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In the presence of dislocations, the elastic deformation tensor F is not a gradient but satisfies the condition Curl $F = \Lambda_{\mathscr{L}}^{\mathrm{T}}$ (with the dislocation density $\Lambda_{\mathscr{L}}$ a tensor-valued measure concentrated in the dislocation $\mathscr{L}$). Then $F \in L^p$ with $1 \leq p < 2$. This peculiarity is at the origin of the mathematical difficulties encountered by dislocations at the mesoscopic scale, which are here modeled by integral 1-currents free to form complex geometries in the bulk. In this paper, we first consider an energy-minimization problem among the couples $(F, \mathscr{L})$ of strains and dislocations, and then we exhibit a *constraint reaction* field arising at minimality due to the satisfaction of the condition on the deformation curl, hence providing explicit expressions of the Piola–Kirchhoff stress and Peach–Koehler force. Moreover, it is shown that the Peach–Koehler force is balanced by a defect-induced configurational force, a sort of line tension. The functional spaces needed to mathematically represent dislocations and strains are also analyzed and described in a preliminary part of the paper.

1. Introduction

Dislocations in elastic bodies are at the origin of dissipative phenomena, and in particular, their motion is responsible for the plastic behavior 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 perfectly elastic. This scale of matter description is called the *mesoscopic* or the *continuum scale*. 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 cannot 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., [Acharya 2003; Scala and Van Goethem 2016]). Therefore, dislocation location and field singularity are bound notions.
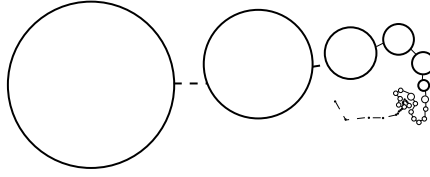
Figure 1. Example of a continuum dislocation cluster.

Specifically, the support of the curl of the deformation field (which in the presence of dislocations 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 fundamentally different from those encountered in the mathematical modeling of fracture mechanics. In particular, the displacement is not an appropriate model variable as opposed to most of solid mechanics problems. Furthermore, the stress and strain fields are not square-integrable and so the less-tractable L^p spaces with $1 \le p < 2$ must be considered, and bounds on the model fields are given in terms of the curl and the divergence (in place of the full gradient) 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 networks (see Figure 1) are observed [Zaiser 2004], one can hardly rely on the assumption of a periodic array of straight dislocations. Therefore, one is forced to build specific mathematical tools step by step, which should provide

- an appropriate functional framework and
- a geometric description of the lines.

To achieve the latter, the mathematical formalism of currents as briefly described in Section 1.2 has been proposed. In this framework, a cluster as depicted in Figure 1 is modeled as a continuum dislocation [Scala and Van Goethem 2016]. The formalism of currents to study and model dislocation clusters has been introduced in the pioneering works [Hochrainer and Zaiser 2005; Hochrainer 2013] and then adopted in more recent contributions to the theory of continuum dislocations as in [Conti et al. 2015a; 2015b]. The notion of integral current with coefficient in a group, also adopted in the companion paper [Scala and Van Goethem 2016; 2015], is the main tool to treat dislocation networks. This is due, principally, to the ability of dislocation lines to annihilate, sum, and form complex structures with specific rules for summing the Burgers vectors, which belong to a specific group. Moreover, the formalism of currents in general has proven to be useful in treating variational

problems in the theory of continuum dislocations [Scala and Van Goethem 2016; 2015]. Restricting ourselves to a quasistatic regime, we assume that the optimal networks result from minimization laws (note that such minimization states are reached very fast in actual crystals such as pure copper, where resistance to dislocation motion is negligible [Berdichevsky 2006]).

Therefore, the first purpose of this paper is to establish the functional setting appropriate to describe mesoscopic dislocations. The main features are that, when Sobolev spaces $W^{1,p}$ are considered, exponent p is in the "bad range" $1 \leq p < \frac{3}{2}$ and that the second grade variable is the curl instead of the gradient and the curl must be a concentrated Radon measure. Minimization problems in this range are considered in [Scala and Van Goethem 2016], where, aware of [Müller and Palombaro 2008], the main tools used are integral currents and Cartesian maps.

We shall provide elements for an analysis of the space of L^p-tensors whose curl is bounded in a measure space and in particular bring to light and 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. The second purpose is to compute the first variation of the energy with respect to the strain and the dislocation-associated density. These 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–Koehler force.

1.2. *A quick survey on currents and dislocations at the continuum scale.* In [Scala and Van Goethem 2016], we proposed a mathematical model for a countable family of dislocations in an elastic body Ω, here considered the current (as opposed to "reference") configuration. Motivated by physical reasons [Hirth and Lothe 1982; Müller et al. 2004; Zaiser 2004; Zubov 1997], 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. Since the dislocation loop is the singularity set for stress and strain, the deformation gradient field F is incompatible, meaning[1]

$$- \operatorname{Curl} F = \Lambda^{\mathrm{T}} \neq 0 \quad \text{in } \Omega, \tag{1-1}$$

with F the (inverse) deformation tensor and where the dislocation density Λ is a Radon measure in $\mathcal{M}(\overline{\Omega}, \mathbb{M}^3)$ concentrated on the dislocation set L. Here, L is a dislocation network in the current (i.e., deformed) configuration. Clearly if $\Lambda = 0$, then F is a gradient and there are no dislocations in the bulk. Moreover, conservation properties for dislocations imply that their density is solenoidal:

$$\operatorname{Div} \Lambda^{\mathrm{T}} = 0. \tag{1-2}$$

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

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 [Federer 1969]) are used to describe dislocations at the mesoscopic scale. 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 (1-2), implying that every dislocation is a loop or ends at the crystal boundary. A brief survey of the mathematical formalism can be found in Section 3.1 while for details we refer to [Scala and Van Goethem 2016]. For a so-called dislocation current $\mathscr{L}$, we will denote the associated density by $\Lambda = \Lambda_{\mathscr{L}}$. Whatever the model may be, in this paper, we are merely concerned with variations at optimality; thus, modeling and existence issues are not discussed.

The starting point of the present work is the minimum problem

$$\min_{(F,\mathscr{L}) \in \mathscr{A}} \mathscr{W}(F, \Lambda_{\mathscr{L}}), \tag{1-3}$$

where the energy

$$\mathscr{W}(F, \Lambda_{\mathscr{L}}) = \mathscr{W}_{\mathrm{e}}(F) + \mathscr{W}_{\mathrm{dislo}}(\Lambda_{\mathscr{L}}) \tag{1-4}$$

satisfies some appropriate convexity and coerciveness conditions while $\mathscr{A}$ is the space of admissible couples of deformation and dislocation currents. Among the properties of admissibility, we require that F and $\mathscr{L}$ be related by condition (1-1) and that F be the gradient of a Cartesian map away from L. Therefore, both F and $\mathscr{L}$ are represented by particular types of integral currents.

In dislocation gauge theory, an energy like (1-4) was used in [Lazar and Anastassiadis 2008; Agiasofitou and Lazar 2010], where the decomposition in an elastic and a dislocation part is given. From a mathematical viewpoint, that is, with variational techniques in appropriate functional spaces, problem (1-3) has been discussed and was first solved in [Müller and Palombaro 2008] with a single fixed dislocation loop in the crystal bulk (thus implying a minimization in F only) and later extended in [Scala and Van Goethem 2016] for an unfixed countable family of dislocation currents satisfying certain boundary conditions. Existence of minimizers is based on the assumption (classical in fracture mechanics) that the number of clusters is bounded.

1.3. *Formal derivation of the Peach–Koehler force.* From the standpoint of configurational force theory (as in [Gurtin 2000]) or as a result of invariance properties and Noether's theorem (as proposed by [Agiasofitou and Lazar 2010]), the Eshelby stress $\mathscr{E} = W\mathbb{I} - F^{\mathrm{T}}\mathbb{P}$ appears as a crucial quantity with W the energy density and $\mathbb{P}$ the first Piola–Kirchhoff stress. Assuming that $\mathrm{Div}\,\mathbb{P} = 0$, i.e., that static

equilibrium holds, one immediately finds that

$$\text{Peach–Koehler force} = \text{Div}\,\mathscr{E} = \langle \Lambda_{\mathscr{L}}^{\mathrm{T}} \times \mathbb{P} \rangle, \tag{1-5}$$

where the brackets emphasize that the vector product takes place in a certain function space as a duality product. Equation (1-5) is known as the Peach–Koehler force (see, e.g., [Hirth and Lothe 1982] for a straight dislocation); it is a force due to the equilibrium between the dislocation and the adjacent elastic medium. In particular, the functional choice is provided by the physics considered, that is, in the case of dislocations, whether one considers the macroscale (with Sobolev fields and no line singularity) or on the contrary the mesoscale, as in this work, where geometric measure theory and related functional spaces must be considered. Let us remark that the strong form $\text{Div}\,\mathbb{P} = 0$ is classically obtained by the Euler–Lagrange equation $\int_{\Omega} \mathbb{P} \cdot \nabla u\, dx = 0$ for all test functions u, provided the integration by parts is valid. The point is that, at our scale of matter description, $\mathbb{P}$ turns out to belong to a Lebesgue space, and thus, $\mathbb{P}N$ is not defined at the boundary, precluding the use of the divergence theorem. For this reason, $\text{Div}\,\mathbb{P} = 0$ must follow from another procedure; namely, $\mathbb{P}$ will be defined as the curl of a constraint reaction $\mathbb{L}$ (in the sense of [Fosdick and Royer-Carfagni 2004]), in appropriate function space, and due to the satisfaction of (1-1).

On the other hand, observe that the rightmost member of (1-5) has no rigorous meaning at the mesoscale since $\Lambda_{\mathscr{L}}$ is a measure and $\mathbb{P}$ a Lebesgue-integrable field.

1.4. *Scope of the work.* It is the goal of the present work to elucidate the functional setting allowing one to mathematically establish (1-5). To the knowledge of the authors, such a proof was nonexistent in the literature since the variational problem was unsolved until [Scala and Van Goethem 2016] at the mesoscale, in finite-strain elasticity, and for curved dislocations (i.e., loops) and dislocation networks. In this respect, it has to be emphasized that our point of view is completely different from that of [Agiasofitou and Lazar 2010], where the relation (1-5) is derived within the framework of gauge field theory of dislocations using the Noether theorem.

Considering the existence of minimizers of problem (1-3), in the present paper, we analyze the variation of $\mathscr{W}$ at the minimum points with respect to L, which by a formal chain rule can be written as

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

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

The first aim of this paper is of a theoretical nature: basically, it consists of giving a precise meaning to $\delta_L F$ and $\delta_L \Lambda_{\mathscr{L}}$ that will be achieved by proving a series of preliminary results. As far as the second term is concerned, the geometric analysis made in [Scala and Van Goethem 2016] and synthesized in Section 3.1 is used as a basis but here completed by putting the concentrated measure $\Lambda_{\mathscr{L}}$ in duality with a certain continuous tensor, called the *constraint reaction*. One difficulty is related to the identification of the dual space of Radon measures which are concentrated in closed lines since in general it is not true that this set is a subspace of continuous functions. This first result will in particular require inverting the curl operator. As far as the deformation part of the energy is concerned, we have already mentioned that it is not a gradient since to satisfy constraint (1-1) it must read $F = \nabla u + \mathrm{Curl}\, V$ (an expression recognized as a tensor Helmholtz–Weyl-type decomposition). As a matter of fact, F will depend on L through the solution of $-\mathrm{Curl}\,\mathrm{Curl}\, V = \Lambda_{\mathscr{L}}^{\mathrm{T}}$, 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., [Kozono and Yanagisawa 2009; Galdi 2011]), where by Maxwell these are intended estimates of vectors/tensors with respect to their curl and divergence [Neff et al. 2012b; 2012a; 2015b; Yanagisawa 2007], the crucial fact being that, by (1-1), the L^p-norm of the deformation gradient is estimated by the dislocation density norm, here intended as total variation of the Radon measure.

A direct consequence of the results in this work, discussed in Section 4.5, is setting the basis of a model of evolution in time of dislocations, in the sense that computing $\delta_L \mathscr{W}$ amounts to considering that a certain (configurational) force exerted on the dislocations is vanishing. Therefore, a moving dislocation will evolve with a velocity proportional to this force, as documented in dislocation theories [Hirth and Lothe 1982; Acharya 2003], and originating from the variation of the deformation part of the energy. In the final Theorem 26, we show that, at optimality, there is a balance of forces, one of which is the well-known Peach–Koehler force $\mathscr{F}$, while the other is a line-tension term, $\mathscr{G}$, provided by the variation of the defect part of the energy (see also [Conti et al. 2011]). In fact, the identity

$$\mathscr{F} = -\mathscr{G},$$

holding at minimality, might be considered a constitutive law for $\mathscr{F}$ since $\mathscr{G}$ is given explicitly in terms of the dislocation energy density and the line curvature and normal and tangent vectors. Let us emphasize that time evolution per se is not considered in the present work.

1.5. *Structure of the paper.* In Section 2, the theoretical results required as preliminaries are stated and proved, unless their proofs are found elsewhere in the

literature. An important result is the existence of a constraint reaction, given in
Section 2.4, relying on the important result on the invertibility of the curl operator
as found in Section 2.3. Section 3 contains three subsections where the mathemat-
ical properties of a dislocation model in this setting are given and discussed. In
particular, the functional relations between the deformation and the defect variables
are given (important relations are here (3-13) and (3-14)), 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 goal here is to compute the first variation of the energy at the minimum
points, eventually yielding the Peach–Koehler force expression in Section 4.3. In
Section 4.4, a shape-optimization view of minimality provides a balance of con-
figurational forces, which is applied to an example. All preliminary results of this
paper are required to derive this force expression, collected in Theorem 26.

1.6. *A remark.* This paper has been written in two parts; the first, Section 2, is
where all theoretical results are stated and proved without even referring to disloca-
tions. 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 previous
statements are particularized. Moreover, in order to be self-contained, the essence
of [Scala and Van Goethem 2016] is recalled in simple terms in Section 3.1.

2. Theoretical setting and preliminary results

2.1. *Notation and conventions.* The class of 3×3 matrices is denoted by $\mathbb{M}^3 :=$
$\mathbb{R}^{3\times3}$. 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.
The 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 $\mathcal{R}$-valued
solenoidal finite Radon measures on an open set $X \subset \mathbb{R}^3$ reads

$$\mathcal{M}_{\mathrm{div}}(X, \mathcal{R}) := \{\mu \in \mathcal{M}(X, \mathcal{R}) : \langle \mu, D\varphi \rangle = 0 \text{ for all } \varphi \in \mathscr{C}_0^1(X, \mathcal{R}')\}, \qquad (2\text{-}1)$$

where the product (here intended in the sense of finite Radon measures) yields, in
the case $\mathcal{R} = \mathbb{M}^3$, a real tensor whose components read $(\langle \mu_{ij}, D_j\varphi_k \rangle)_{ik}$. Recall
that $\varphi \in \mathscr{C}_0^1(X, \mathcal{R}')$ if it is of class $\mathscr{C}^1$ and if for every $\epsilon > 0$ there exists a compact
set $K \subset X$ such that $|\varphi(x)|$ and $|D\varphi(x)|$ are smaller than ϵ for any $x \in X \setminus K$.

Observe that $\mathcal{M}_{\mathrm{div}}(X, \mathcal{R})$ is a closed subspace of $\mathcal{M}(X, \mathcal{R})$ and hence is a Banach
space, endowed with the total variation norm $|\mu|(X) = \sup\{\langle \mu, \varphi \rangle : \varphi \in \mathscr{C}(X, \mathcal{R}),$
$\|\varphi\|_\infty \le 1\}$ (see [Ambrosio et al. 2000] for details on vector- and tensor-valued
Radon measures on metric spaces). A particular subclass of $\mathcal{M}_{\mathrm{div}}(X, \mathcal{R})$ will be

the family of (the transpose of) the dislocation densities[2] $(\Lambda^\star)^T \in \mathcal{M}_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3)$, where $\widehat{\Omega} \supset \Omega$ is an open set containing only dislocation loops.

For a tensor A and vector N, we use the convention $(N \times A)_{ij} = -(A \times N)_{ij} = -\epsilon_{jkl} A_{ik} N_l$. Further, the curl of a tensor A is defined componentwise as $(\mathrm{Curl}\, A)_{ij} = \epsilon_{jkl} D_k A_{il}$. As a consequence,

$$\langle \mathrm{Curl}\, A, \psi \rangle = -\langle A_{il}, \epsilon_{jkl} D_k \psi_{ij} \rangle = \langle A_{il}, \epsilon_{lkj} D_k \psi_{ij} \rangle = \langle A, \mathrm{Curl}\, \psi \rangle, \qquad (2\text{-}2)$$

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

$$\langle \mathrm{Curl}\, A, \psi \rangle = \langle A, \mathrm{Curl}\, \psi \rangle + \int_{\partial\Omega} (N \times A) \cdot \psi \, dS. \qquad (2\text{-}3)$$

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

The following lemma characterizes the dislocation measures as a particular subclass of the solenoidal measures.

Lemma 1. *Let $\mu \in \mathcal{M}_{\mathrm{div}}(\Omega, \mathbb{R}^{3\times3})$ be a measure that is absolutely continuous with respect to the $\mathcal{H}^1$-measure restricted on a simple Lipschitz curve L with tangent vector τ and such that 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*

$$\mu = b \otimes \tau \mathcal{H}^1_{\llcorner L}. \qquad (2\text{-}4)$$

We omit the proof, which is quite simple, and refer to [Scala and Van Goethem 2015]. Let us denote by $\mathcal{M}_{\mathrm{dislo}}(\Omega, \mathbb{M}^3)$ the class of the transpose of such measure as (2-4).

Let $1 \le p < \infty$, and let $\Omega \subset \mathbb{R}^3$ be an arbitrary open set. We introduce the vector space of tensor-valued fields

$$\mathcal{BC}^p(\Omega, \mathbb{R}^{3\times3}) := \{F \in L^p(\Omega, \mathbb{R}^{3\times3}) : \mathrm{Curl}\, F \in \mathcal{M}_{\mathrm{div}}(\Omega, \mathbb{R}^{3\times3})\}, \qquad (2\text{-}5)$$

which, as endowed with the norm

$$\|F\|_{\mathcal{BC}^p} := \|F\|_p + |\mathrm{Curl}\, F|(\Omega), \qquad (2\text{-}6)$$

turns out to be a Banach space.

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[2]The transpose is taken to be consistent with Van Goethem's references on dislocations [Van Goethem and Dupret 2012b]. This convention was originally taken from Kröner [1981].

[3]In this paper, we therefore follow the transpose of Gurtin's notation convention [Cermelli and Gurtin 2001], but care must be payed since the curl and divergence of tensor fields are given alternative definitions in the literature (including [Van Goethem and Dupret 2012b; Van Goethem 2014] where the current curl would give $\mathrm{Curl}\, A = -A \times \nabla$).

Remark 2. One might define $\mathscr{B}\mathscr{C}^p(\Omega, \mathbb{M}^3)$ by only specifying Curl $F \in \mathcal{M}(\Omega, \mathbb{M}^3)$ and considering the solenoidal property of μ as a direct consequence of the distributional identity Div Curl $F = 0$ in Ω.

2.2. *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 $\mathscr{C}^1$ boundary. There exists a unique solution (up to a constant) $\phi \in W^{1,p}(\Omega, \mathbb{R}^3)$ of*

$$\begin{cases} -\Delta\phi = \operatorname{Div} G & in \ \Omega, \\ \partial_N \phi = -GN & on \ \partial\Omega. \end{cases} \tag{2-7}$$

Moreover, such a solution satisfies $\|D\phi\|_p \le C\|G\|_p$.

Proof. This lemma is a direct tensor extension of the theorems of existence and uniqueness of the Neumann problem as shown in [Simader and Sohr 1996] (see also [Galdi 2011, Lemma III.1.2, Theorem III.1.2]). $\square$

Note that (2-7) is a formal strong form meaning that the following weak form is solved [Yanagisawa 2007]:

$$-\langle \nabla\phi, \nabla\varphi \rangle = \langle G, \nabla\varphi \rangle \quad \text{for all } \varphi \in W^{1,p'}(\Omega, \mathbb{M}^3). \tag{2-8}$$

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

$$L^p_{\operatorname{div}}(\Omega, \mathbb{M}^3) := \{F \in L^p(\Omega, \mathbb{M}^3) : \operatorname{Div} F = 0\}, \tag{2-9}$$

$$L^p_{\operatorname{curl}}(\Omega, \mathbb{M}^3) := \{F \in L^p(\Omega, \mathbb{M}^3) : \operatorname{Curl} F = 0\}. \tag{2-10}$$

The following result can be proven [Van Goethem 2015].

Lemma 4. *Let $\Omega \subset \mathbb{R}^3$ be a bounded open set with boundary of class $\mathscr{C}^1$, and let $F \in L^p(\Omega, \mathbb{R}^{3\times3})$ be such that $\operatorname{Div} F \in L^p(\Omega, \mathbb{R}^3)$. Let us define the distribution FN as*

$$\langle FN, \gamma(\varphi) \rangle := \langle \operatorname{Div} F, \varphi \rangle + \langle F, D\varphi \rangle \tag{2-11}$$

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, where $\langle \cdot, \cdot \rangle$ always means the duality product in appropriate spaces. Then $FN \in W^{-1/p,p}(\partial\Omega, \mathbb{R}^3) := (W^{1/p,p'}(\partial\Omega, \mathbb{R}^3))'$.

Similarly, the following holds true:

Lemma 5. *Let $\Omega \subset \mathbb{R}^3$ be a bounded open set with boundary of class $\mathscr{C}^1$, and let $F \in L^p(\Omega, \mathbb{R}^{3\times3})$ be such that $\operatorname{Curl} F \in L^p(\Omega, \mathbb{R}^{3\times3})$.*
  Then $F \times N \in W^{-1/p,p}(\partial\Omega, \mathbb{R}^3) := (W^{1/p,p'}(\partial\Omega, \mathbb{R}^3))'$ is defined as

$$\langle F \times N, \gamma(\varphi) \rangle := \langle \operatorname{Curl} F, \varphi \rangle - \langle F, \operatorname{Curl} \varphi \rangle \tag{2-12}$$

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 $1 < p < \infty$. In virtue of the previous two lemmas, if $V \in L^p(\Omega, \mathbb{R}^3)$ is such that $\mathrm{Div}\, V \in L^p(\Omega, \mathbb{R})$, then it is well-defined and its normal trace $VN \in W^{-1/p,p}(\partial\Omega) := (W^{1/p,p'}(\partial\Omega))'$ on $\partial\Omega$. Similarly, if $V \in L^p(\Omega, \mathbb{R}^3)$ with $\mathrm{Curl}\, V \in L^p(\Omega, \mathbb{R}^3)$, then its antinormal trace on $\partial\Omega$ is $V \times N \in W^{-1/p,p}(\partial\Omega, \mathbb{R}^3)$ and is defined as in (2-12). These properties can be straightforwardly applied to tensor-valued maps $V \in L^p(\Omega, \mathbb{M}^3)$ so that, if $\mathrm{Div}\, V \in L^p(\Omega, \mathbb{R}^3)$, it is well-defined and its normal trace $VN \in W^{-1/p,p}(\partial\Omega, \mathbb{R}^3)$ on $\partial\Omega$ (componentwise, $(VN)_i = V_{ij}N_j$). Similarly for the antinormal trace $V \times N$ (componentwise, $\epsilon_{jlp}V_{il}N_p$), it belongs to $W^{-1/p,p}(\partial\Omega, \mathbb{M}^3)$ as soon as $\mathrm{Curl}\, V \in L^p(\Omega, \mathbb{M}^3)$ (see also [Kozono and Yanagisawa 2009] and references therein).

Let us introduce the spaces

$$\mathcal{V}^p(\Omega) := \{V \in L^p_{\mathrm{div}}(\Omega, \mathbb{M}^3) : \mathrm{Curl}\, V \in L^p(\Omega, \mathbb{M}^3), V \times N = 0 \text{ on } \partial\Omega\}, \quad (2\text{-}13)$$

$$\widetilde{\mathcal{V}}^p(\Omega) := \{V \in L^p_{\mathrm{div}}(\Omega, \mathbb{M}^3) : \mathrm{Curl}\, V \in L^p(\Omega, \mathbb{M}^3), VN = 0 \text{ on } \partial\Omega\}. \quad (2\text{-}14)$$

The following estimate can be found in [Kozono and Yanagisawa 2009].

Lemma 6. *Let $\Omega \subset \mathbb{R}^3$ be a bounded open set with boundary of class $\mathscr{C}^1$, and assume $F \in \mathcal{V}^p(\Omega)$ or $F \in \widetilde{\mathcal{V}}^p(\Omega)$. Then $F \in W^{1,p}(\Omega, \mathbb{R}^{3\times 3})$, and there exists a positive constant $C = C(\Omega)$ such that*

$$\|\nabla F\|_p \leq C(\|\mathrm{Curl}\, F\|_p + \|F\|_p). \quad (2\text{-}15)$$

This shows that $\mathcal{V}^p(\Omega)$ and $\widetilde{\mathcal{V}}^p(\Omega)$ 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 [von Wahl 1992]. Note that the following is a classical result for smooth functions with compact support [von Wahl 1992]:

Lemma 7. *Let Ω be a simply connected and bounded domain, and let $F \in \mathcal{V}^p(\Omega)$ or $F \in \widetilde{\mathcal{V}}^p(\Omega)$. Then*

$$\|\nabla F\|_p \leq C\|\mathrm{Curl}\, F\|_p. \quad (2\text{-}16)$$

As a direct consequence, the following result holds.

Lemma 8. *Let Ω be a simply connected and bounded domain, and let $F \in \mathcal{V}^p(\Omega)$ or $F \in \widetilde{\mathcal{V}}^p(\Omega)$. Then $\mathrm{Curl}\, F = 0$ if and only if $F = 0$.*

We remark that, when $F \in \widetilde{\mathcal{V}}^p(\Omega)$, Lemma 8 amounts to proving the uniqueness property of Lemma 3. Moreover, in [Kozono and Yanagisawa 2009], a more general statement is established without the simply connectedness assumption. In general, for Ω a smooth and bounded subset of $\mathbb{R}^3$, $\mathrm{Curl}\, F = \mathrm{Div}\, F = 0$ has a nontrivial solution. In particular, Kozono and Yanagisawa [Yanagisawa 2007] show that the solutions belong to a subspace of $\mathscr{C}^\infty(\overline{\Omega}, \mathbb{M}^3)$ with positive finite dimension, depending on the Betti numbers 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 the help of Lemma 3 (for a complete proof, see [Kozono and Yanagisawa 2009; Yanagisawa 2007] and also [Galdi 2011; Neff et al. 2012a]).

Theorem 9 (Helmholtz, Weyl, Hodge, and 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 $V \in \widetilde{\mathcal{V}}^p(\Omega)$ such that*

$$F = Du_0 + \operatorname{Curl} V \quad \left(L^p(\Omega, \mathbb{M}^3) = \nabla W_0^{1,p}(\Omega, \mathbb{R}^3) \oplus \operatorname{Curl} \widetilde{\mathcal{V}}^p(\Omega) \right). \quad (2\text{-}17)$$

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

$$F = Du + \operatorname{Curl} V_0 \quad \left(L^p(\Omega, \mathbb{M}^3) = \nabla W^{1,p}(\Omega, \mathbb{R}^3) \oplus \operatorname{Curl} \mathcal{V}^p(\Omega) \right). \quad (2\text{-}18)$$

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

Remark 10. When F is smooth with compact support, decompositions such as (2-17) and (2-18) are classically given by the Stokes theorem and explicit formulae involving the divergence and curl of F [von Wahl 1992; Bolik and von Wahl 1997].

Remark 11. Let F be of class $\mathscr{C}^1$. 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 $u \in \mathscr{C}^2(\Omega, \mathbb{R}^3)$ satisfying $F = Du$. This result extends for $F \in L^p$ with $1 < p < +\infty$ as shown in [Galdi 2011]. See [Kozono and Yanagisawa 2009] for a complete treatment of Helmholtz decomposition in L^p, relying on the pioneering paper [Fujiwara and Morimoto 1977]. Moreover, if $\operatorname{Div} F = 0$, then by Theorem 9, $F = \operatorname{Curl} V$ with $V \in \widetilde{\mathcal{V}}^p(\Omega)$. Note that, for smooth functions F, this result holds for any simply connected domain with Lipschitz boundary.

Remark 12. Smoothness of the boundary is a strong requirement which is needed for the following reason: (2-17) and (2-18) require in principle solving a Poisson equation $\Delta u = \operatorname{Div} F$ with the right-hand side in some distributional (that is, Sobolev–Besov) space for which smoothness of the boundary is needed. It is known [Fabes et al. 1998] that for a Lipschitz boundary the solution holds for restricted p (namely $\frac{3}{2} - \epsilon \leq p \leq 3 + \epsilon$) for some $\epsilon = \epsilon(\Omega) > 0$. Note that for $p = 2$ a Lipschitz boundary would be sufficient.

Lemma 13. *Let $\Omega \subset \mathbb{R}^3$ be a bounded open set with boundary of class $\mathscr{C}^1$, and let $V \in \mathcal{V}^p(\Omega)$. Then $(\operatorname{Curl} V)N = 0$ in the sense of Lemma 4.*

Proof. Take any $\varphi \in W^{1,p'}(\Omega, \mathbb{R}^3)$. With by-parts integration ((2-11) and (2-12)), it holds that

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

Since φ is arbitrary, the proof is done. $\square$

By Lemma 13, the function u of (2-18) is found by solving (2-7) with $\phi = u$ and $G = -F$. This also gives a meaning to the condition $\partial_N u = FN$.

2.3. *Invertibility of the curl.*

Notation 14. Unless otherwise specified, the domains Ω we consider are bounded, smooth, and simply connected subsets of $\mathbb{R}^3$, with outward unit normal N.

Let us introduce the following notation.

Notation 15. Given Ω, we denote by $\widehat{\Omega}$ another domain satisfying Notation 14 and such that $\Omega \Subset \widehat{\Omega}$.

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

$$\begin{cases} -\mathrm{Curl}\, F = \mu^{\mathrm{T}} & \text{in } \widehat{\Omega}, \\ \mathrm{Div}\, F = 0 & \text{in } \widehat{\Omega}, \\ FN = 0 & \text{on } \partial\widehat{\Omega}, \end{cases} \tag{2-19}$$

with μ^{T} a Radon measure in $\mathcal{M}_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3)$. Note that the transpose is put here for convenience. In fact, the right-hand side is a general tensor-valued solenoidal bounded Radon measure. Existence and uniqueness of a solution is given by Theorem 16 below, for the proof of which Lemma 3 (or Lemma 8) will be required.

The following result is first given for general solenoidal measures and then slightly improved for dislocation measures. The existence part is a straightforward consequence of the main result of [Bourgain and Brezis 2004], whereas some further details can be found in [Scala and Van Goethem 2015, Appendix].

Theorem 16 (Biot and Savart). *Let μ be a tensor-valued Radon measure such that $\mu^{\mathrm{T}} \in \mathcal{M}_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3)$. Then there exists a unique F in $\mathcal{BC}^1_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3)$ that is a solution of (2-19). Moreover, F belongs to $\mathcal{BC}^p_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3)$ for all p with $1 \le p < \frac{3}{2}$, and for all such p, there exists a constant $C > 0$ satisfying*

$$\|F\|_p \le C|\mu|(\widehat{\Omega}). \tag{2-20}$$

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

Let us remark that the regularity assumption on the curve L is necessary here since there exist examples of a measure concentrated on a rectifiable curve such

that the associated deformation F is not in L^p with $\frac{3}{2} < p < 2$, as shown in [Conti et al. 2015b].

By uniqueness, there exists a linear one-to-one and onto correspondence between the spaces $\mathcal{M}_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3)$ and $\mathcal{B}\mathcal{C}^p_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3)$. Thus, the map

$$\mathrm{Curl}^{-1} : \mathcal{M}_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3) \to \mathcal{B}\mathcal{C}^p_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3), \quad \nu \mapsto F = -\mathrm{Curl}^{-1}(\nu), \qquad (2\text{-}21)$$

is well-defined and linear. Therefore, we may write

$$\mathcal{B}\mathcal{C}^p_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3) := \mathrm{Curl}^{-1}(\mathcal{M}_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3)). \qquad (2\text{-}22)$$

Moreover, for any $F \in \mathcal{B}\mathcal{C}^p_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3)$, we recover by (2-20) the L^p-counterpart of the Maxwell relation in L^2 [Neff et al. 2012a], that is,

$$\|F\|_p \le C |\mathrm{Curl}\, F|(\widehat{\Omega}). \qquad (2\text{-}23)$$

Remark 17. In case Ω is not simply connected, the uniqueness of the solution of problem (2-19) does not hold. In such a case, Lemma 8 would also not hold since the problem might exhibit nontrivial solutions, as shown in [Yanagisawa 2007].

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

$$\Phi : \mathcal{B}\mathcal{C}^p(\widehat{\Omega}, \mathbb{M}^3) \to \mathbb{R}, \qquad (2\text{-}24)$$

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

$$L^p_{\mathrm{curl}}(\widehat{\Omega}, \mathbb{M}^3) \subset \ker \Phi. \qquad (2\text{-}25)$$

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

Theorem 18. *Let* $1 < p < \frac{3}{2}$, *and let* Φ *be a linear and continuous map on* $L^p(\widehat{\Omega}, \mathbb{M}^3)$ *satisfying* $\Phi(Du) = 0$ *for every* $u \in W^{1,p}(\widehat{\Omega}, \mathbb{R}^3)$. *Then there exist two maps* $\mathbb{L}$ *and* $\tilde{\mathbb{L}}$ *belonging to* $\mathcal{C}(\overline{\widehat{\Omega}}, \mathbb{M}^3) \cap W^{1,p'}(\widehat{\Omega}, \mathbb{M}^3)$, *with* $3 < p' < \infty$, $1/p + 1/p' = 1$, *such that, for every* $F \in \mathcal{B}\mathcal{C}^p(\widehat{\Omega}, \mathbb{M}^3)$,

$$\Phi(F) = \langle \mathrm{Curl}\, \tilde{\mathbb{L}}, F \rangle = \langle \mathrm{Curl}\, \mathbb{L}, F \rangle = \langle \mathbb{L}, \mathrm{Curl}\, F \rangle \qquad (2\text{-}26)$$

and satisfying $\mathrm{Div}\,\mathbb{L} = \mathrm{Div}\,\tilde{\mathbb{L}} = 0$ *in* $\widehat{\Omega}$, $N \times \mathbb{L} = 0$, *and* $\tilde{\mathbb{L}}N = 0$ *on* $\partial\widehat{\Omega}$.

Proof. Since Φ is linear and continuous,

$$\Phi(F) = \langle \mathbb{T}, F \rangle, \qquad (2\text{-}27)$$

for some $\mathbb{T} \in L^{p'}(\widehat{\Omega}, \mathbb{M}^3)$. Now for every $\varphi \in \mathcal{C}^\infty(\widehat{\Omega}, \mathbb{R}^3)$, we have $\langle \mathbb{T}, D\varphi \rangle = \Phi(D\varphi) = 0$, proving that $\mathrm{Div}\,\mathbb{T} = 0$ in $\widehat{\Omega}$ and, integrating by parts, that $\mathbb{T}N = 0$ on $\partial\widehat{\Omega}$. By Theorem 9 ((2-17) or (2-18)), there exist a unique $\mathbb{L} \in L^{p'}_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3)$

satisfying $N \times \mathbb{L} = 0$ on $\partial\widehat{\Omega}$ and a unique $\tilde{\mathbb{L}} \in L^{p'}_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3)$ with $\tilde{\mathbb{L}}N = 0$ on $\partial\widehat{\Omega}$ such that

$$\mathrm{Curl}\,\mathbb{L} + Du = \mathrm{Curl}\,\tilde{\mathbb{L}} + Du_0 = \mathbb{T}, \tag{2-28}$$

for some u and u_0 as in Theorem 9. Since $\mathrm{Div}\,\mathbb{T} = 0$ in $\widehat{\Omega}$, one has $u_0 = 0$ and, from $\mathrm{Curl}\,\mathbb{L}N = \mathbb{T}N = 0$ on $\partial\widehat{\Omega}$, $Du = 0$. By the Maxwell–Friedrich-type inequality (i.e., the generalization of (2-15) [Yanagisawa 2007]), i.e.,

$$\|\nabla\mathbb{L}\|_{p'} \leq C(\|\mathrm{Curl}\,\mathbb{L}\|_{p'} + \|\mathrm{Div}\,\mathbb{L}\|_{p'} + \|\mathbb{L}\|_{p'}), \tag{2-29}$$

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

$$\mathbb{L} \in \mathscr{C}(\overline{\widehat{\Omega}}, \mathbb{M}^3). \tag{2-30}$$

The same is true for $\tilde{\mathbb{L}}$. Integrating by parts the identities (2-26), we get, since $N \times \mathbb{L} = 0$ on $\partial\widehat{\Omega}$,

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

completing the proof. □

In the applications, Φ will be the first variation of the 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.

3. Energy minimization of dislocation networks

The key point of this work is 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 18. In principle, variations can be made with respect to F, the dislocation density Λ, and 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, with respect to infinitesimal Lipschitz variations of 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 $\Lambda = \Lambda_{\mathscr{L}}$ (see (3-4)). In the case of F, the dependence is implicit since

$$F = \nabla u + F^\circ, \tag{3-1}$$

where F depends on L through the relation $\operatorname{Curl} F^\circ = -(\Lambda_{\mathscr{L}})^{\mathrm{T}}$. Therefore, since the energy consists of one term in F and another in Λ, variations of the energy with respect to $\mathscr{L}$ (that is, with respect to its support 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 [Scala and Van Goethem 2016] are first recalled while rewritten in a concise form. We refer to [Scala and Van Goethem 2016; 2015] for a full discussion of the results and of the models. In the next two subsections, the results from Section 2 are applied to continuum dislocations. The main results are relations (3-13) and (3-14).

3.1. *Dislocation density measures.*

In the sequel, we will adopt Notations 14 and 15. In order to perform variations in F and Λ, we introduce an appropriate subspace of $\mathscr{M}_{\mathrm{div}}(\overline{\Omega}, \mathbb{M}^3)$ called the set of dislocation density measures and based upon the notion of integer-multiplicity (or integral) 1-currents.

In many applications, the Burgers vector is constrained by crystallographic 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

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

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

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

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

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

A dislocation can be described using the notion of the integer-multiplicity 1-current. For every Burgers vector $b \in \mathbb{Z}^3$, we introduce the *regular b-dislocation* in $\widehat{\Omega}$ as the closed integral 1-current $\widehat{\mathscr{L}}^b := \{\hat{L}^b, \tau^b, \theta^b\}$, where $\hat{L}^b$ represents the union of a finite family of Lipschitz and closed curves in $\widehat{\Omega}$, τ^b its oriented unit tangent vector, and θ^b an integer-valued function on $\hat{L}^b$ called multiplicity. We define the regular b-dislocation $\mathscr{L}^b := \{L^b, \tau^b, \theta^b\}$ in Ω as the restriction of $\widehat{\mathscr{L}}^b$ to $\overline{\Omega}$, i.e., $\mathscr{L}^b(\omega) := \int_{\hat{L}^b \cap \overline{\Omega}} \langle \omega, \tau^b \rangle \theta^b(x) \, d\mathscr{H}^1(x)$ for every compactly supported and smooth 1-form ω defined in $\widehat{\Omega}$. Associated to any b-dislocation in $\widehat{\Omega}$ is its density,

that is, the measure $\hat{\Lambda}_{\mathscr{L}^b} \in \mathcal{M}(\widehat{\Omega}, \mathbb{M}^3)$, defined by

$$\langle \Lambda_{\widehat{\mathscr{L}}^b}, w \rangle := \widehat{\mathscr{L}}^b((wb)^*), \qquad (3\text{-}2)$$

for every $w \in \mathscr{D}(\widehat{\Omega}, \mathbb{M}^3)$, where in the right-hand side $\omega := (wb)^*$ is the covector $(wb)^* := w_{kj}b_j dx_k$. If we identify test functions $w \in \mathscr{D}(\widehat{\Omega}, \mathbb{M}^3)$ with 1-forms in $\mathscr{D}^1(\widehat{\Omega}, \bigwedge \mathbb{R}^3)^3$, then we can also identify the density $\Lambda_{\widehat{\mathscr{L}}^b}$ with an integral 1-current with coefficients in the group $\mathbb{Z}^3$, as in (3-2). We will use the notation

$$\Lambda_{\widehat{\mathscr{L}}^b} = \widehat{\mathscr{L}}^b \otimes b.$$

Its counterpart in $\overline{\Omega}$ is the restriction of $\Lambda_{\widehat{\mathscr{L}}^b}$ to $\overline{\Omega}$, denoted by $\Lambda_{\mathscr{L}^b}$ and characterized by

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

A general dislocation $\widehat{\mathscr{L}}$ is a sequence of b-dislocations $\{\widehat{\mathscr{L}}^b\}_{b \in \mathbb{Z}^3}$. The associated dislocation densities in $\widehat{\Omega}$ and $\overline{\Omega}$ are given by

$$\Lambda_{\widehat{\mathscr{L}}} = \sum_{b \in \mathbb{Z}^3} \Lambda_{\widehat{\mathscr{L}}^b} \quad \text{and} \quad \Lambda_{\mathscr{L}} = \sum_{b \in \mathbb{Z}^3} \Lambda_{\mathscr{L}^b}, \qquad (3\text{-}3)$$

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 $\mathscr{L}$ can be split in the basis of $\mathbb{R}^3$, as the sum of three integral 1-currents (called *canonical dislocation currents*) $\mathscr{L} = \mathscr{L}_1 + \mathscr{L}_2 + \mathscr{L}_3$, in such a way that $\Lambda_{\mathscr{L}_i} = \Lambda_i = \mathscr{L}_i \otimes e_i$ for $i = 1, 2, 3$ and that $\Lambda_{\mathscr{L}} = \Lambda_1 + \Lambda_2 + \Lambda_3$. With the notation $\mathscr{L}_i = \{L_i, \tau^i, \theta_i\}$, we call $L := \bigcup_i L_i$ the dislocation set, which corresponds to the support of $\mathscr{L}$ as shown in [Scala and Van Goethem 2016].

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

3.2. *Functional space representation of dislocation networks.* We will restrict our attention to the class of *continuum dislocations* (c.d.), defined as follows: $\mathscr{L}$ is a continuum dislocation if, for $i = 1, 2, 3$, there exists a 1-Lipschitz map $\lambda^i : [0, M^i] \to \widehat{\Omega}$ such that $\widehat{\mathscr{L}}_i = \lambda^i_\sharp [\![0, M^i]\!]$, the push-forward by λ^i of the standard current given by integration on the interval $[0, M^i]$; see [Scala and Van Goethem 2016, §2] for details (note that this definition is equivalent to the original one given in the reference thanks to Theorem 4.5 therein). 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

descriptions allow for the formation of complex curves. 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

$$\Lambda_{\mathscr{L}} = \sum_{i=1}^{3} \Lambda_i = \sum_{i=1}^{3} \lambda_\sharp^i [\![S^1]\!]_{\llcorner \bar{\Omega}} \otimes e_i, \tag{3-4}$$

which can be equivalently written as $\Lambda_i = (\dot{\lambda}^i \otimes e_i)\lambda_\sharp^i \mathcal{H}^1$, where $\lambda_\sharp^i \mathcal{H}^1$ is the push-forward of the 1-dimensional Hausdorff measure on S^1 through λ^i (see, e.g., [Krantz and Parks 2008] for this notion).

If $\mathscr{L}$ is a continuum dislocation, then there exists a set $\mathscr{C}_{\mathscr{L}} \subset \widehat{\Omega}$ containing the support of the density $\Lambda_{\widehat{\mathscr{L}}}$ 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, $\mathscr{C}_{\mathscr{L}} = \bigcup_{i=1}^{3} \lambda^i(S^1)$.

Let us introduce the class of *dislocation density measures* with compact support in $\widehat{\Omega}$ as

$$\mathcal{M}_\Lambda(\widehat{\Omega}, \mathbb{M}^3) := \{\hat{\mu} \in \mathcal{M}(\widehat{\Omega}, \mathbb{M}^3) : \text{there exists } \widehat{\mathscr{L}}, \text{ c.d., with density } -(\Lambda_{\widehat{\mathscr{L}}})^{\mathrm{T}} = \hat{\mu}\}. \tag{3-5}$$

Let $\lambda \in W^{1,1}(S^1, \mathbb{M}^3)$, with $L := \bigcup_{i=1}^{3} \lambda^i(S^1)$. We introduce

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

for every $P \in L$, which stands for the multiplicity of the dislocation with Burgers vector e_i, where the symbol # denotes the cardinality of a set (the subtraction is due to overlapping loops with reverse orientations).

For every $\varphi \in \mathscr{C}_c(\widehat{\Omega}, \mathbb{M}^3)$, the density $\hat{\mu}_\lambda := -(\Lambda_{\widehat{\mathscr{L}}})^{\mathrm{T}}$ which is associated to λ satisfies

$$-\langle \hat{\mu}_\lambda, \varphi \rangle = \sum_{k=1}^{3} \int_{S^1} \varphi(\lambda^k(s)) \cdot (e_k \otimes \dot{\lambda}^k(s)) \, d\mathcal{H}^1(s)$$

$$= \sum_{k=1}^{3} \int_{S^1} (\varphi \circ \lambda^k)_{kj}(s)(\dot{\lambda}^k)_j(s) \, ds. \tag{3-6}$$

The latter equality can also be seen as the integration on the image L^i of the curve λ^i counted with its multiplicity θ_i. It turns out that

$$-\langle \hat{\mu}_\lambda, \varphi \rangle = \int_L \varphi_{ij}(P)\tau_j^i(P)\theta_i(P) \, d\mathcal{H}^1(P). \tag{3-7}$$

Here

$$\tau_j^i \theta_i \, d\mathcal{H}^1 = (\dot{\lambda}^i)_j \, ds. \tag{3-8}$$

The counterpart of $\hat{\mu}_\lambda$ in $\overline{\Omega}$ is $\mu_\lambda = \hat{\mu}_{\lambda,\overline{\Omega}}$. The correspondence between the arcs λ and the Burgers vectors of the dislocation will appear clearer in the following:

Remark 19. When we deal with a dislocation $\mathscr{L}$ generated by a single 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 $\mathscr{L} = \gamma^b_\sharp [\![S^1]\!]_{\llcorner\overline{\Omega}}$ and $-\mu^T_{\gamma^b} = \Lambda_\mathscr{L} = \mathscr{L} \otimes b$, that is, the measure such that

$$
-\langle \mu_{\gamma^b}, \varphi \rangle = \int_{S^1} \varphi(\gamma^b(s)) \cdot (b \otimes \dot{\gamma}^b(s)) \, ds = \int_{S^1} \varphi_{ij}(\gamma^b(s)) b_i \dot{\gamma}^b_j(s) \, ds
$$

$$
= \int_L \varphi_{ij} \tau^i_j b_i \theta \, d\mathscr{H}^1, \tag{3-9}
$$

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

$$
\theta(P) := \#\left\{ s \in (\gamma^b)^{-1}(P) : \frac{\dot{\gamma}^b}{|\gamma^b|}(s) = \tau(P) \right\} - \#\left\{ s \in (\gamma^b)^{-1}(P) : \frac{\dot{\gamma}^b}{|\gamma^b|}(s) = -\tau(P) \right\}. \tag{3-10}
$$

For every $\mu \in \mathscr{M}_\Lambda(\widehat{\Omega}, \mathbb{M}^3)$, it is easy to check that $\mathrm{Div}\,\mu = 0$ in $\widehat{\Omega}$ since $\mathscr{L}_i$ are closed integral currents. In fact for all $\psi \in \mathscr{D}(\widehat{\Omega}, \mathbb{R}^3)$, one has

$$
-\langle D\psi, \mu \rangle = \left\langle D\psi, \sum_{k=1}^3 e_k \otimes \dot{\lambda}^k(\lambda^k_\sharp \mathscr{H}^1) \right\rangle = \sum_{i=1}^3 \int_{S^1} D_j(\psi_i \circ \lambda^i) \dot{\lambda}^i_j \, ds
$$

$$
= \int_{S^1} D_t(\psi_k \circ \lambda^k) \, dt = 0.
$$

We then get $\mathscr{M}_\Lambda(\widehat{\Omega}, \mathbb{M}^3) \subset \mathscr{M}_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3)$. We can now identify the space $\mathscr{M}_\Lambda(\widehat{\Omega}, \mathbb{M}^3)$ with $W^{1,1}(S^1, \widehat{\Omega}^3)$ through the map

$$
T : W^{1,1}(S^1, \widehat{\Omega}^3) \to \mathscr{M}_\Lambda(\widehat{\Omega}, \mathbb{M}^3) \quad \text{such that } T(\lambda) = -\hat{\mu}_\lambda \text{ defined in (3-6).} \tag{3-11}
$$

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

$$
\|T(\lambda)\|_{\mathscr{M}} \leq \|\dot{\lambda}\|_{L^1}, \tag{3-12}
$$

implying the continuity of T. In general, T is not an injective map, but it is injective up to an equivalence relation $\sim$ in $W^{1,1}(S^1, \widehat{\Omega}^3)$ (namely, $\lambda \sim \lambda'$ if and only if $T(\lambda) = T(\lambda')$ as measures). As a consequence,

$$
T(W^{1,1}(S^1, \widehat{\Omega}^3)) = \mathscr{M}_\Lambda(\widehat{\Omega}, \mathbb{M}^3), \tag{3-13}
$$

$$
T^{-1}(\mathscr{M}_\Lambda(\widehat{\Omega}, \mathbb{M}^3)) = W^{1,1}(S^1, \widehat{\Omega}^3). \tag{3-14}
$$

3.3. *Class of admissible deformations and existence of minimizers.* In this subsection, we exhibit an existence result for minimizers of energies $\mathcal{W}$ satisfying some particular assumptions. For the proofs, we refer to [Scala and Van Goethem 2016]. Let us introduce

$$\mathcal{BC}^{p,\Lambda}(\widehat{\Omega}, \mathbb{M}^3) := \{F \in \mathcal{BC}^p(\widehat{\Omega}, \mathbb{M}^3) : \operatorname{Curl} F \in \mathcal{M}_\Lambda(\widehat{\Omega}, \mathbb{M}^3)\}, \tag{3-15}$$

$$\mathcal{BC}^{p,\Lambda}(\Omega, \mathbb{M}^3) := \{F \in \mathcal{BC}^p(\Omega, \mathbb{M}^3)$$
$$: \text{there exists } \widehat{F} \in \mathcal{BC}^{p,\Lambda}(\widehat{\Omega}, \mathbb{M}^3) \text{ with } F = \widehat{F}_{\llcorner\Omega}\} \tag{3-16}$$

and its proper subspace

$$\mathcal{BC}^{p,\Lambda}_{\operatorname{div}}(\widehat{\Omega}, \mathbb{M}^3) := \{F \in \mathcal{BC}^p_{\operatorname{div}}(\widehat{\Omega}, \mathbb{M}^3) : \operatorname{Curl} F \in \mathcal{M}_\Lambda(\widehat{\Omega}, \mathbb{M}^3)\} \tag{3-17}$$

in such a way that, by Theorem 16 and (3-13),

$$\mathcal{BC}^{p,\Lambda}_{\operatorname{div}}(\widehat{\Omega}, \mathbb{M}^3) := \operatorname{Curl}^{-1}(\mathcal{M}_\Lambda(\widehat{\Omega}, \mathbb{M}^3)) = \operatorname{Curl}^{-1}(T(W^{1,1}(S^1, \widehat{\Omega}^3))). \tag{3-18}$$

In [Scala and Van Goethem 2016], we consider deformations $F \in \mathcal{BC}^{p,\Lambda}(\Omega, \mathbb{M}^3)$ which also satisfy some regularity conditions outside the continuum dislocation set $\mathcal{C}_{\mathscr{L}}$ of the dislocation $\Lambda_{\mathscr{L}} \in \mathcal{M}_\Lambda(\overline{\Omega}, \mathbb{M}^3)$. If F is an admissible deformation, we assume that F satisfies the following property:

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

Let us recall the meaning of $\operatorname{Cart}^p(B, \mathbb{R}^3)$. If U is an open set on $\mathbb{R}^3$, the space of Cartesian maps on U, denoted by $\operatorname{Cart}^p(U, \mathbb{R}^3)$, 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 conditions that $\operatorname{adj}(Du)$ and $\det(Du)$ 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 [Giaquinta et al. 1998]. We denote by

$$\mathcal{AD}^p(\widehat{\Omega}) := \{F \in \mathcal{BC}^{p,\Lambda}(\widehat{\Omega}, \mathbb{M}^3) : F \text{ satisfies (P) above}\}, \tag{3-19}$$

$$\mathcal{AD}^p(\Omega) := \{F \in \mathcal{BC}^p(\Omega, \mathbb{M}^3) : \text{there exists } \widehat{F} \in \mathcal{AD}^p(\widehat{\Omega}) \text{ with } F = \widehat{F}_{\llcorner\Omega}\}. \tag{3-20}$$

Notation 20. Let $\widehat{\Omega}$ be the open set introduced in Notation 15, and let α be a boundary condition in $V = \widehat{\Omega} \setminus \overline{\Omega}$ (i.e., $\alpha = \mathscr{L}_{\llcorner V}$ for a closed dislocation current $\widehat{\mathscr{L}}$ in $\widehat{\Omega}$). We then fix $\widehat{F} \in \mathcal{AD}^p(\widehat{\Omega})$ such that $-\operatorname{Curl} \widehat{F} = (\Lambda_{\widehat{\mathscr{L}}})^{\mathrm{T}}$ and define

$$\mathcal{F}_\alpha := \{F \in \mathcal{AD}^p(\Omega), \ 1 \le p < 2 : \widetilde{F} := F\chi_\Omega + \widehat{F}\chi_V \in \mathcal{AD}^p(\widehat{\Omega}), \ -\operatorname{Curl} \widetilde{F} = (\Lambda_{\widehat{\mathscr{L}}})^{\mathrm{T}}$$
$$\text{in } \widehat{\Omega} \text{ for some closed dislocation current } \widehat{\mathscr{L}} \text{ in } \widehat{\Omega}\}. \tag{3-21}$$

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

Assumptions on the energy. We make the assumption on the elastic energy

$$\mathcal{W}(F, \Lambda_{\mathscr{L}}) := \mathcal{W}_{\mathrm{e}}(F) + \mathcal{W}_{\mathrm{dislo}}(\Lambda_{\mathscr{L}}), \tag{3-22}$$

with

$$\mathcal{W}_{\mathrm{e}}(F) := \int_{\Omega} W_{\mathrm{e}}(F) \, dx. \tag{3-23}$$

As for the dislocation part, we assume that

$$\mathcal{W}_{\mathrm{dislo}}(\Lambda_{\mathscr{L}}) = \mathcal{W}^1_{\mathrm{dislo}}(\Lambda_{\mathscr{L}}) + \mathcal{W}^2_{\mathrm{dislo}}(\Lambda_{\mathscr{L}}), \tag{3-24}$$

where the precise continuity, growth properties on the bulk, and defect energies are discussed and motivated in [Scala and Van Goethem 2016]. Let us stress that following [Conti et al. 2015a] (where no variational problem is solved), an expression for the line tension $\mathcal{W}^1_{\mathrm{dislo}}$ is here taken as

$$\mathcal{W}^1_{\mathrm{dislo}}(\mu) = \int_{L} \psi(\theta b, \tau) \, d\mathcal{H}^1, \tag{3-25}$$

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 nonnegative function satisfying $\psi(0, \cdot) = 0$ and $\psi(b, t) \geq c\|b\|$ for a constant $c > 0$.

As for the term $\mathcal{W}^2_{\mathrm{dislo}}(\Lambda_{\mathscr{L}})$, it is remarkable that, under the hypotheses needed to get existence of minimizers, it does not depend on small perturbations of the dislocation line set L. This will be strongly used in the subsequent section.

Now the existence theorem is the following:

Theorem 21. *Under Notation 20 and suitable hypotheses on the energy $\mathcal{W}$ in (3-22) (see [Scala and Van Goethem 2016] for details), there exists a minimizer $F^{\star}$ of the problem*

$$\min_{F \in \mathscr{F}_{\alpha}} \mathcal{W}(F, \Lambda_{\mathscr{L}}). \tag{3-26}$$

We write $\mathrm{Curl}\, F^{\star} = \Lambda^{\mathrm{T}}_{\mathscr{L}^{\star}}$ with $\mathscr{L}^{\star}$ being the optimal dislocation network, whose support is denoted by $L^{\star}$. It should be remarked that, due to the Dirichlet condition $F = \widehat{F}$ on $\widehat{\Omega} \setminus \Omega$ for the admissible deformations gradients, the minimizer is not trivial and must satisfy $-\mathrm{Curl}\, F = \Lambda_{\mathscr{L}}$ for some closed dislocation current $\mathscr{L}$ coinciding with α in $\widehat{\Omega} \setminus \Omega$. An explicit example showing the nontriviality of the solution can be found in [Scala and Van Goethem 2016, §5.4]. Note that such energies at the macroscale are considered in [Neff et al. 2015a], where a variational problem is solved.

4. Configurational forces at optimal dislocation networks

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. They are related to the presence of microstructure, here dislocations, in an otherwise static elastic medium in equilibrium. All the results of the previous sections will allow us to prove Theorem 26, which consists of a balance of forces at minimality. Furthermore, minimality will entail Euler–Lagrange equations which physically correspond to the balance of forces and to the vanishing of virtual work done by the configurational force, recognized as the Peach–Koehler force.

4.1. *Shape variation at optimality.* Let $F^\star$ be a minimizer of $\mathcal{W}(F)$. By Theorem 9 and (3-13),

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

where Curl^{-1} is the solution of (2-19), for some $\lambda^\star \in W^{1,1}(S^1, \widehat{\Omega}^3)$. Let $-(\Lambda^\star)^{\mathrm{T}} := T(\lambda^\star) = -\mathrm{Curl}\, F^\star$ on $\widehat{\Omega}$.

Define the linear map

$$S : W^{1,1}(S^1, \widehat{\Omega}^3) \to \mathcal{BC}^{p,\Lambda}_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3), \quad S = \mathrm{Curl}^{-1} \circ T. \tag{4-1}$$

We first prove the following preliminary result.

Lemma 22. *The map* $S : W^{1,1}(S^1, \widehat{\Omega}^3) \to \mathcal{BC}^{p,\Lambda}_{\mathrm{div}}(\widehat{\Omega}, \mathbb{M}^3)$ *is Gâteaux differentiable at* $\lambda^\star$ *in all directions* λ. *In particular,* $DS(\lambda^\star)[\lambda] \in \mathcal{M}(\widehat{\Omega}, \mathbb{M}^3)$, *for every* $W^{1,1}(S^1, (\mathbb{R}^3)^3)$-*variation* λ, *and*

$$\langle DS(\lambda^\star)[\lambda], \varphi \rangle = \sum_{i=1}^{3} \int_{S^1} \epsilon_{jkm}(\varphi \circ \lambda^\star)_{im}(s)(\dot{\lambda}^\star)^i_k(s)\lambda^i_j(s)\, ds \tag{4-2}$$

for every $\varphi \in \mathcal{C}_c(\Omega, \mathbb{M}^3)$ *such that* $\mathrm{Div}\,\varphi = 0$.

Proof. Let $\Psi \in \mathcal{D}(\Omega, \mathbb{M}^3)$. From (3-6) and (3-11), we infer by a Taylor expansion of Ψ that the directional derivative of T at $\lambda^\star$ along a variation $\lambda \in W^{1,1}(S^1, (\mathbb{R}^3)^3)$ reads

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

Integrating the last expression by parts, we get

$$
\begin{aligned}
\langle DT(\lambda^\star)[\lambda], \Psi\rangle &= \sum_{i=1}^{3} \int_{S^1} \big(D_k(\Psi \circ \lambda^\star)_{ij}(s)(\dot{\lambda}^\star)^i_j(s)\lambda^i_k(s) \\
&\qquad\qquad\qquad - D_k(\Psi \circ \lambda^\star)_{ij}(s)(\dot{\lambda}^\star)^i_k(s)\lambda^i_j(s)\big)\,ds \\
&= \sum_{i=1}^{3} \int_{S^1} \big(D_j(\Psi \circ \lambda^\star)_{ik}(s) - D_k(\Psi \circ \lambda^\star)_{ij}(s)\big)(\dot{\lambda}^\star)^i_k(s)\lambda^i_j(s)\,ds \\
&= \sum_{i=1}^{3} \int_{S^1} \epsilon_{jkm}\epsilon_{mpq} D_p(\Psi \circ \lambda^\star)_{iq}(s)(\dot{\lambda}^\star)^i_k(s)\lambda^i_j(s)\,ds. \qquad (4\text{-}3)
\end{aligned}
$$

Let us now compute DS. Let $\varphi \in \mathscr{C}_c(\Omega, \mathbb{M}^3)$ such that $\mathrm{Div}\,\varphi = 0$. Then $\varphi = \mathrm{Curl}\,\Psi$ for some $\Psi \in C^1(\Omega, \mathbb{M}^3)$, and hence, by Theorem 16,

$$
\begin{aligned}
\frac{1}{\epsilon}\langle S(\lambda^\star + \epsilon\lambda) - S(\lambda^\star), \mathrm{Curl}\,\Psi\rangle &= \frac{1}{\epsilon}\langle \mathrm{Curl}^{-1}(T(\lambda^\star + \epsilon\lambda) - T(\lambda^\star)), \mathrm{Curl}\,\Psi\rangle \\
&= \frac{1}{\epsilon}\langle (T(\lambda^\star + \epsilon\lambda) - T(\lambda^\star)), \Psi\rangle.
\end{aligned}
$$

Letting $\epsilon \to 0$ yields the result by (4-3). $\qquad\qquad\qquad\qquad\qquad\square$

4.2. *First Euler–Lagrange equation and the static equilibrium.* In this subsection, we make variations of the deformation at minimality, assuming the optimal line fixed, and derive the classical strong form of finite-strain elasticity.

Regularity assumption on the energy. We make the assumption that the energy $\mathscr{W}_e : L^p(\widehat{\Omega}) \to \mathbb{R}$ in (3-23) is Fréchet differentiable in $L^p(\widehat{\Omega})$ with the Fréchet derivative of $F \mapsto \mathscr{W}(F, \Lambda^\star)$ denoted by $W_F \in L^{p'}(\widehat{\Omega})$. As a consequence, for every $F \in L^p(\widehat{\Omega})$,

(A$_1$) $\delta\mathscr{W}(F^\star)[F] := \frac{d}{d\epsilon}\mathscr{W}(F^\star + \epsilon F, \Lambda^\star)_{|\epsilon=0} = \int_{\widehat{\Omega}} W_F^\star \cdot F\,dx = \delta\mathscr{W}_e(F^\star)[F]$ with
$\quad\;\; W_F^\star := W_F(F^\star, \Lambda^\star) = \delta\mathscr{W}_e(F^\star) \in L^{p'}(\widehat{\Omega}).$

Note that this assumption is rather general and is about the least we can assume on $\mathscr{W}_e$.

Variations F of deformation $F^\star$ still satisfying the constraint $-\mathrm{Curl}(F^\star + \epsilon F) = (\Lambda^\star)^{\mathrm{T}}$ must belong to $\mathscr{AD}^p_{\mathrm{curl}}(\widehat{\Omega}) := \{F \in \mathscr{AD}^p(\widehat{\Omega}) : \mathrm{Curl}\,F = 0\}$. Moreover, such variations at the minimum points of the energy $\mathscr{W}$ must provide a vanishing variation of $\mathscr{W}$. Thus, $F^\star$ being such a solution, for every curl-free $F = Du \in L^p(\widehat{\Omega})$, it must hold that

$$
\delta\mathscr{W}^\star(Du) = \delta\mathscr{W}_e(F^\star)[Du] = 0. \qquad (4\text{-}4)
$$

From (A_1), (4-4), and Theorem 18, it follows that there exists $\mathbb{L}^\star$ continuous such that

$$\mathbb{P}^\star := W_F^\star = \delta W_e(F^\star) = \operatorname{Curl} \mathbb{L}^\star \in L^{p'}(\widehat{\Omega}) \tag{4-5}$$

satisfying the strong form

$$\begin{cases} -\operatorname{Div} \mathbb{P}^\star = 0 & \text{in } \widehat{\Omega}, \\ \mathbb{P}^\star N = 0 & \text{on } \partial\widehat{\Omega}. \end{cases} \tag{4-6}$$

One could wonder why (4-6) is not immediate from the relation $\int_\Omega W_F^\star \cdot \nabla u \, dx = 0$, which is Euler–Lagrange in weak form. In fact, the integration by parts which is classically used in this context is not legitimate in the present case simply because the divergence theorem does not hold for L^p-fields since $\mathbb{P}^\star N$ has no meaning at the boundary. This is the reason why Theorem 18 is called and $\mathbb{P}^\star$ is obtained as the curl of constraint reaction $\mathbb{L}^\star$, being therefore automatically divergence-free, while $\mathbb{P}^\star N$ has a meaning by Lemma 13 and Theorem 18.

Remark 23. By (4-6), $\mathbb{P}^\star := W_F^\star$ is identified with the first Piola–Kirchhoff stress. $\mathbb{P}^\star$ being in $L^{p'}(\widehat{\Omega})$, and recalling that $F \in L^p(\widehat{\Omega})$, means that the Kirchhoff stress $\mathbb{P}^\star F$ is in $L^1(\widehat{\Omega})$.

4.3. *The Peach–Koehler force as a stationary condition.* In this subsection, we derive the second Euler–Lagrange equation of the system in equilibrium.

Regularity assumption on the stress. Regularity of the minimizers is a well-known open problem in mathematical elasticity. Indeed, almost no results exist, even with an energy growth with $p \geq 2$ (i.e., without dislocations), as reported by J. Ball [2002]. A related problem is the regularity of the Piola–Kirchhoff stress $\mathbb{P}^\star$. In order to derive the subsequent formulae, which are well-established by physicists, we will also appeal to an assumption, not on $F^\star$, but rather on some components of $\mathbb{P}^\star$.

Let us consider the orthonormal curvilinear basis $(\tau^\star, \sigma^\star, \nu^\star)$ on the optimal dislocation set $L^\star$, with $\tau^\star$ the unit tangent vector to $L^\star$. Let us decompose $\mathbb{P}^\star$ in this basis; i.e., $\mathbb{P}^\star = \mathbb{P}^\star \tau^\star \otimes \tau^\star + \widetilde{\mathbb{P}}^\star$. Physically, $\mathbb{P}^\star \tau^\star$ represents the force $d\mathscr{F}$ exerted on a facet dS of normal $\tau^\star$, that is, on a section of the tubular neighborhood of the dislocation $L^\star$; namely, $d\mathscr{F} = \mathbb{P}^\star \tau^\star dS$. Since all such facets are crossed by the dislocation, they presumably correspond to singular forces, in such a way that no regularity assumption can be made on these components. We will therefore make a regularity assumption on the remaining components $\widetilde{\mathbb{P}}^\star$. Let us emphasize that the optimal deformation tensor $F^\star$ is smooth in $\Omega \setminus L^\star$, and hence, by (4-6), $\mathbb{P}^\star$ will also be smooth in $\Omega \setminus L^\star$. Therefore, it is assumed that

(A_2) $\widetilde{\mathbb{P}}^\star$ is continuous in a neighborhood of $L^\star$.

In fact, lack of continuity of these components would mean that the contact forces $d\mathscr{F}$ tend to infinity at $L^\star$.

Validity of Assumption (A_2). First, we remark that in linearized elasticity the stress behaves as $\sim 1/r$ and following [Hirth and Lothe 1982; Van Goethem and Dupret 2012a] one has $\widetilde{\mathbb{P}}^{\star}_{\text{screw}} = 0$ whereas $\widetilde{\mathbb{P}}^{\star}_{\text{edge}} \to \infty$ as $r \to 0$. Hence, obviously, one must consider finite strain elasticity to discuss Assumption (A_2). Here again, the situation is not evident since nonlinear stresses depend on the choice of the material (i.e., of the energy W_{e}) and on the physics which takes place at the singular line. We will thus follow L. Zubov, who has reported the current state of the art in [Zubov 1997]. About the screw dislocation, he first points out that, for a *Mooney* (and neo-Hookean) incompressible material, one has divergence of $\widetilde{\mathbb{P}}^{\star}_{\text{screw}}$ at the singularity, but he discards this case as being nonphysical, i.e., not suitable for the creation of a screw dislocation [Zubov 1997, p. 74]. Then he considers the *Bartenev–Khazanovich* among two other incompressible materials and finds $\widetilde{\mathbb{P}}^{\star}_{\text{screw}} \sim \ln r$, hence again lacking continuity though showing better integrability properties. However, incompressibility is not assumed in general and in particular not in the present paper (indeed, it would imply another constraint reaction [Fosdick and Royer-Carfagni 2005]). Therefore, following Zubov again, one considers a *Blatz–Ko* material together with the physical observation that the creation of a screw dislocation takes place together with a cylindrical cavity, and this implies continuity of $\widetilde{\mathbb{P}}^{\star}_{\text{screw}}$ at the singularity [Zubov 1997, (3.2.12), (3.2.16), (3.2.24), (3.2.28), p. 76], whereas $\mathbb{P} - \widetilde{\mathbb{P}}$ must not be continuous [Zubov 1997, (3.2.12), p. 76]. Because the technical difficulties are huge, Zubov does not compute in extenso the edge dislocation with a cavitation, but nonetheless we consider the following physical interpretation, as based on Zubov's aforementioned results and physical evidence of dislocation nucleation as reported by, e.g., [Cottrell 1964; Berezhkova 1969]:

> Assumption (A_2) *holds true for a compressible material where a cavitation is found along any dislocation loop.*

In practice, Assumption (A_2) allows one to have a finite radius R in the reference configuration corresponding to $r = 0$ in the deformed configuration Ω. Furthermore, Zubov shows that $R(0)$ is proportional, on the order of 10% of the Burgers vector.

Note that the creation of such a cavity in single crystals is due to the nucleation process of dislocation loops resulting from the collapse of a void, i.e., a cluster of vacancies which has become unstable.

The Peach–Koehler force. We write $F = Du + \text{Curl}^{-1}(-\Lambda^{\text{T}}) = Du + S(\lambda)$ for all $F \in \mathcal{BC}^p(\widehat{\Omega}, \mathbb{R}^{3\times 3})$ with $u \in W^{1,p}(\widehat{\Omega}, \mathbb{R}^3)$ (by Theorem 9 and (4-1)). Following this formalism, it is thus assumed that the energy $\mathcal{W}$ depends on the dislocation path $\lambda \in W^{1,1}(S^1, \widehat{\Omega}^3)$ as defined in (3-11), that is,

$$\mathcal{W}^{\circ}(Du, \lambda) := \mathcal{W}(Du + S(\lambda), -T(\lambda)), \tag{4-7}$$

and then $\mathcal{W}^\circ(Du, \lambda) = \mathcal{W}(F, \Lambda)$ with $\Lambda^T = -\operatorname{Curl} F$ if $\lambda \in T^{-1}(-\Lambda^T)$. Let us consider the energy at its minimum $F^\star$:

$$
\begin{aligned}
\mathcal{W}^\circ(Du^\star, \lambda^\star) &:= \mathcal{W}(Du^\star + S(\lambda^\star), -T(\lambda^\star)) \\
&= \mathcal{W}_e(Du^\star + S(\lambda^\star)) + \mathcal{W}_{\text{defect}}(-T(\lambda^\star)) \\
&=: \mathcal{W}_e^\circ(\lambda^\star) + \mathcal{W}_{\text{defect}}^\circ(\lambda^\star).
\end{aligned}
\tag{4-8}
$$

Let us denote the variation of the energy $\mathcal{W}_e$ by $\delta^\circ \mathcal{W}_e(F^\star) := \delta \mathcal{W}_e^\circ(\lambda^\star)$. The expression of the variation of the energy is then given by the following main result.

Theorem 24 (work done by the Peach–Koehler force). *Under the assumptions of Theorem 21 and hypotheses* (A$_1$) *and* (A$_2$), *one has*

$$
\langle \delta^\circ \mathcal{W}_e(F^\star), \lambda \rangle = \sum_{i=1}^{3} \int_{L^\star} (\mathbb{P}^\star \times \tau^i)^T \theta_i \cdot \lambda^i \circ (\lambda^\star)^{-1} \, d\mathcal{H}^1,
\tag{4-9}
$$

where we have employed notation (3-7).

Proof. We want to perform variations $\lambda \in W^{1,1}(S^1, (\mathbb{R}^3)^3)$ of $\mathcal{W}_e^\circ(\lambda^\star)$. Identifying $W_F^\star$ with the Piola–Kirchhoff $\mathbb{P}^\star$ as in (4-5), using Lemma 22 with $\varphi = \widetilde{\mathbb{P}}$, one has

$$
\begin{aligned}
\delta \mathcal{W}_e^\circ(\lambda^\star)[\lambda] &= \sum_{i=1}^{3} \int_{S^1} \lambda_j^i \epsilon_{jkm} (\dot{\lambda}^\star)_k^i \widetilde{\mathbb{P}}_{im}^\star \circ \lambda^\star \, ds \\
&= \sum_{i=1}^{3} \int_{S^1} \lambda_j^i \epsilon_{jkm} (\dot{\lambda}^\star)_k^i \mathbb{P}_{im}^\star \circ \lambda^\star \, ds,
\end{aligned}
\tag{4-10}
$$

where Assumption (A$_2$) gives a meaning to $\widetilde{\mathbb{P}}_{im}^\star$ on $L^\star$ (i.e., to $\widetilde{\mathbb{P}}_{im}^\star \circ \lambda^\star$ on S^1) and hence to the duality pairing

$$
\delta \mathcal{W}_e^\circ(\lambda^\star)[\lambda] = \langle W_F^\star, DS(\lambda^\star)[\lambda] \rangle,
\tag{4-11}
$$

completing the proof. $\qquad\square$

The integrand in the right-hand side of (4-9) is recognized as the Peach–Koehler force. Theorem 24 simply says that at minimality the virtual work done by the Peach–Koehler force must vanish.

Remark 25. The duality pairing (4-11) holds as soon as one considers a mollification of $W_F^\star$, that is, if $W_F^\star$ is assumed continuous. However, this assumption is stronger than (A$_2$), which requires only the continuity of some physically relevant components (related to the formation of a cavitation at the line singularity). Furthermore, nothing guarantees that the variation with any mollification of $W_F^\star$ would vanish since it is strictly speaking not the minimum point. Thus, at the mesoscopic scale, the best assumption found is (A$_2$) in order to be able to merely define the Peach–Koehler force as related to minimality.

According to Remark 25, the following subsection shows how the Peach–Koehler force would formally be recovered.

Formal derivation of the Peach–Koehler force from the Eshelby tensor. Recalling (3-23), we introduce the Eshelby tensor $\mathscr{E}$ componentwise as

$$\mathscr{E}_{ij} = \delta_{ij} W_{\mathrm{e}} - F_{ki} \mathbb{P}_{kj}. \tag{4-12}$$

Then, assuming that F and $\mathbb{P}$ are smooth enough,

$$\partial_j \mathscr{E}_{ij} = \partial_i W_{\mathrm{e}} - \partial_j F_{ki} \mathbb{P}_{kj} - F_{ki} \partial_j \mathbb{P}_{kj}. \tag{4-13}$$

At minimality, one has $\partial_j \mathbb{P}_{kj} = 0$ and hence

$$\partial_j \mathscr{E}_{ij}^{\star} = \partial_i W_{\mathrm{e}}^{\star} - \partial_j F_{ki}^{\star} \mathbb{P}_{kj}^{\star} = \partial_i W_{\mathrm{e}}^{\star} - (\partial_j F_{ki}^{\star} - \partial_i F_{kj}^{\star}) \mathbb{P}_{kj}^{\star} - \partial_i F_{kj}^{\star} (W_F^{\star})_{kj}, \quad \text{(4-14)}$$

where the first and last terms of the right-hand side mutually cancel, whence

$$\partial_j \mathscr{E}_{ij}^{\star} = -(\partial_j F_{ki}^{\star} - \partial_i F_{kj}^{\star}) \mathbb{P}_{kj}^{\star} = \epsilon_{ijl} \epsilon_{lmn} \partial_m F_{kn}^{\star} \mathbb{P}_{kj}^{\star} = \epsilon_{ijl} (\mathrm{Curl}\, F^{\star})_{kl} \mathbb{P}_{kj}^{\star}, \quad \text{(4-15)}$$

that is

$$\partial_j \mathscr{E}_{ij}^{\star} = \langle \epsilon_{ilj} \Lambda_{lk}^{\star}, \mathbb{P}_{kj}^{\star} \rangle. \tag{4-16}$$

Note that (4-16) has no rigorous meaning in our setting, i.e., at the mesoscale, since, $\Lambda^{\star}$ being a Radon measure but $\mathbb{P}^{\star}$ not being continuous, the duality pairing (4-16) is undefined. This is the reason why the Peach–Koehler force is established in our work by means of Assumption (A$_2$).

4.4. *Configurational balance.* Let $L = \gamma^{\star}(S^1)$ be a single smooth-enough dislocation loop with tangent vector τ, normal vector ν, curvature κ, and total Burgers vector B. This is assumed for simplicity of exposition, but similar results can be stated for general $\lambda^{\star} \in W^{1,1}(S^1, \widehat{\Omega}^3)$. We introduce

$$\mathscr{F} := (\mathbb{P}^{\star} \times \tau)^{\mathrm{T}} B \delta_L,$$
$$\mathscr{G} := \kappa \big(\psi(b, \tau) - \nabla \psi(b, \tau) \cdot \tau + \nabla\nabla \psi(b, \tau) \cdot \nu \otimes \nu \big) \nu \| \dot{\gamma}^{\star} \|^{-1} \delta_L,$$

the so-called Peach–Koehler force and line tension, respectively, where ψ is the energy density as introduced in (3-25).

Deriving strong forms of equilibrium from a variational problem is classically done provided some regularity of the minimizers is assumed, as summarized in the following theorem. Note that restricting to a single generating loop with Burgers vector b is chosen for simplicity of exposition. 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$_3$) $\gamma^{\star} \in W^{2,1}(S^1, \widehat{\Omega})$.

Theorem 26. *Under the assumptions of Theorem 21, assuming $\psi, \bar{\psi} : \mathbb{Z}^3 \times \mathbb{R}^3 \to \mathbb{R}^+$ are of class $\mathscr{C}^2$ and that the optimal dislocation network satisfies (A_3) and is associated to a single Burgers vector b, then minimality implies equilibrium of configurational forces, in the sense that the Peach–Koehler force $\mathscr{F}^\star$ is balanced by the line tension $\mathscr{G}^\star$ in $L^\star$, i.e.,*

$$\mathscr{F}^\star + \mathscr{G}^\star = 0. \tag{4-17}$$

Proof. Let us particularize (4-10) to the case where the density $\Lambda^\star$ is generated by one single loop $\gamma^\star \in W^{1,1}(S^1, \widehat{\Omega})$ with Burgers vector $b = \beta_i e_i$, $\beta_i \in \mathbb{Z}$ ($b \neq 0$) (see Remark 19). For variations of the form $\gamma^\star + \epsilon\gamma$ with $\gamma \in W^{1,\infty}(S^1, \widehat{\Omega})$, (4-10) becomes

$$\delta W_{\mathrm{e}}^\circ(\gamma^\star)[\gamma] = \int_{S^1} \epsilon_{kjm}(\mathbb{P}^\star \circ \gamma^\star(s))_{im} \tau_k b_i \gamma_j(s) \|\dot{\gamma}^\star(s)\| \, ds$$

$$= \int_{L^\star} \epsilon_{kjm} \mathbb{P}_{im}^\star \tau_k b_i \gamma_j \, d\mathscr{H}^1 = \int_{\widehat{\Omega}} \epsilon_{kjm} \mathbb{P}_{im}^\star \gamma_j \, d\Lambda_{ki}^\star. \tag{4-18}$$

Using the notation introduced in (4-8), we write

$$\mathscr{W}^\circ(\gamma^\star + \epsilon\gamma) = \mathscr{W}_{\mathrm{e}}^\circ(\gamma^\star + \epsilon\gamma) + \mathscr{W}_{\mathrm{defect}}^\circ(\gamma^\star + \epsilon\gamma), \tag{4-19}$$

We have

$$\delta\mathscr{W}^\circ(\gamma^\star)[\gamma] = \delta\mathscr{W}_{\mathrm{e}}^\circ(\gamma^\star)[\gamma] + \delta\mathscr{W}_{\mathrm{defect}}^\circ(\gamma^\star)[\gamma]. \tag{4-20}$$

Let us now compute the variation of the defect part of the energy. For a dislocation density of the form $\mu = b \otimes \gamma_\sharp[\![S^1]\!]$, (3-25) can be written as

$$\mathscr{W}_{\mathrm{defect}}^1(\mu) = \int_{S^1} \psi\left(b, \frac{\dot{\gamma}}{\|\dot{\gamma}\|}(s)\right) \|\dot{\gamma}(s)\| \, ds. \tag{4-21}$$

Taking into account that the term $\mathscr{W}_{\mathrm{defect}}^2(\mu)$ does not change for small perturbations of the dislocation line, the first variation of (4-21) at the point $\gamma^\star \in W^{1,1}(S^1, \widehat{\Omega})$ can be explicitly computed and will coincide with $\delta\mathscr{W}_{\mathrm{defect}}^\circ(\gamma^\star)[\gamma]$. It holds that

$$\delta\mathscr{W}_{\mathrm{defect}}^\circ(\gamma^\star)[\gamma] = \int_{S^1} \left(D_k\psi\left(b, \frac{\dot{\gamma}^\star}{\|\dot{\gamma}^\star\|}(s)\right) \left(\frac{\dot{\gamma}_k\|\dot{\gamma}^\star\|^2 - \dot{\gamma}_k^\star\dot{\gamma}_j^\star\dot{\gamma}_j}{\|\dot{\gamma}^\star\|^2}(s)\right) \right.$$

$$\left. + \psi\left(b, \frac{\dot{\gamma}^\star}{\|\dot{\gamma}^\star\|}(s)\right) \left(\frac{\dot{\gamma}_j^\star\dot{\gamma}_j}{\|\dot{\gamma}^\star\|}(s)\right) \right) ds, \quad (4\text{-}22)$$

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

$$\delta\widehat{W}_{\mathrm{defect}}(\gamma^\star)[\gamma] = -\int_{S^1} \left(\psi(b, \tau)\dot{\tau}_j - D_k\psi(b, \tau)\tau_k\dot{\tau}_j \right.$$

$$\left. + D_j D_k\psi(b, \tau)\dot{\tau}_k - D_p D_k\psi(b, \tau)\dot{\tau}_k\tau_p\tau_j \right)\gamma_j \, ds,$$

where we dropped the variable s. Equivalently, recalling that $\dot{\tau}_i = \kappa \nu_i$ and since $D_j D_k \psi(b, \tau) \dot{\tau}_k = \tau_j^i \tau_p^i D_p D_k \psi(b, \tau) \dot{\tau}_k + \nu_j \nu_p D_p D_k \psi(b, \tau) \dot{\tau}_k$,

$$
\begin{aligned}
g_j^\star[b] &:= \psi(b, \tau) \dot{\tau}_j^i - D_k \psi(b, \tau) \tau_k \dot{\tau}_j^i + D_j D_k \psi(b, \tau) \dot{\tau}_k - D_p D_k \psi(b, \tau) \dot{\tau}_k \tau_p^i \tau_j^i \\
&= \psi(b, \tau) \dot{\tau}_j^i - D_k \psi(b, \tau) \tau_k \dot{\tau}_j^i + D_p D_k \psi(b, \tau) \dot{\tau}_k \nu_p \nu_j \\
&= \kappa \big(\psi(b, \tau) - D_k \psi(b, \tau) \tau_k + D_p D_k \psi(b, \tau) \nu_p \nu_k \big) \nu_j.
\end{aligned}
\tag{4-23}
$$

Plugging the last expression into (4-20) and using (4-18), we obtain

$$
\delta \mathcal{W}^\circ(\gamma^\star)[\gamma] = \int_{S^1} \big(\epsilon_{kjm} (\mathbb{P}^\star \circ \gamma^\star)_{im}(s) b_i \dot{\gamma}_k^\star(s) - g_j^\star[b](s) \big) \gamma_j(s) \, ds.
\tag{4-24}
$$

From the condition

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

due to the minimality of $\gamma^\star$, we then get from (4-24) $\mathscr{F}_j^\star + \mathscr{G}_j^\star = 0$, with

$$
\mathscr{F}_j^\star := \epsilon_{kjm} (\mathbb{P}^\star)_{im} B_i \tau_k \delta_{L^\star} \quad \text{and} \quad \mathscr{G}_j^\star := \rho_{\mathrm{dislo}}(B) \nu_j \delta_{L^\star},
$$

where

$$
\rho_{\mathrm{dislo}}(B) := -g^\star[B] \varepsilon^{-1}
\tag{4-25}
$$

with $g^\star := g_j^\star \nu_j$, $\varepsilon = \varepsilon(P) := \| \dot{\gamma}^\star \circ {\gamma^\star}^{-1}(P) \|$, the local deformation of the curve at $P \in L^\star$,

$$
B := \theta(P) b,
$$

the total Burgers vector, and $\theta(P)$ as defined by (3-10), the multiplicity of the dislocation (accounting for the loops of the cluster whose Burgers vector is a multiple of b). □

Remark 27. Actually, (4-17) 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 orthogonal vector ν.

In the case where $\theta = 1$ and the dislocation is parametrized by arc length ($|\dot{\gamma}^\star| = 1$), the balance of forces can be rewritten as

$$
\epsilon_{kjm} \mathbb{P}_{im}^\star b_i \tau_k = g_j^\star[b] \quad \text{on } L^\star.
$$

A modeling example. Conti et al. [2015a] consider a potential $\mathcal{W}_{\mathrm{dislo}}^1$ of the form (3-25) with

$$
\psi(b, \tau) := |b|^2 + \eta \langle b, \tau \rangle^2,
\tag{4-26}
$$

where $\eta > 0$ is a constant.

In the particular case where $b = \beta e_1$, $\beta \geq 1$, it is shown that such energy is also lower-semicontinuous.

In such a case, the above computations entail that

$$\mathscr{G}_j^\star(P) = (|b|^2 - \eta\langle b, \tau\rangle^2 + 2\eta\langle b, \nu\rangle^2)\kappa\nu_j$$

so that at the minimum of the energy

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

4.5. *Some additional remarks.*

Formal balance of configurational forces. Equation (4-18) yields, by (4-16) and a slight abuse of notation,

$$\delta\mathscr{W}_{\mathrm{e}}^\circ(\gamma^\star)[\gamma] = \int_{\widehat{\Omega}} -\partial_k\mathscr{E}_{jk}^\star\gamma_j\,dx. \tag{4-27}$$

Therefore, (4-24) and (4-27) can be rewritten as the virtual configurational work balance at minimality, i.e.,

$$-\operatorname{Div}\mathscr{E}^\star = \mathscr{G}^\star, \tag{4-28}$$

where $\mathscr{E}^\star$ and $\mathscr{G}^\star$ stand for the configurational stress and the internal configurational force [Gurtin 2000, p. 34]. In our case, $\mathscr{G}^\star := \rho_{\mathrm{dislo}}[B]\nu_j\delta_{L^\star}$. Quoting Gurtin, such force is "related to the material structure of the body $\mathscr{B}$; to each configuration of $\mathscr{B}$ there correspond a distribution of material and internal configurational forces that act to hold the material in place in that configuration. Such forces characterize the resistance of the material to structural changes and are basic when discussing temporal changes associated with phenomena such as the breaking of atomic bonds during fracture [and during dislocation motion]".

Let us note that Agiasofitou and Lazar [2010] have also derived a relation such as (4-28) in the framework of dislocation gauge theory by means of invariance properties and the Noether theorem (without considering a minimization problem as done here). These authors showed that the translational balance laws of the elastic and dislocation parts give rise to the Peach–Koehler force and also give the interpretation that "the Peach–Koehler force is the interaction force between the elastic subsystem and the dislocation subsystem" (see also (5.39) in [Lazar and Anastassiadis 2008]).

A brief glance at the dynamic problem. So far, we have identified the stationarity condition as a balance of configurational work. This happens when minimality is reached.

Consider now a time-evolution problem involving dislocation lines. In principle, no variational problem drives its evolution instantaneously, but minimality might be reached as $t \to \infty$ [Berdichevsky 2006]. So a first remark is that, before minimality

is reached, one has Div $\mathscr{E}^\star + g^\star \neq 0$, by definition, and hence there exists a nonzero momentum p such that, according to [Gurtin 2000, p. 46],

$$-F^{\mathrm{T}}\dot{p} = \mathrm{Div}\,\mathscr{E}^\star + \mathscr{G}^\star. \qquad (4\text{-}29)$$

Hence, one might determine the motion of the line towards equilibrium, i.e., until $\dot{p} = 0$.

Now, Gurtin [2000, p. 11] further says that as far as $\dot{p} = 0$ the internal configurational force remains "indeterminate when and only when the associated structures are fixed in the material". This is similar to the constraint forces in classical mechanics (as the line tension of the pendulum) which do not need to be determined to establish the motion equation. In particular, no constitutive law for these forces is required in general.

However, we would like to emphasize that we have derived a constitutive law since (4-28) can be rewritten as

$$\text{Peach–Koehler force} = \mathrm{Div}\,\mathscr{E}^\star = -\rho_{\mathrm{dislo}}[B]v_j\delta_{L^\star}, \qquad (4\text{-}30)$$

where ρ_{dislo} is given in extenso by (4-23) and (4-25) in terms of the dislocation energy.

Second Euler–Lagrange equation and the dislocation equation. With the view of establishing an equation relating dislocation density and stress, the second Euler–Lagrange equation for our minimum problem should be derived; that is, the differential of the total energy should be computed with respect to divergence-free deformations G (recall that curl-free deformations were considered for the first Euler–Lagrange equation in Section 4.2). We would like to point out serious mathematical issues in order to give a meaning to a vanishing of such a variation, $0 = \delta\mathscr{W}(F^\star)[G]$. The principal reason (and the only which we discuss here) is that the differential $\frac{d}{d\epsilon}\mathscr{W}_{\mathrm{dislo}}(\Lambda^\star + \epsilon\Lambda)_{|\epsilon=0}$ has no meaning in $\mathcal{M}_\Lambda(\widehat{\Omega}, \mathbb{M}^3)$, this space not being linear, due to the fact that, as ϵ tends to zero, the resulting Burgers vector might not be an integer, whereas the minimum is achieved in this class of measures, with a crystallographic Burgers vector.

5. Concluding remarks

On the way to mathematically understanding time evolution of dislocations, the work achieved in [Scala and Van Goethem 2016] 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 26 introduces two forces balancing each other at optimality, the first deriving from the elastic part of the energy and named after Peach and Koehler (well-known in dislocation models [Hirth

and Lothe 1982]) 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 on the line. Such a force and such a balance of forces could be derived at the mesoscopic scale, without the required mathematical formalism, since there is subtle interplay between concentrated measures and Sobolev functions.

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 [Acharya 2003]). Of course, a nonvanishing velocity, i.e., a nonzero force, means that the solution does not coincide with energy minimization, as is well-known for evolution problems. In future work, our task is to determine the dissipative effects and the balance equations and to analyze in detail the evolutionary scheme.

The force we derived here yields an important output in terms of modeling, but to achieve a proof of Theorem 26, 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 considered at the mesoscale in appropriate 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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