KRÖNER'S FORMULA FOR DISLOCATION LOOPS REVISITED

NICOLAS VAN GOETHEM

1. Introduction

Several dislocation theories coexist in the literature and in general each emphasizes a particular aspect of the physics of dislocations and disclinations. For a physical approach let us refer to [1,2,5–7]. In engineering practice, empirical models are for instance used in the context of single crystal growing from the melt [9, 10]. These models are in general rather crude extensions of models available for polycrystals, whereas the physics of single crystals which we here consider is radically different for one main reason. Since the dislocations satisfy a conservation law and since there are no internal boundaries, dislocation may form curves which are comparable with the characteristic length of the crystal. So, separation of scales can hardly be done, and one is forced to analyze the properties of dislocations and/or disclination curves, even if a macroscopic thermomechanical model is adopted.

As soon as the mesoscale is considered[1] (thus also at the macroscale, cf. [15]), one crucial governing equation holding for both static and dynamic descriptions of dislocations, is what we called in a previous contributions [12, 14, 16] the "Kröner's formula". This formula relates the linear elastic strain incompatibility to dislocation and disclination densities. This means that as soon as these densities are known, the strain $\mathcal{E}^\star$ must satisfy a geometrical constraint, which can roughly be stated as follows: the Ricci (curvature) tensor asscociated to the elastic metric $g = I - 2\mathcal{E}^\star$ is directly related to the contortion curl, being the contortion $\kappa^\star$ another tensorial expression of the dislocation density. For a discussion on the non-Riemannian nature of the dislocated crystal, see [5] and the recent contributions [2,4,7,8,12]. Let us emphasize that in, e.g., [3,5] the "Kröner's formula", namely $\operatorname{inc}\mathcal{E}^\star = -\kappa^\star \times \nabla$, follows in a straightforward manner from an "elastic-plastic" displacement gradient (or distortion) decomposition postulate, which itself requires the selection of a particular reference configuration[2]. Therefore, it is not admissible in our approach which avoids any such arbitrary reference body prescription.

In [14] a new "Kröner's formula" was proven in the absence of disclinations and under precise field assumptions for a finite set of skew isolated (i.e., with no accumulation sets) rectilinear defects. It turned out that the formula we proved was not the formula classically reported [3, 5], since an additional term generated by the edge segments of a dislocation curve happens to be directly related to the scalar curvature of g, or, equivalently, to the trace of $\kappa^\star$.

In this communication, our aim is to respond to open questions which arose from [14]: (i) does the new formula hold for a dislocation loop? (ii) which new terms appear due to the line curvature? Therefore, the main part of the present work is devoted to verify by complete calculation of distributional type that a general Kröner's formula (i.e., an extension of that proven in [14], which we here state as Conjecture 1) holds true for two classical examples of dislocation loops.

Let us emphasize that Kröner's formulae are crucial since they relate the *mechanical* to the *defect internal variables* in any complete thermodynamic model of dislocations. Whereas it could seem artificial to consider sets of rectilinear dislocation lines, as in [14, 16, 17], this is no more the case for the dislocation loops, which are the most common type of dislocations observed in single crystal

[1]In our approach, mesoscopic fields are identified with a $\star$-superscript, which is removed as their macroscopic counterparts are considered [15].

[2]Elastic and plastic decomposition of the strain can classically be considered. However, no rigourous such decomposition holds for the distortion since in the absence of a well-defined *privileged* reference configuration, there is no constitutive law which would define the elastic and plastic parts of the rotation tensor.

growing from the melt. So, the topic of this paper has a potential scientific impact for engineer and technology-oriented applications [10].

2. Preliminary results at the mesoscale: the basis of the distributional approach

The basis of the distributional approach can be found with more detail in the two references [16,17], where the defect lines were assumed parallel to the z-axis, with a resulting elastic strain independent of z (in fact, those lines are the edge and screw dislocations and the wedge disclination). Hence they could be treated as a set of points in the plane. These two introductory works paved the way for the first application of the theory to $3D$ dislocations in an elastic medium [14], where the lines were not assumed parallel anymore and where in addition to the 3 above-mentioned families of defects, we included the twist disclination. The main results of these three papers are first recalled. Let us emphasize that in the present work, disclinations, which is a rarer kind of defects in single crystals growing from the melt, are not considered.

Notations 1. *For a second-order tensor E, we introduce the left (resp. right) curl operator $\nabla\times$ (resp. $\times\nabla$), i.e., $(\nabla\times E)_{ij}=\epsilon_{ikl}\partial_k E_{lj}$ and*[3] *$(E\times\nabla)_{ij}=\epsilon_{lkj}\partial_k E_{il}$ (otherwise written, $(E\times\nabla)^T=-\nabla\times E^T$), where E^T denotes the transpose of E.*

The incompatibility tensor associated to the symmetric second-order tensor E writes as

$$\text{inc } E := -\nabla\times E\times\nabla = \nabla\times(\nabla\times E)^T,$$

i.e., written componentwise, $(\text{inc } E)_{ij}=\epsilon_{ikm}\epsilon_{jln}\partial_k\partial_l E_{mn}$.

The assumed open and connected domain is denoted by $\Omega^\star$, the defect line(s) are indicated by $\mathcal{L}\subset\Omega^\star$, and $\Omega^\star_{\mathcal{L}}$ stands for $\Omega^\star\setminus\mathcal{L}$.

In the sequel, we say that a symmetric tensor E_{mn} is compatible on $U\subset\Omega^\star$ if $\epsilon_{kpm}\epsilon_{lqn}\partial_p\partial_q E_{mn}$ vanishes on U. Moreover, as soon as $E\in L^1_{loc}(\Omega^\star,\mathbb{R}^{3\times3})$, the incompatibility of E, inc E is a distribution [11], that is, a linear and continous form on the space of test functions $\mathcal{C}^\infty_c(\Omega^\star)$.

Assumption 1 ($3D$ elastic strain)**.** *Let $\mathcal{L}\subset\Omega$ be a dislocation loop with a Lipschitz continuous tangent vector*[4]*. The linear strain $\mathcal{E}^\star_{mn}$ is a given symmetric $L^s_{loc}(\Omega^\star)$-tensor compatible on $\Omega^\star_{\mathcal{L}}$, with $1\le s<2$. In other words, the incompatibility tensor, as defined by the distribution $\eta^\star_{kl}:=\epsilon_{kpm}\epsilon_{lqn}\partial_p\partial_q\mathcal{E}^\star_{mn}$, vanishes everywhere on $\Omega^\star_{\mathcal{L}}$.*

Definition 1 (Dislocation densities)**.**

DISLOCATION DENSITY: $$\alpha^\star := \tau\delta_{\mathcal{L}}\otimes B^\star \quad \left(\alpha^\star_{ij}:=\tau_i B^\star_j\delta_{\mathcal{L}}\right) \tag{2.1}$$

MESOSCOPIC CONTORTION: $$\kappa^\star := \alpha^\star - \frac{I}{2}\text{tr }\alpha^\star \quad \left(\kappa^\star_{ij}:=\alpha^\star_{ij}-\frac{1}{2}\delta_{ij}\alpha^\star_{kk}\right). \tag{2.2}$$

where $\delta_{\mathcal{L}}$ denotes the 1-dimensional Hausdorff measure concentrated on $\mathcal{L}$, and τ the unit tangent vector to $\mathcal{L}$.

The following classical theorem iare clasically proven from the relation $\partial_i\alpha^{\star\mathcal{L}}_{ij}=0$ (see, eg. [3]).

Theorem 1 (Conservation laws)**.** *Isolated defect lines are either closed or end at the boundary of $\Omega^\star$.*

It has been proven in [16] that at the mesoscale and for a set parallel rectilinear defects, strain incompatibility satisfies the following theorem.

Theorem 2 (Incompatibility of Volterra dislocations)**.** *For a set of isolated parallel dislocations $\mathcal{L}$, incompatibility is the following first-order symmetric tensor distribution,*

KRÖNER'S FORMULA: $$\tilde\eta = \text{inc }\mathcal{E}^\star = -\kappa^\star\times\nabla = \nabla\times(\kappa^\star)^T. \tag{2.3}$$

This result correspond to the Kröner's formula as reported in, e.g., [3, 5].

Moreover, it turns out that this formula is no longer true without a correction term if the lines are not parallel. It has been proven in [14] that at the mesoscale and for a set of skew rectilinear defects, strain incompatibility satisfies the following theorem.

[3] This notation is preferred to the other as found in [13, 14] with the opposite sign convention for the $\times\nabla$ operator.

[4] Therefore its curvature is bounded

Theorem 3 (Incompatibility of a set of skew defect lines)**.** *Under Assumptions 1, for a set Υ of isolated skew (rectilinear) defect lines L, incompatibility is the following first-order symmetric tensor distribution:*

$$\eta^\star_{mn} = \mathrm{inc}_{mn}\left(\mathcal{E}^\star\right) := \epsilon_{mkp}\epsilon_{nlq}\partial_k\partial_l\mathcal{E}^\star_{pq} = \sum_{L\in\Upsilon}\left[\tau^L_m\tau^L_k\hat{\eta}^{\star L}_{kn}\right]_{m\leftrightarrow n}, \tag{2.4}$$

where the Einstein tensor reads

$$\hat{\eta}^{\star L}_{kn} = \tilde{\eta}^{\star L}_{kn} - \frac{\delta_{kn}}{2}\tilde{\eta}^{\star L}_{pp}, \tag{2.5}$$

the Kröner's tensor is defined by

$$\tilde{\eta}^{\star L}_{kn} = \epsilon_{kij}\partial_i\kappa^{\star L}_{nj}, \tag{2.6}$$

with the defect contortion $\kappa^\star$ as given by Definition 1, and with symbol $A_{m\leftrightarrow n}$ meaning that sum of tensor A_{mn} and its transposed A_{nm} is taken. Moreover, τ^L indicates the tangent vector of L (here understood as multiplied by a unit cut-off function around L).

Remark 1 (Link with Kröner's formula)**.** *In 2D elasticity (i.e., when the strain is independent of z) and for a single dislocation L along the z-axis, Kröner's formula, $\eta^\star = -\kappa^\star \times \nabla$ (cf. [3, 5]) is easily recovered from the general formula (2.4) (cf. [14, 16]).*

3. The corrected Kröner's formulae for dislocation loops

Let ν be the inward normal to the loop $\mathcal{L}$ and introduce the normal vector $\sigma := \nu \times \tau$ in such a way that the right-handed orthonormal basis $\{\sigma, \nu, \tau\}$ is defined and satisfy the usual Frenet's formulae on $\mathcal{L}$: in particular we recall that $\partial_s\tau = \chi\nu$ with s the curvilinear abcissa of $\mathcal{L}$ and χ the curvature of $\mathcal{L}$.

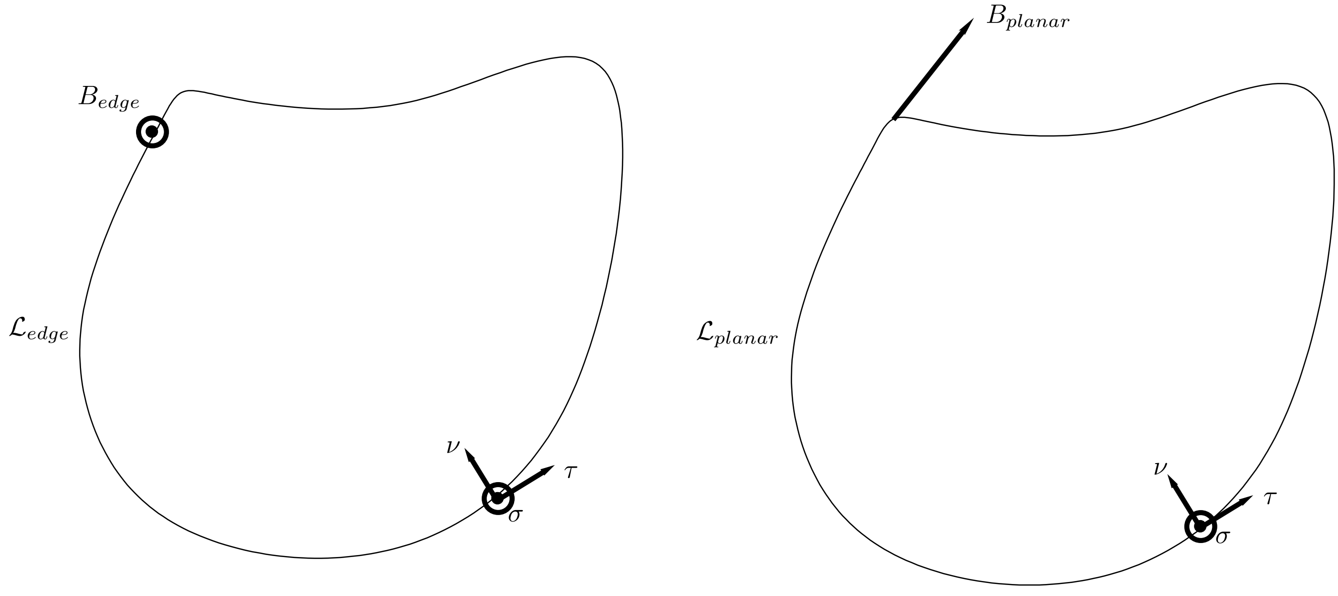

Figure 1. Left: pure edge dislocation loop. Right: the planar loop dislocation. The out-of-plane normal σ is pointing downwards.

The aim of this paper is to generalize Eq. (2.4) for a loop. However, it is beyond the scope of this communication to give a complete proof of this formula. Let us nevertheless gather some hints towards the general formula by scrutating the proof of Theorem 3 of [14]. First of all, let us remark that a loop is a limit of countable skew segments, whereby Theorem 3 appears as a first step.

As a first adaptation, if the dislocation is a curve it must be closed by Theorem 1 in such a way that all quantities which appear at the segment end-points mutually cancel. The second modification comes from identity $\tau_n\partial_i\alpha^\star_{kj} = \tau_k\partial_i\alpha^\star_{nj}$ (cf. Eq. (4.10) in [14]) which does not hold anymore if the line is curved, unless replaced by

$$\tau_n\partial_i\alpha^\star_{kj} = \tau_k\partial_i\alpha^\star_{nj} - \chi\tau_i\epsilon_{nkl}\sigma_l B^\star_j\delta_{\mathcal{L}}. \tag{3.1}$$

Briefly stated, the line curvature comes into play (at least for the – non conservative[5] edge dislocation loop) and the formula for a loop is inferred as follows.

Conjecture 1 (Incompatibility of planar loops)**.** *For a planar loop $\mathcal{L}$, incompatibility is the following first-order symmetric tensor distribution*

$$\eta^\star_{mn} = \mathrm{inc}_{mn}(\mathcal{E}^\star) = \left[\tau_m\tau_k\hat{\eta}^\star_{kn} + \tau_m\tau_n\frac{1}{2}\left(B^\star_k\sigma_k\right)\chi\delta_{\mathcal{L}}\right]_{m\leftrightarrow n} \tag{3.2}$$

where $\hat{\eta}^\star_{kn} = \tilde{\eta}^\star_{kn} - \frac{\delta_{kn}}{2}\tilde{\eta}^\star_{pp}$ and $\tilde{\eta}^\star_{kn} = \epsilon_{kij}\partial_i\kappa^\star_{nj}$ are defined by (2.5) *and* (2.6)*, and with τ the tangent vector of $\mathcal{L}$ (here understood, as χ, as multiplied by a unit cut-off function around $\mathcal{L}$).*

Formula (3.2) will be verified by complete hand calculation in Section 4 on two examples of dislocation loops, namely the conservative planar loop (i.e., with vanishing out-of-plane Burgers vector component), and the pure edge dislocation loop. In a first step, let us determine the differences between this formula and the classical Kröner's formula.

3.1. **Case A. The pure edge dislocation loop.** Let us consider a loop dislocation $\mathcal{L}$ lying on the $e_1 - e_2$ plane, with Burgers vector $B^\star_3$ with e_3 the normal vector to the plane.

Contortion of the pure edge dislocation loop: one has $\alpha^\star_{ij} = B^\star_j\tau_i\delta_{\mathcal{L}}$, $\alpha^\star_{kk} = 0$ and hence $\kappa^\star_{ij} = \alpha^\star_{ij}$.

Difference between Kröner's and corrected Kröner's formula: it follows that $\tilde{\eta}^\star_{ij} = B^\star_z\left(\epsilon_{ipz}\partial_p(\tau_j\delta_{\mathcal{L}})\right)$ and $\tilde{\eta}^\star_{iz} = 0$. Moreover since $\epsilon_{\alpha\gamma}\tau_\gamma = \nu_\alpha$ we compute

$$\tilde{\eta}^\star_{\alpha\beta} = B^\star_z\left(\epsilon_{\alpha\gamma}\tau_\beta\partial_\gamma\delta_{\mathcal{L}} + \nu_\alpha\nu_\beta\chi\delta_{\mathcal{L}}\right)$$

and $\tilde{\eta}^\star_{\kappa\kappa} = B^\star_z\left(-\nu_\kappa\partial_\kappa\delta_{\mathcal{L}} + \chi\delta_{\mathcal{L}}\right)$. It results that $\hat{\eta}^\star_{\alpha\beta} = \tilde{\eta}^\star_{\alpha\beta} - \frac{1}{2}\delta_{\alpha\beta}\tilde{\eta}^\star_{\kappa\kappa} = B^\star_z(\epsilon_{\alpha\gamma}\tau_\beta\partial_\gamma\delta_{\mathcal{L}} + \nu_\alpha\nu_\beta\chi\delta_{\mathcal{L}}) + \frac{1}{2}\delta_{\alpha\beta}B^\star_z\left(\nu_\kappa\partial_\kappa\delta_{\mathcal{L}} - \chi\delta_{\mathcal{L}}\right)$.

Then, the corrected Kröner's formula, as given by Eq. (3.2) of Conjecture 1 writes as

$$\eta^\star_{\alpha\beta} = \left[\tau_\alpha\tau_\kappa\hat{\eta}^\star_{\kappa\beta}\right]_{\alpha\leftrightarrow\beta} + \tau_\alpha\tau_\beta B^\star_z\chi\delta_{\mathcal{L}} = -\tau_\alpha\tau_\beta B^\star_z\nu_\kappa\partial_\kappa\delta_{\mathcal{L}}. \tag{3.3}$$

3.2. **Case B. The conservative planar loop: (a) $\alpha\beta$ and zz-components.** *Contortion of the conservative planar loop:* let us consider a loop dislocation $\mathcal{L}$ lying on the $e_1 - e_2$ plane with Burgers vector $B^\star_i = B^\star_\gamma$ (the antiplanar component $B^\star_z = 0$–here Greek indices take their values in $\{1, 2\}$). We have $\alpha^\star_{ij} = B^\star_\gamma\tau_i\delta_{\gamma j}\delta_{\mathcal{L}}$, $\alpha^\star_{kk} = B^\star_\gamma\tau_\gamma\delta_{\mathcal{L}}$ and hence

$$\kappa^\star_{ij} = \alpha^\star_{ij} - \frac{1}{2}\delta_{ij}\alpha^\star_{kk} = B^\star_\gamma\tau_i\delta_{\gamma j}\delta_{\mathcal{L}} - \frac{1}{2}\delta_{ij}B^\star_\gamma\tau_\gamma\delta_{\mathcal{L}}. \tag{3.4}$$

Difference between Kröner's and corrected Kröner's formula: from (3.4), the planar components of Kröner's formula read $\tilde{\eta}^\star_{\alpha\beta} = \epsilon_{\alpha pq}\partial_p\kappa^\star_{\beta q} = -\epsilon_{\alpha\gamma}\partial_z\kappa^\star_{\beta\gamma}$ (since $\kappa^\star_{\beta z} = 0$) and hence

$$\tilde{\eta}^\star_{\alpha\beta} = B^\star_\gamma\partial_z\delta_{\mathcal{L}}\left(-\epsilon_{\alpha\gamma}\tau_\beta + \frac{1}{2}\tau_\gamma\epsilon_{\alpha\beta}\right)$$

with its trace (recall that $\nu_\alpha = \epsilon_{\alpha\gamma}\tau_\gamma$) $\tilde{\eta}^\star_{\kappa\kappa} = \nu_\kappa B^\star_\kappa\partial_z\delta_{\mathcal{L}}$. It results that

$$\hat{\eta}^\star_{\alpha\beta} = \tilde{\eta}^\star_{\alpha\beta} - \frac{1}{2}\tilde{\eta}^\star_{\kappa\kappa}\delta_{\alpha\beta} = B^\star_\gamma\partial_z\delta_{\mathcal{L}}\left(-\epsilon_{\alpha\gamma}\tau_\beta + \frac{1}{2}\tau_\gamma\epsilon_{\alpha\beta} - \frac{1}{2}\delta_{\alpha\beta}\nu_\kappa B^\star_\kappa\right).$$

The corrected Kröner's formula, as given by Eq. (3.2) of Conjecture 1 thus reads

$$\eta^\star_{\alpha\beta} = \left(\tau_\alpha\tau_\beta(B^\star_\kappa\nu_\kappa) - (\tau_\alpha\nu_\beta + \tau_\beta\nu_\alpha)\frac{B^\star_\kappa\tau_\kappa}{2}\right)\partial_z\delta_{\mathcal{L}}. \tag{3.5}$$

Moreover $\eta^\star_{zz} = 0$ since $\tau_z = 0$ while $\tilde{\eta}^\star_{zz} = \epsilon_{\gamma\xi}\partial_\gamma\kappa^\star_{z\xi} = 0$ since $\kappa^\star_{z\xi} = 0$.

[5] Meaning that the out-of-plane Burgers vector component does not vanish.

3.3. **Case B. the conservative planar loop: (b) αz-components.** Since $\kappa^\star_{zz} = -\frac{1}{2}B^\star_\kappa \tau_\kappa \delta_\mathcal{L}$, we compute from (3.4) the antiplane components of Kröner's formula, viz., $\tilde{\eta}^\star_{\gamma z} = \epsilon_{\gamma\beta}\partial_\beta \left(-\frac{1}{2}B^\star_\kappa \tau_\kappa \delta_\mathcal{L}\right) = \epsilon_{\gamma\beta}\left(-\frac{1}{2}B^\star_\kappa \tau_\kappa \partial_\beta \delta_\mathcal{L} - \frac{1}{2}B^\star_\kappa \tau_\beta \chi \nu_\kappa \delta_\mathcal{L}\right)$ while $\tilde{\eta}^\star_{\kappa\kappa} = 0$. It results that $\hat{\eta}^\star_{\alpha z} = \tilde{\eta}^\star_{\alpha z}$. Incompatibility as given by Eq. (3.2) of Conjecture 1 reads (recall that $\tau_\gamma \epsilon_{\gamma\beta} = -\nu_\beta$)

$$\eta^\star_{\alpha z} = \tau_\alpha \frac{B^\star_\kappa \tau_\kappa}{2} \nu_\beta \partial_\beta \delta_\mathcal{L}. \tag{3.6}$$

4. Validation of the corrected Kröner's formulae

We must verify that

$$\eta^\star_{mn} = \mathrm{inc}_{mn}(\mathcal{E}^\star) := \epsilon_{mpi}\epsilon_{nqj}\partial_p\partial_q \mathcal{E}^\star_{ij} \tag{4.1}$$

is a concentrated distribution on $\mathcal{L}$ and coincides with Eqs. (3.3), (3.5), and (3.6).

In the spirit of our distributional approach, Eq. (3.5) can be verified by hand computations as soon as an expression $\mathcal{E}^\star$ of the strain associated to the conservative planar dislocation is known. Referring to Kleinert [3], the strain expression for any curve $\mathcal{L}$ reads

$$\begin{aligned}\mathcal{E}^\star_{ij}(x) &= \frac{B^\star_r}{8\pi}\epsilon_{uvr}[\epsilon_{j\kappa l}\epsilon_{vil}]_{i\leftrightarrow j} \oint_\mathcal{L} \tau_\kappa(\hat{x})\partial_u\left(1/|x-x'|\right) dL(x') \\ &+ \frac{B^\star_r}{8\pi(1-\nu)}\epsilon_{klr}\oint_\mathcal{L}\tau_\kappa(x')\partial_i\partial_j\partial_l\left(1/|x-x'|\right) dL(x')\end{aligned} \tag{4.2}$$

where ∂ refers to the derivation with respect to x. Of course, the strain as expressed by (4.2) is compatible outside $\mathcal{L}$. However, as a $L^1_{loc}(\Omega^\star)$-function, it is a concentrated distribution at $\mathcal{L}$ as the following distributional expression of incompatibility will show:

$$\begin{aligned}\langle \eta^\star_{mn}, \varphi\rangle &= \langle \mathcal{E}^\star_{ij}, \epsilon_{mpi}\epsilon_{nqj}\partial_p\partial_q\varphi\rangle = -\frac{B^\star_r}{8\pi}\epsilon_{uvr}\epsilon_{mpi}\epsilon_{nqj}[\epsilon_{j\kappa l}\epsilon_{vil}]_{i\leftrightarrow j}\langle \oint_\mathcal{L}\tau_\kappa(x')\left(1/|x-x'|\right) dL(x'), \partial_p\partial_u\partial_q\varphi\rangle \\ &+ \langle \frac{B^\star_r}{8\pi(1-\nu)}\epsilon_{mpi}\epsilon_{nqj}\epsilon_{klr}\oint_\mathcal{L}\tau_\kappa(x')\partial_l\left(1/|x-x'|\right) dL(x'), \partial_p\partial_q\partial_i\partial_j\varphi\rangle,\end{aligned} \tag{4.3}$$

where the last term identically vanishes by the smoothness of φ.

Let us denote $\|x-x'\|$ by R, $\tau_\kappa(x')dL(x')$ by dx'_κ, $-\nu_\kappa(x')dL(x')$ by dC'_κ, and recall that in $3D$,

$$\Delta\frac{1}{R} = \partial_i^2\frac{1}{R} = 4\pi\delta_{x'}(x) = \Delta'\frac{1}{R} = \partial_i'^2\frac{1}{R} = 4\pi\delta_x(x'), \tag{4.4}$$

where the $'$ symbol in Δ', or in general in ∂', refers to a derivation with respect to x' (and of course, ∂_i indicates the derivative with respect to x_i, with x_i the ith Cartesian coordinates). We recall that $\delta_{x'}(x)$ is the shifted Dirac delta satisfying $\langle\delta_{x'}, \varphi\rangle = \varphi(x')$ for every test function φ. Moreover, φ will always denote a $3D$ test function with compact support in $\Omega^\star$.

Local basis components are also used, by which we mean the following. Consider a smooth planar loop $\mathcal{L}$ in the $3D$ space and $x_\mathcal{L}$, a point of $\mathcal{L}$ with tangent vector $\tau(x_\mathcal{L})$ and its two orthonormal unit vector $\sigma(x_\mathcal{L})$ and $\nu(x_\mathcal{L})$ such that $\{\underline{\tau}, \underline{\sigma}, \underline{\nu}\}$ form a direct orthonormal *local* basis at $x_\mathcal{L}$ (i.e., with ν pointing inwards the loop). The planar components of $\underline{\tau}$ and $\underline{\nu}$ will in the sequel be denoted by τ_α and ν_β with $\epsilon_{\beta\alpha}\tau_\alpha = \nu_\beta$ and $\alpha, \beta \in \{1,2\}$ (or any other dumb Greek index except τ and ν which are kept to designate the tangent and normal vectors).

We adopt the notation $r := (x_i - x_{\mathcal{L}i})\nu_i(x_\mathcal{L})$ and $z := (x_i - x_{\mathcal{L}i})\sigma_i(x_\mathcal{L})$. Moreover, $\partial_r := \nu_\gamma\partial_\gamma$ and $\partial_s := \tau_\gamma\partial_\gamma$ with the arc parameter denoted by s such that $ds = \tau'_i dx'_i$ where $\tau'_i = \tau_i(x')$. So, in the local basis at $x_\mathcal{L}$, with $x_\mathcal{L}$ the projection of x on $\mathcal{L}$ (with $\tau(x_\mathcal{L})\cdot(x-x_\mathcal{L}) = 0$), $R^2(x, x_\mathcal{L}) = \|x-x_\mathcal{L}\|^2 = z^2+r^2$ is independent of s. In particular the following expression for the Laplacian holds in the polar base $\{\underline{\tau}, \underline{\sigma}, \underline{\nu}\}$ with polar coordinates $\{s, z, r\}$ and for a scalar function f :

$$\Delta f = \partial_r^2 f + \frac{1}{r}\partial_r f + \frac{1}{r^2}\partial_s f + \partial_z^2 f. \tag{4.5}$$

4.1. **Case A. Validation the pure edge dislocation loop.** For the planar pure edge dislocation loop, $r = 3(\text{“} = z\text{“})$, and hence

$$\langle \eta^\star_{mn}, \varphi\rangle = \frac{-B^\star_z}{8\pi}\epsilon_{\xi\eta}\epsilon_{mpi}\epsilon_{nqj}[\epsilon_{j\kappa l}\epsilon_{\eta il}]_{i\leftrightarrow j}\langle \oint_{\mathcal{L}} \frac{dx'_\kappa}{R}, \partial_p\partial_q\partial_\xi\varphi\rangle. \tag{4.6}$$

Observe from the identity (with the convention $\epsilon_{ab} := \epsilon_{zab}$)

$$\begin{aligned}\epsilon_{\xi\eta}\epsilon_{mpi}\epsilon_{nqj}[\epsilon_{j\kappa l}\epsilon_{\eta il}]_{i\leftrightarrow j} &= \delta_{\kappa q}(\delta_{pn}\epsilon_{\xi m} - \delta_{mn}\epsilon_{\xi p}) + \delta_{\kappa p}(\delta_{qm}\epsilon_{\xi n} - \delta_{mn}\epsilon_{\xi q})\\ &+\epsilon_{\xi p}\delta_{mq}\delta_{n\kappa} + \epsilon_{\xi q}\delta_{m\kappa}\delta_{np} + \delta_{pq}(\epsilon_{n\xi}\delta_{m\kappa} + \epsilon_{m\xi}\delta_{n\kappa})\end{aligned}$$

that the first two terms (i.e., with $\delta_{\kappa q}$ and $\delta_{\kappa p}$) provide a vanishing contribution because the curve is a loop, and that the second two (i.e., with $\epsilon_{\xi p}$ and $\epsilon_{\xi q}$) also provide a vanishing contribution by the smoothness of the test-function, in such a way that (4.6) simply rewrites as

$$\langle \eta^\star_{mn}, \varphi\rangle = \frac{-B^\star_z}{8\pi}(\epsilon_{n\xi}\delta_{m\kappa} + \epsilon_{m\xi}\delta_{n\kappa})\langle \oint_{\mathcal{L}} \Delta\frac{1}{R}dx'_\kappa, \partial_\xi\varphi\rangle.$$

On the one hand, observe that $\eta^\star_{zn}$ and η_{mz} identically vanish, and on the other that also the terms $\eta^\star_{mn}\nu_n$ and $\nu_m\eta^\star_{mn}$ do vanish since by (4.4),

$$\epsilon_{m\xi}\delta_{n\kappa}\langle \oint_{\mathcal{L}} \Delta\frac{1}{R}dx'_\kappa, \nu_n\partial_\xi\varphi\rangle = 4\pi\epsilon_{m\xi}\oint_{\mathcal{L}} \nu'_\kappa\partial'_\xi\varphi dx'_\kappa = 0$$

while, in the local basis (recall that $\partial_s = \tau_\xi\partial_\xi$),

$$\epsilon_{n\xi}\delta_{m\kappa}\langle \nu_n\oint_{\mathcal{L}} \Delta\frac{1}{R}dx'_\kappa, \partial_\xi\varphi\rangle = -\langle \tau_\xi\partial_\xi\oint_{\mathcal{L}} \frac{1}{R}dx'_m, \Delta\varphi\rangle = 0.$$

So, the only nonzero component is $\eta^\star_{mn}\tau_m\tau_n$ with (recall that $\tau_n\epsilon_{n\xi} = -\nu_\xi$ and $\tau'_k dx'_k = ds'$)

$$\langle \eta^\star_{mn}\tau_m\tau_n, \varphi\rangle = B^\star_z\oint_{\mathcal{L}} \partial'_\nu\varphi ds',$$

in such a way that

$$\eta^\star_{\alpha\beta} = -B^\star_z\tau_\alpha\tau_\beta\nu_\xi\partial_\xi\delta_{\mathcal{L}}, \tag{4.7}$$

where we recall that $\eta^\star_{mz} = 0$. Therefore, by (4.7), the announced Eq. (3.3) is recovered.

4.2. **Case B. Validation of the conservative planar loop: (a) $\alpha\beta$ and zz-components.** For the planar dislocation loop, consider (4.3) with $r = \xi$. Moreover we shall consider the planar components of incompatibility, i.e., take $m = \alpha$ and $n = \beta$. Let us decompose the computations in subterms:

$$\eta^\star_{\alpha\beta} = \overbrace{\eta^{\star\{1\}}_{\alpha\beta}}^{\texttt{take } u=z \texttt{ in (4.3)}} + \overbrace{\eta^{\star\{2\}}_{\alpha\beta}}^{\texttt{take } u=\gamma \texttt{ in (4.3)}} = \overbrace{\eta^{\star\{11\}}_{\alpha\beta} + \eta^{\star\{12\}}_{\alpha\beta}}^{\texttt{take } u=z \texttt{ in (4.3)}} + \overbrace{\eta^{\star\{21\}}_{\alpha\beta} + \eta^{\star\{22\}}_{mn}}^{\texttt{take } u=\gamma \texttt{ in (4.3)}}$$

and compute each term separately.
For $u = z$, (we have consequently set $v = \eta$),

$$\langle \eta^{\star\{1\}}_{mn}, \varphi\rangle = \frac{B^\star_\xi}{8\pi}\epsilon_{\xi\eta}\epsilon_{mpi}\epsilon_{nqj}[\epsilon_{j\kappa l}\epsilon_{\eta il}]_{i\leftrightarrow j}\langle \oint_{\mathcal{L}} \frac{dx'_\kappa}{R}, \partial_p\partial_q\partial_z\varphi\rangle.$$

From the identity

$$\begin{aligned}\epsilon_{\xi\eta}\epsilon_{mpi}\epsilon_{nqj}[\epsilon_{j\kappa l}\epsilon_{\eta il}]_{i\leftrightarrow j} &= \delta_{\kappa q}(\delta_{pn}\epsilon_{\xi m} - \delta_{mn}\epsilon_{\xi p}) + \delta_{\kappa p}(\delta_{qm}\epsilon_{\xi n} - \delta_{mn}\epsilon_{\xi q})\\ &+\epsilon_{\xi p}\delta_{mq}\delta_{n\kappa} + \epsilon_{\xi q}\delta_{m\kappa}\delta_{np} + \delta_{pq}(\epsilon_{n\xi}\delta_{m\kappa} + \epsilon_{m\xi}\delta_{n\kappa}),\end{aligned} \tag{4.8}$$

it can be observed that the first two terms provide a vanishing contribution because the curve is a loop. Observe first that $\eta^\star_{zz}$ identically vanishes by (4.8).

The last one provides the $\{11\}$-contribution, namely

$$\frac{B^\star_\xi}{8\pi}(\epsilon_{n\xi}\delta_{m\kappa} + \epsilon_{m\xi}\delta_{n\kappa})\langle \oint_{\mathcal{L}} \Delta\frac{1}{R}dx'_\kappa, \partial_z\varphi\rangle = \frac{B^\star_\xi}{2}(\epsilon_{n\xi}\delta_{m\kappa} + \epsilon_{m\xi}\delta_{n\kappa})\oint_{\mathcal{L}} \partial'_z\varphi(x')dx'_\kappa,$$

and hence, in the local basis, $\eta^{\star\{11\}}_{mz} = 0$ and from $\nu_\alpha = \epsilon_{\alpha\xi}\tau_\xi$,

$$\eta^{\star\{11\}}_{\alpha\beta} = \tau_\alpha\tau_\beta\left(B^\star_\xi\nu_\xi\right)\partial_z\delta_{\mathcal{L}} - (\tau_\alpha\nu_\beta + \tau_\beta\nu_\alpha)\frac{B^\star_\xi\tau_\xi}{2}\partial_z\delta_{\mathcal{L}}. \tag{4.9}$$

Moreover, the two central terms term of (4.8), collectively labelled by $\{12\}$, yield

$$\langle \eta^{\star\{12\}}_{mn}, \varphi\rangle = -\frac{B^\star_\xi}{8\pi}[\langle \oint_{\mathcal{L}} \epsilon_{\xi p}\partial'_p \frac{1}{R} dx'_n, \partial_m \partial_z \varphi\rangle]_{m\leftrightarrow n}. \tag{4.10}$$

Observe on the one hand that its trace

$$\langle \eta^{\star\{12\}}_{kk}, \varphi\rangle = -\frac{B^\star_\xi}{4\pi}\langle \oint_{\mathcal{L}} \partial'_k \frac{1}{R} dx'_k, \epsilon_{\xi p}\partial_p \partial_z \varphi\rangle$$

identically vanishes, since the curve is a loop, while the first diagonal entry,

$$\langle \eta^{\star\{12\}}_{mn}\tau_m\tau_n, \varphi\rangle = \frac{B^\star_\xi}{8\pi}[\langle \tau_n \partial_s \oint_{\mathcal{L}} \frac{1}{R} dx'_n, \epsilon_{\xi p}\partial_p \partial_z \varphi\rangle]_{m\leftrightarrow n},$$

vanishes (because ∂_s of the integral vanishes), whereby all diagonal terms vanish since $dx'_z = 0$.

Moreover the off-diagonal component of (4.10) writes in the local basis as (recall that $\partial_r = \nu_\gamma\partial_\gamma$)

$$\langle \eta^{\star\{12\}}_{mn}\nu_m\tau_n, \varphi\rangle = -\frac{B^\star_\xi}{8\pi}\epsilon_{\xi p}\langle \tau_n\partial_p \oint_{\mathcal{L}} \frac{1}{R} dx'_n, \partial_r \partial_z \varphi\rangle$$

showing only one non-vanishing contribution for $\partial_p = \nu_p\partial_r$. Hence, recalling (4.5) with $f = R$,

$$\begin{aligned}
\langle \eta^{\star\{12\}}_{mn}\nu_m\tau_n, \varphi\rangle &= \frac{B^\star_\xi}{8\pi}\langle \tau_\xi\tau_n \oint_{\mathcal{L}} \partial_r^2 \frac{1}{R} dx'_n, \partial_z \varphi\rangle \\
&= \frac{B^\star_\xi}{8\pi}\langle \tau_\xi\tau_n \oint_{\mathcal{L}} \left(\Delta\frac{1}{R} + \left(\frac{1}{R^3} - \partial_z^2\frac{1}{R}\right) - \frac{1}{R^2}\partial_s^2\frac{1}{R}\right) dx'_n, \partial_z \varphi\rangle \\
&= \frac{B^\star_\xi}{8\pi}\langle \tau_\xi\tau_n \oint_{\mathcal{L}} \Delta\frac{1}{R} dx'_n, \partial_z \varphi\rangle = \frac{B^\star_\xi}{8\pi}\langle \tau_\xi \oint_{\mathcal{L}} \Delta\frac{1}{R} dx'_n, \tau_n\partial_z \varphi\rangle
\end{aligned}$$

yielding by (4.4),

$$\eta^{\star\{12\}}_{\alpha\beta} = -\frac{B^\star_\xi\tau_\xi}{2}\left(\tau_\alpha\nu_\beta + \tau_\beta\nu_\alpha\right)\partial_z\delta_{\mathcal{L}}. \tag{4.11}$$

For $u = \gamma$, while $r = \xi$, $m = \alpha$ and $n = \beta$ (and where we have consequently set $v = z$), one obtains from the identity (where the last term vanishes since $\delta_{\kappa z} = 0$)

$$[\epsilon_{j\kappa l}\epsilon_{vil}]_{i\leftrightarrow j} = \delta_{jv}\delta_{\kappa i} + \delta_{iv}\delta_{\kappa j} - 2\delta_{ij}\delta_{\kappa v},$$

that

$$\langle \eta^{\star\{2\}}_{\alpha\beta}, \varphi\rangle = \frac{B^\star_\xi}{8\pi}\epsilon_{\gamma\xi}\epsilon_{\alpha\kappa}\epsilon_{\beta\zeta}\langle \oint_{\mathcal{L}} \partial_\zeta\frac{1}{R}dx'_\kappa + \partial_\kappa\frac{1}{R}dx'_\zeta, \partial_\gamma\partial_z\varphi\rangle,$$

and hence, by the identity $\epsilon_{\alpha\kappa}\epsilon_{\beta\zeta} = \delta_{\alpha\beta}\delta_{\kappa\zeta} - \delta_{\alpha\zeta}\delta_{\kappa\beta}$, the definition $dC'_\zeta = -\nu_\zeta dL(x')$ (i.e., $dx'_\beta = \epsilon_{\beta\kappa}dC'_\kappa$) with $\tau_\beta = -\epsilon_{\beta\kappa}\nu_\kappa$ and since $\mathcal{L}$ is a loop,

$$\langle \eta^{\star\{2\}}_{\alpha\beta}, \varphi\rangle = -\frac{B^\star_\xi}{8\pi}\langle \oint_{\mathcal{L}} \epsilon_{\gamma\xi}\left(\epsilon_{\kappa\beta}\partial'_\alpha\frac{1}{R} + \epsilon_{\kappa\alpha}\partial'_\beta\frac{1}{R}\right)dC'_\kappa, \partial_\gamma\partial_z\varphi\rangle.$$

Noticing that since $dC'_z = 0$, i must be equal to z, one rewrites

$$\langle \eta^{\star\{2\}}_{\alpha\beta}, \varphi\rangle = -\frac{B^\star_q}{8\pi}\langle \oint_{\mathcal{L}} \epsilon_{jpq}\left(\epsilon_{ikn}\partial'_m\frac{1}{R} + \epsilon_{ikm}\partial'_n\frac{1}{R}\right)dC'_k, \partial_p\partial_i\varphi\rangle\delta_{m\alpha}\delta_{n\beta}\delta_{jz} \tag{4.12}$$

which by the identity (since k must be equal to κ) $\epsilon_{jpq}\epsilon_{ikn} = \delta_{ji}(\delta_{pk}\delta_{qn} - \delta_{pn}\delta_{qk}) = \delta_{pk}\delta_{qn} - \delta_{pn}\delta_{qk}$ and by the Divergence theorem yields

$$\begin{aligned}
\langle \eta^{\star\{2\}}_{\alpha\beta}, \varphi\rangle &= -\frac{B^\star_q}{8\pi}\langle \oint_{\mathcal{L}} \partial'_k\partial'_p\frac{1}{R}dS', \left((\delta_{pk}\delta_{q\beta} - \delta_{p\beta}\delta_{qk})\partial_\alpha + (\delta_{pk}\delta_{q\alpha} - \delta_{p\alpha}\delta_{qk})\partial_\beta\right)\partial_z\varphi\rangle \\
&= \frac{-B^\star_q}{8\pi}\langle \int_{B_{\mathcal{L}}} \Delta'\frac{1}{R}dS', \left(\delta_{q\beta}\partial_\alpha + \epsilon_{q\alpha}\partial_\beta\right)\partial_z\varphi\rangle + \frac{B^\star_q}{4\pi}\langle \oint_{\mathcal{L}} \partial'_\alpha\partial'_\beta\frac{1}{R}dS', \partial_q\partial_z\varphi\rangle.
\end{aligned} \tag{4.13}$$

Let us introduce χ_A the characteristic function of the set A and ν_j the inwards normal of its boundary ∂A. Recall the relation

$$\int_A \delta_x(x')dS(x') = \chi_A \quad \text{with} \quad \partial_j\chi_A = -\nu_j\delta_{\partial A}. \tag{4.14}$$

Then, (4.13) rewrites as

$$\begin{aligned}\langle\eta^{\star\{2\}}_{\alpha\beta},\varphi\rangle &= \frac{B^\star_\xi}{2}\langle((\delta_{\xi\beta}\partial_\alpha+\delta_{\xi\alpha}\partial_\beta)\chi_{B_\mathcal{L}}(x),\partial_z\varphi\rangle+\frac{B^\star_\xi}{4\pi}\langle\int_{B_\mathcal{L}}\partial'_\alpha\partial'_\beta\frac{1}{R}dS',\partial_\xi\partial_z\varphi\rangle\\ &= -\frac{B^\star_\xi}{2}\langle((\delta_{\xi\beta}\nu_\alpha+\delta_{\xi\alpha}\nu_\beta)\delta_\mathcal{L},\partial_z\varphi\rangle+\frac{B^\star_\xi}{4\pi}\langle\int_{B_\mathcal{L}}\partial'_\alpha\partial'_\beta\frac{1}{R}dS',\partial_\xi\partial_z\varphi\rangle \qquad (4.15)\\ &= \frac{B^\star_\xi}{2}\langle((\delta_{\xi\beta}\nu_\alpha+\delta_{\xi\alpha}\nu_\beta)\partial_z\delta_\mathcal{L},\varphi\rangle-\frac{B^\star_\xi}{4\pi}\langle\partial_\alpha\oint_\mathcal{L}\frac{1}{R}dC'_\beta,\partial_\xi\partial_z\varphi\rangle, \qquad (4.16)\end{aligned}$$

whose first term as labeled by $\{21\}$ rewrites as

$$\eta^{\star\{21\}}_{\alpha\beta}=(\tau_\beta\nu_\alpha+\tau_\alpha\nu_\beta)\frac{B^\star_\xi\tau_\xi}{2}\partial_z\delta_\mathcal{L}+\nu_\alpha\nu_\beta\left(B^\star_\xi\nu_\xi\right)\partial_z\delta_\mathcal{L}. \qquad (4.17)$$

Concerning the second term of (4.15) (or (4.16)), labeled by $\{22\}$, it can be observed that it is symmetric with, as expressed in the local basis, vanishing entries along τ. Moreover, its trace reads

$$\langle\eta^{\star\{22\}}_{\alpha\alpha},\varphi\rangle=B^\star_\xi\langle\chi_{B_\mathcal{L}},\partial_\xi\partial_z\varphi\rangle=-B^\star_\xi\langle\nu_\xi\partial_z\delta_\mathcal{L},\varphi\rangle,$$

and equals the only non vanishing diagonal entry in the local basis, i.e., the $\nu_\alpha\nu_\beta$-entry, and hence

$$\eta^{\star\{22\}}_{\alpha\beta}=-\nu_\alpha\nu_\beta\left(B^\star_\xi\nu_\xi\right)\partial_z\delta_\mathcal{L}. \qquad (4.18)$$

Hence, summing (4.9), (4.11), (4.17) and (4.18) entails

$$\eta^\star_{\alpha\beta}=\tau_\alpha\tau_\beta\left(B^\star_\gamma\nu_\gamma\right)\partial_z\delta_\mathcal{L}-(\tau_\alpha\nu_\beta+\tau_\beta\nu_\alpha)\frac{B^\star_\gamma\tau_\gamma}{2}\partial_z\delta_\mathcal{L}, \qquad (4.19)$$

which is recognized as Eq. (3.5), achieving this second verification.

4.3. **Case B. Validation of the conservative planar loop: (b) αz-components.** For the planar dislocation loop, $r=\xi$, it results that for $m=3=z,n=\beta$, one has $p=\zeta,i=\alpha$ and hence

$$\langle\eta^\star_{z\beta},\varphi\rangle=\frac{-B^\star_\xi}{8\pi}\epsilon_{uv\xi}\epsilon_{\zeta\alpha}\epsilon_{\beta qj}[\delta_{jv}\delta_{\kappa\alpha}+\delta_{\alpha v}\delta_{\kappa j}-2\delta_{\alpha j}\delta_{\kappa v}]\langle\oint_\mathcal{L}\frac{dx'_\kappa}{R},\partial_\zeta\partial_q\partial_u\varphi\rangle. \qquad (4.20)$$

For $u=3=z$, $v=\eta$ and since $j\neq 3$ (otherwise all terms inside the bracket would vanish), q must be equal to 3 (i.e., $q=z$). Let us analyze separately each of the 3 terms of (4.20) arising from the 3 terms inside the bracket of (4.20):

$$\begin{array}{llcl}(i) & \dfrac{B^\star_\xi}{8\pi}\epsilon_{\zeta\alpha}(\epsilon_{\eta\xi}\epsilon_{\beta\eta})\langle\oint_\mathcal{L}\dfrac{dx'_\alpha}{R},\partial_\zeta\partial^2_z\varphi\rangle &=& \dfrac{B^\star_\beta}{8\pi}\langle\oint_\mathcal{L}\dfrac{dC'_p}{R},\partial_p\partial^2_z\varphi\rangle\\ & &=& \dfrac{B^\star_\beta}{2}\langle\int_{B_\mathcal{L}}\delta_x(x')dS',\partial^2_z\varphi\rangle\\ (ii) & \dfrac{B^\star_\xi}{8\pi}(\epsilon_{\eta\xi}\epsilon_{\zeta\eta})\epsilon_{\beta\kappa}\langle\oint_\mathcal{L}\dfrac{dx'_\kappa}{R},\partial_\zeta\partial^2_z\varphi\rangle &=& \dfrac{B^\star_\xi}{8\pi}\langle\oint_\mathcal{L}\dfrac{dC'_\beta}{R},\partial_\xi\partial^2_z\varphi\rangle\\ (iii) & \dfrac{-B^\star_\xi}{4\pi}\epsilon_{\eta\xi}(\epsilon_{\zeta\alpha}\epsilon_{\beta\alpha})\langle\oint_\mathcal{L}\dfrac{dx'_\eta}{R},\partial_\zeta\partial^2_z\varphi\rangle &=& \dfrac{-B^\star_\xi}{4\pi}\langle\oint_\mathcal{L}\dfrac{dC'_\xi}{R},\partial_\beta\partial^2_z\varphi\rangle,\end{array}$$

whereby the sum of these three terms (i.e., $(i)+(ii)+(iii)$) reads

$$\langle\eta^{\star\{1\}}_{z\beta},\varphi\rangle=\frac{B^\star_\beta}{2}\langle\chi_{B_\mathcal{L}},\partial^2_z\varphi\rangle-\frac{B^\star_\xi}{8\pi}\langle\int_{B_\mathcal{L}}\partial'_\xi\partial'_\beta\frac{1}{R}dS',\partial^2_z\varphi\rangle. \qquad (4.21)$$

Observe that the first term of the RHS of (4.21) vanishes by (4.14), and hence

$$\langle\eta^{\star\{1\}}_{z\beta},\varphi\rangle=-\frac{B^\star_\xi}{8\pi}\langle\int_{B_\mathcal{L}}\partial'_\xi\partial'_\beta\frac{1}{R}dS',\partial^2_z\varphi\rangle. \qquad (4.22)$$

Moreover, $\langle\int_{B_\mathcal{L}}\partial'_\xi\partial'_\beta\frac{1}{R}dS',\partial^2_z\varphi\rangle=\langle\int_{B_\mathcal{L}}\partial'_\beta\frac{1}{R}dS',\partial_\xi\partial^2_z\varphi\rangle=-\langle\partial_\xi\int_{B_\mathcal{L}}\partial'_\beta\frac{1}{R}dS',\partial^2_z\varphi\rangle$ is symmetric with, as expressed in the local basis, vanishing entries along τ_ξ (because ∂_s of the integral vanishes). Moreover, its trace vanishes by (4.14), $\langle 4\pi\chi_{B_\mathcal{L}},\partial^2_z\varphi\rangle=0$, implying that the whole term (4.22) vanishes.

For $u = \eta$, $v = 3 = z$, one is left with (we have chosen $q = \gamma$, since $j = 3$)

$$\langle \eta^{\star\{2\}}_{z\beta}, \varphi\rangle = \frac{B^\star_\xi}{8\pi}(\epsilon_{\eta\xi}\epsilon_{\zeta\kappa})\epsilon_{\beta\gamma}\langle \oint_{\mathcal{L}} \frac{1}{R} dx'_\kappa, \partial_\eta\partial_\zeta\partial_\gamma\varphi\rangle = \frac{B^\star_\xi}{8\pi}(\epsilon_{\eta\xi}\epsilon_{\zeta\kappa})\epsilon_{\beta\gamma}\langle \oint_{\mathcal{L}} \partial'_\eta \frac{1}{R} dx'_\kappa, \partial_\zeta\partial_\gamma\varphi\rangle$$

which from $\epsilon_{\eta\xi}\epsilon_{\zeta\kappa} = \delta_{\eta\zeta}\delta_{\xi\kappa} - \delta_{\eta\kappa}\delta_{\xi\zeta}$ (and $\tau'_\xi dx_\xi = ds'$) rewrites as

$$\langle \eta^{\star\{2\}}_{z\beta}, \varphi\rangle = -\frac{B^\star_\xi}{8\pi}\epsilon_{\beta\gamma}\langle \partial_\gamma \oint_{\mathcal{L}} \frac{1}{R} dx'_\xi, \Delta\varphi\rangle,$$

whose projection along ν,

$$\langle \eta^{\star\{2\}}_{z\beta}\nu_\beta, \varphi\rangle = \frac{-B^\star_\xi}{8\pi}\langle \tau_\gamma\partial_\gamma \oint_{\mathcal{L}} \frac{1}{R} dx'_\xi, \Delta\varphi\rangle,$$

vanishes. Moreover, its projection along ν reads (recall that $\epsilon_{\beta\gamma}\tau_\beta = -\nu_\gamma$)

$$\langle \eta^{\star\{2\}}_{z\beta}\tau_\beta, \varphi\rangle \quad = \quad \frac{B^\star_\xi}{8\pi}\langle \tau_\beta\epsilon_{\beta\gamma} \oint_{\mathcal{L}} \Delta\frac{1}{R} dx'_\xi, \partial_\gamma\varphi\rangle = \frac{B^\star_\xi}{2}\langle \oint_{\mathcal{L}} \delta_x(x') dx'_\xi, -\nu_\gamma\partial_\gamma\varphi\rangle$$

yielding

$$\eta^{\star\{2\}}_{z\beta} = \tau_\beta \frac{\tau_\xi B^\star_\xi}{2}\nu_\gamma\partial_\gamma\delta_{\mathcal{L}}. \tag{4.23}$$

By summing (4.22) and (4.23) and since $\eta^\star_{\alpha z} = \eta^\star_{z\alpha}$, we recover the announced Eq. (3.6).

5. Concluding remarks

In the first part of this communication, that is Section 3, a general Kröner's formula, stated as Conjecture 1 and holding for a dislocation loop, has been inferred, directly from a previously established result as found in [14]. This formula basically relates the elastic strain incompatibility inc $\mathcal{E}^\star$ to a projection on the dislocation line $\mathcal{L}$ of the semi-deviatoric part of the (right-) curl of the contortion tensor, viz. $\kappa^\star \times \nabla$, where we recall that $\kappa^\star$ is related to the dislocation density $\alpha^\star$ by the (semi-deviatoric) relation $\kappa^\star = \alpha^\star - \frac{I}{2}\,\mathrm{tr}\ \alpha^\star$. Moreover, in this new formula, a curvature-dependent term appears which however vanishes if the dislocation has no climb component, i.e., is *conservative*.

In a second part, that is Section 4, the explicit differences between this new formula and the classically reported Kröner's formula has been exhibited for two types of dislocation loops, namely the pure edge dislocation loop (with an out-of-plane Burgers vector, thereby sometimes referred to as non conservative), and the planar loop with planar Burgers vector. In particular, it happens that the new terms appearing in Conjecture 1 are mandatory as soon as the dislocation exhibits a planar Burgers vector.

Finally, the last part of this communication consisted in a direct validation of the new formula as based on the theory of distributions. This rather technical part is the core of the present contribution.

We believe that this new formula can have an impact for crystal growth practice, since in the presence of dislocations, scale separation can hardly be done in any realistic thermodynamic model accounting for dislocation creation and/or movement (cf., e.g., [18]) outside equilibrium. Therefore, even at the macroscale, dislocation loops may appear while intracting with any other defect types. In fact, the established formula explicitely relates the elastic strain (also taking into account its evolution in time) to the dislocation density dynamics.

A crucial step to reach crystal growth models is to homogenize, to define the macroscale, the results obtained here at the mesoscale. This will be considered in a forthcoming work in the spirit of [13,15].

Acknowledgements. The author has been supported by Fundação para a Ciência e a Tecnologia (Ciência 2007, PEst OE/MAT/UI0209/2011 & FCT Project: PTDC/EME-PME/108751/2008).

References

[1] C. Dascalu and G. A. Maugin. The energy of elastic defects: A distributional approach. *Proc. R. Soc. Lond. A*, 445:23–37, 1994.
[2] F. W. Hehl and Y.N. Obukhov. Élie cartan's torsion in geometry and in field theory, an essay. *Annales de la Fondation Louis de Broglie*, 32(2-3):157–194, 2007.
[3] H. Kleinert. *Gauge fields in condensed matter, Vol.1.* World Scientific Publishing, Singapore, 1989.
[4] H. Kleinert. New gauge symmetry in gravity and the evanescent role of torsion. *Electronic Journal of Theoretical Physics*, 7(24):28–298, 2010.

[5] E. Kröner. Continuum theory of defects. In R. Balian, editor, *Physiques des défauts, Les Houches session XXXV (Course 3).* North-Holland, Amsterdam, 1980.
[6] M. Lazar. On the screw dislocation in a functionally graded material. *Mechanics Research Communications*, 34:305–311, 2007.
[7] M. Lazar and F. W. Hehl. Cartan's spiral staircase in physics and, in particular, in the gauge theory of dislocations. *Foundations of Physics*, 40:1298–1325, 2010.
[8] G. Maugin. Geometry and thermomechanics of structural rearrangements: Ekkehart Kröner's legacy. *ZAMM*, 83(2):75–84, 2003.
[9] G. Müller and J. Friedrich. Challenges in modeling of bulk crystal growth. *J. Cryst. Growth*, 266(1-3):1–19, 2004.
[10] G. Müller, J. J. Métois, and P. Rudolph, editors. *Crystal Growth-From fundamentals to technology.* Elsevier, 2004.
[11] L. Schwartz. *Théorie des distributions*. Hermann, Paris, 1957.
[12] N. Van Goethem. The non-Riemannian dislocated crystal: a tribute to Ekkehart Kröner's (1919-2000). *J. Geom. Mech.*, 2(3), 2010.
[13] N. Van Goethem. Shape optimization for a time-dependent 4th-order equation in a dislocation model. *C. R. Acad. Sci. Paris, Ser. I 340*, 349:923–927, 2011.
[14] N. Van Goethem. Strain incompatibility in single crystals: Kröner's formula revisited. *J. Elast.*, 103(1):95–111, 2011.
[15] N. Van Goethem. A multiscale model for dislocations: from mesoscopic elasticity to macroscopic plasticity. *ZAMM*, 92(7):514 – 535, 2012.
[16] N. Van Goethem and F. Dupret. A distributional approach to $2D$ volterra dislocations at the continuum scale. *Europ. Jnl. Appl. Math.*, 23(3):417–439, 2012.
[17] N. Van Goethem and F. Dupret. A distributional approach to the geometry of $2D$ dislocations at the continuum scale. *Ann. Univ. Ferrara*, 58(2), 2012.
[18] H.M. Zbib, M. Hiratani, and M. Shehadeh. Multiscale discrete dislocation dynamics plasticity. In D. Raabe, editor, *Continuum Scale Simulation of Engineering Materials*. Wiley, 2005.

Nicolas Van Goethem. Email: vangoeth@ptmat.fc.ul.pt. Address: Universidade de Lisboa, Faculdade de Ciências, Departamento de Matemática, CMAF, Av. Prof. Gama Pinto 2, 1649-003 Lisboa, Portugal.