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On Nye's lattice curvature tensor

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ABSTRACT

We revisit Nye's lattice curvature tensor in the light of Cartan's moving frames. Nye's definition of lattice curvature is based on the assumption that the dislocated body is stress-free, and therefore, it makes sense only for zero-stress (impotent) dislocation distributions. Motivated by the works of Bilby and others, Nye's construction is extended to arbitrary dislocation distributions. We provide a material definition of the lattice curvature in the form of a triplet of vectors, that are obtained from the material covariant derivative of the lattice frame along its integral curves. While the dislocation density tensor is related to the torsion tensor associated with the Weitzenböck connection, the lattice curvature is related to the contorsion tensor. We also show that under Nye's assumption, the material lattice curvature is the pull-back of Nye's curvature tensor via the relaxation map. Moreover, the lattice curvature tensor can be used to express the Riemann curvature of the material manifold in the linearized approximation.

1. Introduction

The definitions of the dislocation density tensor and the lattice curvature tensor are both due to Nye [1]. Nye's seminal work was motivated by the observation that "when a single crystal deforms by glide which is unevenly distributed over the glide surfaces the lattice becomes curved". The dislocation density tensor $\boldsymbol{\alpha}$ is then defined as the operator that assigns to a unit vector $\boldsymbol{l}$ the Burgers vector $\boldsymbol{B}$ associated with a circuit of unit area that is normal to $\boldsymbol{l}$, i.e., $B_i = \alpha_{ij} l_j$, and it results from the distribution of dislocations in the lattice. Nye also showed that this tensor carries information on the change of the orientation of the lattice directions along the coordinate $\mathrm{d}x_j$ described by the infinitesimal axial vector $\mathrm{d}\phi_i$ via the relation $\mathrm{d}\phi_i = \kappa_{ij}\mathrm{d}x_j$, where $\boldsymbol{\kappa}$ is a tensor that is related to the dislocation density tensor as $\kappa_{ij} = \alpha_{ji} - \frac{1}{2}\alpha_{kk}\delta_{ij}$. Nye called $\boldsymbol{\kappa}$ the curvature tensor, but since in the geometric setting the expression "curvature tensor" usually implies the Riemannian curvature associated with the material metric, we will be referring to $\boldsymbol{\kappa}$ as the lattice curvature tensor as in Kröner [2] (where the lattice curvature tensor is defined with the opposite sign).

To prove the relation between $\boldsymbol{\alpha}$ and $\boldsymbol{\kappa}$, Nye looked at the deformed configuration of lattice directions and planes and through the use of graphic techniques he was able to calculate their curvature. His study was carried out under the assumption of negligible elastic deformations: "when real crystals are distorted plastically they do in fact contain large-scale distributions of residual strains, which contribute to the lattice curvature". In the absence of external loads, elastic deformations develop to restore compatibility of the total strain in the crystal, inducing residual stresses. This difficulty can be avoided by considering impotent plastic deformations, i.e., plastic deformations that, albeit incompatible in the sense that they are not associated with any configuration map, still allow the crystal to relax locally into a stress-free configuration. In the language of modern dislocation theory, the absence of residual elastic strains is equivalent to the assumption of plastic deformations inducing a Euclidean material metric. This state is the same as Noll's contorted aeolotropy [3], sometimes referred to as zero-stress or impotent dislocation distributions [4–6]. This ensures the existence of a local isometric embedding of the material manifold into the ambient space, so that the plastic deformation of the material can be relaxed into a stress-free configuration. The lattice curvature tensor has been studied by other researchers from a more geometric perspective. Bilby et al. [7] and Bilby and Smith [8] reviewed Nye's construction, and provided a material version of the notion of lattice curvature, showing that it is related to the Ricci rotation coefficients. Steinmann [9] established a relation between the contorsion tensor and Nye's lattice curvature.

In this paper we revisit Nye's lattice curvature tensor in the light of modern differential geometry, and particularly, Cartan's moving frames [10,11], and teleparallelism. The material nature of Nye's tensor will be shown without assuming the absence of residual stresses. We do this by using a notion of lattice curvature due

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to Bilby and Smith [8], which is purely material and relies on the Riemannian structure inherited by the metric defined on the material manifold, without the need of a Euclidean material metric. More specifically, the lattice curvature is defined starting from the material covariant derivative of the lattice moving frame along the frame itself, a quantity that is independent of any mapping of the material manifold into the ambient space. In our approach, using Cartan's moving frames, the lattice curvature is represented by a triplet of vectors. We show that starting from this more general definition of curvature, the material variant of Nye's tensor is the object that encodes it. As a matter of fact, while the material dislocation density tensor is related to the torsion tensor associated with the Weitzenböck connection, the material lattice curvature tensor can be obtained from the contorsion tensor in a similar way. Carrying information on both the Weitzenböck and the Levi–Civita connections, the lattice curvature tensor can be used to express the Riemann curvature of the material manifold in the linearized approximation.

This paper is organized as follows. In Section 2 we introduce the notion of lattice frame in a dislocated solid and define all the geometric quantities associated with it. In Section 3 we review the dislocation density tensor. In Section 4 we introduce a material definition of lattice curvature, show its relation with the contorsion tensor and, in the linear approximation, with the Einstein tensor.

2. The dislocated lattice

We work in the framework of continuum mechanics and consider smooth embeddings $\varphi:\mathcal{B}\to\mathcal{S}$ representing spatial configurations of a material body $\mathcal{B}$ in the ambient space $\mathcal{S}$. The ambient space is endowed with a Euclidean metric $\boldsymbol{g}$, expressing the standard scalar product in the ambient space. Crystalline solids carry additional information on the order with which particles are arranged. In a geometric continuum theory this information is encoded in a moving frame $\{\boldsymbol{e}_\beta\}$ on $\mathcal{B}$ [6], that we call lattice frame. Alternatively, one can use the associated lattice coframe $\{\boldsymbol{\vartheta}^\beta\}$, i.e., a field of three 1-forms such that $\langle\boldsymbol{\vartheta}^\beta,\boldsymbol{e}_\gamma\rangle=\delta^\beta_\gamma$. The material metric $\boldsymbol{G}$ representing the natural distances in the lattice is then defined as

$$\boldsymbol{G}=\delta_{\alpha\beta}\,\boldsymbol{\vartheta}^\alpha\otimes\boldsymbol{\vartheta}^\beta\,. \tag{2.1}$$

This means that the lattice frame $\{\boldsymbol{e}_\alpha\}$ is orthonormal with respect to $\boldsymbol{G}$, i.e., $\langle\!\langle\boldsymbol{e}_\alpha,\boldsymbol{e}_\beta\rangle\!\rangle_{\boldsymbol{G}}=\delta_{\alpha\beta}$. In other words, the lattice frame represents an internal observer that is unaware of the plastic slip occurring in the solid [12,13].

The presence of dislocations in solids is associated with the anholonomicity of the lattice frame. A frame $\{\boldsymbol{e}_\beta\}$ is holonomic if there exist local coordinates $\{Y^\beta\}$ such that $\boldsymbol{e}_\beta=\frac{\partial}{\partial Y^\beta}$. This is equivalent to the vanishing of the Lie bracket $[\boldsymbol{e}_\alpha,\boldsymbol{e}_\beta]$ for all α,β [14–17]. Holonomicity of the lattice frame can also be expressed in terms of its coframe as $\boldsymbol{\vartheta}^\beta=\mathrm{d}Y^\beta$, which is equivalent to requiring the lattice forms to be closed.[1] As a matter of fact one has

$$\mathrm{d}\boldsymbol{\vartheta}^\gamma(\boldsymbol{e}_\alpha,\boldsymbol{e}_\beta)=-\langle\boldsymbol{\vartheta}^\gamma,[\boldsymbol{e}_\alpha,\boldsymbol{e}_\beta]\rangle\,. \tag{2.2}$$

The presence of distributed dislocations can be detected by calculating the circulation of the lattice coframe along a closed curve γ, viz.

$$B^\beta[\gamma]=\int_{\varphi(\gamma)}\varphi_*\boldsymbol{\vartheta}^\beta=\int_\gamma\boldsymbol{\vartheta}^\beta\,. \tag{2.3}$$

[1] A k-form α on $\mathcal{B}$ is closed if $\mathrm{d}\alpha=\mathbf{0}$, and is exact if there exists a $k-1$-form $\boldsymbol{\chi}$ such that $\alpha=\mathrm{d}\boldsymbol{\chi}$. An exact k-form is necessarily closed, while the converse holds only when the k-th de Rham cohomology group is trivial [18]. Since closedness can be seen as the local version of exactness, holonomicity becomes quite clear: the existence of local coordinates $\{Y^\beta\}$ such that $\boldsymbol{\vartheta}^\beta=\mathrm{d}Y^\beta$ is guaranteed whenever the lattice forms are closed.

The scalars $B^\beta[\gamma]$ represent the Burgers vector associated with γ. If γ is the only component of the boundary of a surface Σ, i.e., $\gamma=\partial\Sigma$, invoking Stokes' theorem one can write (2.3) as

$$B^\beta[\gamma]=\int_\Sigma i^*\mathrm{d}\boldsymbol{\vartheta}^\beta\,, \tag{2.4}$$

where $i:\Sigma\hookrightarrow\mathcal{B}$ is the inclusion map.

Remark 2.1. The dislocation-free case implies the existence of local coordinates $\{Y^\beta\}$ such that $\boldsymbol{\vartheta}^\beta=\mathrm{d}Y^\beta$, and hence, from (2.1) one obtains $\boldsymbol{G}=\delta_{\alpha\beta}\,\mathrm{d}Y^\alpha\otimes\mathrm{d}Y^\beta$. This means that there exists a map $\varphi:\mathcal{B}\to\mathcal{S}$ whose Cartesian coordinate representation is $\{Y^\beta\}$ and such that $\boldsymbol{G}=\varphi^*\boldsymbol{g}$ locally, i.e., a local isometric embedding. Such a map can be seen as a local relaxation for the body.

We define a Weitzenböck connection $\hat{\nabla}$ on $\mathcal{B}$ that parallelizes the lattice frame $\{\boldsymbol{e}_\alpha\}$. As a derivative operator, it acts on a tensor as the ordinary derivative of the components of the tensor with respect to the lattice frame, whence the vanishing of the Weitzenböck derivative of the material metric $\boldsymbol{G}$. Its torsion can be calculated by using Cartan's formalism [6,14] and expressing the first structural equation in terms of the lattice frame, viz.

$$\mathcal{T}^\beta=\mathrm{d}\boldsymbol{\vartheta}^\beta+\boldsymbol{\omega}^\beta{}_\gamma\wedge\boldsymbol{\vartheta}^\gamma\,, \tag{2.5}$$

where $\boldsymbol{\omega}^\beta{}_\gamma$ are the connection 1-forms and $\mathcal{T}^\beta$ are the torsion 2-forms. As the Weitzenböck connection parallelizes $\boldsymbol{\vartheta}^\beta$, one sets $\boldsymbol{\omega}^\beta{}_\gamma=0$ to obtain $\mathcal{T}^\beta=\mathrm{d}\boldsymbol{\vartheta}^\beta$, and hence $\boldsymbol{T}$ has the expression $\boldsymbol{T}=\boldsymbol{e}_\beta\otimes\mathrm{d}\boldsymbol{\vartheta}^\beta$. The first Bianchi identity is obtained by differentiating the first structural equation and reads $\mathrm{d}\mathcal{T}^\beta=0$, as $\mathrm{d}\mathrm{d}\boldsymbol{\vartheta}^\beta=0$. By construction, $\hat{\nabla}$ has zero curvature [19].

We denote with ∇ the Levi–Civita connection associated with $\boldsymbol{G}$, having zero torsion by construction and non-vanishing curvature $\boldsymbol{R}$. The contorsion tensor $\boldsymbol{K}$ is defined as the difference between the Weitzenböck and the Levi–Civita connections, i.e.,

$$\boldsymbol{K}(\boldsymbol{X},\boldsymbol{Y})=\hat{\nabla}_{\boldsymbol{X}}\boldsymbol{Y}-\nabla_{\boldsymbol{X}}\boldsymbol{Y}\,, \tag{2.6}$$

for all vectors $\boldsymbol{X},\boldsymbol{Y}$. In components with respect to a coordinate chart $\{X^A\}$ on $\mathcal{B}$, one has

$$K^A{}_{BC}=\frac{1}{2}\left(T^A{}_{BC}+T_B{}^A{}_C+T_C{}^A{}_B\right), \tag{2.7}$$

where indices are lowered and raised using $\boldsymbol{G}$.

Remark 2.2. It is straightforward to prove that when torsion $\boldsymbol{T}$ of the Weitzenböck connection vanishes (dislocation-free case of Remark 2.1), the Levi–Civita connection has zero curvature (absence of residual stresses). The converse does not hold: there exist distributions of dislocations (i.e., $\boldsymbol{T}\neq\mathbf{0}$) associated with a lattice frame inducing a Euclidean material metric $\boldsymbol{G}$, i.e., such that $\boldsymbol{R}=\mathbf{0}$. In this case, the existence of a local isometric embedding is still guaranteed by the Test Case theorem [14], and therefore the body is allowed to locally relax. In other words, the plastic slips are $\{\boldsymbol{\vartheta}^\beta\}$-incompatible but $\mathbf{G}$-compatible. These are called zero-stress or impotent dislocations by Mura [5], or contorted aeolotropy by Noll [3]. As was mentioned earlier, the study by Nye [1] is carried out under this assumption. It should also be noted that in this case the lattice frame can be obtained through a rotation field superimposed to a defect-free lattice frame. Hence, the stress-free state that Nye works with cannot be achieved by pure plastic rotations, as was claimed in [20]. This can be shown by considering the example of plastic bending of a slab presented by Nye, which is a process that requires a change in length of the material fibers, and not just a change in their orientation. However, by reparametrizing the material manifold via the relaxation map φ, i.e., working with $\varphi(\mathcal{B})$ as reference configuration, one would be able to express the lattice structure through a field of rotations of the Cartesian frame.

3. The dislocation density tensor

The volume form $\boldsymbol{\mu}$ associated with $\boldsymbol{G}$ is called the material volume form and has components $\mu_{ABC} = G^{\frac{1}{2}}\,\epsilon_{ABC}$, where $G = \det \boldsymbol{G}$ and ϵ is the permutation symbol. This object can be used to relate vectors and 2-forms through the raised Hodge operator $\star^\sharp$. Given a 2-form $\boldsymbol{\beta}$, the vector $\star^\sharp\boldsymbol{\beta}$ is defined as $\boldsymbol{\beta} = \iota_{\star^\sharp\boldsymbol{\beta}}\boldsymbol{\mu}$ (ι is the interior product operator), which in components reads $\beta_{AB} = \mu_{ABC}(\star^\sharp\beta)^C$. The inverse relation is written as $(\star^\sharp\beta)^A = \frac{1}{2}\mu^{ABC}\beta_{BC}$, with $\mu^{ABC} = G^{-\frac{1}{2}}\,\epsilon^{ABC}$.[2] A volume form allows one to define the divergence of a vector field $\boldsymbol{V}$ as $(\mathrm{Div}\,\boldsymbol{V})\,\boldsymbol{\mu} = \mathfrak{L}_{\boldsymbol{V}}\boldsymbol{\mu} = \mathrm{d}\iota_{\boldsymbol{V}}\boldsymbol{\mu}$.[3] When $\boldsymbol{\mu}$ is induced by a metric $\boldsymbol{G}$ one also has $\mathrm{Div}\,\boldsymbol{V} = \mathrm{tr}\,\nabla\boldsymbol{V}$, where ∇ is the Levi–Civita connection associated with $\boldsymbol{G}$. Exterior derivative, raised Hodge operator and divergence operator are related as

$$\mathrm{d}\boldsymbol{\beta} = \mathrm{Div}(\star^\sharp\boldsymbol{\beta})\,\boldsymbol{\mu}\,, \tag{3.1}$$

for any 2-form $\boldsymbol{\beta}$.

Geometric definitions of the dislocation density tensor using the notion of holonomicity and torsion are due to Kondo [21], Bilby et al. [7], and Kröner [22]. We define the dislocation density as the triplet of vectors $\{\boldsymbol{\alpha}^\beta\}$ given by

$$\boldsymbol{\alpha}^\beta = \star^\sharp\mathrm{d}\boldsymbol{\vartheta}^\beta\,, \tag{3.2}$$

or $\boldsymbol{\alpha}^\beta = \star^\sharp\boldsymbol{\mathcal{T}}^\beta$ in Cartan's formalism, where $\star^\sharp$ is the raised Hodge operator associated to $\boldsymbol{G}$. Note that since $\mathrm{d}\boldsymbol{\mathcal{T}}^\beta = \mathrm{d}\mathrm{d}\boldsymbol{\vartheta}^\beta = 0$, from (3.1) one necessarily has $\mathrm{Div}\,\boldsymbol{\alpha}^\beta = 0$. Thus, $\mathrm{Div}\,\boldsymbol{\alpha}^\beta = 0$ can also be seen as a consequence of the first Bianchi identity for the Weitzenböck connection. The tensorial variant of the dislocation density is defined as the tensor $\boldsymbol{\alpha} = \boldsymbol{e}_\beta \otimes \boldsymbol{\alpha}^\beta$ of type (2,0), or equivalently, as $\boldsymbol{\alpha} = \star^\sharp\boldsymbol{T}$, where the raised Hodge operator acts on the lower indices. Note that denoting the extension of the divergence operator to double contravariant tensors with Div (acting on the second index), one has

$$\mathrm{Div}\,\boldsymbol{\alpha} = (\mathrm{Div}\,\boldsymbol{\alpha}^\beta)\,\boldsymbol{e}_\beta + \nabla_{\boldsymbol{\alpha}^\beta}\boldsymbol{e}_\beta = \nabla_{\boldsymbol{\alpha}^\beta}\boldsymbol{e}_\beta\,, \tag{3.3}$$

which in general does not vanish.[4] This can also be written as $\nabla_B\alpha^{AB} = -K^A{}_{BC}\alpha^{CB}$. It should be noted that by linearizing around a defect-free lattice coframe (see Section 4), where both $\boldsymbol{\alpha}^\beta$ and $\nabla\boldsymbol{e}_\beta$ vanish, one obtains

$$\mathrm{Div}\,\delta\boldsymbol{\alpha} = \mathrm{Div}(\delta\boldsymbol{\alpha}^\beta)\,\boldsymbol{e}_\beta = \delta(\mathrm{Div}\,\boldsymbol{\alpha}^\beta)\,\boldsymbol{e}_\beta\,, \tag{3.4}$$

and hence, one recovers the classic identity $\mathrm{Div}\,\delta\boldsymbol{\alpha} = \boldsymbol{0}$.

The dislocation density tensor can be used to express the Burgers vector associated with a closed curve $\gamma = \partial\Sigma$. Denoting with $\boldsymbol{N}$ the unit normal on Σ, and with $\boldsymbol{\nu}$ the area 2-form induced by $\boldsymbol{G}$ on Σ, both induced by $\boldsymbol{G}$, one can rewrite (2.3) as

$$B^\beta[\gamma] = \int_\Sigma \langle\!\langle \boldsymbol{\alpha}^\beta, \boldsymbol{N}\rangle\!\rangle_{\boldsymbol{G}}\;\boldsymbol{\nu}\,, \tag{3.5}$$

meaning that each $B^\beta[\gamma]$ is given by the flux of the corresponding vector $\boldsymbol{\alpha}^\beta$ across Σ.

[2] In general, the Hodge operator assigns to a k-form $\boldsymbol{\beta}$ the $(n-k)$-form $\star\boldsymbol{\beta}$ such that for any $\boldsymbol{G}$-orthonormal frame $\{\boldsymbol{X}_\alpha\}$ one has $(\star\boldsymbol{\beta})(\boldsymbol{X}_{I_1},\ldots,\boldsymbol{X}_{I_k}) = \boldsymbol{\beta}(\boldsymbol{X}_{I_{k+1}},\ldots,\boldsymbol{X}_{I_n})$. The raised Hodge operator is defined by raising all the indices of the Hodge star operator, i.e., $\star^\sharp\boldsymbol{\beta} = (\star\boldsymbol{\beta})^\sharp$. The result is an alternating contravariant tensor.

[3] The second equality is a consequence of Cartan's formula $\mathfrak{L}_{\boldsymbol{V}}\boldsymbol{\mu} = \mathrm{d}\iota_{\boldsymbol{V}}\boldsymbol{\mu} + \iota_{\boldsymbol{V}}\mathrm{d}\boldsymbol{\mu}$, and $\mathrm{d}\boldsymbol{\mu} = 0$, where $\mathfrak{L}$ is the Lie derivative operator.

[4] This might seem to disagree with what was obtained by Yavari and Goriely [6], i.e., that the dislocation density tensor is divergence-free. In that work, however, Cartan's exterior covariant derivative was used to define a divergence operator for tensors of type (2,0) that only operates on the second index. Therefore, this extended divergence operation is equivalent to taking the divergences of triplets of vectors and assembling them together. As a matter of fact, it is straightforward to prove that if one denotes with $\widetilde{\mathrm{Div}}$ the divergence operator defined by Yavari and Goriely [6], then $\widetilde{\mathrm{Div}}\boldsymbol{\alpha} = (\mathrm{Div}\,\boldsymbol{\alpha}^\beta)\,\boldsymbol{e}_\beta$. Thus, our result agrees with what was obtained by Yavari and Goriely [6].

4. Nye's lattice curvature tensor

The incompatibility of the lattice structure can be described by Nye's lattice curvature tensor as well. This object is equivalent to the dislocation density tensor, but instead of being associated with the circulation of the lattice coframe, it represents the way the lattice frame changes along its own integral curves. We start by providing three equivalent definitions of the lattice curvature tensor in the material manifold. We will also discuss their geometric interpretations. First, we introduce the lattice curvature as a triplet of vectors $\{\boldsymbol{\kappa}_\beta\}$ defined by

$$\boldsymbol{\kappa}_\beta = \boldsymbol{\alpha}_\beta - \frac{1}{2}\langle\boldsymbol{\vartheta}^\gamma, \boldsymbol{\alpha}_\gamma\rangle\,\boldsymbol{e}_\beta\,, \tag{4.1}$$

where $\boldsymbol{\alpha}_\beta = \delta_{\beta\eta}\boldsymbol{\alpha}^\eta$ is a simple reindexing of the triplet $\{\boldsymbol{\alpha}^\beta\}$. The lattice curvature can also be defined as a tensor $\boldsymbol{\kappa}$ of type (2,0) as

$$\boldsymbol{\kappa} = \boldsymbol{\alpha} - \frac{1}{2}(\mathrm{Tr}_{\boldsymbol{G}}\,\boldsymbol{\alpha})\,\boldsymbol{G}^\sharp\,. \tag{4.2}$$

In components, $\kappa^{AB} = \alpha^{AB} - \frac{1}{2}\alpha_H{}^H\,G^{AB}$. It can also be written as $\boldsymbol{\kappa} = \delta^{\alpha\beta}\,\boldsymbol{e}_\alpha \otimes \boldsymbol{\kappa}_\beta$. Finally, a definition very similar to that of Nye [1] is the following tensor of type (1,1):

$$\mathsf{k} = \boldsymbol{\alpha}^{\flat_1} - \frac{1}{2}(\mathrm{Tr}_{\boldsymbol{G}}\,\boldsymbol{\alpha})\,\mathsf{I}\,, \tag{4.3}$$

where $\flat_1$ denotes the lowering of the first index, while I is the identity operator. In components, one has $\mathsf{k}^A{}_B = \alpha_B{}^A - \frac{1}{2}\alpha_H{}^H\,\delta^A_B$. It can be written as $\mathsf{k} = \boldsymbol{\vartheta}^\beta \otimes \boldsymbol{\kappa}_\beta$, and vice versa $\boldsymbol{\kappa}_\beta = \mathsf{k}\boldsymbol{e}_\beta$. The (1,1) and (2,0) variants are related as $\mathsf{k} = \boldsymbol{\kappa}^{\flat_1}$, i.e., $\mathsf{k}^A{}_B = \kappa_B{}^A$.

Next we provide a geometric interpretation of Nye's construction. Instead of assuming the existence of a relaxed configuration and expressing all the quantities with respect to it, we carry out our analysis entirely in the material manifold. Let us consider an arbitrary curve γ in the material manifold $\mathcal{B}$, with $\boldsymbol{G}$-unit tangent vector $\mathbf{t}$. Then, $\nabla_{\mathbf{t}}$ indicates covariant derivative along γ corresponding to an arc-length parametrization, where ∇ is the Levi–Civita connection associated with $\boldsymbol{G}$. Let us define the following symbols

$$\Lambda_{\mu\nu} = \langle\!\langle \nabla_{\mathbf{t}}\boldsymbol{e}_\mu, \boldsymbol{e}_\nu\rangle\!\rangle_{\boldsymbol{G}}\,, \tag{4.4}$$

representing the way $\boldsymbol{e}_\mu$ changes along γ with respect to $\boldsymbol{e}_\nu$. It is straightforward to check that since the lattice frame $\{\boldsymbol{e}_\beta\}$ is orthonormal with respect to $\boldsymbol{G}$, by construction, one has $\Lambda_{\mu\nu} = -\Lambda_{\nu\mu}$. Therefore, the coefficients (4.4) represent the infinitesimal rotation that the lattice frame undergoes while moving by ds along the curve γ in the material manifold. Using the coefficients $\Lambda_{\mu\nu}$ one defines the 2-form $\boldsymbol{\Lambda} = \Lambda_{\mu\nu}\boldsymbol{\vartheta}^\mu \otimes \boldsymbol{\vartheta}^\nu$. The axial vector associated with $\boldsymbol{\Lambda}$ is defined through the raised Hodge operator as $\boldsymbol{W} = \star^\sharp\boldsymbol{\Lambda}$.

Remark 4.1. We emphasize that the coefficients $\Lambda_{\mu\nu}$ do not transform tensorially with the frame that is used to define them. As a matter of fact, if one considers a different frame $\boldsymbol{f}_\beta$, related to $\boldsymbol{e}_\beta$ as $\boldsymbol{e}_\beta = A^\omega{}_\beta\boldsymbol{f}_\omega$, then one can easily see that

$$\langle\!\langle \nabla_{\mathbf{t}}\boldsymbol{e}_\mu, \boldsymbol{e}_\nu\rangle\!\rangle = A^\rho{}_\mu A^\sigma{}_\nu\langle\!\langle \nabla_{\mathbf{t}}\boldsymbol{f}_\rho, \boldsymbol{f}_\sigma\rangle\!\rangle + \nabla_{\mathbf{t}}A^\rho{}_\mu\,\delta_{\rho\sigma}A^\sigma{}_\nu\,. \tag{4.5}$$

If one considers the Frenet frame $\{\boldsymbol{f}_\beta\} = \{\mathbf{t},\mathbf{n},\mathbf{b}\}$ associated with a curve γ, where $\mathbf{n}$ and $\mathbf{b}$ are respectively the normal and binormal unit vectors, the coefficients $\langle\!\langle \nabla_{\mathbf{t}}\boldsymbol{f}_\mu, \boldsymbol{f}_\nu\rangle\!\rangle$ have the following representation:

$$\Big[\langle\!\langle \nabla_{\mathbf{t}}\boldsymbol{f}_\mu, \boldsymbol{f}_\nu\rangle\!\rangle\Big] = \begin{bmatrix} 0 & \kappa & 0 \\ -\kappa & 0 & \tau \\ 0 & -\tau & 0 \end{bmatrix}, \tag{4.6}$$

where κ and τ are, respectively, the curvature and torsion of γ (here the torsion of a curve should not be confused with the torsion of a connection). The axial vector associated to the Frenet frame $\{\mathbf{t}, \mathbf{n}, \mathbf{b}\}$ is $\boldsymbol{W} = \tau\mathbf{t} + \kappa\mathbf{b}$.

Next we let the curve γ be an integral curve for the lattice vector $\boldsymbol{e}_\beta$, i.e., we assume $\mathbf{t} = \boldsymbol{e}_\beta$. This means that we are looking at infinitesimal rotations of the lattice frame along its own integral curves. Hence, we define the triplet of 2-forms $\{\mathcal{H}_\beta\}$ as the analogue of (4.4), with components

$$(\mathcal{H}_\beta)_{\mu\nu} = \langle\!\langle \nabla_{\boldsymbol{e}_\beta}\boldsymbol{e}_\mu, \boldsymbol{e}_\nu \rangle\!\rangle_{\boldsymbol{G}} = \Gamma_{\nu\beta\mu}\,, \tag{4.7}$$

where $\Gamma_{\nu\beta\mu}$ are the Christoffel symbols of the first kind of $\boldsymbol{G}$ in the moving frame $\{\boldsymbol{e}_\beta\}$. The $(\mathcal{H}_\beta)_{\mu\nu}$'s represent Ricci rotation coefficients [23] associated with the frame $\{\boldsymbol{e}_\beta\}$. It should be noted that from the orthonormality of the lattice frame one has

$$\begin{aligned}\Gamma_{\mu\beta\nu} &= -\langle\!\langle \nabla_{\boldsymbol{e}_\beta}\boldsymbol{e}_\nu, \boldsymbol{e}_\mu \rangle\!\rangle_{\boldsymbol{G}} = -\langle\!\langle \hat{\nabla}_{\boldsymbol{e}_\beta}\boldsymbol{e}_\nu - \boldsymbol{K}(\boldsymbol{e}_\beta, \boldsymbol{e}_\nu), \boldsymbol{e}_\mu \rangle\!\rangle_{\boldsymbol{G}} \\ &= \langle\!\langle \boldsymbol{K}(\boldsymbol{e}_\beta, \boldsymbol{e}_\nu), \boldsymbol{e}_\mu \rangle\!\rangle_{\boldsymbol{G}} = K_{\mu\beta\nu}\,,\end{aligned} \tag{4.8}$$

where use was made of the definition of the contorsion tensor (2.6) and the fact that the Weitzenböck derivative of the lattice frame vectors vanishes. In other words, the contorsion tensor can be used to express the Ricci rotation coefficients. Hence, we define the symbols $H_{\beta\nu\mu} = (\mathcal{H}_\beta)_{\mu\nu} = K_{\mu\beta\nu}$. This allows us to define the tensor $\boldsymbol{H}$ as

$$\langle\!\langle \boldsymbol{H}(\boldsymbol{X}, \boldsymbol{Y}), \boldsymbol{e}_\beta \rangle\!\rangle_{\boldsymbol{G}} = \mathcal{H}_\beta(\boldsymbol{X}, \boldsymbol{Y})\,, \tag{4.9}$$

or

$$\langle\!\langle \boldsymbol{H}(\boldsymbol{X}, \boldsymbol{Y}), \boldsymbol{Z} \rangle\!\rangle_{\boldsymbol{G}} = \langle\!\langle \boldsymbol{K}(\boldsymbol{Z}, \boldsymbol{Y}), \boldsymbol{Z} \rangle\!\rangle_{\boldsymbol{G}}\,. \tag{4.10}$$

In coordinate components $H^A{}_{BC} = K_B{}^A{}_C = G_{BD}G^{AF}K^D{}_{FC}$. It should be noted that the anti-simmetry in the lower indices of $\boldsymbol{H}$ coming from the orthonormality of $\{\boldsymbol{e}_\beta\}$ can be verified by using (2.7), viz.

$$\begin{aligned}H^A{}_{BC} &= \frac{1}{2}\left(T_B{}^A{}_C + T^A{}_{BC} + T_{CB}{}^A\right) = -\frac{1}{2}\left(T_C{}^A{}_B + T^A{}_{CB} + T_{BC}{}^A\right) \\ &= -K_C{}^A{}_B = -H^A{}_{CB}\,.\end{aligned} \tag{4.11}$$

The following proposition shows that the lattice curvature tensor of Nye can be obtained from the permutated contorsion tensor.

Proposition 4.2. *The lattice curvature tensor is the axial vector associated with the permutated contorsion tensor, i.e.,* $\boldsymbol{\kappa} = \star^\sharp\boldsymbol{H}$ *and* $\boldsymbol{\kappa}_\beta = \star^\sharp\mathcal{H}_\beta$.

Proof. We use components, and invoke (2.7) and (4.11) to write

$$\begin{aligned}H^A{}_{CD} &= \frac{1}{2}\left(T_C{}^A{}_D + T^A{}_{CD} + T_{DC}{}^A\right) \\ &= \frac{1}{2}\left(\mu^A{}_{DF}\,\alpha_C{}^F + \mu_{CDF}\,\alpha^{AF} + \mu_C{}^A{}_F\,\alpha_D{}^F\right),\end{aligned} \tag{4.12}$$

where use was made of the relation $T^A{}_{BC} = \mu_{BCD}\,\alpha^{AD}$. Therefore, we can calculate $\star^\sharp\boldsymbol{H}$ as

$$\begin{aligned}\frac{1}{2}\mu^{BCD}H^A{}_{CD} &= \frac{1}{4}\left(\mu^{BCD}\mu^A{}_{DF}\,\alpha_C{}^F + \mu^{BCD}\mu_{CDF}\,\alpha^{AF} + \mu^{BCD}\mu_C{}^A{}_F\,\alpha_D{}^F\right) \\ &= \frac{1}{4}\left(\alpha^{AB} - \alpha_H{}^H G^{AB} + 2\alpha^{AB} + \alpha^{AB} - \alpha_H{}^H G^{AB}\right) \\ &= \alpha^{AB} - \frac{1}{2}\alpha_H{}^H G^{AB}\,,\end{aligned} \tag{4.13}$$

which coincides with (4.2). The expression for $\boldsymbol{\kappa}_\beta$ can be obtained by lowering the first index of $\boldsymbol{\kappa}$ and contracting it with $\boldsymbol{e}_\beta$. □

Proposition 4.2 implies that the lattice curvature tensor can be obtained from $\mathcal{H}_\beta$ and $\boldsymbol{H}$ in the same way that the dislocation density tensor is obtained from $\mathcal{T}^\beta$ and $\boldsymbol{T}$. This also shows that the lattice curvature tensor represents rotations of the lattice frame. In particular, the geometric interpretation of the operator $\mathbf{k}$ is the following: given a vector field $\boldsymbol{Z}$ on $\mathcal{B}$, the vector $\mathbf{k}\boldsymbol{Z}$ is the axial vector describing the rotation of the lattice along integral curves of $\boldsymbol{Z}$. Similarly, the vector $\boldsymbol{\kappa}_\beta$ is the axial vector associated with the rotation of the lattice along integral curves of the lattice vector $\boldsymbol{e}_\beta$.

Remark 4.3. Under the assumption of a stress-free crystal, Nye's work was carried out entirely in the deformed (relaxed) configuration. In geometric terms, Nye studied the deformed lattice structure on $\varphi(\mathcal{B})$ represented by $\{\varphi_*\boldsymbol{e}_\beta\}$ with respect to the metric $\boldsymbol{g}$. Although not explicitly stated by Nye, this approach consists of defining the following spatial dislocation density tensor and lattice curvature tensor:

$$\bar{\boldsymbol{\alpha}}^\beta = \star_{\boldsymbol{g}}^\sharp \mathrm{d}\varphi_*\boldsymbol{\vartheta}^\beta\,, \qquad \bar{\boldsymbol{\kappa}}_\beta = \bar{\boldsymbol{\alpha}}_\beta - \frac{1}{2}\langle \varphi_*\boldsymbol{\vartheta}^\gamma, \bar{\boldsymbol{\alpha}}_\gamma\rangle\,\varphi_*\boldsymbol{e}_\beta\,, \tag{4.14}$$

where $\star_{\boldsymbol{g}}^\sharp$ denotes the raised Hodge operator in the ambient space induced by the metric $\boldsymbol{g}$, and φ is a configuration map. The quantities defined in (4.14) are the spatial analogues of (3.2) and (4.1), and describe the deformed lattice structure with respect to the metric $\boldsymbol{g}$. Under Nye's assumption, the configuration map φ is a local isometric embedding, and hence $\boldsymbol{g} = \varphi_*\boldsymbol{G}$ (see Remark 2.2). This means that all the quantities involved in the definition of $\bar{\boldsymbol{\alpha}}^\beta$ and $\bar{\boldsymbol{\kappa}}_\beta$ (metric, covariant derivative, Hodge operator) are preserved by the tangent map $T\varphi$, and hence, they coincide with their material counterparts, i.e., $\bar{\boldsymbol{\alpha}}^\beta = \varphi_*\boldsymbol{\alpha}^\beta$ and $\bar{\boldsymbol{\kappa}}^\beta = \varphi_*\boldsymbol{\kappa}^\beta$ (note that d and φ_* commute).

Next we look at the lattice curvature tensor in the linearized approximation. In nonlinear elasticity compatibility can be expressed in terms of the strain field as the vanishing of the curvature tensor associated with the pulled-back metric $\boldsymbol{C}$ [24]. These conditions can be linearized to obtain the compatibility equations in terms of the infinitesimal strain $\boldsymbol{\epsilon} = \frac{1}{2}\delta\boldsymbol{C}$ in the linearized setting [25]. It should be noted that in dimension three, curvature can be expressed by several equivalent tensors [26]. In particular, the linearization of the Einstein tensor allows one to obtain compatibility as $\mathrm{curl}\circ\mathrm{curl}\,\boldsymbol{\epsilon} = \mathbf{0}$ [24]. In a similar way, the compatibility of plastic deformations can be written in terms of the material metric $\boldsymbol{G}$ as the vanishing of the curvature $\boldsymbol{R}$ associated with $\boldsymbol{G}$. As was mentioned in Remark 2.2, this does not ensure the absence of dislocations, but the lack of residual stresses. An incompatibility object for the plastic deformation is usually defined by linearizing the curvature tensor [27].

According to Kröner [2], the lattice curvature tensor can be used to express the incompatibility content of the plastic strain. Therefore, we would like to recover Kröner's result in our geometric approach via the linearization of the Einstein tensor. We linearize around a defect-free lattice coframe, inducing a Euclidean material metric and a Weitzenböck connection that coincides with the flat Levi–Civita connection. This means that the initial plastic deformation is compatible, while we look at a small plastic deformation carrying the entire dislocation content. Therefore, in this zeroth-order structure, the tensors $\boldsymbol{T}$, $\boldsymbol{K}$, $\boldsymbol{\alpha}$, $\boldsymbol{\kappa}$ and $\boldsymbol{R}$ vanish. We start by linearizing the Riemann curvature tensor. As all the second-order terms vanish, one can write [28]

$$\begin{aligned}\delta R^A{}_{BCD} &= \delta\Gamma^A{}_{DB|C} - \delta\Gamma^A{}_{CB|D} \\ &= \delta\hat{\Gamma}^A{}_{DB|C} - \delta K^A{}_{DB|C} - \delta\hat{\Gamma}^A{}_{CB|D} + \delta K^A{}_{CB|D} \\ &= \delta K^A{}_{CB|D} - \delta K^A{}_{DB|C}\,,\end{aligned} \tag{4.15}$$

where $\Gamma^A{}_{BC} = \hat{\Gamma}^A{}_{BC} - K^A{}_{DB}$, and a vertical bar denotes the covariant derivative ∇. Recalling the definition of permuted contorsion tensor $\boldsymbol{H}$ and the lattice curvature tensor $\boldsymbol{\kappa}$, one writes

$$\delta R^A{}_{BCD} = \delta H_C{}^A{}_{B|D} - \delta H_D{}^A{}_{B|C} = \mu^A{}_{BF}\left(\delta\kappa_C{}^F{}_{|D} - \delta\kappa_D{}^F{}_{|C}\right). \tag{4.16}$$

Next, we linearize the relation

$$\mathsf{Ein}^{AB} = -\frac{1}{4}\mu^{AMN}\,\mu^{BPQ}\,R_{MNPQ}\,, \tag{4.17}$$

for the raised Einstein tensor,[5] and recalling that all the defect-related zeroth-order quantities vanish, (4.15) can be written as

$$\begin{aligned}\delta\mathsf{Ein}^{AB} &= -\frac{1}{4}\mu^{AMN}\,\mu^{BPQ}\,\mu_{MNF}\left(\delta\kappa_P{}^F{}_{|Q} - \delta\kappa_Q{}^F{}_{|P}\right)\\ &= \frac{1}{2}\mu^{BQP}\left(\delta\kappa_P{}^A{}_{|Q} - \delta\kappa_Q{}^A{}_{|P}\right) = \mu^{BQP}\delta\kappa_P{}^A{}_{|Q}\,.\end{aligned} \tag{4.18}$$

One can also write (4.18) as $\delta\mathsf{Ein}^{AB} = \mu^{BQP}\delta\mathsf{K}^A{}_{P|Q}$. This coincides with what was obtained by Kröner [2].

5. Conclusions

In this paper we revisited Nye's lattice curvature tensor and presented a modern perspective. While Nye's construction is based on the assumption of no residual stresses, motivated by the works of Bilby and others the notion of lattice curvature was extended to arbitrary dislocation distributions. In the framework of Cartan's moving frames, the lattice curvature is a representation of the rotation of the lattice moving frame with respect to an affine connection. In particular, the lattice curvature is related to the Ricci rotation coefficients associated with the lattice frame and is therefore a purely material object. We started by expressing the material version of Nye's lattice curvature as a triplet of vectors, and showed that it can be obtained from the contorsion tensor via the raised Hodge operator. It was also shown that if one works under Nye's assumption of a Euclidean material metric (i.e., zero-stress dislocations), which ensures the existence of a (local) stress-free reference configuration in which the material metric is preserved, the material and the spatial definitions of $\boldsymbol{\kappa}$ coincide. As a matter of fact, since all the quantities involved in its geometric definition—metric, covariant derivative, and Hodge operator—are preserved, the spatial lattice curvature is the push forward of the material lattice curvature via the relaxation map. Moreover, we were able to show that in the linearized approximation the lattice curvature tensor can be used to express the Riemann curvature of the material manifold. In particular, its curl is equal to the linearization of the Einstein tensor.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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[5] This can be found in Fosdick [26] with the opposite sign coming from a different definition of the Ricci curvature.

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