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DISLOCATIONS AT THE CONTINUUM SCALE: FUNCTIONAL SETTING AND VARIATIONAL PROPERTIES

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Abstract. Considering the existence of solutions to a minimum problem for dislocations in finite elasticity [21], in the present paper we first exhibit a constraint reaction field, due to the geometrical constraint that the deformation curl is a concentrated measure. The appropriate functional spaces and their properties needed to describe dislocations are then established. Following the preceding theoretical developments, the first variation of the energy at the minimum points with respect to Lipschitz variations of the lines and to curl-free deformations is carried on. Our first purpose is to show that the constraint reaction provides explicit expressions of the Piola-Kirchhoff stress and Peach-Köhler force. Then, equilibrium at optimality shows that the latter force is balanced by a defect-induced configurational force. Our main result is to establish that the Peach-Köhler force is a concentrated Radon measure in the dislocation. In the modeling application, in order to consider complex structures such as dislocation clusters, countable families of dislocations are represented by means of integer-valued 1-currents at the continuum scale in the spirit of [21].

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1. Introduction

Dislocations in elastic bodies are at the origin of dissipative phenomena, and in particular their motion is responsible for the plastic behaviour of single crystals. A dislocation loop L is a closed curve in $\bar{\Omega}$. Outside the dislocation, i.e. in $\bar{\Omega} \setminus L$, the body is considered as perfectly elastic. This scale of matter description is called the *mesoscopic*, or the *continuum scale*. Motivated by physical reasons [15, 18, 32, 33], we consider finite elasticity near the line with a less-than-quadratic strain energy, while linear elasticity is a valid assumption away from the dislocations. Nonetheless, it is not easy to understand the physical nature of a mesoscopic dislocation. In fact, it is not a material line, since it can be equivalently generated by an excess or a lack of lattice atoms. Moreover, contrarily to fracture, it can not even be defined as a mere singularity in the reference configuration where deformation fields would be unbounded. In fact, a dislocation must be viewed as a singularity of the deformation field whose support lies in the current configuration (see, e.g., [1, 21]). Therefore, dislocation location and field singularity are bound notions. Specifically, the support of the curl of the deformation field (which in general is not a gradient) is identified with the dislocation density field. This definition is at the basis of the present work, since a constraint reaction will be generated by the satisfaction of the latter relation between model variables.

1.1. Mathematical and physical properties of dislocations.

The intrinsic mathematical difficulties generated by dislocations are fundamentaly different from those encountered in the mathematical modeling of fracture mechanics: (i) dislocations are $\mathcal{H}^{N-2}$ field singularities; (ii) dislocations are free to mutually annihilate, recombine, split, spontaneously appear, and hence form complex geometrical structures, without any law such as irreversibility; (iii) there is no natural reference configuration and hence intrinsic approaches must be preferred. In particular, the displacement is not an appropriate model variable, as opposed to most of Solid Mechanics problems; (iv) the stress and strain fields are not square-integrable and so the less tractable L^p spaces with $1 \leq p < 2$ must be considered; (v) bounds on the model fields are given in terms of the curl and the divergence, in place of the full gradient; (vi) these curl and divergence are found in measure spaces instead of Sobolev spaces. Moreover, we believe that in order to model single crystals with dislocations, where complex geometries such as dislocation clusters (cf. Fig. 1) are observed [32], one can hardly rely on the assumption of a period array of dislocations. Therefore, one is forced to build a specific mathematical framework step by step, which should provide

(i) An appropriate functional framework.
(ii) A geometric description of the lines.

To achieve (ii), the mathematical formalism of currents as briefly described in Section 1.2 has been proposed. In this framework, a cluster as depicted in Fig. 1 is modelled as a continuum dislocation [21]. Moreover this formalism introduces in a natural way the notions of geometrically necessary and unnecessary dislocations, which are well known to engineers. Restricting ourselves to a quasi-static regime, in this work we assume that the crystal obeys minimization laws (note that such minimization states are reached very fast in actual crystals such as pure copper, where resistence to dislocation motion is negligible [3]).

The first step we should achieve is thus to establish the functional setting appropriate to describe mesoscopic (otherwise called *continuum*) dislocations. The main features are that (i) when Sobolev spaces $W^{1,p}$ are considered, exponent p is in the "bad range" $1 \leq p < 3/2$, and (ii) the second grade variable is the curl instead of the gradient, and the curl must be a concentrated Radon measure. Minimization

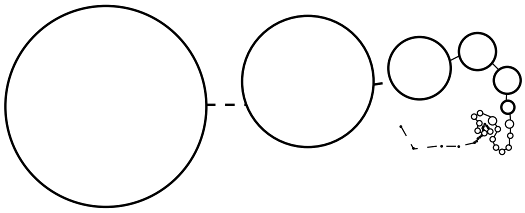

FIGURE 1. Example of a continuum dislocation cluster.

problems in this range are considered in [21] where, awared of [20], the main tool used was Cartesian maps.

In the present work, the purpose is to provide elements for an analysis of the space of L^p-tensors whose curl is bounded in a measure space, and in particular to study the homeomorphism between this space and the space of solenoidal Radon measures, which in the model application will be the space of dislocation densities. These two spaces and their properties will allow us to determine a configurational force, capable of driving the dislocations outside equilibrium, which as far as the deformation part of the energy is concerned, is the well-known Peach-Köhler force. In contrast, no such generic formula could be derived for the defect part of the energy, since the functional dual of L^p-tensors with measure curl could not be found explicitely. Nevertheless, we have based our derivations on a model example as found in [7], which was sufficient for our application purpose.

1.2. **A quick survey on currents and dislocations at the continuum scale.** In [21] we proposed a mathematical model for a countable family of dislocations in an elastic body Ω, here considered as the *current* (as opposed to *reference*) configuration. Since the dislocation loop is the singularity set for the extensive fields such as stress and strain, the deformation gradient field F is incompatible, meaning that[1]

$$-\operatorname{Curl} F = \Lambda^{\mathrm{T}} \quad \text{in } \Omega, \tag{1.1}$$

with F the (inverse) deformation tensor, and where the dislocation density Λ is a Radon measure in $\mathcal{M}(\bar{\Omega}, \mathbb{M}^3)$ concentrated on the dislocation set L. Clearly if $\Lambda = 0$ then F is a gradient. Moreover, conservation properties for dislocations imply that their density is solenoidal (i.e., divergence free),

$$\operatorname{Div} \Lambda^{\mathrm{T}} = 0. \tag{1.2}$$

The explicit formula for Λ shows a linear dependence on the line orientation τ and on the Burgers vector B (i.e., $\Lambda = \tau \otimes B\delta_L$), where for crystallographic reasons, the value of the Burgers vector is constrained to belong to a countable lattice in $\mathbb{R}^3$.

In the proposed formalism, *currents* (for which the main reference is [11]) are used to describe dislocations at the mesoscopic scale. In brief, a current is a linear and continuous functional acting on differential forms, thereby generalizing the notion of distributions [25]. Specifically, dislocations are described by integer-multiplicity 1-currents, which are mathematical objects generalizing the concept of curves, and are assumed closed to account for the property that by (1.2) every dislocation is a loop or ends at the single-crystal boundary. A brief survey of the mathematical formalism can be found in Section 3.1, while for detail we refer to [21]. The use of currents suits rather well the analysis and modeling of dislocations in single crystals. Indeed, when dislocation currents intersect or overlap, they sum according to the Frank rule [15]. Moreover, in case the generating loops are countably many, the closure theorem for integer-multiplicity currents provides

[1] Componentwise, $(\operatorname{Curl} F)_{ij} = \epsilon_{jkl}\partial_k F_{il}$ and $\Lambda_{ij} = \tau_i b_j \delta_{\mathcal{L}}$.

direct proofs of existence of minimizers for a large class of potential energies. Note also that the use of currents may also be convenient in order to study the time evolution of dislocations. For a so-called dislocation curent $\mathcal{L}$ we will denote the associated density by $\Lambda = \Lambda_{\mathcal{L}}$. In case L, the support of $\mathcal{L}$, does not coincide with $L^\star$, the support of $\Lambda_{\mathcal{L}}$, the difference $L \setminus L^\star$ is called the geometrically nonnecessary part.

The starting point of the present work is the the minimum problem

$$\min_{(F,\mathcal{L})\in\mathcal{A}} \mathcal{W}(F, \Lambda_{\mathcal{L}}), \tag{1.3}$$

where the energy $\mathcal{W}$ satisfies some appropriate convexity and coerciveness conditions, while $\mathcal{A}$ is the space of admissible couples of deformation and dislocation currents. Among the properties of admissibility, we require that F and $\mathcal{L}$ be related by condition (1.1), and that F be the gradient of a Cartesian map away from L. Therefore, both F and $\mathcal{L}$ are represented by particular types of currents. Problems (1.3) has been proposed and first studied in [20] with a single fixed dislocation loop in the crystal bulk (thus implying a minimization in F only), and later extend in [21] for an unfixed countable family of dislocation currents satisfying certain boundary conditions. Existence of minimizers will be recalled in Section 3.4.

Let us emphasize that the assumption $1 \le p < 2$ is at the origin of the difficulties encountered to solve (1.3) (see also [23, 24]). Moreover, the case $1 \le p < 3/2$ is even more puzzling, but cannot be discarded for convenience, since physical understanding of dislocations tells us that relevant and striking phenomena, such as cavitation, only occur with such kind of singular deformations. In fact dislocation nucleation follows from cavitation, that is, from the collapse of a void (i.e., a cluster of vacancies) which has become unstable or too big.

1.3. **Scope of the work.** Considering the existence of minimizers of Problem (1.3), in the present paper we analyze the variation of $\mathcal{W}$ at the minimum points with respect to L, which by a formal chain rule writes as

$$\delta_L \mathcal{W}(F, \Lambda_{\mathcal{L}}) = \delta_F \mathcal{W}(F, \Lambda_{\mathcal{L}})\delta_L F + \delta_\Lambda \mathcal{W}(F, \Lambda_{\mathcal{L}})\delta_L \Lambda_{\mathcal{L}}.$$

Note first that $\mathcal{W}$ writes as the sum of a deformation and a defect part, the first depending on F, the second on $\Lambda_{\mathcal{L}} = -\left(\text{Curl } F\right)^{\mathrm{T}}$. However both variables are related to L in a specific manner, and hence a precise meaning must be given to the above chain rule expression.

The first aim of this paper is of theoretical nature: it consists in giving a precise meaning to $\delta_L F$ and $\delta_L \Lambda_{\mathcal{L}}$, and will be achieved by proving a series of preliminary result. As far as the second term is concerned, the geometric analysis made in [21] and synthetized in Section 3.1 is used as basis, but here completed by putting the concentrated measure $\Lambda_{\mathcal{L}}$ in duality with a certain continuous tensor, called the *constraint reaction*. One difficulty is related to the identification of the dual space such Radon measures which are concentrated in closed lines, since in general it is not true that this set be a subspace of continuous functions. This will in particular require to invert the curl operator. As far as the deformation part of the energy is concerned, we have already mentioned that it was not a gradient, since to satisfy constraint (1.1), it must read as $F = \nabla u + \text{Curl } V$, which is recognized as a tensor Helmholtz-Weyl type decomposition. As a matter of fact, F will depend on L through the solution of $-\text{Curl Curl } V = (\Lambda_{\mathcal{L}})^{\mathrm{T}}$, which is an equation to consider with care, since it is not an elliptic PDE. In this paper, use will also be made of Helmholtz and Friedrich/Maxwell type decompositions in L^p (see, e.g., [13, 16]), where by Maxwell it is intended boundedness properties of a vector/tensor with respect to their curl and divergence [19, 31]. The crucial fact being that since dislocation densities are solenoidal fields, the L^p-norm of the deformation gradient is, by (1.1), estimated by a simple bound of the dislocation density norm, here intended as total variation of the Radon measure.

The second aim of this paper is about modeling, and is thought with a view to model the evolution in time of dislocations, in the sense that computing $\delta_{\mathcal{L}} W$ amounts to consider that a certain (configurational) force exerted on the dislocations is vanishing. Therefore, a moving dislocation will evolve with a velocity proportional to this force, very well known in dislocation theories [1, 15], and originating from the variation of the deformation part of the energy. In the final Theorem 7 we show that at optimality, there is a balance of forces, one of which being the Peach-Köhler force, while the other is a line-tension term provided by variation of the defect part of the energy (see also [8]). However, time evolution *per se* is not considered in the present work.

1.4. **Main result.** The paper main result is the existence of a single continuous *constraint reaction* field from which the Newtonian and configurational forces exerted on the dislocation at equilibrium are derived. Whereas the Piola-Kirchhoff stress shows high integrability property, the Peach-Köhler force, which is a priori a first-order distribution, is proved to be a Radon measure.

Main Theorem: Under the assumptions of existence to Problem (1.3), and the hypothesis that (i) the elastic part of the energy $\mathcal{W}_e$ is Fréchet differentiable, and (ii) that the optimal lines $\mathcal{L}^\star := \lambda^\star(S^1)$ are $W^{2,1}(S^1)$, there exists a continuous constraint reaction $\mathbb{L}^\star$ such that

- the derivative $W_F^\star$ of $\mathcal{W}_e$ at the optimal $F^\star$ writes as $W_F^\star = \operatorname{Curl} \mathbb{L}^\star$ and is recognized as the *Piola Kirchhoff stress*.
- the first variation of $\mathcal{W}_e$ with respect to the dislocation line $L^\star$ is such that
$$\delta^\circ \mathcal{W}_{\mathrm{e}}(F^\star) \in \mathcal{M}(L^\star, \mathbb{R}^3),$$
with, for every $\lambda \in W^{1,1}(S^1)$, the *Peach-Köhler force* $\delta^\circ \mathcal{W}_{\mathrm{e}}(F^\star)$ writing for a single dislocation $\mathcal{L}$ with Burgers vector b as
$$\langle \delta^\circ \mathcal{W}_{\mathrm{e}}(F^\star), \lambda \rangle = -\int_{\mathcal{L}} \left((W_F^\star \times \tau)^{\mathrm{T}}\, b \right) \cdot \lambda d\mathcal{H}^1. \tag{1.4}$$
Note that the precise meaning of (1.4) is at the heart of this paper, since $W_F^\star = \operatorname{Curl} \mathbb{L}^\star$ is a mere distribution at this stage.

Proof outine:
- Helmholtz decomposition (Theorem 1) and Inversion of the curl operator (Theorem 2) $\Rightarrow$ Existence of a constraint reaction (Theorem 3)
- Functional space representation of dislocations (Theorem 4) and Existence results (Theorem 5) $\Rightarrow$ Main result (Theorem 6).

Moreover, as an application: Theorems 1-6 $\Rightarrow$ Balance of configurational forces (Theorem 7).

1.5. **Structure of the paper.** In Section 2, the theoretical results required as preliminaries are stated and proved, unless their proof is found elsewhere in the literature. An important result is the existence of a constraint reaction, given in Section 2.5, but the main result is the inversion of the curl operator as found in Section 2.4. Section 3 contains three subsections where the mathematical properties of a dislocation model in this setting are given and discussed. In particular, the functional relations between the deformation and defect variables are given (important relations are here (3.13) and (3.14) and Theorem 4), their admissibility is studied, and minimization results in appropriate spaces are recalled. In Section 4, the generic results of previous sections are applied to a more specific dislocation model. The final scope is to compute the first variation of the energy at the minimum points, to the aim of which a crucial result is Lemma 10 of Section 4.1. As a matter of fact, in Sections 4.2 and 4.3, a shape optimization view of minimality provides a balance of configurational forces, which is applied to an example in Section 4.3.1. All preliminary results of this paper are required to derive this force expression, collected in Theorem 7.

1.6. **A remark.** This paper has been written in two parts, the first, i.e., Section 2, where all theoretical results are stated and proved without even referring to dislocations. Indeed, the functional spaces described in this section are broader than those needed for dislocations, and hence the results more general. Instead, Sections 3 and 4 are specifically devoted to the study of dislocations, and hence the previously proved results are particularized. Moreover, in order to be self-contained, the essence of [21] is recalled in simple terms in Section 3.1.

2. Theoretical setting and preliminary results

2.1. **Notations and conventions.** The class of 3×3 matrices are denoted by $\mathbb{M}^3 := \mathbb{R}^{3\times 3}$. In the following definitions the codomain space $\mathcal{R}$ is either tensor valued, $\mathcal{R} = \mathbb{M}^3$, or vector valued, $\mathcal{R} = \mathbb{R}^3$. Then $\mathcal{R}'$ stands for $\mathbb{R}^3$ or $\mathbb{R}$, respectively. Symbol $\mathcal{M}$ stands for finite Radon measures, while $\mathcal{D}$ denotes the topological vector space of smooth functions with compact support. The subset of solenoidal finite Radon measures in $X \subset \mathbb{R}^3$ reads

$$\mathcal{M}_{\rm div}(X,\mathcal{R}) := \{\mu \in \mathcal{M}(X,\mathcal{R}) \quad \text{s.t.} \quad \langle \mu, D\varphi\rangle = 0 \quad \forall \varphi \quad \text{in} \quad \mathcal{C}^1_0(X,\mathcal{R}')\}, \tag{2.1}$$

with D denoting the distributional derivative, and where the duality product (here intended in the sense of finite Radon measures) yields a real-valued tensor whose components read $(\langle \mu_{ij}, D_j\varphi_k\rangle)_{ik}$. Recall that $\varphi \in \mathcal{C}^1_0(X,\mathcal{R}')$ if φ and $D\varphi$ are continuous and if for every $\epsilon > 0$ there exists a compact K such that $\|\varphi(x)\|$ and $\|D\varphi(x)\|$ are smaller than ϵ for any $x \in X \setminus K$. In particular, the transpose of the dislocation density[2] $(\Lambda^\star)^T \in \mathcal{M}_{\rm div}(\hat\Omega, \mathbb{M}^3)$, where $\hat\Omega \supset \Omega$ is an open set containing only dislocations loops. Observe that $\mathcal{M}_{\rm div}(X,\mathcal{R})$ is a closed subset of $\mathcal{M}(X,\mathcal{R})$ an hence is a Banach space, endowed with the total variation norm $|\mu|(X) = \sup\{\langle \mu,\varphi\rangle : \varphi \in \mathcal{C}(X,\mathcal{R}), \|\varphi\|_\infty \le 1\}$ (see [2] for details on vector- and tensor-valued Radon measures on metric spaces). For a tensor A we use the convention that $(N \times A)_{ij} = -(A\times N)_{ij} = -\epsilon_{jkl}A_{ik}N_l$. Moreover the curl of a tensor A will be defined componentwise as $(\operatorname{Curl} A)_{ij} = \epsilon_{jkl}D_kA_{il}$. In particular, one has

$$\langle \operatorname{Curl} A, \psi\rangle = -\langle A_{il}, \epsilon_{jkl}D_k\psi_{ij}\rangle = \langle A_{il}, \epsilon_{lkj}D_k\psi_{ij}\rangle = \langle A, \operatorname{Curl}\psi\rangle, \tag{2.2}$$

for every $\psi \in \mathcal{D}(\Omega,\mathbb{M}^3)$. In general, if ψ has not compact support, it holds

$$\langle \operatorname{Curl} A, \psi\rangle = \langle A, \operatorname{Curl}\psi\rangle + \int_{\partial\Omega} (N\times A)\cdot\psi dS. \tag{2.3}$$

Note that with this convention one has $\operatorname{Div}\ \operatorname{Curl} A = 0$ in the sense of distributions, since componentwise the divergence is classicaly defined as $(\operatorname{Div} A)_i = D_jA_{ij}$.[3]

[2]The transpose is taken to be consistent to the second author's references on dislocations [**?**, 27, 29]. This convention was originally taken from Kröner [17].

[3]In this paper we therefore follow the transpose of Gurtin's notation convention [6] but care must be payed since the curl and divergence of tensor fields are given alternative definitions in the literature (including the second author references [**?**, 29] where the current curl would write $\operatorname{Curl} A = -A \times \nabla$).

2.2. **L^p-fields with bounded measure curl.** Let $1 \leq p < \infty$ and let $\Omega \subset \mathbb{R}^3$ be an arbitrary open set. We introduce the vector space of tensor-valued fields

$$\mathcal{BC}^p(\Omega, \mathbb{R}^{3\times 3}) := \{F \in L^p(\Omega, \mathbb{R}^{3\times 3}) \text{ s.t. } \operatorname{Curl} F \in \mathcal{M}_{\rm div}(\Omega, \mathbb{R}^{3\times 3})\}, \tag{2.4}$$

which, as endowed with norm

$$\|F\|_{\mathcal{BC}^p} := \|F\|_p + |\operatorname{Curl} F|(\Omega), \tag{2.5}$$

turns out to be a Banach space. Here the curl of $F \in \mathcal{BC}^p(\Omega, \mathbb{R}^{3\times 3})$ is intended in the sense of distributions.

Remark 1. *One could define $\mathcal{BC}^p(\hat{\Omega}, \mathbb{M}^3)$ by specifying only that* $\operatorname{Curl} F \in \mathcal{M}(\hat{\Omega}, \mathbb{M}^3)$ *and considering the solenoidal property of μ as a direct consequence of the distributional identity* $\operatorname{Div} \operatorname{Curl} F = 0$ *in $\hat{\Omega}$.*

Lemma 1. *Let $\mu \in \mathcal{M}_{\rm div}(\Omega, \mathbb{R}^{3\times 3})\}$ be a measure that is abosolutely continuous with respect to the $\mathcal{H}^1$-measure restricted on a simple Lipschitz curve $\mathcal{L}$ with tangent vector τ and such that $\mathcal{L}$ is either closed or ends at the boundary. Then μ is a dislocation-measure, that is, there exists a constant vector b such that*

$$\mu = b \otimes \tau \mathcal{H}^1_{\llcorner \mathcal{L}}.$$

Proof. By definition $\langle \mu, \varphi\rangle = \int_{\mathcal{L}} M(z) \cdot \varphi(z) d\mathcal{H}^1(z)$ with $M \in L^1(\mathcal{L}, \mathbb{M}^3)$ for every $\varphi \in \mathcal{D}(\Omega, \mathbb{M}^3)$. Moreover $\langle \mu, D\psi\rangle = 0$ for every $\psi \in \mathcal{D}(\Omega, \mathbb{R}^3)$. Let $\{\nu, \sigma, \tau\}$ be a local orthogonal basis attached to $\mathcal{L}$. By orthogonal decomposition, $M_{ij} = M_{ik}\tau_k\tau_j + M_{ik}\nu_k\nu_j + M_{ik}\sigma_k\sigma_j$ and $\varphi_{ij} = \varphi_{ik}\tau_k\tau_j + \varphi_{ik}\nu_k\nu_j + \varphi_{ik}\sigma_k\sigma_j$. It is easy to see that we can always choose $\varphi_{ij} = D_j\psi_i$ such that $\partial_\tau \psi_{i|\mathcal{L}} = D_j\psi_i\tau_j = 0, \partial_\nu\psi_{i|\mathcal{L}} = \eta_i, \partial_\sigma\psi_{i|\mathcal{L}} = \xi_i$ for arbitrary smooth η and ξ on $\mathcal{L}$, so that one has $0 = \int_{\mathcal{L}} M(z) \cdot D\psi(z) d\mathcal{H}^1 = \int_{\mathcal{L}} (M_{ij}\eta_i\nu_j + \xi_i M_{ij}\sigma_j)\, d\mathcal{H}^1$, and hence $M_{ij} = b_i\tau_j$ with $b_i := M_{ik}\tau_k$. Taking now $\varphi = D\psi$, it results from the closeness property of $\mathcal{L}$ and the compact support of ψ that $0 = \int_{\mathcal{L}} b \cdot \partial_\tau \psi_{|\mathcal{L}} d\mathcal{H}^1 = -\int_{\mathcal{L}} \partial_\tau b \cdot \psi d\mathcal{H}^1$, and b is constant. $\square$

The following result is required to give a meaning to the boundary trace of a L^p function whose curl is a Radon measure (in case the full gradient is a Radon measure, the statement is a classical properties of functions of bounded variation). For simplicity of presentation, it is stated for the vector case, but tensor extension is straightforward.

Lemma 2 (Trace operator)**.** *Let $1 \leq p < \infty$ and Ω be a smooth bounded subset of $\mathbb{R}^3$. There exists a linear and bounded operator $\tau : \mathcal{BC}^p_{\rm div}(\Omega, \mathbb{R}^3) \to H^{-1/2}(\partial\Omega, \mathbb{R}^3)$ such that, for $f \in \mathcal{BC}^p_{\rm div}(\Omega, \mathbb{R}^3)$*

$$\langle f, \nabla \times \varphi\rangle = \langle \nabla \times f, \varphi\rangle + \langle \tau(f), \varphi\rangle_{\partial\Omega} \qquad \forall \varphi \in C^1(\Omega, \mathbb{R}^3). \tag{2.6}$$

For smooth f, $\tau(f) = f \times N$ where N is the outer unit normal vector to $\partial\Omega$.

Remark 2. *The "antinormal" tensor $F \times N = (F\tau_A) \otimes \tau^B - (F\tau_B) \otimes \tau^A$ is distinct from the tangent projection $F - FN \otimes N = (F\tau_A) \otimes \tau^A + (F\tau_B) \otimes \tau^B$ with (τ^A, τ^B) the 2 tangent vectors of $\partial\Omega$.*

2.3. **Helmholtz decomposition for tensor fields.**

Lemma 3. *Let $G \in L^p(\Omega, \mathbb{M}^3)$ with $1 < p < \infty$ and Ω be a bounded open and simply-connected set with C^1 boundary. There exists a unique solution (up to a constant) $\phi \in W^{1,p}(\Omega, \mathbb{R}^3)$ of*

$$\left\{ \begin{array}{rcll} -\Delta\phi & = & \operatorname{Div} G & \textit{in} \quad \Omega \\ \partial_N \phi & = & -GN & \textit{on} \quad \partial\Omega \end{array} \right. . \tag{2.7}$$

Moreover such solution satisfies $\|D\phi\|_p \leq C\|G\|_p$.

Proof. This Lemma is a direct tensor extension of the theorems of existence and uniqueness of Neumann problem as shown in [26] (see also [13, Lemma III.1.2 and Theorem III.1.2]).

□

Remark that Eq. (2.7) is a formal strong form meaning that the following weak form is solved [31]:

$$-\langle \nabla\phi, \nabla\varphi\rangle = \langle G, \nabla\varphi\rangle \quad \forall \varphi \in W^{1,p'}(\Omega, \mathbb{M}^3). \tag{2.8}$$

In particular, observe that the GN is not well defined on the domain boundary. This issue will be addressed by Lemma 4. Let us define

$$\begin{aligned} L^p_{\rm div}(\Omega, \mathbb{M}^3) &:= \{F \in L^p(\Omega, \mathbb{M}^3) \quad \text{s.t.} \quad \text{Div } F = 0\} \\ &= \text{adh}_{L^p}\{F \in \mathcal{C}^\infty(\bar\Omega, \mathbb{M}^3) \quad \text{s.t.} \quad \text{div}F = 0\}, \end{aligned} \tag{2.9}$$

$$\begin{aligned} L^p_{\rm curl}(\Omega, \mathbb{M}^3) &:= \{F \in L^p(\Omega, \mathbb{M}^3) \quad \text{s.t.} \quad \text{Curl } F = 0\} \\ &= \text{adh}_{L^p}\{F \in \mathcal{C}^\infty(\bar\Omega, \mathbb{M}^3) \quad \text{s.t.} \quad \text{curl}F = 0\}. \end{aligned} \tag{2.10}$$

Let $1 < p < \infty$. If $V \in L^p(\Omega, \mathbb{R}^3)$ is such that $\text{Div } V \in L^p(\Omega, \mathbb{R})$, then there exists $VN \in W^{-1/p,p}(\partial\Omega) := \left(W^{1/p,p'}(\partial\Omega)\right)'$. Moreover, if $V \in L^p(\Omega, \mathbb{R}^3)$ with $\text{Curl } V \in L^p(\Omega, \mathbb{R}^3)$, there exists $V \times N \in W^{-1/p,p}(\partial\Omega, \mathbb{R}^3)$. These properties straightforwardly apply to tensor valued maps, where VN (componentwise, $V_{ij}N_j$) and $V \times N$ (componentwise, $\epsilon_{jlp}V_{il}N_p$) mean with an abuse of notations the bounded normal and antinormal traces in $W^{-1/p,p}(\partial\Omega, \mathbb{R}^3)$ and $W^{-1/p,p}(\partial\Omega, \mathbb{M}^3)$ respectively. In particular, these traces are well defined for tensors belonging to the spaces $L^p_{\rm div}(\Omega, \mathbb{M}^3)$ and $L^p_{\rm curl}(\Omega, \mathbb{M}^3)$ (see [16] and references therein). Specifically, the following can be proven.

Lemma 4. *Let $\Omega \subset \mathbb{R}^3$ be a bounded open set with boundary of class C^1 and let $F \in L^p(\Omega, \mathbb{R}^{3\times 3})$ be such that* $\text{Div } F \in L^p(\Omega, \mathbb{R}^3)$*. Then there exists $FN \in W^{-1/p,p}(\partial\Omega, \mathbb{R}^3) := \left(W^{1/p,p'}(\partial\Omega, \mathbb{R}^3)\right)'$ such that*

$$\langle FN, \gamma(\varphi)\rangle := \langle \text{ Div } F, \varphi\rangle + \langle F, D\varphi\rangle \tag{2.11}$$

for all $\varphi \in W^{1,p'}(\Omega, \mathbb{R}^3)$, with $\gamma(\varphi) \in W^{1/p,p'}(\partial\Omega, \mathbb{R}^3)$ the boundary trace of φ, and where $\langle\cdot\rangle$ always mean the duality product in appropriate spaces.

Similarly:

Lemma 5. *Let $\Omega \subset \mathbb{R}^3$ be a bounded open set with boundary of class C^1 and let $F \in L^p(\Omega, \mathbb{R}^{3\times 3})$ be such that* $\text{Curl } F \in L^p(\Omega, \mathbb{R}^{3\times 3})$*. Then there exists $F \times N \in W^{-1/p,p}(\partial\Omega, \mathbb{R}^3) := \left(W^{1/p,p'}(\partial\Omega, \mathbb{R}^3)\right)'$ such that*

$$\langle F \times N, \gamma(\varphi)\rangle := \langle \text{ Curl } F, \varphi\rangle - \langle F, \text{ Curl } \varphi\rangle \tag{2.12}$$

for all $\varphi \in W^{1,p'}(\Omega, \mathbb{R}^3)$, with $\gamma(\varphi) \in W^{1/p,p'}(\partial\Omega, \mathbb{R}^3)$ the boundary trace of φ.

Let us introduce the spaces

$$\mathcal{V}^p(\Omega) := \left\{V \in L^p_{\rm div}(\Omega, \mathbb{M}^3) \text{ s.t. } \text{Curl } V \in L^p(\Omega, \mathbb{M}^3), V \times N = 0 \text{ on } \partial\Omega\right\}, \tag{2.13}$$

$$\tilde{\mathcal{V}}^p(\Omega) := \left\{V \in L^p_{\rm div}(\Omega, \mathbb{M}^3) \text{ s.t. } \text{Curl } V \in L^p(\Omega, \mathbb{M}^3), VN = 0 \text{ on } \partial\Omega\right\}. \tag{2.14}$$

The following estimate can be found in [16].

Lemma 6 (Kozono-Yanagisawa). *Let $\Omega \subset \mathbb{R}^3$ be a bounded open set with boundary of class C^1 and assume $F \in \mathcal{V}^p(\Omega)$ or $F \in \tilde{\mathcal{V}}^p(\Omega)$. Then $F \in W^{1,p}(\Omega, \mathbb{R}^{3\times 3})$ and it holds*

$$\|\nabla F\|_p \leq C\left(\| \operatorname{Curl} F\|_p + \|F\|_p\right). \tag{2.15}$$

This shows that $\mathcal{V}^p(\Omega)$ and $\tilde{\mathcal{V}}^p(\Omega)$ are closed subspaces in $W^{1,p}(\Omega, \mathbb{M}^3)$. By virtue of Lemma 6 and for simply connected and bounded domains, a better estimate can be found in [30]. Note that the following is a classical result for smooth functions with compact support.

Lemma 7 (von Wahl). *Let Ω be a simply-connected and bounded domain and let $F \in \mathcal{V}^p(\Omega)$ or $F \in \tilde{\mathcal{V}}^p(\Omega)$. Then it holds*

$$\|\nabla F\|_p \leq C\| \operatorname{Curl} F\|_p. \tag{2.16}$$

As a direct consequence the following result holds.

Lemma 8. *Let $F \in \mathcal{V}^p(\Omega)$ or $F \in \tilde{\mathcal{V}}^p(\Omega)$. Then* $\operatorname{Curl} F = 0 \iff F = 0$.

We remark that, when $F \in \tilde{\mathcal{V}}^p(\Omega)$, Lemma 8 amounts to proving the uniqueness property of Lemma 3. Moreover, in [16], a more general statement is established without the simply-connectedness assumption. In general, for Ω a smooth and bounded subset of $\mathbb{R}^3$, $\operatorname{Curl} F = \operatorname{Div} F = 0$ has a non-trivial solution. In particular Kozono and Yanagisawa [31] show that the solutions belong to a subspace of $C^\infty(\bar{\Omega}, \mathbb{M}^3)$ with positive finite dimension, depending on the Betti number of Ω.

The following result is well known in the Hilbertian case L^2 but is not classical for the general Banach space L^p. It is basically proven with help of Lemma 3 (for a complete proof see [16,31], cf. also [13,19]).

Theorem 1 (Helmholtz-Weyl-Hodge-Yanagisawa). *Let $1 < p < \infty$ and let Ω be a bounded, simply-connected and smooth open set in $\mathbb{R}^3$. For every $F \in L^p(\Omega, \mathbb{M}^3)$, there exist $u_0 \in W_0^{1,p}(\Omega, \mathbb{R}^3)$ and a solenoidal $V \in \tilde{\mathcal{V}}^p(\Omega)$, such that*

$$F = Du_0 + \operatorname{Curl} V, \quad \left(L^p(\Omega, \mathbb{M}^3) = \nabla W_0^{1,p}(\Omega, \mathbb{R}^3) \oplus \operatorname{Curl} \tilde{\mathcal{V}}^p(\Omega)\right), \tag{2.17}$$

Alternatively, there exist $u \in W^{1,p}(\Omega, \mathbb{R}^3)$, and a solenoidal $V_0 \in \mathcal{V}^p(\Omega)$, such that

$$F = Du + \operatorname{Curl} V_0, \quad \left(L^p(\Omega, \mathbb{M}^3) = \nabla W^{1,p}(\Omega, \mathbb{R}^3) \oplus \operatorname{Curl} \mathcal{V}^p(\Omega)\right), \tag{2.18}$$

Moreover the decompositions are unique, in the sense that u_0, V, V_0 are uniquely determined, while u is unique up to a constant, and it holds $\|Du_0\|_p, \|Du\|_p \leq C\|F\|_p$, respectively.

Remark 3. *When F is smooth with compact support, decompositions such as* (2.17) *and* (2.18) *are classically given by Stokes theorem and explicit formulae involving the divergence and the curl of F (see [30], [4]). Notice that no boundary datum for F is here given.*

Remark 4. *Let F be of class C^1. In the particular case* $\operatorname{Curl} F = 0$ *the Helmholtz decomposition is trivial when Ω is a simply-connected domain. Indeed it is well-known that in such a case there exists $u \in \mathcal{C}^2(\Omega, \mathbb{R}^3)$ satisfying $F = Du$. This result extends for $F \in L^p$ with $1 < p < +\infty$ as shown in [13]. See [16] for a complete treatment of Helmholtz decomposition in L^p, relying on the pioneer paper [12]. Moreover, if* $\operatorname{Div} F = 0$ *then, by Theorem 1, $F =$* $\operatorname{Curl} V$ *with $V \in \tilde{\mathcal{V}}^p(\Omega)$. Remark that for smooth functions F, this result holds for any simply-connected domain with Lipschitz boundary.*

Remark 5. *Smoothness of the boundary is a strong requirement which is needed for the following reason:* (2.17) *and* (2.18) *require in principle to solve a Poisson* *equation $\Delta u = \operatorname{Div} F$ with the RHS in some distributional (viz., Sobolev-Besov space) for which smoothness of the boundary is needed. It is known [10] that for a Lipschitz boundary the solution holds for restricted p (namely $3/2-\epsilon \le p \le 3+\epsilon$) for some $\epsilon=\epsilon(\Omega)>0$. Note that for $p=2$ a Lipschitz boundary would be sufficient.*

Lemma 9. *Let $\Omega \subset \mathbb{R}^3$ be a bounded open set with boundary of class C^1 and $V \in \mathcal{V}^p(\Omega)$. Then $(\operatorname{Curl} V)N = 0$ in the sense of Lemma 4.*

Proof. Take any $\varphi \in W^{1,p'}(\Omega,\mathbb{R}^3)$. By part integration (equations (2.11) and (2.12)), it holds

$$\langle (\operatorname{Curl} V)N, \varphi\rangle_{\partial\Omega} = \langle \operatorname{Curl} V, D\varphi\rangle = \langle V \times N, D\varphi\rangle_{\partial\Omega} = 0.$$

Since φ is arbitrary, the proof is achieved. □

By Lemma 9, the potential u of (2.18) is found by solving (2.7) with $\phi = u$ and $G = -F$, this also gives a meaning to the condition $\partial_N u = FN$.

2.4. Invertibility of the curl.

Assumption 1. *Unless otherwise specified, the domains Ω we consider are bounded, smooth and simply connected subsets of $\mathbb{R}^3$, with outward unit normal N.*

Assumption 2. *Given Ω, we denote by $\hat\Omega$ another domain satisfying Assumption 1 and such that $\Omega \subset\subset \hat\Omega$.*

A key equation behind the results of this work is the following system:

$$\begin{cases} -\operatorname{Curl} F &= \mu^{\mathrm{T}} & \text{in } \hat\Omega \\ \operatorname{Div} F &= 0 & \text{in } \hat\Omega \\ FN &= 0 & \text{on } \partial\hat\Omega, \end{cases} \tag{2.19}$$

with μ^{T} a Radon measure in $\mathcal{M}_{\mathrm{div}}(\hat\Omega,\mathbb{M}^3)$. Existence and uniqueness of a solution is given by the following Theorem 2, for which Lemma 3 (or Lemma 8) will be required.

The following result generalizes to the case of measures the result in [5].

Theorem 2 (Biot-Savart)**.** *Let μ be a tensor-valued Radon measure such that $\mu^{\mathrm{T}} \in \mathcal{M}_{\mathrm{div}}(\hat\Omega,\, \mathbb{M}^3)$, and let it be extended by zero outside $\hat\Omega$. Then there exists a unique F in $\mathcal{BC}^1_{\mathrm{div}}(\hat\Omega,\mathbb{M}^3)$ solution of (2.19). Moreover F belongs to $\mathcal{BC}^p_{\mathrm{div}}(\hat\Omega,\mathbb{M}^3)$ for all p with $1 \le p < 3/2$ and for all such p there exists a constant $C>0$ satisfying*

$$\|F\|_p \le C|\mu|(\hat\Omega). \tag{2.20}$$

Moreover, if $\mu = b \otimes \tau\, \mathcal{H}^1 \llcorner_C$, for some $b \in \mathbb{R}^3$ and a C^2-closed curve C in $\hat\Omega$ with unit tangent vector τ, then the solution F belongs to $\mathcal{BC}^p_{\mathrm{div}}(\hat\Omega,\mathbb{M}^3)$ for all p with $1 \le p < 2$.

Proof. **Step 1:** tensor computations with product of measures.

Let $\varphi \in \mathcal{C}^\infty_c(\mathbb{R}^3,\mathbb{R})$ and denote by $\langle\cdot\rangle$ the duality product (for measures, distributions, etc.). It holds

$$\int_{\mathbb{R}^3} \varphi(x)d\mu_{ij}(x) = \langle \mu_{ij},\varphi\rangle = \langle \mu^x_{ij}, \langle \Delta\Phi(x-\xi),\varphi(\xi)\rangle\rangle, \tag{2.21}$$

where Φ is the fundamental solution of the Laplacian in $\mathbb{R}^3$ (i.e., $\Delta\Phi = \delta_0$). The subscript x, y or ξ means that the field on which it is apended is a function of x, y or $\xi := x+y$. Dropping these subscripts will be allowed if no ambiguity results from this simplification.

Let $\bar\varphi(x) := D\Phi \star \varphi(x) = \int_{\mathbb{R}^3} D\Phi(x-\xi)\varphi(\xi)d\xi = -\int_{\mathbb{R}^3} D\Phi(\xi-x)\varphi(\xi)d\xi = -\int_{\mathbb{R}^3} D\Phi(y)\varphi(x+y)dy \in \mathcal{C}^1_0(\mathbb{R}^3,\mathbb{R}^3)$, where we have used the odd and asymptotically decreasing properties of $D\Phi$. By solenoidal property of μ^{T}, one has

$\langle\mu_{ij}, D_i\bar\varphi_k\rangle = 0$, and recalling that $\epsilon_{iqm}\epsilon_{mkl} = \delta_{ik}\delta_{ql} - \delta_{il}\delta_{qk}$ while $D\Phi(\xi - x) = -D\Phi(\xi - x)$, we rewrite (2.21) as

$$\begin{aligned}\langle\mu_{ij},\varphi\rangle &= -\langle\mu_{kj}, \epsilon_{iqm}\epsilon_{mkl}D_q\bar\varphi_l\rangle = \langle\mu^x_{kj}, \epsilon_{iqm}\epsilon_{mkl}\langle D_l\Phi(y), D_q\varphi(y+x)\rangle\rangle \\ &= \epsilon_{iqm}\epsilon_{mkl}\int_{\mathbb{R}^3} d\mu_{kj}(x)\int_{\mathbb{R}^3} D_l\Phi(y)D_q\varphi(x+y)dy \\ &= \langle\epsilon_{mkl}D_l\Phi\mu^x_{kj}, \epsilon_{iqm}D_q\varphi(x+y)\rangle,\end{aligned}$$

which by definition of the convolution between distributions (cf. [25, Théorème 1,VI,2;5]) reads

$$\langle\epsilon_{mkl}D_l\Phi\star\mu_{kj}, \epsilon_{iqm}D_q\varphi\rangle = \langle\epsilon_{iqm}D_q\left(\epsilon_{mlk}D_l\Phi\star\mu_{kj}\right), \varphi\rangle, \tag{2.22}$$

implying that $\mu_{ij} = \epsilon_{iqm}D_q\left(\epsilon_{mlk}D_l\Phi\star\mu_{kj}\right)$ as a distribution.

Step 2: explicit expression of a solution.

Therefore the solution G writes componentwise as

$$G_{jm}(x) := -\epsilon_{mlk}\left(D_l\Phi\star\mu_{kj}\right)(x) = \int_{\mathbb{R}^3}\epsilon_{mlk}D_l\Phi(\xi - x)d\mu_{kj}(\xi), \tag{2.23}$$

satisfies, by (2.22),

$$-\operatorname{Curl} G = \mu^{\mathrm{T}} \quad \text{in} \quad \hat\Omega. \tag{2.24}$$

Step 3: boundedness and solenoidal properties of G.

First observe that $D\Phi \in L^p(\mathbb{R}^3, \mathbb{M}^3)$ with $1 \le p < 3/2$, since $D\Phi(x) = O(|x|^{-2})$, and hence, posing $R := |x - y|$, while $\bar R$ is the radius of a ball centered in 0 and containing $\bar\Omega$,

$$\|D\Phi\|_p^p \le \int_0^{\bar R} R^{-2p}R^2 dR, \tag{2.25}$$

where the last factor in the RHS is bounded as long as $1 \le p < 3/2$. The boundedness in L^p (hence the continuity) now follows from Minkowski's inequality since for some $C > 0$, it holds (see also [25, VI.I;4]),

$$\|G\|_p \le C|\mu|(\hat\Omega).$$

Now, taking $\psi \in W^{1,p'}(\mathbb{R}^3, \mathbb{R}^3))$ yields $\operatorname{Div} G = 0$ since componentwise,

$$\begin{aligned}\langle G_{jm}, D_m\psi_j\rangle &= \langle\epsilon_{mlk}\langle D^y_l\Phi(\xi - x), \mu_{kj}(\xi)\rangle, D_m\psi_j(x)\rangle \\ &= -\int_{\mathbb{R}^3}\epsilon_{mlk}\langle D_l\Phi(\xi - x), D_m\psi_j(x)\rangle d\mu_{kj}(\xi) \\ &= \int_{\mathbb{R}^3}\epsilon_{mlk}\langle D_mD_l\Phi(\xi - x), \psi_j(x)\rangle d\mu_{kj}(\xi) = 0,\end{aligned}$$

where the last equality follows from the smoothness of Φ.

Step 4: vanishing of FN.

By Lemma 4 (with $\hat\Omega$ in place of Ω), since $\operatorname{Div} G = 0$ the normal trace of G, denoted as GN, exists as an element of $W^{-1/p,p}(\partial\hat\Omega, \mathbb{R}^3)$ and satisfies

$$\langle GN, \varphi\rangle_{\partial\hat\Omega} := \langle G, \nabla\varphi\rangle + \langle\operatorname{Div} G, \varphi\rangle = \langle G, \nabla\varphi\rangle \quad \forall\varphi \in W^{1,p'}(\mathbb{R}^3, \mathbb{R}^3). \tag{2.26}$$

If $\phi \in W^{1,p}(\hat\Omega)$ we have that $F := G + D\phi$ also satisfies $-\operatorname{Curl} F = \mu^{\mathrm{T}}$. Thus, Lemma 3 (with $\hat\Omega$ in place of Ω) provides a solution ϕ such that $\operatorname{Div} F = 0$ in $\hat\Omega$, $FN = 0$ on $\partial\hat\Omega$, and such that (2.20) holds.

Step 5: uniqueness.

Assume that there exist two solutions and denote by $H \in L^p$ their difference, one has $\text{Curl } H = \text{Div } H = 0$ in $\hat{\Omega}$ while $HN = 0$ on $\partial\hat{\Omega}$. From Remark 4 there exists $u \in W^{1,p}(\hat{\Omega}, \mathbb{R}^3)$ such that $H = \nabla u$. Taking the divergence one gets $\Delta u = 0$ in Ω. Moreover from $HN = 0$ we also have $\partial_N u = 0$ on $\partial\hat{\Omega}$. By Lemma 3 this implies that there is a constant c with $u \equiv c$ in $\hat{\Omega}$, whereby $H = 0$, achieving the proof of uniqueness.

Step 6: sharp result for a smooth curve.

Let $\mu_{\mathcal{L}}$ be concentrated on a smooth curve $\mathcal{L} \subset \hat{\Omega}$. By its regularity, there exists a tube $\mathcal{T}_{\mathcal{L}}$ with nonvanishing radius around $\mathcal{L}$ whose sections never mutually intersect (see [28] for a proof). On each sections S_z a local coordinates system is used, where z denotes the curvilinear abcissa, and $\tilde{x}$ the planar Cartesian coordinates. Moreover, we can assume that the support of the test functions φ lie in $\mathcal{T}_{\mathcal{L}}$. One has

$$\begin{aligned}
\frac{\Pi}{2\pi} = \langle \mu_{\mathcal{L}}, \varphi \rangle &= \langle \mu, \varphi \rangle = \int_{\mathcal{L}} M(z) \cdot \varphi(0, z) d\mathcal{H}^1(z) \\
&= \int_{\mathcal{L}} M(z) \cdot \ll \delta_z, \varphi(\tilde{x}, z) \gg d\mathcal{H}^1(z) \\
&= \frac{1}{2\pi} \int_{\mathcal{L}} M_{ij}(z) \ll \Delta_P \ln_z(\cdot), \varphi_{ij}(\tilde{x}, z) \gg d\mathcal{H}^1(z),
\end{aligned}$$

where $\ln_z(\cdot) := \ln r_z$, with $r_z := \|(\cdot, z) - (0, z)\|$ and where Δ_P denotes the planar Laplacian operator, and $M_{ij}(z) = b_i \tau_j(z)$ with constant b_i by Lemma 1. Then $\Delta = \Delta_P + \partial_z^2$ is the $3D$ Laplacian. By the identity $\epsilon_{mkn}\epsilon_{nlp} D_k D_l A_{jp} = D_p D_m A_{jp} - \Delta A_{jm}$ with $A_{jm} = \ln_z(\cdot)\delta_{jm}$, we have that

$$\begin{aligned}
\Pi &= \int_{\mathcal{L}} b_i \tau_j \ll (D_j D_m - \epsilon_{mkn}\epsilon_{nlj} D_k D_l) \ln_z(\cdot), \varphi_{im}(\tilde{x}, z) \gg d\mathcal{H}^1(z) \\
&- \int_{\mathcal{L}} M_{ij} \ll \partial_z^2 \ln_z(\cdot), \varphi_{ij}(\tilde{x}, z) \gg d\mathcal{H}^1(z).
\end{aligned}$$

Since by the curve smoothness, it holds $\partial_z^2 \ln_z(\cdot) = \partial_{r_z}^2 \ln_z(r_z)(\partial_z r_z)^2 + \partial_{r_z} \ln_z(r_z) \partial_z^2 r_z$ $= \partial_{r_z}(\partial_{r_z} \ln_z(r_z)(\partial_z r_z)^2 + \ln_z(r_z)\partial_z^2 r_z)$, part integration (of $\tau_j D_j$ in $\mathcal{L}$ and ∂_{r_s} in S_z), the fact that $\mathcal{L}$ is closed or ends at the boundary, with constant b, and that $\varphi(\cdot, z)$ has compact support in S_z entail that

$$\begin{aligned}
\Pi &= \int_{\mathcal{L}} b_i \tau_j \ll \epsilon_{mkn} D_k \left(\epsilon_{jln} D_l \ln_z(\cdot)\right), \varphi_{im}(\tilde{x}, z) \gg d\mathcal{H}^1(z) \\
&= \langle \epsilon_{mkn} D_k \left(b_i \tau_j \epsilon_{jln} D_l \ln_z(\cdot)\right), \varphi_{im} \rangle \\
&- \int_{\mathcal{T}_{\mathcal{L}}} b_i \epsilon_{mkn} \tau_k \kappa \nu_j \epsilon_{jln} D_l \ln_z(\tilde{x}) \varphi_{im}(\tilde{x}, z) d\mathcal{H}^3.
\end{aligned} \tag{2.27}$$

By previous steps, $\Pi = \langle \text{Curl } G_{\mathcal{L}}, \varphi \rangle$ for some $G_{\mathcal{L}} \in L^1(\Omega; \mathbb{M}^3)$. Hence, in the last term in the RHS of (2.27),

$$b_i \epsilon_{mkn} \tau_k \kappa \nu_j \epsilon_{jln} D_l \ln_z(\tilde{x}) = (\text{Curl } V)_{im},$$

belongs to $L^p(\Omega; \mathbb{M}^3)$ with $1 \le p < 2$, with $V = b_i \tau_j \epsilon_{jln} D_l \ln_z(\cdot) - G_{\mathcal{L}} \in L^p(\Omega; \mathbb{M}^3)$ with (by Remark 4) $1 \le p < 2$. Therefore, $G_{\mathcal{L}} \in L^p(\Omega; \mathbb{M}^3)$ with $1 \le p < 2$ and

$$\Pi = 2\pi \langle \mu_{\mathcal{L}}, \varphi \rangle = \langle \text{Curl } G_{\mathcal{L}}.\varphi \rangle,$$

Now, repeating twice Step 4 (i.e., the addition of a gradient field to $G_{\mathcal{L}}$) provides a solenoidal tensor $F_{\mathcal{L}}$ whose normal component vanishes on the boundary, while Step 5 yields uniqueness. The proof is achieved. □

By uniqueness, there exists a linear one-to-one and onto correspondance between $\nu \in \mathcal{M}_{\mathrm{div}}(\hat{\Omega}, \mathbb{M}^3)$ and $F \in \mathcal{BC}^p_{\mathrm{div}}(\hat{\Omega}, \mathbb{M}^3)$. Thus the map

$$\text{Curl}^{-1} : \mathcal{M}_{\mathrm{div}}(\hat{\Omega}, \mathbb{M}^3) \to \mathcal{BC}^p_{\mathrm{div}}(\hat{\Omega}, \mathbb{M}^3), \quad \nu \mapsto F = -\text{Curl}^{-1}(\nu), \tag{2.28}$$

is well defined and linear. Therefore, we may write

$$\mathcal{BC}^p_{\mathrm{div}}(\hat{\Omega}, \mathbb{M}^3) := \text{Curl}^{-1}\left(\mathcal{M}_{\mathrm{div}}(\hat{\Omega}, \mathbb{M}^3)\right). \tag{2.29}$$

Moreover, for any $F \in \mathcal{BC}^p_{\mathrm{div}}(\hat{\Omega}, \mathbb{M}^3)$ we recover by Eq. (2.20) the L^p-counterpart of Maxwell relation in L^2 [19], that is,

$$\|F\|_p \leq C|\,\text{Curl}\, F|(\hat{\Omega}). \tag{2.30}$$

Remark 6. *In case Ω is not simply-connected the uniqueness of solution of problem* (2.19) *does not hold. In such a case, Lemma 8 would also not hold, since the problem might exhibit non-trivial solutions, as shown in [31].*

2.5. **Existence of a constraint reaction.** In the next sections we will deal with a linear and continuous map,

$$\Phi : \mathcal{BC}^p(\hat{\Omega}, \mathbb{M}^3) \to \mathbb{R}, \tag{2.31}$$

that is such that $|\Phi(F)| \leq C\|F\|_p$ for some $C > 0$, and satisfying

$$L^p_{\mathrm{curl}}(\hat{\Omega}, \mathbb{M}^3) \subset \ker \Phi. \tag{2.32}$$

An important result for map of this kind is now stated and proved.

Theorem 3. *Let $1 < p < 3/2$ and let Φ be a linear and continuous map on $L^p(\hat{\Omega}, \mathbb{M}^3)$ satisfying $\Phi(Du) = 0$ for every $u \in W^{1,p}(\hat{\Omega}, \mathbb{R}^3)$. Then there exist two linear and continuous maps $\mathbb{L},\ \tilde{\mathbb{L}} : \mathcal{M}_{\mathrm{div}}(\hat{\Omega}, \mathbb{M}^3) \to \mathbb{R}$ belonging to $C(\bar{\hat{\Omega}}, \mathbb{M}^3) \cap W^{1,p'}(\hat{\Omega}, \mathbb{M}^3)$, where $3 < p' < \infty$ satisfies $1/p + 1/p' = 1$, such that, for every $F \in \mathcal{BC}^p(\hat{\Omega}, \mathbb{M}^3)$,*

$$\Phi(F) = \langle\,\text{Curl}\,\mathbb{L}, F\rangle = \langle\,\text{Curl}\,\tilde{\mathbb{L}}, F\rangle, \tag{2.33}$$

and satisfying $\text{Div}\,\mathbb{L} = \text{Div}\,\tilde{\mathbb{L}} = 0$ *in $\hat{\Omega}$, $N \times \mathbb{L} = 0$ and $\tilde{\mathbb{L}}N = 0$ on $\partial\hat{\Omega}$. Moreover it holds*

$$\Phi(F) = \langle \mathbb{L}, \text{Curl}\, F\rangle = \langle \tilde{\mathbb{L}}, \text{Curl}\, F\rangle + \langle \tilde{\mathbb{L}}, F \times N\rangle_{\partial\hat{\Omega}}. \tag{2.34}$$

Proof. Since Φ is linear and continuous it holds

$$\Phi(F) = \langle \mathbb{T}, F\rangle, \tag{2.35}$$

for some $\mathbb{T} \in L^{p'}(\hat{\Omega}, \mathbb{M}^3)$. Now, for every $\varphi \in \mathcal{C}^\infty(\hat{\Omega}, \mathbb{R}^3)$ we have $\langle \mathbb{T}, D\varphi\rangle = \Phi(D\varphi) = 0$, proving that (i) $\text{Div}\,\mathbb{T} = 0$ in $\hat{\Omega}$ and, by integration by parts, that (ii) $\mathbb{T}N = 0$ on $\partial\hat{\Omega}$. By Theorem 1 (Eq. (2.17) or (2.18)), there exist a unique $\mathbb{L} \in L^{p'}_{\mathrm{div}}(\hat{\Omega}, \mathbb{M}^3)$ satisfying $N \times \mathbb{L} = 0$ on $\partial\hat{\Omega}$ and a unique $\tilde{\mathbb{L}} \in L^{p'}_{\mathrm{div}}(\hat{\Omega}, \mathbb{M}^3)$ with $\tilde{\mathbb{L}}N = 0$ on $\partial\hat{\Omega}$, such that (u and u_0 are those of Theorem 1)

$$\text{Curl}\,\mathbb{L} + Du = \text{Curl}\,\tilde{\mathbb{L}} + Du_0 = \mathbb{T}. \tag{2.36}$$

Since $\text{Div}\,\mathbb{T} = 0$ in $\hat{\Omega}$, one has $u_0 = 0$ and from $\text{Curl}\,\mathbb{L}N = \mathbb{T}N = 0$ on $\partial\hat{\Omega}$, $Du = 0$. By Maxwell-Friedrich-type inequality (i.e., the generalization of (2.15), see [31]), i.e.,

$$\|\nabla\mathbb{L}\|_{p'} \leq C\left(\|\,\text{Curl}\,\mathbb{L}\|_{p'} + \|\,\text{Div}\,\mathbb{L}\|_{p'} + \|\mathbb{L}\|_{p'}\right), \tag{2.37}$$

the fact that $\mathbb{L} \in L^{p'}(\hat{\Omega}, \mathbb{M}^3)$ with $\text{Curl}\,\mathbb{L} \in L^{p'}(\hat{\Omega}, \mathbb{M}^3)$ and $\text{Div}\,\mathbb{L} = 0$, implies that $\mathbb{L} \in W^{1,p'}(\hat{\Omega}, \mathbb{M}^3)$, which since $3 < p' \leq \infty$ entails by Sobolev embedding that

$$\mathbb{L} \in \mathcal{C}(\bar{\hat{\Omega}}, \mathbb{M}^3). \tag{2.38}$$

The same is true for $\tilde{\mathbb{L}}$. Integrating by parts the identities (2.33) we get, since $N \times \mathbb{L} = 0$ on $\partial\hat{\Omega}$,

$$\Phi(F) = \langle \operatorname{Curl} \mathbb{L}, F\rangle = \langle \mathbb{L}, \operatorname{Curl} F\rangle,$$

and similarly

$$\Phi(F) = \langle \operatorname{Curl} \tilde{\mathbb{L}}, F\rangle = \langle \tilde{\mathbb{L}}, \operatorname{Curl} F\rangle + \langle \tilde{\mathbb{L}}, F \times N\rangle_{\partial\hat{\Omega}},$$

achieving the proof by (2.36). □

In the applications, Φ will be the first variation of deformation part of the energy. In the sequel we will restrict to those variations whose deformation curl is concentrated in a closed curve, and, specifically, is associated to some dislocation density measure. This latter notion will be made clear in Section 3.1. In particular an appropriate subspace of $\mathcal{BC}^p(\hat{\Omega}, \mathbb{M}^3)$ will be introduced and its properties studied.

3. Minimizers of a continuum dislocation energy

The keypoint of this work is to to perform variations around the minima of Problem (1.3) in the largest possible functional spaces. As far as the deformation part of the energy is concerned, this amounts to proving the existence of an appropriate Lagrange multiplier to account for the constraint (1.1). This will be achieved thanks to Theorem 3. For the defect part, a crucial result is given in Theorem 4 of Section 3.3. In principle, variations can be made with respect to (i) F, (ii) the dislocation density Λ and (iii) the dislocation set L. In the first case one recovers the equilibrium equations, where the Piola-Kirchhoff stress is written as the curl of the constraint reaction. The second case is more delicate since the space of variations is not a linear space (due to the so-called crystallographic assumption), thus creating a series of difficulties which we do not address further. Most interesting is the variation with respect to the line, that is, w.r.t to infinitesimal Lipschitz variations at the optimal dislocation cluster $L^\star$. The difficulty here is that both F and Λ depend on L. In the case of Λ, the dependence is explicit since L is in some sense the support of $\Lambda = \Lambda_{\mathcal{L}}$ (see (3.4)). In the case of F, the dependence is implicit since it holds

$$F = \nabla u + F^\circ, \tag{3.1}$$

where F implicitely depends on $\mathcal{L}$ through F° solution of $\operatorname{Curl} F^\circ = -(\Lambda_{\mathcal{L}})^{\mathrm{T}}$. Therefore, since the energy consists of one term in F and another in Λ, variation of the energy w.r.t. to $\mathcal{L}$ will require an appropriate version of the chain rule. This computation is the main objective of Section 4, which to be carried out carefully requires a series of preliminary steps, collected in the present section. In order to be self-contained, results from [21] are first recalled, while rewritten in a concise form. In the next two sections, the results from Section 2 are applied to continuum dislocations. The main results are relations (3.13) and (3.14) and Theorem 4.

3.1. **Dislocation density measures.** In order to perform variations in F and Λ, in this section we introduce an appropriate subspace of $\mathcal{M}_{\mathrm{div}}(\bar{\Omega}, \mathbb{M}^3)$ called the set of dislocation density measures and based upon the notion of integer multiplicity 1-currents.

In the following we will suppose that Assumptions 1 and 2 hold.

In many applications, the Burgers vector is constrained by crystollagraphic properties to belong to a lattice. For simplicity this lattice will be assumed isomorphic to $\mathbb{Z}^3$. Let the lattice basis $\{\bar{b}_1, \bar{b}_2, \bar{b}_3\}$ be fixed, and define the set of *admissible Burgers vectors* as

$$\mathcal{B} := \{b \in \mathbb{R}^3 : \exists \beta \in \mathbb{Z}^3 \text{ such that } b = \beta_i \bar{b}_i\}.$$

In the sequel we will adopt the non-restrictive and simple choice $\mathcal{B} = \mathbb{Z}^3$, i.e., $\bar{b}_i = e_i$, the ith Euclidean base vector. In the sequel we will write $b \in \mathbb{Z}^3$ to mean $b \in \mathcal{B}$.

Let L be a $\mathcal{H}^1$-rectifiable subset of $\hat{\Omega}$, $\tau \in T_x L$ the unit vector defined $\mathcal{H}^1$-a.e. on L, and $\theta : L \to \mathbb{Z}$ a $\mathcal{H}^1$-integrable integer-valued function. Then the integer multiplicity 1-current $\mathcal{L}$ denoted by $\mathcal{L} := \{L, \tau, \theta\}$ is defined as

$$\mathcal{L}(\omega) := \int_L \langle \omega, \tau \rangle \theta(x) d\mathcal{H}^1(x)$$

for every compactly supported and smooth 1-form ω defined in $\hat{\Omega}$. The (topological vector) space of such forms is denoted by $\mathcal{D}^1(\hat{\Omega}, \bigwedge \mathbb{R}^3)$.

A dislocation can be described using the notion of integer multiplicity 1-currents with coefficients in the group $\mathbb{Z}^3$. For every Burgers vector $b \in \mathbb{Z}^3$, we introduce the *regular b-dislocation* in $\hat{\Omega}$ as the closed integral 1-current $\hat{\mathcal{L}}^b := \{\hat{L}^b, \tau^b, \theta^b\}$, where $\hat{L}^b$ represents a finite family of Lipschitz and closed curves in $\hat{\Omega}$ (otherwise said, $\hat{\mathcal{L}}^b$ are closed currents in $\hat{\Omega}$). We define the regular b-dislocation $\mathcal{L}^b := \{L^b, \tau^b, \theta^b\}$ in Ω as the restriction of $\hat{\mathcal{L}}^b$ to $\bar{\Omega}$, i.e., $\mathcal{L}^b(\omega) := \int_{\hat{L}^b \cap \bar{\Omega}} \langle \omega, \tau^b \rangle \theta^b(x) d\mathcal{H}^1(x)$ for every compactly supported and smooth 1-form ω defined in $\hat{\Omega}$. Associated to any b-dislocation in $\hat{\Omega}$ is its density, that is the measure $\hat{\Lambda}_{\mathcal{L}^b} \in \mathcal{M}(\hat{\Omega}, \mathbb{M}^3)$, defined by

$$\langle \Lambda_{\hat{\mathcal{L}}^b}, w \rangle := \hat{\mathcal{L}}^b((wb)^*), \tag{3.2}$$

for every $w \in \mathcal{D}(\hat{\Omega}, \mathbb{M}^3)$, where in the right-hand side $\omega := (wb)^*$ is the covector $(wb)^* := w_{kj} b_j dx_k$. If we identify test functions $w \in \mathcal{D}(\hat{\Omega}, \mathbb{M}^3)$ with 1-forms in $\mathcal{D}^1(\hat{\Omega}, \bigwedge \mathbb{R}^3)^3$, then we can also identify the density $\Lambda_{\hat{\mathcal{L}}^b}$ with an integral 1-current with coefficients in the group $\mathbb{Z}^3$, as (3.2). In particular we can use the notation

$$\Lambda_{\hat{\mathcal{L}}^b} = \hat{\mathcal{L}}^b \otimes b.$$

Its counterpart in $\bar{\Omega}$ is the restriction of $\Lambda_{\hat{\mathcal{L}}^b}$ in $\bar{\Omega}$, denoted by $\Lambda_{\mathcal{L}^b}$, and characterized by

$$\Lambda_{\mathcal{L}^b} = \mathcal{L}^b \otimes b = \tau^b \otimes b \theta^b \ \mathcal{H}^1 \llcorner L^b.$$

A *dislocation current* in $\hat{\Omega}$ is a map $\hat{\mathcal{L}} : \mathcal{D}^1(\hat{\Omega}, \bigwedge \mathbb{R}^3) \times \mathbb{Z}^3 \to \mathbb{R}$ such that for $b \in \mathbb{Z}^3$, $\hat{\mathcal{L}}(\cdot, b) = \{\hat{L}^b, \tau^b, \theta^b\}$ is a b-dislocation current in $\hat{\Omega}$.

The dislocations densities in $\hat{\Omega}$ and $\bar{\Omega}$ are given by

$$\Lambda_{\hat{\mathcal{L}}} = \sum_{b \in \mathbb{Z}^3} \Lambda_{\hat{\mathcal{L}}(\cdot, b)} \quad \text{and} \quad \Lambda_{\mathcal{L}} = \sum_{b \in \mathbb{Z}^3} \Lambda_{\mathcal{L}(\cdot, b)}, \tag{3.3}$$

respectively. These definitions allow us to describe any dislocation showing a finite or countable family of Burgers vectors. However it can be shown that actually any dislocation current $\mathcal{L}$ can be split in the basis of $\mathbb{R}^3$, as the sum of three integral 1-currents (called *canonical dislocation currents*) $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3$, in such a way that $\Lambda_{\mathcal{L}_i} = \Lambda_i = \mathcal{L}_i \otimes e_i$ for $i = 1,\ 2,\ 3$, and that $\Lambda_{\mathcal{L}} = \Lambda_1 + \Lambda_2 + \Lambda_3$. With the notation $\mathcal{L}_i = \{L_i, \tau^i, \theta_i\}$, we call $L := \cup_i L_i$ the dislocation set.

A dislocation current α in $V := \hat{\Omega} \setminus \bar{\Omega}$ is a boundary condition if it is the restriction to V of a closed dislocation current α in $\hat{\Omega}$. We finally define the class of admissible dislocations in $\bar{\Omega}$ with respect to a given boundary condition α as the set of all dislocation currents $\mathcal{L}$ which are the restrictions to $\bar{\Omega}$ of some closed dislocation current $\hat{\mathcal{L}}$ in $\hat{\Omega}$ such that $\hat{\mathcal{L}} \llcorner_V = \alpha$. In the sequel we will always suppose that dislocation currents are admissible for a fixed boundary datum.

3.2. **Functional space representation of continuum dislocations.** We will restrict our attention to the class of *continuum dislocations* (c.d.), defined as follows: $\mathcal{L}$ is a continuum dislocation if for $i = 1, 2, 3$, there exists a 1-Lipschitz map $\lambda^i : [0, M^i] \to \hat{\Omega}$ such that $\hat{\mathcal{L}}_i = \lambda^i_\sharp [\![0, M^i]\!]$ (note that the latter definition is equivalent to the original one given in [21], thanks to [21, Theorem 4.5]). Moreover, since all such currents are boundaryless by definition, we can rescale the functions λ^i and suppose they are defined on S^1. These dislocations might be called clusters because their Lipschitz description allow for the formation of complex such geometries. Their counterparts in $\bar{\Omega}$ are defined as above. In such a case, the density of a continuum dislocation in $\bar{\Omega}$ can be written as the sum of the three measures

$$\Lambda_{\mathcal{L}} = \sum_{i=1}^{3} \Lambda_i = \sum_{i=1}^{3} \lambda^i_\sharp [\![S^1]\!]_{\llcorner \bar{\Omega}} \otimes e_i, \tag{3.4}$$

that we can equivalently write as $\Lambda_i = (\dot{\lambda}^i \otimes e_i)\lambda^i_\sharp \mathcal{H}^1$, where $\lambda^i_\sharp \mathcal{H}^1$ is the push-forward of the 1-dimensional Hausdorff measure on S^1 through λ^i.

If $\mathcal{L}$ is a continuum dislocation, then there exists a set $\mathcal{C}_{\mathcal{L}} \subset \hat{\Omega}$ containing the support of the density $\Lambda_{\hat{\mathcal{L}}}$ which is a continuum, i.e., a finite union of connected compact sets with finite 1-dimensional Hausdorff measure. Note that such a set is not unique, and that we can always take, for example, $\mathcal{C}_{\mathcal{L}} = \cup_{i=1}^3 \lambda^i(S^1)$.

We then introduce the class of *dislocation density measures* with compact support in $\hat{\Omega}$ as

$$\mathcal{M}_\Lambda(\hat{\Omega}, \mathbb{M}^3) := \{\hat{\nu} \in \mathcal{M}(\hat{\Omega}, \mathbb{M}^3) : \exists\ \hat{\mathcal{L}} \ \text{ c.d. with density } -(\Lambda_{\hat{\mathcal{L}}})^{\mathrm{T}} = \hat{\nu}\}. \tag{3.5}$$

Setting $\varphi^\lambda_{ij}(s) := \varphi_{ij}(\lambda^i(s))$ for every $\varphi \in \mathcal{C}_c(\hat{\Omega}, \mathbb{M}^3)$ (with no sum in i), the density $\hat{\mu}_\lambda := -(\Lambda_{\hat{\mathcal{L}}})^{\mathrm{T}}$ which is associated to λ reads

$$\begin{aligned}\langle T(\lambda), \varphi\rangle := -\langle \hat{\mu}_\lambda, \varphi\rangle &= \sum_{k=1}^{3} \int_{S^1} \varphi(\lambda^k(s)) \cdot (e_k \otimes \dot{\lambda}^k(s)) d\mathcal{H}^1(s) \\ &= \sum_{k=1}^{3} \int_{S^1} \varphi^\lambda_{ij}(s) \left(\dot{\lambda}^i\right)_j (s) ds = \sum_{k=1}^{3} \int_L \varphi_{ij} \tau^i_j \theta_i d\mathcal{H}^1. \end{aligned} \tag{3.6}$$

Its counterpart in $\bar{\Omega}$ is $\mu_\lambda = \hat{\mu}_{\lambda \llcorner \bar{\Omega}}$. In (3.6), we have introduced

$$\theta_i(P) := \sharp\{s \in (\lambda^i)^{-1}(P) : \frac{\dot{\lambda}^i}{|\dot{\lambda}^i|}(s) = \tau(P)\} - \sharp\{s \in (\lambda^i)^{-1}(P) : \frac{\dot{\lambda}^i}{|\dot{\lambda}^i|}(s) = -\tau(P)\},$$

for every $P \in L$, which stands for the multiplicity of the dislocation with Burgers vector e_i. Here

$$\tau^i_j \theta_i d\mathcal{H}^1 = (\dot{\lambda}^i)_j ds. \tag{3.7}$$

The correspondance between the arcs λ and the Burgers vectors of the dislocation will appear clearer in the following Remark.

Remark 7. *When we deal with a dislocation $\mathcal{L}$ generated by only one loop with Burgers vector $b = (\beta_1, \beta_2, \beta_3) = \beta_i e_i, \beta_i \in \mathbb{Z}$ $(b \neq 0)$, then we have a Lipschitz function $\gamma^b \in W^{1,1}(S^1, \mathbb{R}^3)$ such that $\mathcal{L} = \gamma^b_\sharp [\![S^1]\!]_{\llcorner \bar{\Omega}}$ and $-\mu^{\mathrm{T}}_{\gamma^b} = \Lambda_{\mathcal{L}} = \mathcal{L} \otimes b$, that is the measure such that*

$$\begin{aligned}-\langle \mu_{\gamma^b}, \varphi\rangle &= \int_{S^1} \varphi(\gamma^b(s)) \cdot (b \otimes \dot{\gamma}^b(s)) ds = \int_{S^1} \varphi_{ij}(\gamma^b(s)) b_i \dot{\gamma}^b_j(s) ds \\ &= \int_L \varphi_{ij} \tau^i_j b_i \theta d\mathcal{H}^1, \end{aligned} \tag{3.8}$$

where $\theta(P)$ represents the multiplicity of the dislocation and is defined for every $P \in L$ as

$$\theta(P) := \sharp\{s \in (\gamma^b)^{-1}(P) : \frac{\dot{\gamma}^b}{|\gamma^b|}(s) = \tau(P)\} - \sharp\{s \in (\gamma^b)^{-1}(P) : \frac{\dot{\gamma}^b}{|\gamma^b|}(s) = -\tau(P)\}. \tag{3.9}$$

For every $\mu \in \mathcal{M}_\Lambda(\hat{\Omega}, \mathbb{M}^3)$ it is easy to check that Div $\mu = 0$ in $\hat{\Omega}$, since $\mathcal{L}_i$ are closed integral currents. In fact for all $\psi \in \mathcal{D}(\hat{\Omega}, \mathbb{R}^3)$ one has $-\langle D\psi, \mu\rangle = \langle D\psi, \sum_{k=1}^3 e_k \otimes \dot{\lambda}^k(\lambda^k_\sharp \mathcal{H}^1)\rangle = \sum_{i=1}^3 \int_{S^1} D_j\psi_i(\lambda^i)\dot{\lambda}^i_j ds = \int_{S^1} D_t\psi_k(\lambda^k)dt = 0$. We then get $\mathcal{M}_\Lambda(\hat{\Omega}, \mathbb{M}^3) \subset \mathcal{M}_{\rm div}(\hat{\Omega}, \mathbb{M}^3)$. We can now identify the space $\mathcal{M}_\Lambda(\hat{\Omega}, \mathbb{M}^3)$ with $W^{1,1}(S^1, \hat{\Omega}^3)$, through the map

$$T : W^{1,1}(S^1, \hat{\Omega}^3) \to \mathcal{M}_\Lambda(\hat{\Omega}, \mathbb{M}^3) \quad \text{s.t.} \quad T(\lambda) = -\hat{\mu}_\lambda \text{ defined in (3.6).} \tag{3.10}$$

The map T is by definition onto, while for every $\lambda \in W^{1,1}(S^1, \hat{\Omega}^3)$ it holds

$$\|T(\lambda)\|_{\mathcal{M}} \leq \|\dot{\lambda}\|_{L^1}, \tag{3.11}$$

implying the continuity of T. However T is not an injective map. We now define an equivalence relation $\sim$ in $W^{1,1}(S^1, \hat{\Omega}^3)$ by writing $\lambda \sim \lambda'$ if and only if $T(\lambda) = T(\lambda')$. Then we set $\dot{W}^{1,1}(S^1, \hat{\Omega}^3) := W^{1,1}(S^1, \hat{\Omega}^3)/\sim\ = W^{1,1}(S^1, \hat{\Omega}^3)/\ker(T)$, and so we may define the inverse of T as $T^{-1} : \mathcal{M}_\Lambda(\hat{\Omega}, \mathbb{M}^3) \to \dot{W}^{1,1}(S^1, \hat{\Omega}^3))$. If we define a new norm $\|\cdot\|_\sim$ on $\dot{W}^{1,1}(S^1, \hat{\Omega}^3)$, given by $\|\lambda\|_\sim = \inf_{\lambda' \sim \lambda} \|\dot{\lambda}'\|_{L^1}$ then by virtue of the open mapping theorem, T^{-1} is also linear and bounded, whereas with the norm of $W^{1,1}(S^1, \hat{\Omega}^3)$ an inverse of T is in general not continuous. For every $\mu \in \mathcal{M}_\Lambda(\hat{\Omega}, \mathbb{M}^3)$ we set

$$m(\mu) := \inf_{\lambda' \sim \lambda} \|\dot{\lambda}'\|_{L^1} = \|\lambda\|_\sim, \tag{3.12}$$

where the infimum is taken over all $\lambda \in T^{-1}(\mu)$.

As a consequence, the following functional relations will show crucial:

$$T\left(\dot{W}^{1,1}(S^1, \hat{\Omega}^3)\right) = \mathcal{M}_\Lambda(\hat{\Omega}, \mathbb{M}^3), \tag{3.13}$$

$$T^{-1}\left(\mathcal{M}_\Lambda(\hat{\Omega}, \mathbb{M}^3)\right) = \dot{W}^{1,1}(S^1, \hat{\Omega}^3). \tag{3.14}$$

Let us introduce also

$$\mathcal{BC}^{p,\Lambda}(\hat{\Omega}, \mathbb{M}^3) := \{F \in \mathcal{BC}^p(\hat{\Omega}, \mathbb{M}^3) \text{ s.t. Curl } F \in \mathcal{M}_\Lambda(\hat{\Omega}, \mathbb{M}^3)\}, \tag{3.15}$$

and its proper subspace

$$\mathcal{BC}^{p,\Lambda}_{\rm div}(\hat{\Omega}, \mathbb{M}^3) := \{F \in \mathcal{BC}^p_{\rm div}(\hat{\Omega}, \mathbb{M}^3) \text{ s.t. Curl } F \in \mathcal{M}_\Lambda(\hat{\Omega}, \mathbb{M}^3)\} \tag{3.16}$$

in such a way that by Theorem 2 and Eq. (3.13), it holds

$$\mathcal{BC}^{p,\Lambda}_{\rm div}(\hat{\Omega}, \mathbb{M}^3) := \text{Curl }^{-1}\Big(\mathcal{M}_\Lambda(\hat{\Omega}, \mathbb{M}^3)\Big) = \text{Curl }^{-1}\Big(T\Big(\dot{W}^{1,1}(S^1, \hat{\Omega}^3)\Big)\Big). \tag{3.17}$$

Moreover we introduce

$$\mathcal{BC}^{p,\Lambda}(\Omega, \mathbb{M}^3) := \{F \in \mathcal{BC}^p(\Omega, \mathbb{M}^3) \text{ s.t. } \exists \hat{F} \in \mathcal{BC}^{p,\Lambda}(\hat{\Omega}, \mathbb{M}^3) : F = \hat{F}_{\llcorner\Omega}\}. \tag{3.18}$$

3.3. **Class of admissible deformations.** Let U be an open set on $\mathbb{R}^3$, we recall that the space of Cartesian maps on U, denoted by $\mathrm{Cart}^p(U,\mathbb{R}^3)$, is defined as the space of maps $u: U \to \mathbb{R}^3$ belonging to $W^{1,p}(U,\mathbb{R}^3)$ and satisfying the following conditions: $\mathrm{adj}(Du)$, $\det(Du)$ belong to $L^1(U,\mathbb{M}^3)$ and $\partial\mathcal{G}_u = 0$, where $\mathcal{G}_u$ is the rectifiable 3-current in $U\times\mathbb{R}^3$ carried by the graph of u (see [14]). If $F = Du$ is the gradient of a Cartesian map, the distributional determinant $\mathrm{Det}(F)$ and adjoint $\mathrm{Adj}(F)$ of F are elements of $L^1(U,\mathbb{M}^3)$ and coincide with $\det(Du)$ and $\mathrm{adj}(Du)$ respectively. It is also straightforward that smooth functions $u \in C^1(U,\mathbb{R}^3)$ are Cartesian.

In [21] we consider deformations $F \in \mathcal{BC}^{p,\Lambda}(\Omega,\mathbb{M}^3)$ which also satisfy some regularity conditions outside the continuum dislocation set $C_{\mathcal{L}}$ of the dislocation $\Lambda_{\mathcal{L}} \in \mathcal{M}_\Lambda(\bar\Omega,\mathbb{M}^3)$. If F is an admissible deformation, then we assume that F satisfies the following property:

(P) For every ball $B \subset \Omega$ with $B \cap C_{\mathcal{L}} = \varnothing$ there exists a Cartesian map $u \in \mathrm{Cart}^p(B,\mathbb{R}^3)$ such that $F = Du$ in B.

We denote by

$$\mathcal{AD}^p(\hat\Omega) := \{F \in \mathcal{BC}^{p,\Lambda}(\hat\Omega,\mathbb{M}^3) : F \text{ satisfies } (P) \text{ above}\} \tag{3.19}$$

$$\mathcal{AD}^p(\Omega) := \{F \in \mathcal{BC}^p(\Omega,\mathbb{M}^3) \text{ s.t. } \exists \hat F \in \mathcal{AD}^p(\hat\Omega) : F = \hat F_{\llcorner\Omega}\}. \tag{3.20}$$

Remark 8. *As a consequence of the crystallographic assumption, that is, the hypothesis that the Burgers vectors belong to the lattice $\mathbb{Z}^3$, it turns out that $\mathcal{AD}^p(\Omega)$ is not a linear subspace of $\mathcal{BC}^p(\Omega,\mathbb{M}^3)$. Indeed it is easy to see that if $F \in \mathcal{AD}^p(\Omega)$ has density $-(\mathrm{Curl}\ F)^{\mathrm{T}}$, then ηF, with η an irrational real number, has density $-(\eta\,\mathrm{Curl}\ F)^{\mathrm{T}}$ which has not Burgers vectors in $\mathbb{Z}^3$.*

We also introduce the proper subspace of $\mathcal{AD}^p(\hat\Omega)$

$$\mathcal{AD}^p_{\mathrm{div}}(\hat\Omega) := \{F \in \mathcal{BC}^{p,\Lambda}_{\mathrm{div}}(\hat\Omega,\mathbb{M}^3) : F \text{ satisfies } (P) \text{ above}\}. \tag{3.21}$$

The following regularity result holds:

Theorem 4. *Let $\mu \in \mathcal{M}_\Lambda(\hat\Omega,\mathbb{M}^3)$, then the solution $F := \mathrm{Curl}^{-1}(\mu)$ of (2.19) in $\hat\Omega$ satisfies (P). In other words*

$$\mathcal{AD}^p_{\mathrm{div}}(\hat\Omega) \equiv \mathcal{BC}^{p,\Lambda}_{\mathrm{div}}(\hat\Omega,\mathbb{M}^3) = \mathrm{Curl}^{-1}\Big(T\Big(\dot W^{1,1}(S^1,\hat\Omega^3)\Big)\Big).$$

Proof. By hypothesis there is a $\lambda \in W^{1,1}(S^1,\hat\Omega^3)$ such that $\mu^{\mathrm{T}} = -\sum_{i=1}^3 \dot\lambda^i \otimes e^i\lambda^i_\sharp\mathcal{H}^1$. Let $C_\mu = \cup_{i=1}^3\lambda^i(S^1)$, that is a closed set of finite length. Let us fix a ball B with $\bar B \subset (\hat\Omega\setminus C_\mu)$. We first see that the function $x \mapsto G(x)$ defined in (2.23) turns out to be $C^\infty(B)$, thanks to the fact that for fixed x, the map $y \mapsto \nabla\phi(x-y)$ and all its derivatives are uniformly continuous on C_μ. Now $F = G + D\psi$ where ψ is the solution of (2.7) with $\mathrm{Div}\ G = 0$. Since C_μ does not intersect $\partial\hat\Omega$ we see that GN is smooth on $\partial\hat\Omega$, so that ψ is smooth in $\hat\Omega$ and we find out that F is smooth on any ball $B \subset \hat\Omega\setminus C_\mu$. In particular, in any such ball, since F is curl-free, it is the gradient of a smooth map, and thus the gradient of a Cartesian map. The statement is proved by Theorem 2 and Eq. (3.13), that is, by Eq. (3.17). □

3.4. **Existence of minimizers.** In this section, we exhibit some existence results for minimizers of energies $\mathcal{W}$ satisfying some particular assumptions. The proofs essentially are given in [21].

Let $\hat\Omega$ be the open set introduced in 3.1 and let α be a boundary condition in $V = \hat\Omega\setminus\bar\Omega$ (i.e. $\alpha = \hat{\mathcal{L}}_{\llcorner V}$ for a closed dislocation current $\hat{\mathcal{L}}$ on $\hat\Omega$). We then fix

$\hat{F} \in \mathcal{AD}^p(\hat{\Omega})$ such that $-\operatorname{Curl} \hat{F} = \left(\Lambda_{\hat{\mathcal{L}}}\right)^{\mathrm{T}}$ and define

$$\mathcal{F} := \{F \in \mathcal{AD}^p(\Omega) : \tilde{F} := F\chi_\Omega + \hat{F}\chi_V \in \mathcal{AD}^p(\hat{\Omega}), -\operatorname{Curl} \tilde{F} = \left(\Lambda_{\hat{\mathcal{L}}}\right)^{\mathrm{T}} \text{ on } \hat{\Omega} \\ \text{for some closed dislocation current } \hat{\mathcal{L}} \text{ in } \hat{\Omega}\}. \tag{3.22}$$

In particular, note that the dislocation current $\hat{\mathcal{L}}$ in the above definition must coincide with α in V. We denote by $\mathcal{L}$ the restriction to $\bar{\Omega}$ of $\hat{\mathcal{L}}$.

Let us now discuss some technical assumptions on the energy $\mathcal{W} : \mathcal{F} \to \bar{\mathbb{R}}$ in order to get existence of minimizers. We emphasize that these assumptions are not the only possible. For a more detailed description of existence results we refer to [21] and [22].

We assume that there are positive constants C and β for which

$$\begin{aligned} \hat{\mathcal{W}}(F) = \mathcal{W}(F, \Lambda_{\mathcal{L}}) &:= \mathcal{W}_e(F) + \mathcal{W}_{\text{defect}}(\Lambda_{\mathcal{L}}) \\ &\geq C\big(\||M(F)|\|_{L^p} + m(\Lambda_{\mathcal{L}}) + \kappa_{\mathcal{L}}\big) - \beta, \end{aligned} \tag{3.23}$$

with $F \in \mathcal{F}$ and $M(F) = (F, \operatorname{adj} F, \det F)$, where $m(\Lambda_{\mathcal{L}})$ is defined in (3.12) and $\kappa_{\mathcal{L}}$ denotes the number of connected components of $\mathcal{L}$. Moreover it is assumed that

- (W1) $W_e(F) \geq h(\det F)$, for a continuous real function h such that $h(t) \to \infty$ as $t \to 0$,
- (W2) W_e is polyconvex, i.e., there exists a convex function $g : \mathbb{R}^{3\times 3}\times\mathbb{R}^{3\times 3}\times\mathbb{R}^+ \to \bar{\mathbb{R}}$ s.t. $W_e(F) = g(\mathcal{M}(F))$, $\forall F \in \mathcal{F}$,
- (W3) $\mathcal{W}_{\text{defect}}(\Lambda_{\mathcal{L}}) \geq \kappa_1 \displaystyle\sum_{1\leq i\leq k_{\mathcal{L}}} b^i \|\dot{\lambda}^i\|_{L^1} + \kappa_2 k_{\mathcal{L}}$, for some constitutive material parameters κ_1 and κ_2.
- (W4) W_{defect} is weakly* lower semicontinuous, that is $\liminf\limits_{k\rightharpoonup\infty} \mathcal{W}_{\text{defect}}(\Lambda^k) \geq \mathcal{W}_{\text{defect}}(\Lambda)$ as $\Lambda^k \rightharpoonup \Lambda$ weakly* in $\mathcal{M}_b(\bar{\Omega}, \mathbb{R}^{3\times 3})$.

Note that assumption $(W2)$ implies that $\mathcal{W}_e$ is weakly lower semicontinuous, i.e., $\liminf\limits_{k\to\infty} \mathcal{W}_e(F^k) \geq \mathcal{W}_e(F)$ as $\mathcal{M}(F^k) \to \mathcal{M}(F)$ weakly in $L^p(\Omega, \mathbb{R}^{3\times 3})\times L^p(\Omega, \mathbb{R}^{3\times 3})\times L^p(\Omega)$. Note also that a control of the length of the dislocations and of the number of connected components in $(W3)$ is mandatory to prove existence. Without these bounds minimizing sequences might exhibit peculiar limit properties, as space-filling curves, which are to be avoided at the mesoscopic scale. In particular there would be no ball outside the limit set where F is the gradient of a Cartesian map.

Moreover, we may take $\mathcal{W}_{\text{defect}} := \mathcal{W}^1_{\text{defect}} + \mathcal{W}^2_{\text{defect}}$, where for instance, following [7] (where no variational problem is solved) an expression for the line tension $\mathcal{W}^1_{\text{defect}}$ is suggested as

$$\mathcal{W}^1_{\text{defect}}(\mu) = \int_L \psi(\theta b, \tau) d\mathcal{H}^1, \tag{3.24}$$

when $\mu = b \otimes \gamma_\sharp[\![S^1]\!] = b \otimes \theta\tau\mathcal{H}^1 \llcorner L$ is the dislocation density of a cluster generated by the loop $\gamma \in W^{1,1}(S^1, \mathbb{R}^3)$ and Burgers vector $b = \beta_i e_i, \beta_i \in \mathbb{Z}$ $(b \neq 0)$, and takes the value $+\infty$ if μ is not of this type. Here $\psi : \mathbb{Z}^3 \times \mathbb{R}^3 \to \mathbb{R}$ is a non-negative function satisfying $\psi(0, \cdot) = 0$ and $\psi(b, t) \geq c\|b\|$ for a constant $c > 0$. Thus, by (3.7), it holds $\mathcal{W}^1_{\text{defect}}(\mu) \geq m(\mu)$. Note that the first entry of ψ is given by the Burgers vector of the dislocation, that in general does not coincide with b but is a positive multiple since also its multiplicity must be taken into account. We remark that within our formalism the multiplicity, defined in (3.9), depends on the image of the curve γ.

Remark 9. *In general such a $\mathcal{W}_{\text{defect}}$ is not lower semicontinuous. However, the main result of [7] stated that its relaxation also writes in integral form*

$$\overline{\mathcal{W}}_{\text{defect}}(\mu) = \int_L \bar{\psi}(\theta b, \tau) d\mathcal{H}^1, \tag{3.25}$$

and is lower semicontinuous, for a function $\bar{\psi}$ satisfying some properties (see for details [7]).

According to Remark 9, we introduce the following alternative assumptions:

- (W3') $\mathcal{W}_{\text{defect}}(\Lambda_{\mathcal{L}}) := \mathcal{W}^1_{\text{defect}}(\Lambda_{\mathcal{L}}) + \mathcal{W}^2_{\text{defect}}(\Lambda_{\mathcal{L}})$, the second term being bounded from below by $\kappa_{\mathcal{L}}$, and the first beeing of the form (3.24) (if it is already semicontinuous) or (3.25) (else).
- (W4') $\mathcal{W}^2_{\text{defect}}$ is weakly* lower semicontinuous.

Moreover, continuum dislocations must not be necessarily bound to the length of $\lambda^i(S^1)$, since lying in a continuum entails that the following assumptions also yields existence [21]:

- (W3") $\mathcal{W}_{\text{defect}}(\Lambda_{\mathcal{L}})$ is such that

$$\mathcal{W}_{\text{defect}}(\Lambda_{\mathcal{L}}) \geq G(\mathcal{L}) := \kappa_1 \inf_{\mathcal{K} \in \mathcal{C}_{\mathcal{L}}} \left(\mathcal{H}^1(\mathcal{K}) + \kappa_2 \# \mathcal{K} \right), \tag{3.26}$$

where $\#\mathcal{K}$ represents the number of connected components of the embedding continuum $\mathcal{K}$. Note that by Golab theorem G is lower semi-continuous. This lower bound is written in a rather unnatural way from a physical point of view, but it is mathematically mandatory to prove existence without appealing to the description by Lipschitz maps. However, a physical interpretation of $G(\mathcal{L})$ can be proposed: to create a new loop at some finite distance d from the current dislocation $\mathcal{L}$, it is worth to nucleate (i.e., add a connected component) rather than deforming the existent dislocation, as soon as $d > \kappa_2$. It basically means that the continuum dislocation lies in a compact 1-set which keeps as minimal the balance between the number of its connected subsets (of the continuum, not of the dislocation cluster) and its length.

We emphasize that some existence results holding by different hypotheses also exist and are discussed in [22], as for instance adding to $W_e(F)$ a perturbation in Div F (that is, in Δu by Helmholtz decomposition). However, as long as the computation of the Peach-Köhler force (Section 4) is sought, we do not need this generality. We also emphasize that, as we will see, the presence of this term does not change the expression of the Peach-Köhler force, but only guarantees the existence of a minimizer in the class $\mathcal{F}$.

The following theorem is proved in [21, Theorem 6.4]:

Theorem 5. *Let $\hat{\mathcal{W}}$ be a potential satisfying assumptions* (3.23) *and either (W1)-(W4), or (W1)-(W2) and (W3')-(W4'), or (W1)-(W2) and (W3"). Then there exists a minimizer of $\hat{\mathcal{W}}$ in $\mathcal{F}$.*

4. Configurational forces at minimizing dislocation clusters

Certain forces apply on the dislocation clusters, solutions to the above minimization problem. They are due to the combined effect of the deformation and defect part of the energy. The line having no mass, these forces must be understood as being of configurational nature. All the results of the previous section will allow us to prove Theorem 7, which consists of a balance of forces at minimality.

4.1. **Internal variations at minimality.** Within our formalism, it is assumed that the energy $\mathcal{W}$ depends on the density Λ via the $W^{1,1}(S^1,\hat\Omega^3)$-field $\lambda := (\lambda^1,\lambda^2,\lambda^3)$ as defined in Eq. (3.10), viz.,

$$\mathcal{W}(F,\Lambda)=\mathcal{W}^\circ(F,\lambda), \tag{4.1}$$

with $\lambda\in T^{-1}(-\Lambda^{\mathrm{T}})$. Specifically, by (3.17) and Theorem 4, it holds

$$\mathcal{AD}^p_{\mathrm{div}}(\hat\Omega)= \mathrm{Curl}^{\,-1}\Big(T\Big(\dot W^{1,1}(S^1,\hat\Omega^3)\Big)\Big), \tag{4.2}$$

while for any admissible deformation $F\in\mathcal{AD}^p(\hat\Omega)$ it holds by Helmholtz decomposition (Theorem 1) that $F=Du+F^\circ$ with $F^\circ\in\mathcal{AD}^p_{\mathrm{div}}(\hat\Omega)$, so that

$$\hat{\mathcal{W}}(F)=\mathcal{W}(F,\Lambda)=\mathcal{W}_{\mathrm{e}}(Du+F^\circ)+\mathcal{W}^\circ_{\mathrm{defect}}(\mathrm{Curl}\,F^\circ)=:\mathcal{W}^{\circ\circ}(u,\lambda), \tag{4.3}$$

the latter being well defined, since F° is associated to a unique curve λ by (4.2). In the previous formula $\mathcal{W}^\circ_{\mathrm{defect}}$ is defined by $\mathcal{W}^\circ_{\mathrm{defect}}(T):=\mathcal{W}_{\mathrm{defect}}\left(-T^{\mathrm{T}}\right)$.

Let $F^\star$ be a minimizer of $\hat{\mathcal{W}}(F)$. Then by Theorem 4,

$$F^\star=Du^\star+\mathrm{Curl}^{\,-1}\circ T(\gamma^\star).$$

In order to well define tangent and normal vectors, as well as line curvature, the following regularity assumption will be made on the optimal dislocation set $L^\star=\gamma^\star(S_1)$:

$(A^\star)$ $\gamma^\star\in W^{2,1}(S^1,(\hat\Omega^3)^3)$.

Lemma 10. *If $(A^\star)$ holds, then $T: W^{1,1}(S^1,(\mathbb{R}^3)^3)\to\mathcal{M}_{div}(\hat\Omega,\mathbb{M}^3)$ is Fréchet differentiable at λ^*, in particular $DT(\lambda^\star)[\lambda]\in\mathcal{M}_{div}(\hat\Omega,\mathbb{M}^3)$, for every $W^{1,1}(S^1,(\mathbb{R}^3)^3)$-variation λ, and it holds $|DT(\lambda^\star)[\lambda]|\le C\|\lambda\|_{W^{1,1}}$.*

Proof. Let $\varphi\in\mathcal{D}(\Omega,\mathbb{M}^3)$. Let us recall the notation $\varphi^\lambda_{ij}(s):=\varphi_{ij}(\lambda^i(s))$ (with no sum in i), valid for every $\varphi\in\mathcal{D}(\Omega,\mathbb{M}^3)$. From (3.6) and (3.10), we entail by a Taylor expansion of φ that the directional derivative of T at $\lambda^\star$ along a variation $\lambda\in W^{1,1}(S^1,(\mathbb{R}^3)^3)$ reads

$$\langle DT(\lambda^\star)[\lambda],\varphi\rangle \;=\; \sum_{i=1}^3\int_{S^1}\varphi^{\lambda^\star}_{ij}(s)\dot\lambda^i_j(s)+D_k\varphi^{\lambda^\star}_{ij}(s)(\dot\lambda^\star)^i_j(s)\lambda^i_k(s)ds. \tag{4.4}$$

Integrating by parts the last expression we get

$$\begin{aligned}\langle DT(\lambda^\star)[\lambda],\varphi\rangle&=\sum_{i=1}^3\int_{S^1}D_k(\varphi_{ij})^{\lambda^\star}(s)(\dot\lambda^\star)^i_j(s)\lambda^i_k(s)-D_k(\varphi_{ij})^{\lambda^\star}(s)(\dot\lambda^\star)^i_k(s)\lambda^i_j(s)ds\\&=\sum_{i=1}^3\int_{S^1}\Big(D_k(\varphi_{ij})^{\lambda^\star}(s)-D_j(\varphi_{ik})^{\lambda^\star}(s)\Big)(\dot\lambda^\star)^i_k(s)\lambda^i_j(s)ds\\&=\sum_{i=1}^3\int_{S^1}\epsilon_{kjm}\epsilon_{mpq}D_p(\varphi_{iq})^{\lambda^\star}(s)(\dot\lambda^\star)^i_k(s)\lambda^i_j(s)ds.\end{aligned} \tag{4.5}$$

From

$$\frac{d}{ds}(\varphi_{iq})^{\lambda^\star}=D_l(\varphi_{iq})^{\lambda^\star}(\dot\lambda^\star)^i_l(s), \tag{4.6}$$

we get by projections that

$$D_p(\varphi_{iq})^{\lambda^\star}=\frac{d}{ds}(\varphi_{iq})^{\lambda^\star}(\dot\lambda^\star)^i_p+D_l(\varphi_{iq})^{\lambda^\star}(\nu^i_l\nu^i_p+\sigma^i_l\sigma^i_p),$$

where $\{\nu^i,\sigma^i,\tau^i:=\frac{(\dot\lambda^\star)^i}{\|(\dot\lambda^\star)^i\|}\}$ form a local orthogonal basis attached to $C^i:=(\lambda^\star)^i(S^1)$. Moreover, let the basis be naturaly extended (see [9]) in a neighbourhood of the line C^i, that is, the extensions read $\hat\tau^i=\tau^i\circ p_{C^i}$, $\hat\nu^i=\nu^i\circ p_{C^i}$ and

$\hat{\sigma}^i = \sigma^i \circ p_{C^i}$, where p_{C^i} is the orthogonal projection on C^i (in the sequel the $\wedge$ symbol will be removed to denote the extensions). Then, $D_l\{\nu^i, \sigma^i, \tau^i\}$ is purely along τ_l, while again by projections, $\varphi_{iq} = \varphi_{in}(\tau^i_n\tau^i_q + \nu^i_n\nu^i_q + \sigma^i_n\sigma^i_q)$, so that

$$
\begin{aligned}
&\epsilon_{mpq}\left(D_p(\varphi_{iq})^{\lambda^\star} - \frac{d}{ds}(\varphi_{iq})^{\lambda^\star}(\dot{\lambda}^\star)^i_p\right)\\
&= \epsilon_{mpq} D_l\left(\varphi_{in}(\tau^i_n\tau^i_q + \nu^i_n\nu^i_q + \sigma^i_n\sigma^i_q)\right)^{\lambda^\star}(\nu^i_l\nu^i_p + \sigma^i_l\sigma^i_p)\\
&= \epsilon_{mpq} D_l\left(\varphi_{in}\right)^{\lambda^\star}(\tau^i_n\tau^i_q + \nu^i_n\nu^i_q + \sigma^i_n\sigma^i_q)(\nu^i_l\nu^i_p + \sigma^i_l\sigma^i_p)\\
&= D_l\left(\varphi_{in}\right)^{\lambda^\star}(-\sigma^i_m\tau^i_n + \tau^i_m\sigma^i_n)\nu^i_l + D_l\left(\varphi_{in}\right)^{\lambda^\star}(\nu^i_m\tau^i_n - \tau^i_m\nu^i_n)\sigma^i_l.
\end{aligned}
$$

Multiplying this expression by $\epsilon_{mkj}(\dot{\lambda}^\star)^i_k\lambda^i_j$ and since $\epsilon_{mkj}\tau_k\tau_m = 0$ and $\nu_m\sigma_l - \sigma_m\nu_l = \epsilon_{mlp}\tau_p$, the integrand of (4.5) writes as

$$
\begin{aligned}
&\frac{d}{ds}(\varphi_{iq})^{\lambda^\star}\epsilon_{mpq}\epsilon_{mkj}(\dot{\lambda}^\star)^i_p(\dot{\lambda}^\star)^i_k\lambda^i_j + \epsilon_{mkj}(\dot{\lambda}^\star)^i_k\lambda^i_j D_l\left(\varphi_{in}\right)^{\lambda^\star}\tau^i_n(-\sigma^i_m\nu^i_l + \nu^i_m\sigma^i_l)\\
&= \frac{d}{ds}(\varphi_{iq})^{\lambda^\star}\epsilon_{mpq}\epsilon_{mkj}(\dot{\lambda}^\star)^i_p(\dot{\lambda}^\star)^i_k\lambda^i_j + \epsilon_{mkj}(\dot{\lambda}^\star)^i_k\lambda^i_j D_l\left(\varphi_{in}\right)^{\lambda^\star}\tau^i_n\epsilon_{mlp}\tau^i_p.
\end{aligned}
$$

By identity $\epsilon_{mkj}\epsilon_{mpq} = \delta_{kp}\delta_{jq} - \delta_{kq}\delta_{jp}$, and $\tau^i_n(\dot{\lambda}^\star)^i_n = \|(\dot{\lambda}^\star)^i\|$, we have

$$
\begin{aligned}
&\epsilon_{kjm}\epsilon_{mpq}D_p(\varphi_{iq})^{\lambda^\star}(\dot{\lambda}^\star)^i_k\lambda^i_j = \frac{d}{ds}(\varphi_{ij})^{\lambda^\star}(\dot{\lambda}^\star)^i_k(\dot{\lambda}^\star)^i_k\lambda^i_j - \frac{d}{ds}(\varphi_{ik})^{\lambda^\star}(\dot{\lambda}^\star)^i_k(\dot{\lambda}^\star)^i_j\lambda^i_j\\
&+ (\dot{\lambda}^\star)^i_k(s)\lambda^i_j D_k\left(\varphi_{in}\right)^{\lambda^\star}\tau^i_n\tau^i_j - \lambda^i_l D_l\left(\varphi_{in}\right)^{\lambda^\star}\tau^i_n\|(\dot{\lambda}^\star)^i\|, \qquad (4.7)
\end{aligned}
$$

from which it follows that the last term of (4.4) cancels with the last of (4.7), and hence that the sum of (4.4) with (4.5), recalling (4.6), yields

$$
\begin{aligned}
2\langle DT(\lambda^\star)[\lambda],\varphi\rangle &= \sum_{i=1}^3\int_{S^1}\epsilon_{kjm}\epsilon_{mpq}D_p(\varphi_{iq})^{\lambda^\star}(s)(\dot{\lambda}^\star)^i_k(s)\lambda^i_j(s)\\
&+ \varphi^{\lambda^\star}_{ij}(s)\dot{\lambda}^i_j(s) + D_k\varphi^{\lambda^\star}_{ij}(s)(\dot{\lambda}^\star)^i_j(s)\lambda^i_k(s)ds\\
&= \sum_{i=1}^3\int_{S^1}\left(\varphi^{\lambda^\star}_{ij}(s)\dot{\lambda}^i_j(s) + \frac{d}{ds}(\varphi_{ij})^{\lambda^\star}\lambda^i_j\|\dot{\lambda}^\star\|^2\right.\\
&+ \left.\lambda^i_j(s)\frac{d}{ds}\left(\varphi_{in}\right)^{\lambda^\star}\tau^i_n(s)\tau^i_j(s)(1-\|\dot{\lambda}^\star\|^2)\right)ds\\
&= \sum_{i=1}^3\int_{S^1}\left(\varphi^{\lambda^\star}_{ij}(s)\dot{\lambda}^i_j(s)\right.\\
&+ \left.\lambda^i_j(s)\frac{d}{ds}(\varphi_{in})^{\lambda^\star}\left(\delta_{nj}\|\dot{\lambda}^\star\|^2 + \tau^i_n(s)\tau^i_j(s)(1-\|\dot{\lambda}^\star\|^2)\right)\right)ds.
\end{aligned}
$$

Now, integrating by parts the second term of the integrand in the RHS, the last expression becomes

$$
= \sum_{i=1}^3 2\int_{S^1}\lambda^i_j(s)\Sigma^\star_{nj}(s)\left(\varphi_{in}\right)^{\lambda^\star}(s)ds, \qquad (4.8)
$$

where

$$
\Sigma^\star_{nj}(s) := -\frac{1}{2}\frac{d}{ds}\left(\delta_{nj}\|\dot{\lambda}^\star\|^2 + \tau^i_n(s)\tau^i_j(s)(1-\|\dot{\lambda}^\star\|^2)\right). \qquad (4.9)
$$

By the assumed regularity of $\lambda^\star$, $\|\Sigma^\star_{nj}(s)\|_1 = C < +\infty$, so that it holds

$$
|\langle DT(\lambda^\star)[\lambda],\varphi\rangle| \le C\|\varphi\|_\infty\|\lambda\|_\infty \le C\|\varphi\|_\infty\|\lambda\|_\sim \le C\|\varphi\|_\infty\|\lambda\|_{W^{1,1}}, \qquad (4.10)
$$

where we recall (3.12). Hence, the Radon measure property follows at a given λ.

$\square$

The energy functional $\mathcal{W}_e$ defined in (3.23) can be extended to $L^p(\hat\Omega,\mathbb{M}^3)$ as follows: $\mathcal{W}_e(F) := \int_{\hat\Omega} W_e(F)\chi_\Omega dx$. Let us fix $F^\star \in \mathcal{AD}^p(\hat\Omega)$ and $(\Lambda^\star)^{\mathrm{T}} = -\operatorname{Curl} F^\star$ on $\hat\Omega$. We make the assumption that the energy density $\mathcal{W}_{\mathrm{e}} : L^p(\hat\Omega) \to \mathbb{R}$ of (3.23) is Fréchet differentiable in $L^p(\hat\Omega)$ with the Fréchet derivative of $F \mapsto \mathcal{W}(F,\Lambda^\star)$ denoted by $W_F \in L^{p'}(\hat\Omega)$. As a consequence, for every $F \in L^p(\hat\Omega)$, it holds

(A) $\delta\mathcal{W}^\star(F) := \frac{d}{d\epsilon}\mathcal{W}(F^\star+\epsilon F,\Lambda^\star)_{|\epsilon=0} = \int_\Omega W_F^\star \cdot F dx = \delta\mathcal{W}_{\mathrm{e}}(F^\star)[F]$, $W_F^\star := W_F(F^\star,\Lambda^\star) = \delta\mathcal{W}_{\mathrm{e}}(F^\star) \in L^{p'}(\hat\Omega)$.

4.2. **Shape variation at optimality.** Variations F of the deformation $F^\star$ still satisfying the constraint $-\operatorname{Curl}(F^\star+F) = (\Lambda^\star)^{\mathrm{T}}$ must belong to $\mathcal{AD}^p_{\mathrm{curl}}(\hat\Omega) := \{F \in \mathcal{AD}^p(\hat\Omega) \text{ s.t. } \operatorname{Curl} F = 0\}$. Moreover, such variations at the minimum points of the energy $\mathcal{W}$ must provide a vanishing variation of $\mathcal{W}$. Let us denote the derivative of the bulk energy in the space $\mathcal{AD}^p_{\mathrm{curl}}(\hat\Omega)$ by $\mathbb{P} := \delta\mathcal{W}_{\mathrm{e}}(F^\star)$. Moreover we can compute variations λ with respect to the optimal line λ^*. Let us denote the derivative of the bulk energy in $W^{1,1}(S^1,(\mathbb{R}^3)^3)$ by $\delta^\circ\mathcal{W}_{\mathrm{e}}(F^\star)$. We set $F^\circ = S(\lambda) \in \mathcal{AD}^p_{\mathrm{div}}(\hat\Omega)$. By Lemma 10 and since $S = \operatorname{Curl}^{-1}\circ T$, we see that S is Fréchet differentiable at λ^*, and then by (A) one has $\delta\mathcal{W}_{\mathrm{e}}(F^\star) \in L^{p'}(\hat\Omega)$. Moreover by (2.20) and (3.11),

$$\delta^\circ\mathcal{W}_{\mathrm{e}}(F^\star) \in W^{-1,\infty}(S^1,(\mathbb{R}^3)^3). \tag{4.11}$$

From a physical viewpoint $\delta^\circ\mathcal{W}_{\mathrm{e}}(F^\star)$ represents a configurational force, and hence should be represented by an extensible field, that is, by a Radon measure. This is not guaranteed by (4.11) but is proved in the following main theorem.

Theorem 6 (The Peach-Köhler force is a Radon measure)**.** *Under the assumptions of Theorem 5, and hypotheses (A) and (A*),*

$$\delta\mathcal{W}_{\mathrm{e}}(F^\star) \in L^{p'}(\Omega) \quad \textit{and} \quad \delta^\circ\mathcal{W}_{\mathrm{e}}(F^\star) \in W^{-1,\infty}(S^1,(\mathbb{R}^3)^3)\cap\mathcal{M}_b(S^1,(\mathbb{R}^3)^3). \tag{4.12}$$

Moreover, there exists $\mathbb{L}^\star \in \mathcal{C}(\hat\Omega)$ such that, for every $\lambda \in \mathcal{W}^{1,1}(S^1,(\mathbb{R}^3)^3)$,

$$\begin{aligned}\langle\delta^\circ\mathcal{W}_{\mathrm{e}}(F^\star),\lambda\rangle &= \sum_{i=1}^3\int_{S^1}((\mathbb{L}^\star)^i)^{\lambda^\star}(\Sigma^\star)^i\cdot\lambda^i ds \\ &= \sum_{i=1}^3\int_{\mathcal{L}}\left(\operatorname{Curl}\mathbb{L}^\star\times\tau^i\right)^{\mathrm{T}}\theta_i\cdot\lambda^i((\lambda^*)^{-1})d\mathcal{H}^1,\end{aligned} \tag{4.13}$$

where $\Sigma^\star$ writes componentwise (with no sum on i) as,

$$2(\Sigma^\star_{nj})^i = -\kappa(\tau^i_j\nu^i_n+\tau^i_n\nu^i_j)(1-\|\dot\lambda^\star\|^2) - 2(\delta_{jn}-\tau^i_j\tau^i_n)\|\dot\lambda^\star\|^2. \tag{4.14}$$

Moreover, $\mathbb{P} := \operatorname{Curl}\mathbb{L}^\star$ satisfies

$$\begin{cases} -\operatorname{Div}\mathbb{P} &= 0 \quad \textit{in} \quad \hat\Omega \\ \quad \mathbb{P}N &= 0 \quad \textit{on} \quad \partial\hat\Omega \end{cases}. \tag{4.15}$$

Proof. Define the linear map

$$S : W^{1,1}(S^1,(\mathbb{R}^3)^3) \to \mathcal{BC}^{p,\Lambda}_{\mathrm{div}}(\hat\Omega,\mathbb{M}^3) : \quad S = \operatorname{Curl}^{-1}\circ T,$$

where Curl^{-1} is the solution of (2.19). By Theorem 5, let $F^\star \in \mathcal{BC}^{p,\Lambda}(\hat\Omega,\mathbb{M}^3)$ be a minimizer of the energy (4.3) with $\operatorname{Curl} F^\star = T(\lambda^\star)$, where $F^\star = Du^\star + S(\lambda^\star)$ by (2.18), and define $\mathcal{W}^\circ_{\mathrm{e}}(\lambda) := \mathcal{W}_{\mathrm{e}}(Du^\star + S(\lambda))$. We now want to perform variations in $W^{1,1}(S^1,(\mathbb{R}^3)^3)$ of $\mathcal{W}^\circ_e(\lambda^\star)$ and seek an expression of $\delta^\circ\mathcal{W}_{\mathrm{e}}(F^\star) := \delta\mathcal{W}^\circ_{\mathrm{e}}(\lambda^\star)$.

For $\lambda \in W^{1,1}(S^1, (\mathbb{R}^3)^3)$, we have $\delta\mathcal{W}^\circ_{\rm e}(\lambda^\star)[\lambda] = \langle W^\star_F, DS(\lambda^\star)[\lambda]\rangle$, where $DS(\lambda^\star)$ is the Fréchet derivative of S in $\lambda^\star$. Then,

$$DS(\lambda^\star)[\lambda] = \frac{d}{d\epsilon}\left(\text{ Curl }^{-1}(T(\lambda^\star + \epsilon\lambda))\right)_{|\epsilon=0} = \text{ Curl }^{-1}\left(DT(\lambda^\star)[\lambda]\right),$$

where $DT(\lambda^\star)[\lambda]$ is given by Lemma 10. Therefore, it holds

$$\delta\mathcal{W}^\circ_{\rm e}(\lambda^\star)[\lambda] = \langle W^\star_F, \text{ Curl }^{-1}\left(DT(\lambda^\star)[\lambda]\right)\rangle. \tag{4.16}$$

Being $F^\star$ a minimum point, for every curl-free $F = Du \in L^p(\hat\Omega)$, it holds

$$\delta\mathcal{W}^\star(Du) = \delta\mathcal{W}_{\rm e}(F^\star)[Du] = 0. \tag{4.17}$$

From (A), Eq. (4.17) and Theorem 3 it results that there exists $\mathbb{L}^\star$ such that

$$\mathbb{P} := W^\star_F = \delta\mathcal{W}_{\rm e}(F^\star) = \text{ Curl } \mathbb{L}^\star \in L^{p'}(\hat\Omega)$$

satisfying (4.15). Thus (4.16) gives

$$\begin{aligned}\delta\mathcal{W}^\circ_{\rm e}(\lambda^\star)[\lambda] &= \langle DT(\lambda^\star)[\lambda], \mathbb{L}^\star\rangle \\ &= \sum_{i=1}^3 \int_{S^1} \epsilon_{kjm}\epsilon_{mpq} D_p(\mathbb{L}^\star_{iq})^{\lambda^\star}(s)(\dot\lambda^\star)^i_k(s)\lambda^i_j(s)ds, \end{aligned} \tag{4.18}$$

thereby providing (4.13) and (4.14) (with $\varphi = \mathbb{L}^\star$). Moreover, $\delta\mathcal{W}^\circ_{\rm e}(\lambda^\star)$ is a Radon measure in $\mathcal{M}(S^1, (\mathbb{R}^3)^3)$ by the first inequality of (4.10), so that the quantity $\epsilon_{kjm}\epsilon_{mpq} D_p(\mathbb{L}^\star_{iq})^{\lambda^\star}(s)(\dot\lambda^\star)^i_k(s) = \left(\text{Curl } \mathbb{L}^\star \times \tau^i\right)^{\rm T}\theta_i$ (by (3.7)) is well defined as a Radon measure on L, and actually is the push-forward $(\lambda^\star)^i_\sharp(((\mathbb{L}^\star)^i)^{\lambda^\star}(\Sigma^\star)^i)$. This justified (4.13). $\square$

Let us introduce the following notation

$$\mu^i(\mathbb{L}^\star, \lambda^\star) := (\lambda^\star)^i_\sharp(((\mathbb{L}^\star)^i)^{\lambda^\star}(\Sigma^\star)^i), \tag{4.19}$$

so that we write

$$\langle\delta^\circ\mathcal{W}_{\rm e}(F^\star), \lambda\rangle = \sum_{i=1}^3 \int_{L^\star} \mu^i(\mathbb{L}^\star, \lambda^\star)\cdot\lambda^i((\lambda^\star)^{-1})d\mathcal{H}^1. \tag{4.20}$$

Remark 10. *By* (4.15)*,* $\mathbb{P} := W^\star_F$ *is identified with the first Piola-Kirchhoff stress. Being* $\mathbb{P}$ *in* $L^{p'}(\hat\Omega)$*, and recalling that* $F \in L^p(\hat\Omega)$*, means that the Kirchhoff stress*

$$\tau := J\sigma = \mathbb{P}F$$

is in $L^1(\hat\Omega)$*. Thus, for an incompressible body (*$J = \det F = 1$*), the true (Cauchy) stress* $\sigma \in L^1(\hat\Omega)$

Remark 11. *Observe that the first factor of the integrand of the last member of* (4.13) *is recognized as the Peach-Köhler force. Taking* $\lambda^i_j := u^i_j \circ (\lambda^\star)^i$*, and by Eqs.* (4.8) *and* (4.9)*,* (4.13) *is rewritten formaly as*

$$\begin{aligned}\langle\delta\mathcal{W}_{\rm e}(F^\star), \lambda\rangle : &= \sum_{i=1}^3 \int_{L^\star} \left(W^\star_F \times \tau^i\right)^{\rm T}\theta_i \cdot u^i d\mathcal{H}^1 \\ &= \sum_{i=1}^3 \int_{L^\star} \mu^i(\mathbb{L}^\star, \lambda^\star)\cdot u^i d\mathcal{H}^1.\end{aligned}$$

which is the work done by the Peach-Köhler force and the displacement u^i*.*

4.3. **Balance of configurational forces and energy dissipation.** Let $L = \gamma(S^1)$ be a single smooth enough dislocation loop with tangent vector τ, normal vector ν, curvature κ, and total Burgers vector B. We introduce

$$\begin{aligned}\mathcal{F}^\star &:= \left(W_F^\star \times \tau\right)^{\mathrm{T}} B\delta_L,\\ \mathcal{G}^\star &:= \kappa\left(\psi(b,\tau) - \nabla\psi(b,\tau)\cdot\tau + \nabla\nabla\psi(b,\tau)\cdot\nu\otimes\nu\right)\nu\|\dot\gamma\|^{-1}\delta_L,\end{aligned}$$

the so-called deformation-induced Peach-Köhler force and line tension, respectively, where ψ is the energy density as introduced in (3.24).

Deriving strong forms of equilibrium from a variational problem is classicaly done provided some regularity of the minimizers is assumed, as sumarized in the following theorem. Note that restricting to a single generating loop with Burgers vector b is chosen for the simplicity of the exposition.

Theorem 7. *Under the assumptions of Theorem 5, that $\psi, \bar\psi : \mathbb{Z}^3 \times \mathbb{R}^3 \to \mathbb{R}^+$ are of class $\mathcal{C}^2$, and that the optimal dislocation cluster satisfies ($A^\star$) and is associated to a single Burgers vector b, then minimality implies equilibrium of Newtonian and configurational forces, in the sense that the Peach-Köhler force $\mathcal{F}^\star$ is balanced by the line tension $\mathcal{G}^\star$ in $L^\star$, i.e.,*

$$\mathcal{F}^\star + \mathcal{G}^\star = 0. \tag{4.21}$$

Moreover at $F^\star$ it holds $\mathrm{Div}\, W_F^\star = 0$ *in* Ω *and* $W_F^\star N = 0$ *on* $\partial\Omega$.

Proof. Let us particularize (4.18) to the case where the density $\Lambda^\star$ is generated by one single loop $\gamma^\star \in W^{1,1}(S^1, \hat\Omega)$ with Burgers vector $b = \beta_i e_i, \beta_i \in \mathbb{Z}$ ($b \neq 0$) (cf. Remark 7). For variations of the form $\gamma^\star + \epsilon\gamma$ with $\gamma \in W^{1,\infty}(S^1, \hat\Omega)$, (4.18) becomes

$$\begin{aligned}\delta\mathcal{W}_{\mathrm{e}}^\circ(\gamma^\star)[\gamma] &= \int_{S^1} \epsilon_{kjm}\Big(\mathrm{Curl}\ \mathbb{L}^{\gamma^\star}(s)\Big)_{im} \tau_k b_i \gamma_j(s)\|\dot\gamma^\star(s)\|ds\\ &= \int_{L^\star} \epsilon_{kjm}\Big(\mathrm{Curl}\ \mathbb{L}\Big)_{im}\tau_k b_i\gamma_j d\mathcal{H}^1.\end{aligned} \tag{4.22}$$

Define

$$\mathcal{W}^\circ(\lambda) := \mathcal{W}_{\mathrm{e}}^\circ(\lambda) + \mathcal{W}_{\mathrm{defect}}^{\circ\circ}(\lambda), \tag{4.23}$$

where $\mathcal{W}_{\mathrm{defect}}^{\circ\circ}(\lambda) := \mathcal{W}_{\mathrm{defect}}^{\circ}(T(\lambda))$. In particular, $\mathcal{W}^\circ(\lambda^\star) = \mathcal{W}(F^\star)$. We have

$$\delta\mathcal{W}^\circ(\lambda^\star)[\lambda] = \delta\mathcal{W}_{\mathrm{e}}^\circ(\lambda^\star)[\lambda] + \delta\mathcal{W}_{\mathrm{defect}}^{\circ\circ}(\lambda^\star)[\lambda], \tag{4.24}$$

Let us now compute the defect part of the energy. For a dislocation density of the form $\mu = b\otimes\gamma_\sharp[\![S^1]\!]$, (3.24) writes as

$$\mathcal{W}_{\mathrm{defect}}^1(\mu) = \int_{S^1}\psi(b, \frac{\dot\gamma}{\|\dot\gamma\|}(s))\|\dot\gamma(s)\|ds. \tag{4.25}$$

We can now compute the first variation of the energy (4.25) at the point $\gamma^\star \in W^{1,1}(S^1, \hat\Omega)$. Setting $\hat{\mathcal{W}}_{\mathrm{defect}} := \mathcal{W}_{\mathrm{defect}}^1 \circ T$, it holds

$$\begin{aligned}&\delta\hat{\mathcal{W}}_{\mathrm{defect}}(\gamma^\star)[\gamma] =\\ &= \int_{S^1} D_k\psi(b, \frac{\dot\gamma^\star}{\|\dot\gamma^\star\|}(s))\Big(\frac{\dot\gamma_k\|\dot\gamma^\star\|^2 - \dot\gamma_k^\star\dot\gamma_j^\star\dot\gamma_j}{\|\dot\gamma^\star\|^2}(s)\Big) + \psi(b, \frac{\dot\gamma^\star}{\|\dot\gamma^\star\|}(s))\Big(\frac{\dot\gamma_j^\star\dot\gamma_j}{\|\dot\gamma^\star\|}(s)\Big)ds,\end{aligned} \tag{4.26}$$

where $D_k\psi$ is the derivative of ψ with respect to the k-th component of its second variable. Denoting $\tau = \frac{\dot\gamma^\star}{\|\dot\gamma^\star\|}$, we integrate by parts to obtain

$$\begin{aligned}&\delta\hat{\mathcal{W}}_{\mathrm{defect}}(\gamma^\star)[\gamma] =\\ &-\int_{S^1}\Big(\psi(b,\tau)\dot\tau_j - D_k\psi(b,\tau)\tau_k\dot\tau_j + D_jD_k\psi(b,\tau)\dot\tau_k - D_pD_k\psi(b,\tau)\dot\tau_k\tau_p\tau_j\Big)\gamma_j ds,\end{aligned}$$

where we dropped the variable s. Equivalently, recalling that $\dot\tau_i = \kappa\nu_i$ and since $D_jD_k\psi(b,\tau)\dot\tau_k = \tau^i_j\tau^i_p D_pD_k\psi(b,\tau)\dot\tau_k + \nu_j\nu_p D_pD_k\psi(b,\tau)\dot\tau_k$, it holds for every $s \in S^1$ that

$$\begin{aligned}\tilde{\mathcal{G}}^\star_j(b) &:= \psi(b,\tau)\dot\tau^i_j - D_k\psi(b,\tau)\tau_k\dot\tau^i_j + D_jD_k\psi(b,\tau)\dot\tau_k - D_pD_k\psi(b,\tau)\dot\tau_k\tau^i_p\tau^i_j \\ &= \psi(b,\tau)\dot\tau^i_j - D_k\psi(b,\tau)\tau_k\dot\tau^i_j + D_pD_k\psi(b,\tau)\dot\tau_k\nu_p\nu_j \\ &= \kappa\left(\psi(b,\tau) - D_k\psi(b,\tau)\tau_k + D_pD_k\psi(b,\tau)\nu_p\nu_k\right)\nu_j. \end{aligned} \tag{4.27}$$

Plugging the last expression in (4.24) and using (4.22), we obtain

$$\delta\mathcal{W}^\circ(\gamma^\star)[\gamma] = \int_{S^1}\Big(\epsilon_{kjm}(\,\mathrm{Curl}\,\mathbb{L})^{\gamma^\star}_{im}(s)b_i\dot\gamma^\star_k(s) - \tilde{\mathcal{G}}^\star_j(b)(s)\Big)\gamma_j(s)ds. \tag{4.28}$$

From the condition

$$\delta\mathcal{W}^\circ(\gamma^\star)[\gamma] = 0 \qquad \text{for all } \gamma \in W^{1,1}(S^1,\mathbb{R}^3),$$

due to the minimality of $\gamma^\star$, we then get from (4.28), $\mathcal{F}^\star_j + \mathcal{G}^\star_j = 0$, with

$$\mathcal{F}^\star_j := \epsilon_{kjm}(W^\star_F)_{im}B_i\tau_k\delta_L \qquad \text{and} \qquad \mathcal{G}^\star_j := \gamma_{defect}\nu_j\delta_L,$$

where

$$\gamma_{defect} := \tilde{\mathcal{G}}^\star_j(B)\epsilon^{-1},$$

with $\epsilon(P) := \|\dot\gamma^\star \circ {\gamma^\star}^{-1}(P)\|$, the local deformation of the curve, $B := \theta(P)b$, the total Burgers vector, and $\theta(P)$, $P \in L$, as defined by (3.9), the multiplicity of the dislocation (accounting for the loops of the cluster whose Burgers vector is a multiple of b). The proof is achieved. □

Remark 12. *Actually,* (4.21) *holds at $\mathcal{H}^1$-a.e. $P \in L$, and not at all P. This is due to the fact that it might happen that a point $P \in L$ is the overlapping of parts of γ which, although having the same tangent vector τ, do not have the same curvature κ nor the same ortogonal vector ν.*

4.3.1. *A modeling example.* In [7] it is considered a potential $\mathcal{W}_{\mathrm{defect}}$ of the form (3.24) with

$$\psi(b,\tau) := |b|^2 + \eta\langle b,\tau\rangle^2, \tag{4.29}$$

where $\eta > 0$ is a constant.

In the particular case where $b = \beta e_1, \beta \geq 1$, it is shown that ψ and $\bar\psi$ share the same expression up to the multiplicative factor β. In particular, they have the same regularity, i.e., are both smooth. In such a case, the above computations entail that

$$\mathcal{G}^\star_j(P) = \Big(|b|^2 - \eta\langle b,\tau\rangle^2 + 2\eta\langle b,\nu\rangle^2\Big)\kappa\nu_j,$$

so that at minimum of the energy, it holds

$$\theta^2_P\Big((1-\eta)\langle b,\tau\rangle^2 + (1+2\eta)\langle b,\nu\rangle^2\Big)\kappa\nu_j = \epsilon_{jpk}(\,\mathrm{Curl}\,\mathbb{L}^\star)_{ip}(P)\theta_P b_i\tau_k(P).$$

Remark 13. *Let us note that energy* (4.29) *alone does not satisfies the hypothesis* ($W3'$) *necessary to have existence of minimizers among the class $\mathcal{AD}^p(\Omega)$. In particular in such a case $\mathcal{W}^2_{defect} = 0$, that is, such energy does not take account of the number of connected components of the dislocation. However we can always add such a term, and noting that, at least in the hypotheses (W3), (W3'), and (W3"), this will not effect the computation of the first variations (and then the expressions of the Peach-Köhler forse and line tension) since this term is uneffected by infinitesimal variations.*

4.3.2. *Mechanical dissipation.* The mechanical dissipation $\mathcal{D}$ associated to a single dislocation loop with Burgers vector b reads

$$\mathcal{D} + \langle \text{ Curl } \mathbb{L}^\star, \mathbb{N} \rangle = \frac{d}{dt}\mathcal{W}^\circ(\gamma^\star) = \delta\mathcal{W}(\gamma^\star)[\frac{d\gamma^\star}{dt}] = \left(\mathcal{F}_j^\star \nu_j \nu + \gamma_{defect}\right) V_\nu + \mathcal{F}_z^\star V_z$$

where $\mathbb{N}$ is a nucleation potential (see [1] for detail), $V_\tau := \frac{d\gamma^\star}{dt} \cdot \tau\delta_L$ is the tangential velocity, $V_\nu := \frac{d\gamma^\star}{dt} \cdot \nu\delta_L$ is the plane normal velocity, $V_z := \frac{d\gamma^\star}{dt} \cdot \sigma\delta_L$ the out-of-plane velocity.

5. Concluding remarks

On the way to mathematically understand time evolution of dislocations, the work achieved in [21] was the first step, allowing us to describe the geometry of dislocation clusters and to prove existence of solutions to a general variational problem. With the present contribution, our wish was to provide a further decisive step, since the result of Theorem 7 introduces two forces balancing each other at optimality, the first deriving from the elastic part of the energy and named after Peach and Köhler and well-known in dislocation models [15], and the second deriving by shape variation of the defect part of the energy. Here crucial use has been made of the decomposition $F = \nabla u + F^\circ$ where F° and Curl F° depend of the line.

It turns out that the sum of these two forces naturally provides an expression of the velocity of the dislocation (for instance, a linear law is acceptable under certain working assumptions, see [1]). Of course, a nonvanishing velocity, i.e., a nonzero force, means that the solution does not coincide with energy minimization, as well-known for evolution problems. In future work, it is our task to determine the dissipative effects, the balance equations, and analyze in detail the evolutionary scheme.

The force we here derived yields an important output in terms of modeling, but to achieve a proof of Theorem 7, a series of results have appeared about the mathematical nature of functional spaces for dislocation-induced deformations. These should also be considered as contributions to the general aim of understanding dislocation problems in mathematical terms. Moreover, the paper has been written with a first part containing generic results, which are not related to dislocation models.

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