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ON A CLASS OF INVARIANT FUNCTIONALS

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Abstract. A characterization of a class of functionals invariant under isochoric changes of domain is obtained. This class contains strictly the null Lagrangians.

Key words. Crystals with defects, neutral deformations, null Lagrangians.

1. Introduction. In Fonseca and Parry [FP] we studied variational problems for crystals with defects. The model that we followed was proposed by Davini [Dv] and later developed by Davini and Parry [DP1], [DP2]. One of the main contributions of this model is the introduction of a class of defect-preserving deformations, called *neutral*, which generally involve some kind of rearrangement. It was shown in Fonseca and Parry [FP] that a neutral change of state of a perfect crystal corresponds to a lattice matrix

$$L(u(x)) = \nabla u(x)\ \{\nabla v(x)\}^{-1},$$

where $u : \Omega \to \mathbb{R}^3$ is the elastic deformation, Ω is the reference configuration and v represents the slip or plastic deformation with $\det \nabla v = 1$ a. e. in Ω. Clearly, if $\nabla v = \mathbb{1}$ then the deformation is elastic. The total energy is given by

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$$E(L) := \int_\Omega W(\nabla u(x)\{\nabla v(x)\}^{-1})\, dx \qquad (1.1)$$

where W represents the bulk energy density, and we take the viewpoint that equilibria correspond to minimizers of (1.1) with (u, v) in the class of admissible pairs

$$\mathcal{A}(u_0) := \{(u, v) \in W^{1,\infty}(\Omega, \mathbb{R}^3) |\, \det \nabla u > 0 \text{ a. e. in } \Omega,\ u = u_0 \text{ on } \partial\Omega,\ \det \nabla v = 1 \text{ a. e. in } \Omega\}.$$

Existence and smoothness of solutions for this type of problems was discussed in Dacorogna and Fonseca [DF].

We remark that, formally, minimizing E(.) in $\mathcal{A}(u_0)$ involves variations of the reference domain ; indeed, setting $\omega := u \circ v^{-1}$ the integral (1.1) becomes

$$\int_{v(\Omega)} W(\nabla\omega(y))dy.$$

We expect that ∇v will not be too far from the identity at equilibrium, i. e. the state of the crystal will be close to a state elastically related to the reference state and so, we want to understand the effect that penalizations on ∇v may impose on the solution. Consider the perturbed problem

$$E_\varepsilon(L) := \int_\Omega W(\nabla u(x)\{\nabla v(x)\}^{-1})\, dx + \varepsilon \int_\Omega g(\nabla v(x))\, dx$$

where

$$g(\mathbb{1}) = 0 \text{ and } g \geq 0. \qquad (1.2)$$

In Fonseca and Parry [FP], Corollary 2.15, it was proven that the factorization of L into the elastic part ∇u and the slip ∇v is not unique, precisely

$$L(u(x)) = \tilde{L}(\tilde{u}(x)) = \nabla\tilde{u}(x)\ \{\nabla\tilde{v}(x)\}^{-1}$$

if and only if, setting $f := \tilde{u}^{-1} \circ u$, the following hold :

(i) $f(x) = x$ on $\partial\Omega$;

(ii) $\det \nabla f(x) = 1$ a. e. in Ω ;

(iii) $v(x) = \tilde{v}(f(x)) + \text{Cont.}$ a. e. in Ω.

As $E_\varepsilon(.)$ should not depend on the factorization of the lattice matrix L, we seek for a characterization of the class of integrands $g : M^{3\times3} \to \mathbb{R}$ such that

$$\int_{\Omega} g(\nabla v(x))\,dx = \int_{\Omega} g(\nabla(v \circ f)(x))\,dx \tag{1.3}$$

for all Lipschitz functions v and f satisfying (i), (ii). This is accomplished in Theorem 2.1 where we show that

$$g(F) = A.F + B.\mathrm{adj}\,F + \gamma(\det F)^1 \tag{1.4}$$

for some matrices A, B and some smooth function γ. We recall that h is said to be a *null Lagrangian* (see Ball [B1], Dacorogna [Dc], Ericksen [E]) if

$$\int_{\Omega} h(\nabla v(x))\,dx = \int_{\Omega} h(\nabla w(x))\,dx \tag{1.5}$$

whenever v, w $\in W^{1,\infty}(\Omega\,;\mathbb{R}^3)$ are such that v(x) = w(x) on $\partial\Omega$. It is clear that null Lagrangians satisfy (1.3); this is in accordance with (1.4) as it is well known that null Lagragians are linear combinations of the minors of F, i. e. (1.5) holds if and only if there exist A, B $\in M^{3x3}$, c $\in \mathbb{R}$ such that

$$g(F) = A.F + B.\mathrm{adj}\,F + c \det F. \tag{1.6}$$

We conclude that if g satisfies (1.2) and (1.4) then

$$g(F) = \gamma(\det F)$$

in which case the perturbed problem $E_\varepsilon(.)$ reduces to

$$E_\varepsilon(L) := \int_{\Omega} W(\nabla u(x)\{\nabla v(x)\}^{-1})\,dx + \varepsilon\,\gamma(1)\,\mathrm{meas}(\Omega)$$

and so we obtain, up to a constant, the former energy functional. As perturbed problems involving a bulk penalization are reduced, essentially, to (1.1) and as, formally, a change in v corresponds to a variation of the domain, in Fonseca and Parry [FP] we considered instead a surface energy penalization.

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[1]If A, B $\in M^{N\times N}$ then $A.B := \mathrm{tr}(A^TB)$ and adj A is the matrix of cofactors of A, i. e. $(\mathrm{adj}\,A) = \frac{1}{2}\varepsilon_{ipq}\,\varepsilon_{jrs}A_{pr}A_{qs}$. In particular, if A is invertible then $A^{-1} = \frac{(\mathrm{adj}\,A)^T}{\det A}$.

2. Characterization of a class of functionals invariant under isochoric changes of the domain. In what follows $\Omega \subset \mathbb{R}^3$ is an open, bounded domain and M^{3x3} denotes the space of 3x3 real matrices.

Theorem 2.1. Let $g \in C^3(M^{3x3})$. Then

$$\int_\Omega g(\nabla v(x))\, dx = \int_\Omega g(\nabla(v \circ f)(x))\, dx \tag{2.1}$$

for all $v, f \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ such that $\det \nabla f(x) = 1$ a. e. in Ω and $f(x) = x$ on $\partial\Omega$, if and only if

$$g(F) = A.F + B.\mathrm{adj}\, F + \gamma(\det F)$$

for some matrices A, B and some smooth function γ.

Remark 2.2. The function g satisfies (2.1) if and only if

$$\int_\Omega g(\nabla v(x))\, dx = \int_\Omega g(\nabla v(x)\{\nabla h(x)\}^{-1})\, dx \tag{2.2}$$

for all Lipschitz functions v, h such that $\det \nabla h(x) = 1$ a. e. in Ω and $h(x) = x$ on $\partial\Omega$. Indeed, suppose that (2.2) holds and let $f \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ be such that $\det \nabla f(x) = 1$ a. e. in Ω and $f(x) = x$ on $\partial\Omega$. Then (see Ball [B2]) f is invertible, $f^{-1} =: h \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ and

$$\begin{cases} \det \nabla h(y) = 1 & \text{in } \Omega \\ h(y) = y & \text{on } \partial\Omega \end{cases}.$$

Therefore, using the change of variable formula for Sobolev functions (see Ball [B2]) and by (2.2) we conclude that

$$\begin{aligned} \int_\Omega g(\nabla v(x))\, dx &= \int_\Omega g(\nabla v(y)\{\nabla h(y)\}^{-1})\, dy \\ &= \int_{f(\Omega)} g(\nabla v(y)\nabla f(f^{-1}(y)))\, dy \\ &= \int_\Omega g(\nabla v(f(x))\nabla f(x)) \det\nabla f(x)\, dx \\ &= \int_\Omega g(\nabla(v \circ f)(x))\, dx. \end{aligned}$$

Similarly, one can show easily that (2.1) implies (2.2).

We divide the proof of Theorem 2.1 into a series of lemmas. Let

$$H(F) := F^T \frac{\partial g}{\partial F}(F).$$

Lemma 2.3. If g satisfies (2.2) then

$$\frac{\partial}{\partial x_l}\Big[\sum_{j=1}^{3} \frac{\partial}{\partial x_j} H_{ij}(\nabla v(x))\Big] = \frac{\partial}{\partial x_i}\Big[\sum_{j=1}^{3} \frac{\partial}{\partial x_j} H_{lj}(\nabla v(x))\Big] \qquad (2.3)$$

for all $i \neq l$ and for all $v \in C^1(\overline{\Omega}; \mathbb{R}^3)$.

Proof. Let $f \in C^1(\overline{\Omega}; \mathbb{R}^3)$ be such that

$$\begin{cases} \operatorname{div} f(x) = 0 & \text{in } \Omega \\ f(x) = 0 & \text{on } \partial\Omega \end{cases}$$

and for all $x \in \overline{\Omega}$ consider the flow

$$\begin{cases} \frac{d}{dt} X(x,t) = f(X(x,t)) \\ X(x,0) = x \end{cases} .$$

Clearly

$$X(x,t) = x \quad \text{if } x \in \partial\Omega \text{ and for all } t. \qquad (2.4)$$

Also

$$\frac{d}{dt} \det \nabla_x X(x,t) = 0. \qquad (2.5)$$

since

$$\begin{aligned} \frac{d}{dt} \det \nabla_x X(x,t) &= (\operatorname{adj} \nabla_x X)^T . \frac{d}{dt} \nabla_x X(x,t) \\ &= (\operatorname{adj} \nabla X)^T . \nabla_x[f(X(x,t))] \\ &= (\operatorname{adj} \nabla X)^T . \nabla X^T \, \nabla f(X(x,t)) \\ &= \det \nabla_x X \, \mathbb{1} . \nabla f(X(x,t)) \\ &= \det \nabla_x X \, \mathbb{1} . \nabla f(X(x,t)) \operatorname{div} f(X) \\ &= 0. \end{aligned}$$

By (2.4) and (2.5) we deduce that

$$\det \nabla_x X(x,t) = 1$$

and so, by (2.2)

$$0 = \frac{d}{dt}\Big|_{t=0} \int_\Omega g(\nabla v(x)\{\nabla_x X(x,t)\}^{-1})\, dx$$

$$= \int_\Omega \frac{\partial g}{\partial F}(\nabla v(x)).\ \nabla v(x) \frac{d}{dt}\Big|_{t=0} \{\nabla_x X(x,t)\}^{-1}\, dx. \qquad (2.6)$$

By (2.4)

$$0 = \frac{d}{dt}\Big|_{t=0} \left[\nabla_x X(x,t)\{\nabla_x X(x,t)\}^{-1}\right]$$

$$= \nabla_x \left[\frac{d}{dt}\Big|_{t=0} X(x,t)\right] + \frac{d}{dt}\Big|_{t=0}\left[\{\nabla_x X(x,t)\}^{-1}\right]$$

yielding

$$\frac{d}{dt}\Big|_{t=0}\left[\{\nabla_x X(x,t)\}^{-1}\right] = -\nabla f$$

which together with (2.6) implies that

$$0 = \int_\Omega H(\nabla v(x)).\nabla f(x)\, dx.$$

Hence, there exists a function p such that for all $i \in \{1, 2, 3\}$

$$\sum_{j=1}^{3} \frac{\partial}{\partial x_j} H_{ij}(\nabla v(x)) = \frac{\partial p}{\partial x_i}$$

which is equivalent to condition (2.3).

Lemma 2.4. If g verifies (2.3) then the following hold.

1. $\dfrac{\partial H_{li}}{\partial F_{ni}} = 0$ for all $n,\ i \neq l$;
2. $\dfrac{\partial H_{li}}{\partial F_{nl}} = \dfrac{\partial H_{ii}}{\partial F_{ni}} - \dfrac{\partial H_{ll}}{\partial F_{ni}}$ for all $n,\ i \neq l$;
3. $\dfrac{\partial H_{li}}{\partial F_{nm}} = -\dfrac{\partial H_{lm}}{\partial F_{ni}}$ for all n, $\{i, l, m\} = \{1, 2, 3\}$;
4. $\dfrac{\partial^2 H_{li}}{\partial F_{nl}^2} = 0$ for all $n,\ i \neq l$;
5. $\dfrac{\partial^2 H_{li}}{\partial F_{nl}\partial F_{nm}} = 0$ for all n, $\{i, l, m\} = \{1, 2, 3\}$;
6. $\dfrac{\partial^2 (H_{ll} - H_{ii})}{\partial F_{nk}\partial F_{pk}} = 0$ for all $k,\ i \neq l,\ n \neq p$;

7. $\dfrac{\partial^2(H_{ll} - H_{ii})}{\partial F_{nl}\partial F_{pi}} = 0$ for all $i \neq l$, $n \neq p$;

8. $\dfrac{\partial^2(H_{ii} - H_{ll})}{\partial F_{pi}\partial F_{nm}} = \dfrac{\partial^2(H_{mm} - H_{ll})}{\partial F_{pi}\partial F_{nm}}$ for all $n \neq p$, $\{i, l, m\} = \{1, 2, 3\}$.

Proof. By (2.3) we have

$$\frac{\partial}{\partial x_l}\Big[\sum_{j,m,n=1}^{3}\frac{\partial H_{ij}(\nabla v(x))}{\partial F_{nm}}\,\frac{\partial^2 v_n}{\partial x_m \partial x_j}\Big] = \\ = \frac{\partial}{\partial x_i}\Big[\sum_{j,m,n=1}^{3}\frac{\partial H_{lj}(\nabla v(x))}{\partial F_{nm}}\,\frac{\partial^2 v_n}{\partial x_m \partial x_j}\Big]$$

i. e.

$$\frac{\partial^2 H_{ij}}{\partial F_{nm}\partial F_{pq}}\,\frac{\partial^2 v_p}{\partial x_q \partial x_l}\,\frac{\partial^2 v_n}{\partial x_m \partial x_j} + \frac{\partial H_{ij}}{\partial F_{nm}}\,\frac{\partial^3 v_n}{\partial x_m \partial x_j \partial x_l} = \\ = \frac{\partial^2 H_{lj}}{\partial F_{nm}\partial F_{pq}}\,\frac{\partial^2 v_p}{\partial x_q \partial x_i}\,\frac{\partial^2 v_n}{\partial x_m \partial x_j} + \frac{\partial H_{lj}}{\partial F_{nm}}\,\frac{\partial^3 v_n}{\partial x_m \partial x_j \partial x_i}. \tag{2.7}$$

Here we use the convention that repeated indices stand for summation, unless stated otherwise. Setting $D^\alpha v(x_0) = 0$ except $D^3 v(x_0)$, with $a_{mji} := \dfrac{\partial^3 v_n}{\partial x_m \partial x_j \partial x_i}(x_0)$, we deduce that

$$\frac{\partial H_{ij}}{\partial F_{nm}}\, a_{mjl} = \frac{\partial H_{lj}}{\partial F_{nm}}\, a_{mji} \tag{2.8}$$

whenever $a_{mji} = a_{mij} = a_{jmi} = a_{jim} = a_{ijm} = a_{imj}$. Next, if $D^\alpha v(x_0) = 0$ except $D^2 v_n(x_0) = B = B^T$, from (2.7) we have

$$\frac{\partial^2 H_{ij}}{\partial F_{nm}\partial F_{nq}}\, B_{ql}\, B_{mj} = \frac{\partial^2 H_{lj}}{\partial F_{nm}\partial F_{nq}}\, B_{qi}\, B_{mj} \;\; \text{(no summation in n)} \tag{2.9}$$

and finally, if $D^\alpha v(x_0) = 0$ except $D^2 v_p(x_0) = B = B^T$ and $D^2 v_n(x_0) = A = A^T$, with $n \neq p$, by (2.7) and (2.9) we conclude that

$$\frac{\partial^2 H_{ij}}{\partial F_{nm}\partial F_{pq}}\, B_{ql}\, A_{mj} + \frac{\partial^2 H_{ij}}{\partial F_{pm}\partial F_{nq}}\, A_{ql}\, B_{mj} = \frac{\partial^2 H_{lj}}{\partial F_{nm}\partial F_{pq}}\, B_{qi}\, A_{mj} + \frac{\partial^2 H_{lj}}{\partial F_{pm}\partial F_{nq}}\, A_{qi}\, B_{mj}. \tag{2.10}$$

In (2.8) set $a_{ijk} = 0$ except $a_{iii} = 1$. If $i \neq l$ then we obtain property (1), i. e.

$$\frac{\partial H_{li}}{\partial F_{ni}} \text{ (no summation).}$$

If $a_{ijk} = 0$ except $a_{lii} = a_{ili} = a_{iil}$ then

$$\frac{\partial H_{ii}}{\partial F_{ni}} = \frac{\partial H_{li}}{\partial F_{nl}} + \frac{\partial H_{ll}}{\partial F_{ni}} \text{ (no summation)}$$

which is (2). Also, (3) follows from (2.8) where $a_{ijk} = 0$ except for $a_{mii} = 1 = a_{imi} = a_{iim}$.

In (2.9) let $B = e_i \otimes e_l + e_l \otimes e_i$. Then

$$\frac{\partial^2 H_{il}}{\partial F_{ni}^2} + \frac{\partial^2 H_{ii}}{\partial F_{nl}\partial F_{ni}} = \frac{\partial^2 H_{li}}{\partial F_{nl}^2} + \frac{\partial^2 H_{ll}}{\partial F_{ni}\partial F_{nl}}$$

hence

$$\frac{\partial^2 H_{ii}}{\partial F_{nl}\partial F_{ni}} - \frac{\partial^2 H_{ll}}{\partial F_{ni}\partial F_{nl}} = \frac{\partial^2 H_{li}}{\partial F_{nl}^2} - \frac{\partial^2 H_{il}}{\partial F_{ni}^2} \tag{2.11}$$

and by (2)

$$\frac{\partial^2 H_{ii}}{\partial F_{nl}\partial F_{ni}} - \frac{\partial^2 H_{ll}}{\partial F_{ni}\partial F_{nl}} = \frac{\partial}{\partial F_{nl}}\left[\frac{\partial H_{ii}}{\partial F_{ni}} - \frac{\partial H_{ll}}{\partial F_{ni}}\right] = \frac{\partial^2 H_{li}}{\partial F_{nl}^2}$$

which, together with (2.11) yields (4). With $\{i, l, m\} = \{1, 2, 3\}$ and $B = e_l \otimes e_l + e_m \otimes e_i + e_m \otimes e_i$, (2.9) reduces to

$$\frac{\partial^2 H_{ij}}{\partial F_{nk}\partial F_{nl}} B_{kj} = \frac{\partial^2 H_{lj}}{\partial F_{nk}\partial F_{nm}} B_{kj}$$

or

$$\frac{\partial^2 H_{il}}{\partial F_{nl}^2} + \frac{\partial^2 H_{im}}{\partial F_{ni}\partial F_{nl}} + \frac{\partial^2 H_{ii}}{\partial F_{nm}\partial F_{nl}} = \frac{\partial^2 H_{ll}}{\partial F_{nl}\partial F_{nm}} + \frac{\partial^2 H_{lm}}{\partial F_{ni}\partial F_{nm}} + \frac{\partial^2 H_{li}}{\partial F_{nm}^2},$$

which by (1) is equivalent to

$$\frac{\partial^2 H_{im}}{\partial F_{ni}\partial F_{nl}} + \frac{\partial^2 H_{ii}}{\partial F_{nm}\partial F_{nl}} = \frac{\partial^2 H_{ll}}{\partial F_{nl}\partial F_{nm}} + \frac{\partial^2 H_{li}}{\partial F_{nm}^2}. \tag{2.12}$$

On the other hand, by (1) and (3) we have

$$\frac{\partial^2 H_{li}}{\partial F_{nm}{}^2} = - \frac{\partial}{\partial F_{nm}} \frac{\partial H_{lm}}{\partial F_{ni}} = 0$$

and so, from (2.12), (2) and (3) we conclude that

$$\begin{aligned} \frac{\partial^2 H_{im}}{\partial F_{ni}\partial F_{nl}} &= \frac{\partial}{\partial F_{nm}} \frac{\partial}{\partial F_{nl}} \left[H_{ll} - H_{ii}\right] \\ &= \frac{\partial}{\partial F_{nm}} \frac{\partial H_{il}}{\partial F_{ni}} \\ &= - \frac{\partial}{\partial F_{ni}} \frac{\partial H_{im}}{\partial F_{nl}} \end{aligned}$$

proving (5). Replace $B = e_i \otimes e_i$ and $A = e_i \otimes e_l + e_l \otimes e_i$ in (2.10) to obtain

$$\frac{\partial^2 H_{ii}}{\partial F_{pi}\partial F_{ni}} = \frac{\partial^2 H_{ll}}{\partial F_{ni}\partial F_{pi}} + \frac{\partial^2 H_{li}}{\partial F_{nl}\partial F_{pi}} + \frac{\partial^2 H_{li}}{\partial F_{ni}\partial F_{nl}}$$

which, by (1) reduces to

$$\frac{\partial^2 H_{ii}}{\partial F_{pi}\partial F_{ni}} = \frac{\partial^2 H_{ll}}{\partial F_{ni}\partial F_{pi}} . \tag{2.13}$$

With $B = e_m \otimes e_i + e_i \otimes e_m$ and $A = e_m \otimes e_l + e_l \otimes e_m$ we get, again using (1),

$$\frac{\partial^2}{\partial F_{nm}\partial F_{pm}} \left[H_{ii} - H_{ll}\right] = 0$$

which, together with (2.13) yields (6). Equation (7) follows from (2.10) taking $B = e_i \otimes e_i$ and $A = e_l \otimes e_l$. Finally, setting $B = e_i \otimes e_i$ and $A = e_m \otimes e_l + e_l \otimes e_m$, by (2.10) and (2) we deduce

$$\begin{aligned} \frac{\partial^2 H_{ii}}{\partial F_{pi}\partial F_{nm}} &= \frac{\partial^2 H_{ll}}{\partial F_{nm}\partial F_{pi}} + \frac{\partial^2 H_{lm}}{\partial F_{nl}\partial F_{pi}} \\ &= \frac{\partial^2 H_{ll}}{\partial F_{nm}\partial F_{pi}} + \frac{\partial}{\partial F_{pi}} \left[\frac{\partial H_{mm}}{\partial F_{nm}} - \frac{\partial H_{ll}}{\partial F_{nm}}\right] \end{aligned}$$

concluding (8).

Lemma 2.5. If the conditions (1)-(8) of Lemma 2.4 are fullfilled then there exists a matrix M and some constants A_{ijpq}, C_{ij} such that for $i \neq j$

$$H_{ij}(F) = \left\{ F^T \frac{\partial}{\partial F} tr(M \text{ adj } F) \right\}_{ij} + A_{ijpq} F_{pq} + C_{ij}.$$

Proof. For simplicity we set (i, j) = (1, 2). By (1) we have

$$\frac{\partial H_{12}}{\partial F_{n2}} = 0$$

and so

$$H_{12} = H_{12} (\{F_{n1}\}, \{F_{p3}\})$$

We claim that H_{12} is a polynomial of degree less than or equal to 2, i. e.

$$\frac{\partial^3 H_{12}}{\partial F_{ni} \partial F_{pj} \partial F_{kl}} = 0 \text{ for all n, i, p, j, k, l.} \tag{2.14}$$

Clearly, (2.14) holds if $2 \in \{i, j, l\}$. If this is not the case, then two of the indices $\{i, j, l\}$ must be repeated, suppose that $i = j \in \{1, 3\}$. If $i = j = 1$ and $n = p$ then (4) implies that

$$\frac{\partial^2 H_{12}}{\partial F_{n1}^2} = 0 \tag{2.15}$$

in which case (2.14) is satisfied. If $n \neq p$ then by (2) and (7) we have

$$\frac{\partial^2 H_{12}}{\partial F_{n1} \partial F_{p1}} = \frac{\partial}{\partial F_{n1}} \left[\frac{\partial H_{22}}{\partial F_{p2}} - \frac{\partial H_{11}}{\partial F_{p2}}\right]$$
$$= 0 \tag{2.16}$$

thus implying (2.14). Finally, if $i = j = 3$ then (1) and (3) yield

$$\frac{\partial^2 H_{12}}{\partial F_{n3} \partial F_{p3}} = - \frac{\partial}{\partial F_{n3}} \frac{\partial H_{13}}{\partial F_{p2}}$$
$$= 0 \tag{2.17}$$

concluding (2.14). Recall that by (5)

$$\frac{\partial^2 H_{12}}{\partial F_{n1} \partial F_{n3}} = 0$$

which, together with (2.15)-(2.17), implies that

$$H_{12} = \sum_{p \neq r} \alpha_{pr} F_{r1} F_{p3} + A_{12pq} F_{pq} + C_{12} \tag{2.18}$$

and, in a similar way,

$$H_{13} = \sum_{p \neq r} \beta_{pr} F_{r1} F_{p2} + A_{13pq} F_{pq} + C_{13}. \tag{2.19}$$

By (2.18), (2.19) and (3) we must have for all F

$$\sum_{p \neq r} \alpha_{pr} F_{r1} + A_{12p3} = \frac{\partial H_{12}}{\partial F_{p3}}$$

$$= -\frac{\partial H_{13}}{\partial F_{p2}} = - \sum_{p \neq r} \beta_{pr} F_{r1} - A_{13p2}$$

and so

$$\alpha_{pr} = - \beta_{pr} \quad \text{for } r \neq p. \tag{2.20}$$

Note that by (2.18), (2.19), (2.20), (2) and (8) we have

$$\alpha_{pr} = \frac{\partial^2 H_{12}}{\partial F_{r1} \partial F_{p3}} = \frac{\partial}{\partial F_{p3}} \left[\frac{\partial H_{22}}{\partial F_{r2}} - \frac{\partial H_{11}}{\partial F_{r2}}\right]$$

$$= - \frac{\partial}{\partial F_{r2}} \frac{\partial}{\partial F_{p3}} \left[H_{11} - H_{33}\right]$$

$$= \frac{\partial}{\partial F_{r2}} \frac{\partial H_{13}}{\partial F_{p1}}$$

$$= \beta_{rp} = - \alpha_{rp}$$

and so we can rewrite (2.18) and (2.19) as

$$H_{ij} = \sum_{p \neq r} \eta^{ki}_{pr} F_{ri} F_{pk} + A_{ijpq} F_{pq} + C_{ij} \text{ (no summation on k)} \tag{2.21}$$

where $\{i, j, k\} = \{1, 2, 3\}$,

$$\eta^{ki}_{pr} = - \eta^{ki}_{rp} \tag{2.22}$$

and

$$\eta^{ki}_{pr} = - \eta^{ji}_{pr}. \tag{2.23}$$

From (2.22) we deduce that

$$\eta^{ki}_{pr} = \varepsilon_{prs} \theta^{ki}_{s} \tag{2.24}$$

and (2.23) implies that for $\{i, j, k\} = \{1, 2, 3\}$

$$\varepsilon_{prs}\,\theta_s^{ki} = -\,\varepsilon_{prs}\,\theta_s^{ji}.$$

Hence

$$\theta_s^{ki} = \varepsilon_{tkj}\, M_{ts}$$

which, together with (2.21) and (2.24) yields

$$H_{ij} = \varepsilon_{prs}\,\varepsilon_{tkj}\, M_{ts}\, F_{ri}\, F_{pk} + A_{ijpq}\, F_{pq} + C_{ij}$$

where $\{i, j, k\} = \{1, 2, 3\}$, so that there is no summation in k. However, this can be rewritten as

$$H_{ij} = \varepsilon_{prs}\,\varepsilon_{tkj}\, M_{ts}\, F_{ri}\, F_{pk} + A_{ijpq}\, F_{pq} + C_{ij}$$

where the summation convention operates on all repeated indices (including k), and thus

$$H_{ij}(F) = \left\{F^T \frac{\partial}{\partial F}\,\mathrm{tr}(M \text{ adj } F)\right\}_{ij} + A_{ijpq}\, F_{pq} + C_{ij}.$$

Lemma 2.6. If g satisfies the conditions (1) - (8) of Lemma 2.4 then

$$H_{ii}(F) = (M \text{ adj } F)_{ii} + A_{iipq}\, F_{pq} + C_{ii} + p(F)$$

where $p(0) = 0$ and $\partial p/\partial F(0) = 0$.

Proof. We claim that $H_{11} - H_{22}$ is a polynomial of degree at most two, i. e.

$$\frac{\partial^3}{\partial F_{ni}\partial F_{pj}\partial F_{kl}}\left[H_{11} - H_{22}\right] = 0 \text{ for all n, i, p, j, k, l.} \tag{2.25}$$

If $1 \in \{i, j, l\}$ and for simplicity, assume that $i = 1$, then by (2) we have

$$\frac{\partial}{\partial F_{n1}}\left[H_{11} - H_{22}\right] = \frac{\partial H_{21}}{\partial F_{n2}}$$

and so (2.25) follows from Lemma 2.5.

If $1, 2 \notin \{i, j, l\}$ then $i = j = l = 3$. If two of the indices $\{n, p, k\}$ are different then (2.25) follows from (6). If $n = p = k = 3$ then by (2) and (1)

$$\frac{\partial^2\,(H_{11} - H_{22})}{\partial F_{n3}^2} = \frac{\partial^2\,(H_{11} - H_{33})}{\partial F_{n3}^2} + \frac{\partial^2\,(H_{33} - H_{22})}{\partial F_{n3}^2}$$

$$= \frac{\partial}{\partial F_{n3}} \left(-\frac{\partial H_{13}}{\partial F_{n1}}\right) + \frac{\partial}{\partial F_{n3}} \left(\frac{\partial H_{23}}{\partial F_{n2}}\right)$$

$$= 0 \tag{2.26}$$

and once more, (2.25) holds. Next we show that

$$\frac{\partial^2 (H_{11} - H_{22})}{\partial F_{ni} \partial F_{pi}} = 0 \quad \text{for all n, p, i.} \tag{2.27}$$

If $n \neq p$ then (2.27) follows from (6). If $n = p$ and $i = 3$ then (2.27) reduces to (2.26). Finally if $n = p$ and $i = 1$ by (2) and (1)

$$\frac{\partial^2 (H_{11} - H_{22})}{\partial F_{n1}^2} = \frac{\partial}{\partial F_{n1}} \frac{\partial H_{21}}{\partial F_{n2}} = 0.$$

By (2.25) - (2.27) we deduce that

$$H_{11} - H_{22} = \sum_{\{p,q,r\}=\{1,2,3\}} B_{ijr} F_{ip} F_{jq} + L_{pq} F_{pq} + C.$$

In addition, (2) and (4) imply that

$$\frac{\partial^2 (H_{11} - H_{22})}{\partial F_{n2} \partial F_{n1}} = \frac{\partial}{\partial F_{n2}} \frac{\partial H_{21}}{\partial F_{n2}} = 0$$

and by (7)

$$\frac{\partial^2 (H_{11} - H_{22})}{\partial F_{n2} \partial F_{p1}} = 0 \;\; \text{if } n \neq p.$$

Hence, we conclude that

$$H_{11} - H_{22} = \alpha_{ij} F_{i1} F_{j3} + \beta_{ij} F_{i2} F_{j3} + L_{pq} F_{pq} + C. \tag{2.28}$$

From (2) and Lemma 2.5 we have

$$\alpha_{nj} F_{j3} + L_{n1} = \frac{\partial}{\partial F_{n1}} \left[H_{11} - H_{22}\right] = \frac{\partial H_{21}}{\partial F_{n2}}$$

$$= \varepsilon_{pns} \varepsilon_{t31} M_{ts} F_{p3} + A_{21n2}$$

$$= \varepsilon_{jns} M_{2s} F_{j3} + A_{21n2}$$

and so

$$\alpha_{nj} = \varepsilon_{jns} M_{2s}. \tag{2.29}$$

Similarly,

$$\beta_{nj} F_{j3} + L_{n2} = \frac{\partial}{\partial F_{n2}} \left[H_{11} - H_{22}\right] = - \frac{\partial H_{12}}{\partial F_{n1}}$$

$$= - \varepsilon_{pns} \varepsilon_{t32} M_{ts} F_{p3} - A_{12n1}$$

$$= \varepsilon_{jns} M_{1s} F_{j3} - A_{12n1}$$

and so

$$\beta_{nj} = \varepsilon_{jns} M_{1s}$$

which, together with (2.28) and (2.29) implies that

$$H_{11} - H_{22} = \varepsilon_{jis} (M_{2s} F_{i1} F_{j3} + M_{1s} F_{i2} F_{j3}) + L_{pq} F_{pq} + C$$

$$= - (M \text{ adj } F)_{11} + (M \text{ adj } F)_{22} + L_{pq} F_{pq} + C. \tag{2.30}$$

Writing

$$H_{ii} = - (M \text{ adj } F)_{ii} + g_i$$

we have

$$H_{11} - H_{22} = - (M \text{ adj } F)_{11} + (M \text{ adj } F)_{22} + (g_1 - g_2)$$

and by (2.30) we get

$$g_1 - g_2 = L_{pq} F_{pq} + C.$$

Set

$$g_2(F) := p^*(F).$$

Then

$$H_{ii} = - (M \text{ adj } F)_{ii} + p^*(F) + A^*_{iipq} F_{pq} + C^*_{ii}$$

$$= - (M \text{ adj } F)_{ii} + A_{iipq} F_{pq} + C_{ii} + p(F)$$

where

$$p(F) := p^*(F) - p^*(0) - \frac{\partial p^*}{\partial F}(0).F, \quad A_{iipq} := A^*_{iipq} + \frac{\partial p^*}{\partial F_{pq}}(0) \quad \text{and } C_{ii} := C^*_{ii} + p^*(0).$$

Lemma 2.7. Let M be a constant matrix. If $h(F) = -M^T . \operatorname{adj} F = -\operatorname{tr}(M \operatorname{adj} F)$ then

$$F^T \frac{\partial h}{\partial F} = M \operatorname{adj} F - (M^T . \operatorname{adj} F)\mathbb{1}.$$

Proof. Since

$$\frac{\partial h}{\partial F_{ij}} = -\frac{\partial}{\partial F_{ij}} \left[M_{lp} (\operatorname{adj} F)_{pl}\right] = -M_{lp} \frac{\partial (\operatorname{adj} F)_{pl}}{\partial F_{ij}}$$

we get

$$\left(F^T \frac{\partial h}{\partial F}\right)_{kj} = F^T{}_{ki} \frac{\partial h}{\partial F_{ij}} = F_{ik} \frac{\partial h}{\partial F_{ij}} = -M_{lp} \frac{\partial (\operatorname{adj} F)_{pl}}{\partial F_{ij}} F_{ik}. \tag{2.31}$$

We claim that if F is invertible then

$$\frac{\partial (\operatorname{adj} F)_{pl}}{\partial F_{ij}} = -(\operatorname{adj} F)_{ij} F^{-1}_{lp} - (\operatorname{adj} F)_{il} F^{-1}_{jp} \tag{2.32}$$

Indeed

$$(\operatorname{adj} F)_{kl} F_{km} = \det F \, \delta_{lm}$$

and so

$$\frac{\partial (\operatorname{adj} F)_{kl}}{\partial F_{ij}} F_{km} + (\operatorname{adj} F)_{kl} \delta_{ki} \delta_{mj} = (\operatorname{adj} F)_{ij} \delta_{lm}.$$

Multiplying this inequality by F^{-1}_{mp} and adding in m yields (2.32). By (2.31) and (2.32) we obtain

$$\left(F^T \frac{\partial h}{\partial F}\right)_{kj} = -M_{lp} \left[(\operatorname{adj} F)_{ij} F^{-1}_{lp} - (\operatorname{adj} F)_{il} F^{-1}_{jp} \right] F_{ik}$$

$$= -M_{lp} \left[\det F \, F^{-1}_{lp} \delta_{jk} - \det F \, F^{-1}_{jp} \delta_{lk} \right]$$

$$= \left[M \operatorname{adj} F - (M^T . \operatorname{adj} F)\mathbb{1}\right]_{kj}.$$

This relation holds for all matrices F with $\det F \neq 0$ and the result for all matrices follows by density and by continuity.

Lemma 2.8. Let $h : M^{3x3} \to \mathbb{R}$ be a C^1 function. There exists a $\omega \in C^1(\mathbb{R} ; \mathbb{R})$ such that $h(F) = \omega(\det F)$ if and only if $F^T \frac{\partial h}{\partial F}(F) = p(F)\mathbb{1}$ for some function p.

Proof. Suppose that $h(F) = \omega(\det F)$. Then

$$\frac{\partial h}{\partial F}(F) = \omega'(\det F) \operatorname{adj} F$$

and so

$$F^T \frac{\partial h}{\partial F}(F) = \omega'(\det F) \det F \, \mathbb{1}.$$

Conversely, if $F^T \frac{\partial h}{\partial F}(F) = p(F)\mathbb{1}$ we claim that then

i) $h(F) = h(RF)$ for every F and for all rotations R ;

ii) $h(F) = h(F(\mathbb{1} + a\otimes b))$ for every F and for all orthogonal vectors a and b.

In order to prove i), consider the semigroup $\{e^{t\Lambda}\}$ where Λ is a skew-symmetric matrix such that $R = e^{\Lambda}$. Set

$$f(t) := h(F\, e^{t\Lambda}).$$

Then

$$\begin{aligned} f'(t) &= \frac{\partial h}{\partial F}(F\, e^{t\Lambda}) \,.\, F\, e^{t\Lambda}\, \Lambda \\ &= (F\, e^{t\Lambda})^T \frac{\partial h}{\partial F}(F\, e^{t\Lambda}) \,.\, \Lambda \\ &= p(F\, e^{t\Lambda}) \operatorname{trace} \Lambda = 0 \end{aligned}$$

and so f is constant ; in particular $f(1) = f(0)$, i. e.

$$h(F) = h(RF).$$

To prove ii) we define

$$f(t) := h(F(\mathbb{1} + ta\otimes b)).$$

Then

$$\begin{aligned} f'(t) &= \frac{\partial h}{\partial F}(F(\mathbb{1} + ta\otimes b)) \,.\, F\, a\otimes b \\ &= \frac{\partial h}{\partial F}(F(\mathbb{1} + ta\otimes b)) \,.\, F(\mathbb{1} + ta\otimes b)(\mathbb{1} - ta\otimes b)\, a\otimes b \\ &= \left[F(\mathbb{1} + ta\otimes b)\right]^T \frac{\partial h}{\partial F}(F(\mathbb{1} + ta\otimes b)) \,.\, a\otimes b \\ &= p(F(\mathbb{1} + ta\otimes b))\, (a.b) = 0 \end{aligned}$$

and we conclude that f is constant, so that $f(1) = f(0)$.

If $F \in M^{3x3}$ is any matrix with $\det F \neq 0$ then (see Chipot and Kinderlehrer [CK] and Fonseca [F]) F can be written as

$$F = (\det F)^{1/3} R \prod(\mathbb{1} + a_i \otimes b_i), \quad 1 \le i \le 2,$$

where R is a rotation and $a_i . b_i = 0$. Therefore, by i) and ii) we conclude that

$$h(F) = h((\det F)^{1/3} \mathbb{1})$$
$$=: \omega(\det F).$$

The result for arbitrary F follows now from density and continuity.

Finally we prove our main result, Theorem 2.1.

Proof of Theorem 2.1. Suppose that

$$g(F) = A.F + B.\mathrm{adj}\, F + \gamma(\det F).$$

Let $v, f \in W^{1,\infty}(\Omega, \mathbb{R}^3)$ be such that $\det \nabla f(x) = 1$ a. e. in Ω and $f(x) = x$ on $\partial\Omega$. By (1.5) and (1.6) we have

$$\int_\Omega \left[g(\nabla v(x)) - \gamma(\det \nabla v(x))\right] dx = \int_\Omega \left[g(\nabla(v \circ f)(x)) - \gamma(\det \nabla (v \circ f)(x))\right] dx \quad (2.33)$$

and by the change of variables formula for Sobolev functions (see Ball [B2])

$$\int_\Omega \gamma(\det \nabla(v \circ f)(x))\, dx = \int_\Omega \gamma(\det \nabla v(f(x)))\, dx$$
$$= \int_{f(\Omega)} \gamma(\det \nabla v(f(x))) \det \nabla f(x)\, dx$$
$$= \int_\Omega \gamma(\det \nabla v(x))\, dx$$

which, together with (2.33), implies that

$$\int_\Omega g(\nabla v(x))\, dx = \int_\Omega g(\nabla(v \circ f)(x))\, dx .$$

Conversely, if the latter holds then by Remark 2.2, Lemmas 2.3, 2.4, 2.5 and 2.6 we have

$$H_{ij}(F) = -(M\, \mathrm{adj}\, F)_{ij} + A_{ijpq} F_{pq} + C_{ij} + p(F)\, \delta_{ij} \quad (2.34)$$

where $p(0) = 0, \frac{\partial p}{\partial F}(0) = 0$. We claim that (using the summation convention for repeated indices)

$$\frac{\partial H_{sn}}{\partial F_{mj}}(F)\, F_{mi} - H_{in}(F)\, \delta_{sj} = \frac{\partial H_{ij}}{\partial F_{kn}}(F)\ \ F_{ks} - H_{sj}(F)\, \delta_{in}. \tag{2.35}$$

Indeed, as

$$H(F) = F^T \frac{\partial g}{\partial F}(F)$$

and since $g \in C^2$ we obtain

$$\begin{aligned}\frac{\partial H_{sn}}{\partial F_{mj}}\ F_{mi} &= H_{in}\, \delta_{sj} + F_{mi}\, F_{ks} \frac{\partial^2 g}{\partial F_{kn} \partial F_{mj}} \\ &= H_{in}\, \delta_{sj} + F_{ki}\, F_{ms} \frac{\partial^2 g}{\partial F_{mn} \partial F_{kj}} \\ &= H_{in}\, \delta_{sj} + \frac{\partial H_{ij}}{\partial F_{kn}}\ F_{ks} - H_{sj}\, \delta_{in}.\end{aligned}$$

In (2.35) replace F by tF and let $t \to 0$. We deduce that

$$H_{in}(0)\, \delta_{sj} = H_{sj}(0)\, \delta_{in}$$

or, taking into account (2.34)

$$C_{in}\, \delta_{sj} = C_{sj}\, \delta_{in}$$

which implies that

$$C_{ij} = C\, \delta_{ij}$$

and (2.34) reduces to

$$H_{ij}(F) = -\,(M \text{ adj } F)_{ij} + A_{ijpq}\, F_{pq} + C\, \delta_{ij} + p(F)\, \delta_{ij}. \tag{2.36}$$

Again by (2.35) we have

$$\frac{\partial H_{sn}}{\partial F_{mj}}(tF)\ tF_{mj} - \left[H_{jn}(tF) - H_{jn}(0)\right] \delta_{sj} = \frac{\partial H_{ij}}{\partial F_{kn}}(tF)\ \ tF_{ks} - \left[H_{sj}(tF) - H_{sj}(0)\right]\ \delta_{jn}$$

and so, dividing the latter by t and letting $t \to 0$ we obtain

$$\frac{\partial H_{sn}}{\partial F_{mj}}(0)\, F_{mj} - \frac{\partial H_{jn}}{\partial F}(0).F\, \delta_{sj} = \frac{\partial H_{ij}}{\partial F_{kn}}(0)\ \ F_{ks} - \frac{\partial H_{sj}}{\partial F}(0).F\, \delta_{jn}$$

i. e.

$$\frac{\partial H_{sn}}{\partial F_{mj}}(0)\, F_{mj} = \frac{\partial H_{jj}}{\partial F_{kn}}(0)\ \ F_{ks}.$$

From (2.36) we deduce that

$$A_{snmj}\, F_{mj} = A_{jjkn}\, F_{ks} \tag{2.37}$$

and setting[2]

$$A_{qp} := A_{jjpq}$$

we claim that

$$A_{ijpq}\, F_{pq} = \Big(F^T \frac{\partial(\mathrm{trace}\ AF)}{\partial F}\Big)_{ij}. \tag{2.38}$$

In fact, by (2.37)

$$\Big(F^T \frac{\partial(\mathrm{trace}\ AF)}{\partial F}\Big)_{ij} = F^T_{is} \frac{\partial}{\partial F_{sj}} (A_{lm}\, F_{ml})$$

$$= F_{si}\, A_{js} \ = F_{si}\, A_{kksj} = A_{ijpq}\, F_{pq}$$

and so, (2.36) and (2.38) yield

$$H(F) = -\ M\ \mathrm{adj}\ F + (p(F) + C)\ \mathbb{1}\ + F^T \frac{\partial(\mathrm{trace}\ AF)}{\partial F}$$

and by Lemma 2.7 we obtain

$$F^T \frac{\partial}{\partial F} \big[g(F) - M^T.\mathrm{adj}\ F - \mathrm{trace}(AF)\big] \ = \ q(F)\ \mathbb{1}$$

where

$$q(F) := p(F) + C - M^T.\mathrm{adj}\ F.$$

Finally, Lemma 2.8 asserts the existence of a function ω such that

$$g(F) - M^T.\mathrm{adj}\ F - \mathrm{trace}(AF) = \omega\ (\det F)$$

and we conclude that

$$g(F) = \ \ M^T.\mathrm{adj}\ F + A^T.F + \omega\ (\det F).$$

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[2]Here, and unless stated otherwise, the summation convention for repeated indices is used.

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