymbol{X})$ is defined as

$$\boldsymbol{F}(\boldsymbol{X}) = \operatorname{Grad} \boldsymbol{x}(\boldsymbol{X}). \tag{1.1}$$

On the other hand, $\boldsymbol{n}$ is the referencial descriptor of the orientation and length of the nematic molecule associated with a point $\boldsymbol{X}$ in $\mathcal{R}_0$. In [2] only nematic elastomers that consist on inextensible nematic molecules are considered. For such microstructurally inextensible materials we may restrict $\boldsymbol{n}$ to be a unit vector-valued orientation.

The determination of a suitable functional form for the free energy density function ψ is an actual, very active field of research. Two main direction can be followed to develop such material models: the *phenomenological* approach based on the axiomatic theory of continuum mechanics and the *statistical* approach based on molecular concepts. The

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phenomenological approach is for example followed in [7]. The molecular approach is pursued, for example, by the soft matter Cavendish group [16]. In the long and hard way to the determination of effective functional form of the energy density function it is well-known that a precious help that may come from mathematics is the determination of all the *null Lagrangians* associated with the theory. Null Lagrangian is the name given to any energy density that does not contribute to the equilibrium equation for a given energy function. In the classical theory of liquid crystals it is well-known the history of the k_{24} Frank's constant [19]. In 1958 Frank proposed a representation formula for nematics and cholesterics crystals that are quadratic polynomials in $\boldsymbol{G}$. This formula depends on some material moduli which has to be determined experimentally. Estimates of all moduli but one have been made by comparing inverse solution with results of experiments disregarding surface forces and couples. Only for the modulus k_{24} this was impossible. Indeed, Ericksen in [6] shown that the term associated with this material modulus is a null Lagrangian. Therefore, null Lagrangians are fundamental to classify different theories and a recent example of their usefulness is given in [12].

If in the framework of liquid crystals all the null Lagrangians have been computed by a direct method in [6], in nonlinear elasticity all the null Lagrangians can be derived from the general computations by Olver and Sivaloganathan in [14] where a Lagrangian of the form $\psi(\boldsymbol{X}, \boldsymbol{x}, \boldsymbol{F})$. This situation suggests to obtain the null Lagrangians for nematic elastomers by considering a Lagrangian of the form

$$\psi(\boldsymbol{X}, \boldsymbol{x}, \boldsymbol{n}, \boldsymbol{F}, \boldsymbol{G}). \tag{1.2}$$

It is clear that this Lagrangian only in a subcase will be of interest in the theory of nematic elastomers because its general form has to be restricted by *frame indifference* and material symmetry requirements. But here we are more interested in some mathematical speculations about a possible general method for the determination of the complete set of null Lagrangians. This method use the geometrical framework of variational sequences proposed by Anderson, Tulczyjev, Vinogradov and others. This geometrical framework is used not only for academic purposes, but because it allows also to deal with non simply connected domains, or more general topologically non-trivial domains. It is well-known that in liquid crystal theory defects of various kind have an important meaning and literature on defects studied within the classical theory of liquid crystals is huge [19]. It is clear that when we have to cope with defects more refined geometrical methods have to be introduced.

The plan of the paper is the following. In the next section we will introduce the basic settings, such us domains, fields and coordinates. The global computation of null lagrangians will be done in Section 3. Here, in subsection 3.1 we recall basic facts about variational sequences and in the next subsection we compute null Lagrangians in the case when the domain of the fields is 2-dimensional and 3-dimensional. We obtain that, even in the case of a trivial domain, in the 2-dimensional case a topological term appears summed with the local expression that is expected according to [1, 8, 10, 14]. Section 4 will be devoted to concluding remarks.

2. Lagrangians for liquid crystals

The *material space* of our problem, i.e., the space of independent variables, is a regular domain $\mathcal{R}_0 \subset \mathbb{R}^n$, where $n = 2$ (the limit case of a very thin liquid crystal film) or $n = 3$ (the general case). We put (local) coordinates (X^i) on $\mathcal{R}_0$.

The *fields space* is $\mathbb{R}^3 \times S^2$, where $\mathbb{R}^3$ is the space of deformations and S^2 (the unit sphere in $\mathbb{R}^3$) is the space of orientations of the crystals. A *deformation field* is a (local) map $\boldsymbol{x}\colon \mathcal{R}_0 \to \mathbb{R}^3$. An *orientation field* is a (local) map $\boldsymbol{n}\colon \mathcal{R}_0 \to S^2$. We put (local) coordinates (x^j, n^α) on $\mathbb{R}^3 \times S^2$.

The *total space* is $\mathcal{R}_0 \times S^2 \times \mathbb{R}^3$, the product of the material space with the fields space. We put (local) coordinates $(X^i; x^j, n^\alpha)$ on $\mathcal{R}_0 \times S^2 \times \mathbb{R}^3$.

The *velocity space* is $\mathcal{R}_0 \times T^*\mathcal{R}_0 \otimes (T\mathbb{R}^3 \times TS^2)$, the product of the material space with the space of differentials of fields $(\boldsymbol{x}, \boldsymbol{n})\colon \mathcal{R}_0 \to \mathbb{R}^3 \times S^2$. We put (local) coordinates

$$(X^i; x^j, n^\alpha; x^j_i, n^\alpha_i) \quad \text{on} \quad \mathcal{R}_0 \times T^*\mathcal{R}_0 \otimes (T\mathbb{R}^3 \times TS^2).$$

We remark that the velocity space is nothing but the first jet space of the trivial fibering

$$\pi\colon \mathcal{R}_0 \times \mathbb{R}^3 \times S^2 \to \mathcal{R}_0$$

(see [15, 18] about jet spaces). So, we will denote the velocity space by $J^1\pi$, and the velocity of a field $(\boldsymbol{x}, \boldsymbol{n})$ by $j^1(\boldsymbol{x}, \boldsymbol{n})$.

Analogously, the *acceleration space* is $\mathcal{R}_0 \times (T^*\mathcal{R}_0 \odot T^*\mathcal{R}_0) \otimes (T\mathbb{R}^3 \times TS^2)$, the product of the material space with the space of second differentials of fields $(\boldsymbol{x}, \boldsymbol{n})\colon \mathcal{R}_0 \to \mathbb{R}^3 \times S^2$. Again, the acceleration space is the second jet space of π, and is denoted by $J^2\pi$. We put (local) coordinates

$$(X^i; x^j, n^\alpha; x^j_i, n^\alpha_i; x^j_{hk}, n^\alpha_{hk}) \quad \text{on} \quad J^2\pi.$$

We say a (first-order) *Lagrangian* to be a function of the type

$$\psi\colon J_1\pi \to \mathbb{R}.$$

Accordingly, we have the *Lagrangian density* $\psi\,\upsilon$, where υ is the standard volume form on $\mathbb{R}^n$ restricted to $\mathcal{R}_0$. The Lagrangian density is an n-form on $J^1\pi$. It can be integrated over any field $(\boldsymbol{x}, \boldsymbol{n})$ and its derivatives $(\boldsymbol{F}, \boldsymbol{G})$ defined on any compact open subset $U \subset \mathcal{R}_0$ with smooth boundary, producing the *action*

$$\mathcal{A}(\boldsymbol{x}, \boldsymbol{n}; U) = \int_U \psi(\boldsymbol{X}, \boldsymbol{x}(\boldsymbol{X}), \boldsymbol{n}(\boldsymbol{X}), \boldsymbol{F}(\boldsymbol{X}), \boldsymbol{G}(\boldsymbol{X}))\,\upsilon.$$

A standard procedure yields then the (global) *Euler–Lagrange morphism*

$$\mathcal{E}(\psi\upsilon)\colon J^2\pi \to (T^*\mathbb{R}^3 \times T^*S^2) \otimes \wedge^3 T^*\mathcal{R}_0,$$

where $T^*\mathbb{R}^3 \times T^*S^2$ is the dual tangent space to the fields space. Note that the factor $\wedge^3 T^*\mathcal{R}_0$ is present because the Euler–Lagrange morphism is a vector-valued density. The coordinate expression of $\mathcal{E}(\psi\upsilon)$ is the usual one:

$$\mathcal{E}(\psi\upsilon)_\alpha = \frac{\partial\psi}{\partial n^\alpha} - \frac{d}{dX^i}\frac{\partial\psi}{\partial n^\alpha_i}, \qquad \mathcal{E}(\psi\upsilon)_j = \frac{\partial\psi}{\partial x^j} - \frac{d}{dX^i}\frac{\partial\psi}{\partial x^j_i},$$

where

$$\frac{d}{dX^i} = \frac{\partial}{\partial X^i} + x^k_i\frac{\partial}{\partial x^k} + n^\alpha_i\frac{\partial}{\partial n^\alpha} + x^k_{hi}\frac{\partial}{\partial x^k_h} + n^\alpha_{hi}\frac{\partial}{\partial n^\alpha_h}.$$

Admissible fields are assumed to fulfill the *Euler–Lagrange equation*

$$\mathcal{E}(\psi\upsilon)\circ j_2(\boldsymbol{x},\boldsymbol{n})=0.$$

We observe that the Euler–Lagrange morphism $\mathcal{E}(\psi\upsilon)$ can also be regarded as an $(n+1)$-form on $J^2\pi$.

3. Global computation of null Lagrangians

A *null Lagrangian* is a Lagrangian ψ such that $\mathcal{E}(\psi\upsilon)=0$ identically. We want to provide the coordinate expression of the most general first order null Lagrangian in our setting. To this aim, we will use the theory of *variational sequences*. This theory started from the idea that the operation $\mathcal{E}$, which carries any Lagrangian density into the corresponding Euler–Lagrange equations, should be a part of a *complex*. This means that $\mathcal{E}$ behaves like the differential of forms under several viewpoints. For example, we have $\mathcal{E}^2=0$, and, if $\mathcal{E}(\psi\upsilon)=0$, then there exists locally an $(n-1)$-form P (on a star-shaped open subset of $J^1\pi$) such that

$$\mathcal{E}(P)=\psi\upsilon \tag{3.1}$$

(in the given subset). We will clarify in next subsection what is $\mathcal{E}$ on forms of degrees other than n. So, in order to solve our problem, we must provide the expression for the most general form P such that equation (3.1) holds. But it could happen that ψ be *only locally* of the kind of (3.1). So, the solution to our problem is completed by providing a description of the vector space of $\mathcal{E}$-closed Lagrangians modulo $\mathcal{E}$-exact Lagrangians. This is clearly a cohomology class with respect to the differential $\mathcal{E}$, and we will compute it.

Now we recall basic facts from the theory of variational sequences. Then, we apply this theoretical background to our setting in order to classify first order null Lagrangians.

3.1. **Variational sequence.**

We will describe the theory of Vinogradov [18] and his group [3], although our results could also be derived within other theories (for instance Anderson's [1] or Krupka's theory [9]), also in view of the equivalence results of [20, 21]. We will restrict the theory to our first-order model, using results from [8, 10, 21]. Note that the restriction to first-order theories of variational sequences seems to be essential for physical reasons; the standard infinite-order theory would not help us enough in this case. Indeed, higher order Lagrangians can have no physical meaning [19].

Let us denote the space of *k-forms* on $J^1\pi$ by Λ^k_1. We have the distinguished subspace $\mathcal{C}^1\Lambda^k_1\subset\Lambda^k_1$ of *contact k-forms* $\alpha\in\Lambda^k_1$; they are characterised by $(j^1(\boldsymbol{x},\boldsymbol{n}))^*(\alpha)=0$ for all fields $(\boldsymbol{x},\boldsymbol{n})$ (here, * is just the standard pull-back of forms, i. e., the evaluation of the form along the field). In coordinates, contact one-forms are generated by the following one-forms

$$\omega^i=dn^i-n^i_jdX^j,\qquad \theta^k=dx^k-x^k_jdX^j,$$
$$\omega^i_h=dn^i-n^i_{hj}dX^j,\qquad \theta^k_h=dx^k_h-x^k_{hj}dX^j.$$

We consider also he spaces generated by exterior products of two or more contact forms, thus obtaining the spaces $\mathcal{C}^2\Lambda^k_1$, $\mathcal{C}^3\Lambda^k_1$, ... with the obvious sequence of inclusions

(*filtration*, in the terminology of homological algebra)

$$\Lambda^k_1 = \mathcal{C}^0\Lambda^k_1 \supset \mathcal{C}^1\Lambda^k_1 \supset \mathcal{C}^2\Lambda^k_1 \supset \dots \tag{3.2}$$

The differential of forms d preserves $\mathcal{C}^l$ so that on quotient spaces $\mathcal{C}^*\Lambda^*_1/\mathcal{C}^{*+1}\Lambda^*$ it is defined the quotient differential $\mathcal{E}$. This differential, together with (3.2), produces the so-called *first order $\mathcal{C}$-spectral sequence*. Such a construction has been done in [21] taking as a model the standard construction on infinite order jets [3, 18]. The $\mathcal{C}$-spectral sequence yields a lot of interesting facts. We just recall the *first order variational sequence*

$$0 \longrightarrow \mathbb{R} \longrightarrow \bar\Lambda^0_1 \longrightarrow \dots \longrightarrow \bar\Lambda^{n-1}_1 \longrightarrow \bar\Lambda^n_1 \longrightarrow E^1_1 \longrightarrow E^2_1 \longrightarrow \dots \tag{3.3}$$

Here,

(1) $\bar\Lambda^*_1 = \Lambda^*_1/\mathcal{C}^1\Lambda^*_1$. The quotient can be evaluated as follows. Consider the local basis dX^j, dx^i, dn^α, dx^i_j, dn^α_j of one-forms on $J^1\pi$. This can be replaced by the basis dX^j, ω^i, ω^i_h, θ^k, θ^k_h sending dX^j to itself, dn^α in $\omega^\alpha + n^\alpha_j dX^j$, dn^α_h in $\omega^\alpha_h + n^\alpha_{hj}dX^j$, and so on. Then, forms with the derived number of *horizontal* factors dX^j can be taken. This is a global operation denoted by h (*horizontalization*). It can be easily seen that, if $\beta \in \Lambda^k_1$, then the representative $h(\beta) = \alpha \in \bar\Lambda^k_1$ of $[\beta] \in \Lambda^*_1/\mathcal{C}^1\Lambda^*_1$ is

$$\alpha = \alpha_{\lambda_1\dots\lambda_k} dX^1 \wedge \dots \wedge dX^k, \tag{3.4}$$

where $\alpha_{\lambda_1\dots\lambda_k}$ is a polynomial of k-th degree in the second-order derivatives x^i_{hj}, n^α_{hj}.

(2) $\bar\Lambda^n_1$ contains first-order Lagrangian densities, according to the above considerations. We notice that the passage to the quotient space allows us to discard forms β on which the action functional $\int_U (j^1(\boldsymbol{x}, \boldsymbol{n}))^*(\beta)$ would be identically zero. We remark also that the image $\mathcal{E}(\alpha)$ of an $(n-1)$-form $\alpha \in \bar\Lambda^{n-1}_1$ is a trivial Lagrangian density, due to $\mathcal{E}^2 = 0$.

(3) $\bar\Lambda^k_1 \to \bar\Lambda^{k+1}_1$ is just the quotient differential $\mathcal{E}$, defined by $\mathcal{E}(h(\beta)) = h(d\beta)$.

(4) E^1_1 is the quotient of the space $\mathcal{C}^1\Lambda^{n+1}_1/\mathcal{C}^2\Lambda^{n+1}_1$ with the space $\mathcal{E}(\mathcal{C}^1\Lambda^n_1/\mathcal{C}^2\Lambda^n_1)$, hence it is the $n+1$-th cohomology class of the quotient differential $\mathcal{E}$. It contains Euler–Lagrange type forms. Here, the double quotient allows us to discard both forms annihilating on any field and forms that yield a total divergence when computed on the variation $(\delta\boldsymbol{x}, \delta\boldsymbol{n})$ of any field.

(5) $\bar\Lambda^n_1 \to E^1_1$ is the Euler–Lagrange operator, still denoted by $\mathcal{E}$ by an abuse of notation, sending any Lagrangian density into its Euler–Lagrange $(n+1)$-form.

(6) The cohomology of the above sequence is equal to the de Rham cohomology of the total space $\mathcal{R}_0 \times \mathbb{R}^3 \times S^2$ [18]. This means that the variational sequence is locally exact.

3.2. **First-order null lagrangians.** Here we provide the local expression for the most general variationally trivial first-order Lagrangian in our setting. We also solve the problem from a global viewpoint.

First of all, we observe that the space $\bar\Lambda^n_1$ (see the above item 2) does not contain only first-order Lagrangian densities (according to our definition): it is the space of forms of

the type $\bar{\psi}\upsilon$, where

$$\bar{\psi}\colon J^2\pi \to \mathbb{R} \tag{3.5}$$

is a polynomial of n-th degree in second-order derivatives n^α_{hj}, u^i_{hj} of distinguished type [21]. It follows that it is not sufficient to apply the local exactness of the variational sequence (see item 6) to solve our problem. More precisely: if $\alpha \in \bar{\Lambda}^n_1$ is such that $\mathcal{E}(\alpha) = 0$, then there exists (at least locally) $\beta \in \bar{\Lambda}^{n-1}_1$ such that $\mathcal{E}(\beta) = \alpha$. But then (see equation (3.4)) β is a form whose coefficients depend on second-order derivatives. In order to characterize locally first-order null Lagrangians we will use the following theorem.

Theorem 3.1 (local expression)**.** *Let $\psi\upsilon \subset \bar{\Lambda}^n_1$ be a first-order null Lagrangian, i. e., $\mathcal{E}(\psi\upsilon) = 0$. Then there exists* locally *an $(n-1)$-form $P \in \Lambda^{n-1}_0$ (i. e., a form on the total space) such that*

$$\psi\upsilon = \mathcal{E}(h(P)) = h(dP). \tag{3.6}$$

Conversely, any Lagrangian of the local form $\psi\upsilon = \mathcal{E}(h(P)) = h(dP)$ is null.

Proof. This theorem is a classical result (see, *e.g.*, [5]). It has been generalized to arbitrary order Lagrangians in [1, 9, 10, 8]. □

The above theorem solves the problem of finding a minimal order potential for first-order null Lagrangians. At the same time it gives the form of the most general first-order null Lagrangian. We shall provide the coordinate expression for the Lagrangians of the above theorem.

Case n=2. The coordinate expression of P is

$$P = p_i dX^i + p_k dx^k + p_\alpha dn^\alpha, \tag{3.7}$$

where p_i, p_k, p_α, are local functions of (X^j, x^h, n^β). Then we have

$$h(P) = \left(p_i + p_k + x^k_i p_\alpha n^\alpha_i\right) dX^i \tag{3.8}$$

$$\begin{aligned} dP = {} & \frac{\partial p_i}{\partial X_j}\, dX^j \wedge dX^i + \frac{\partial p_\alpha}{\partial n^\beta}\, dn^\beta \wedge dn^\alpha + \frac{\partial p_k}{\partial x^h}\, dx^h \wedge dx^k + \\ & \left(\frac{\partial p_i}{\partial n^\alpha} - \frac{\partial p_\alpha}{\partial X^i}\right) dn^\alpha \wedge dX^i + \left(\frac{\partial p_i}{\partial x^k} - \frac{\partial p_k}{\partial X^i}\right) dx^k \wedge dX^i + \\ & + \left(\frac{\partial p_\alpha}{\partial x^k} - \frac{\partial p_k}{\partial n^\alpha}\right) dx^k \wedge dn^\alpha. \end{aligned} \tag{3.9}$$

Finally, the local expression of a null Lagrangian for $n = 2$ is

$$\begin{aligned} \mathcal{E}(h(P)) = h(dP) = {} & \\ = {} & \left(\frac{\partial p_i}{\partial X_j} + \left(\frac{\partial p_i}{\partial n^\alpha} - \frac{\partial p_\alpha}{\partial X^i}\right) n^\alpha_j + \left(\frac{\partial p_i}{\partial x^k} - \frac{\partial p_k}{\partial X^i}\right) x^k_j + \right. \\ & \left. \frac{\partial p_\alpha}{\partial n^\beta}\, n^\beta_j n^\alpha_i + \left(\frac{\partial p_\alpha}{\partial x^k} - \frac{\partial p_k}{\partial n^\alpha}\right) x^k_j n^\alpha_i + \frac{\partial p_k}{\partial x^h}\, x^h_j x^k_i \right) dX^j \wedge dX^i \end{aligned} \tag{3.10}$$

Case n=3. The coordinate expression of P is

$$P = p_{ji}\, dX^j \wedge dX^i + p_{\beta i}\, dn^\beta \wedge dX^i + p_{hi}\, dx^h \wedge dX^i + p_{\beta\alpha}\, dn^\beta \wedge dn^\alpha + p_{h\alpha}\, dx^h \wedge dn^\alpha + p_{hk}\, dx^h \wedge dx^k, \tag{3.11}$$

where the coefficient functions p are local functions of (X^j, n^β, x^h). Then we have

$$h(P) = \left(p_{ji} + p_{\beta i} n^\beta_j + p_{ki} x^k_j + p_{\beta\alpha} n^\beta_j n^\alpha_i + p_{h\alpha} x^h_j n^\alpha_i + p_{hk} x^h_j x^k_i\right) dX^j \wedge dX^i, \tag{3.12}$$

$$\begin{aligned} dP = {} & \frac{\partial p_{ji}}{\partial X^l}\, dX^l \wedge dX^j \wedge dX^i + \frac{\partial p_{\beta\alpha}}{\partial n^\gamma}\, dn^\gamma \wedge dn^\beta \wedge dn^\alpha + \frac{\partial p_{hk}}{\partial x^t}\, dx^t \wedge dx^h \wedge dx^k + \\ & \left(\frac{\partial p_{ji}}{\partial n^\alpha} - \frac{\partial p_{\alpha i}}{\partial X^j}\right) dn^\alpha \wedge dX^j \wedge dX^i + \left(\frac{\partial p_{ji}}{\partial x^k} - \frac{\partial p_{ki}}{\partial X^j}\right) dx^k \wedge dX^j \wedge dX^i + \\ & \left(\frac{\partial p_{\beta\alpha}}{\partial X^i} + \frac{\partial p_{\alpha i}}{\partial n^\beta}\right) dn^\beta \wedge dn^\alpha \wedge dX^i + \left(\frac{\partial p_{\alpha i}}{\partial x^h} - \frac{\partial p_{hi}}{\partial n^\alpha} + \frac{\partial p_{h\alpha}}{\partial X^i}\right) dx^h \wedge dn^\alpha \wedge dX^i + \\ & \left(\frac{\partial p_{hk}}{\partial X^i} + \frac{\partial p_{ki}}{\partial x^h}\right) dx^h \wedge dx^k \wedge dX^i + \left(\frac{\partial p_{hk}}{\partial n^\alpha} + \frac{\partial p_{k\alpha}}{\partial x^h}\right) dx^h \wedge dx^k \wedge dn^\alpha + \\ & \left(\frac{\partial p_{\beta\alpha}}{\partial x^k} + \frac{\partial p_{h\beta}}{\partial n^\alpha}\right) dx^k \wedge dn^\beta \wedge dn^\alpha. \end{aligned} \tag{3.13}$$

Finally, the local expression of a null Lagrangian for $n = 3$ is

$$\begin{aligned} \mathcal{E}(h(P)) = h(dP) = {} & \left(\frac{\partial p_{ji}}{\partial X^l} + \left(\frac{\partial p_{ji}}{\partial n^\alpha} - \frac{\partial p_{\alpha i}}{\partial X^j}\right) n^\alpha_l + \left(\frac{\partial p_{ji}}{\partial x^k} - \frac{\partial p_{ki}}{\partial X^j}\right) x^k_l + \right. \\ & \left(\frac{\partial p_{\beta\alpha}}{\partial X^i} + \frac{\partial p_{\alpha i}}{\partial n^\beta}\right) n^\beta_l n^\alpha_j + \left(\frac{\partial p_{\alpha i}}{\partial x^h} - \frac{\partial p_{hi}}{\partial n^\alpha} + \frac{\partial p_{h\alpha}}{\partial X^i}\right) x^h_l n^\alpha_j + \\ & + \left(\frac{\partial p_{hk}}{\partial X^i} + \frac{\partial p_{ki}}{\partial x^h}\right) x^h_l x^k_j + \\ & \frac{\partial p_{\beta\alpha}}{\partial n^\gamma} n^\gamma_l n^\beta_j n^\alpha_i + \left(\frac{\partial p_{\beta\alpha}}{\partial x^k} + \frac{\partial p_{h\beta}}{\partial n^\alpha}\right) x^k_l n^\beta_j n^\alpha_i + \left(\frac{\partial p_{hk}}{\partial n^\alpha} + \frac{\partial p_{k\alpha}}{\partial x^h}\right) x^h_l x^k_j n^\alpha_i + \\ & \left. + \frac{\partial p_{hk}}{\partial x^t} x^t_l x^h_j x^k_i \right) dX^l \wedge dX^j \wedge dX^i. \end{aligned} \tag{3.14}$$

Global problem. Here we provide the *global* expression of a null Lagrangian. We explained at the beginning of this section that the global problem depends on the structure of the vector space

$$\bar{H}^n \stackrel{\text{def}}{=} \left.\frac{\ker \mathcal{E}}{\operatorname{Im} \mathcal{E}}\right|_{\bar{\Lambda}^n_1}. \tag{3.15}$$

But $\bar{H}^n$ is just the n-th cohomology space of the variational sequence (3.3), and the variational sequence has the same cohomology as the de Rham cohomology of the total

space $\mathcal{R}_0 \times S^2 \times \mathbb{R}^3$ [3, 18, 21]. Hence,

$$n = 2 \quad \Leftrightarrow \quad \bar{H}^2 = H^2_{\text{de Rham}}(\mathcal{R}_0 \times S^2),$$
$$n = 3 \quad \Leftrightarrow \quad \bar{H}^3 = H^3_{\text{de Rham}}(\mathcal{R}_0 \times S^2)$$

because the total space is contractible to $\mathcal{R}_0 \times S^2$ [4]. The cohomology of $\mathcal{R}_0 \times S^2$ can be computed with the standard Künneth formula, provided that the cohomology of $\mathcal{R}_0$ be finite-dimensional. Note that a basis of the vector space $H^2_{\text{de Rham}}(S^2)$ is the (global) volume form υ_{S^2}, whose expression in spherical coordinates is

$$\upsilon_{S^2} = \sin\theta \, d\theta \wedge d\varphi.$$

In fact, by Stokes'theorem the above form is not exact because the integral of υ_{S^2} over S^2 is equal to the area of S^2.

In the case in which $\mathcal{R}_0$ is a contractible space (for example $\mathbb{R}^n$) our null Lagrangians are globally characterized by the following theorem.

Theorem 3.2 (global expression)**.**

Case $n = 2$**:** *first-order null Lagrangians on* $J^1\pi$ *are of the global form*

$$\psi\upsilon = \mathcal{E}(h(P)) + kh(\upsilon_{S^2}),$$

where $k \in \mathbb{R}$ *is a constant;*

Case $n = 3$**:** *first-order null Lagrangians on* $J^1\pi$ *are of the global form*

$$\psi\upsilon = \mathcal{E}(h(P)).$$

Remark 3.3. It is easy to generalize the above model and computation to the case in which the domain of the deformation x is not $\mathbb{R}^n$, but a regular domain $\mathcal{R}_1 \subset \mathbb{R}^n$. In this case our local results as well as cohomological results still hold. One has just to be careful that the total space is no longer contractible to $\mathcal{R}_0 \times S^2$.

4. Concluding remarks

The findings of our computation may be summarized as follows. First of all, we have determined all the local expression for null Lagrangians when $n = 2$ and $n = 3$. Then, we have shown that if the domain is a contractible space (e.g., $\mathcal{R}_0 = \mathbb{R}^n$) for $n = 2$ it is possible to determine a topological global null Lagrangian, whereas for $n = 3$ there is no topological term. Therefore, for $n = 3$ all local expressions are global. The next step is to use our results in a mechanical framework and especially in the framework of nematic elastomers as we have discussed in the Introduction. From our formulae (3.10), (3.14), it is clear that the classical prototype of the null Lagrangians for nonlinear elasticity, i.e. $\det \boldsymbol{F}$, and for the classical theory of liquid crystals $\operatorname{tr}(\boldsymbol{G})^2 - (\operatorname{div} \boldsymbol{n})^2$ may be recovered. For $\det \boldsymbol{F}$ it is sufficient to consider all the currents to be identically zero but Px, which must be linear in the deformations. For the term $\operatorname{tr}(\boldsymbol{G})^2 - (\operatorname{div} \boldsymbol{n})^2$ the situation is more complex because we have not considered $\boldsymbol{n}$ as a unit vector in the three-space (as in [2, 7, 19, 12]) but the parametrization of this unit vector on the sphere.

Our formulas may be used in a passive or active way. In the passive way given a free energy term it is possible by direct computation to check if this term is a null Lagrangian. In the active way it is possible to generate interesting free energy terms

from the given currents formulas by imposing frame indifference and if necessary other material symmetry requirements. These topics will be the subject of future work.

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