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Continuum elasticity with topological defects, including dislocations and extra-matter

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Abstract

The elasticity of continuous media with topological defects is described naturally by differential geometry, since it relates metric to strain. We construct a geometrical field theory, identifying disclinations, dislocations and extra-matter defects with the curvature, torsion and nonmetricity tensors, respectively. Connection and metric are given explicitly in the presence of dislocations and extra-matter. The density of extra-matter is a scalar source of isotropic strain, described by a local length scale or gauge. The logarithm of the gauge is related to the density of extra-matter by a Poisson equation. The corresponding integral equation, similar to Gauss' law in electrostatics, measures the amount of extra-matter contained inside a contour.

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1. Introduction

Elasticity theory studies the mechanics of solids, described as continuous media. The deformations of the material and the cohesive forces which hold the structure together as an integral unit, are described by strain and stress tensors, respectively (see, e.g., [1]).

In classical elasticity theory, one assumes that strains are small, that the constitutive equations which relate stress and strain tensors are linear and that there are no topological defects. But real solids deform plastically, i.e. permanently, and the necessary yield stress is much weaker than the classical theory's estimate. The concept of dislocation was introduced to account for this discrepancy [2–4]. Dislocations were also shown to be directly responsible for work-hardening, etc (see, e.g., [5–7]).

Dislocations are topological defects. Topological defects can be defined as a generalization of the theorems of Gauss and Ampère in electromagnetism, and of Burgers in elasticity [8–10]. The integral of a field (electric, magnetic or deformation) over a closed contour away from the defect (charge, current or dislocation line), is a signature of this defect,

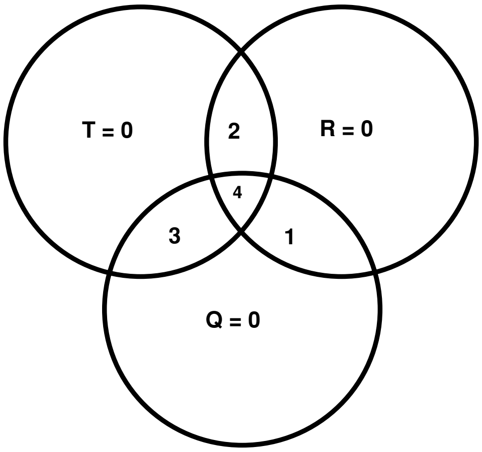

Figure 1. Venn diagram showing that various geometries are defined by the fundamental tensors, R (curvature), T (torsion) and Q (associated with extra-matter). 1: realm of elementary dislocation theory. 3: Riemannian geometry. 4: Euclidean geometry. 2: an example of conformal geometry [17].

independent of the shape or size of the contour which surrounds it. The integral is zero if no defect is enclosed. Examples of topological defects are dislocations in crystals, disclinations in liquid crystals, magnetic flux lines in type II superconductors and vortices in superfluid helium 4.

Dislocations and disclinations have been introduced in elasticity theory through the methods of differential geometry by Kondo [11], Bilby *et al* [12] and Kröner [13–16]. See [17–20] for reviews, and sections 3 and 5 of this paper.

But dislocations and disclinations were introduced one after the other, and in an *ad hoc* fashion, leaving open several questions: Are there any other topological defects? Can they coexist? Why are disclinations absent in three-dimensional crystals [6]? Do they survive in amorphous solids where there is no lattice to *dis*locate [21, 22]? Kröner set the technologically important problem of the coexistence of dislocation lines with impurities or inclusions, and of the pinning of the former by the latter [13]. He showed that the latter were also topological defects, described by a third fundamental tensor, which he called the nonmetricity or Q-tensor. Figure 1 shows the various geometries and topological defects defined by the nonvanishing fundamental tensors R, T and Q. Region 1, $R = 0$, $Q = 0$, is the realm of the classical dislocation theory. Region 3, $T = 0$, $Q = 0$, is Riemannian geometry. Region 4, $R = 0$, $T = 0$, $Q = 0$, is Euclidean geometry, elasticity theory without defects. Region 2, with $R = 0$, $T = 0$ but $Q \neq 0$ deserves more attention. We will discuss this geometry and construct explicitly the appropriate connection.

Weyl's gauge ('calibration') theory [23–25] is, in fact, an example of the region $T = 0$ with nonmetricity and curvature. Some solids may be characterized by a local length scale or gauge: for example, an inclusion made of a material with a thermal expansion coefficient different from that of the matrix in which it is embedded [13]. Another example is a material with ferroelastic inclusions, where a spontaneous strain may develop below the Curie temperature [26]. Conformal crystals, which constitute an example of extra-matter, will be discussed in section 8.

Section 2 of this paper reviews the geometry of elastic continua. Section 3 introduces topological defects from a physical point of view, starting with the dislocation, which is

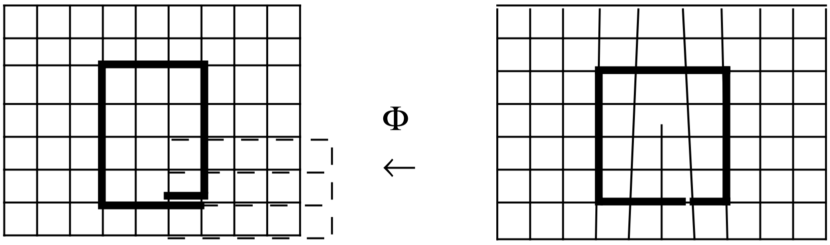

Figure 2. Reference states of an elastic material (left: natural state, right: actual state) and the local mapping between them.

altogether the most common and the most important topological defect technologically. Sections 4 and 6 treat the cases where only one type of defect is present, disclinations and extra-matter, respectively. Section 5, on the differential geometry of topological defects, is the mathematical counterpart of section 3. Sections 6 and 7 contain the main results of this paper, the evaluation of extra-matter enclosed in a contour, and the Poisson equation relating the gauge to its source, the density of extra-matter.

2. The elastic continuum: geometry and strain

The elastic continuum can be described by differential geometry, as a mapping between two states of the material, the actual state and a reference state, each characterized by its own set of coordinates (figure 2).

The *actual*, deformed *state* of the body, is described by holonomic, Euler coordinates x^m, labelled by Latin indices $m = 1, 2, 3$.

The local, relaxed state of the material is characterized by nonholonomic (nonintegrable) Lagrange coordinates $\mathrm{d}X^\alpha$, labelled by Greek indices $\alpha = 1, 2, 3$. This relaxed state is what Kröner [14] calls the *natural state*. It is obtained from the actual, deformed state when one relaxes the elastic strain. Alternatively, the natural state is obtained from a perfect lattice (the ideal state) by plastic deformation (e.g. Volterra construction).

The mapping (Jacobian) matrix ϕ_m^α from actual to natural states,

$$\mathrm{d}X^\alpha = \phi_m^\alpha\, \mathrm{d}x^m \tag{1}$$

contains the physical information. It describes the local geometry of the material. Note that $\phi_m^\alpha = \partial X^\alpha / \partial x^m$ is a gradient only if the coordinates $\mathrm{d}X^\alpha$ are holonomic. (The summation over repeated sub- and superscript indices is implicit by convention.)

The elastic strain tensor e_{mn} is obtained by comparing the distance $\mathrm{d}l'$ between two points separated by an infinitesimal vector $\mathrm{d}x^m$ in the elastically deformed state, with the distance $\mathrm{d}l$ between the same points in the relaxed state, that is, if one had allowed the elastic strain to go to zero

$$\mathrm{d}l'^2 = \mathrm{d}x_m \mathrm{d}x^m = g_{\alpha\beta}\, \mathrm{d}X^\alpha \mathrm{d}X^\beta \qquad \mathrm{d}l^2 = g_{mn} \mathrm{d}x^m \mathrm{d}x^n = \mathrm{d}X^\alpha \mathrm{d}X_\alpha. \tag{2}$$

These equations define the metric g_{mn} of the relaxed state described by the Euler coordinates x^m and the metric $g_{\alpha\beta}$ of the actual state described by the Lagrange coordinates $\mathrm{d}X^\alpha$. Then,

$$\mathrm{d}l'^2 - \mathrm{d}l^2 = 2e_{mn}\, \mathrm{d}x^m \mathrm{d}x^n = 2E_{\alpha\beta} \mathrm{d}X^\alpha \mathrm{d}X^\beta$$

defines the elastic strain tensor

$$e_{mn} = \tfrac{1}{2}(\delta_{mn} - g_{mn}). \tag{3}$$

Both e_{mn} and g_{mn} are symmetric in their indices. Relation (3), is general and fundamental. Since, from (1)

$$g_{mn} = \delta_{\alpha\beta}\phi_m^\alpha \phi_n^\beta \tag{4}$$

equation (3) relates the physical strain to the geometrical mapping (1).

3. Topological defects in an elastic continuum

Consider first the construction of the Burgers vector b^α of a dislocation (see figure 2). Let C be a closed contour in the actual state of the material, characterized by the coordinates x^m. Its image C' in the relaxed state, characterized by the coordinates $\mathrm{d}X^\alpha$, is not closed, the missing amount being the Burgers vector

$$-b^\alpha = \int_{C'} \mathrm{d}X^\alpha = \oint_C \phi_n^\alpha \,\mathrm{d}x^n = \int\!\!\int T_{mn}^\alpha \,\mathrm{d}x^m \wedge \mathrm{d}x^n \tag{5}$$

where the dislocation density

$$T_{mn}^\alpha = \partial_m \phi_n^\alpha - \partial_n \phi_m^\alpha \tag{6}$$

has been obtained through Stokes formula. $T_{mn}^\alpha \,\mathrm{d}x^m \wedge \mathrm{d}x^n$ is a vector-valued two-form in x^m.

Note that the Burgers vector is a property of the whole contour in the natural state of the material. It expresses anholonomy, and is the same, wherever contour C' starts.

The Burgers vector could also be expressed in the actual state, through the use of mapping (1), but only if neither its orientation, nor its length depends on its position. This is only the case if the curvature and nonmetricity tensors vanish inside contour C. If the former condition holds, the material is said to have distant parallelism, or to be free of disclinations. Then, the dislocation density is given by the torsion tensor

$$T_{mn}^s = (\phi^{-1})_\alpha^s T_{mn}^\alpha = \Gamma_{nm}^s - \Gamma_{mn}^s \tag{7}$$

in terms of the connection

$$\Gamma_{nm}^s = (\phi^{-1})_\alpha^s \partial_m \phi_n^\alpha. \tag{8}$$

Disclinations do not occur in crystalline three-dimensional materials. They cost too much elastic energy. Disclination-free crystals have distant parallelism or long-range orientational order. This property can be expressed mathematically through the concept of parallel transport. Parallel transport of a vector v^s between two points separated by $\mathrm{d}x^m$ along the path is given by the formal expression

$$\delta v^s = -\Gamma_{pm}^s v^p \mathrm{d}x^m.$$

Parallel transport of v^s over an arc of a geodesic implies that its covariant derivative

$$D_p v^s = \partial_p v^s + \Gamma_{mp}^s v^m$$

vanishes.

In case of long-range order, any vector v^s returns the same orientation after being transported over an arbitrary closed circuit. The closed circuit decomposed into elementary arcs of geodesics, thus

$$\begin{aligned}\oint \delta v^s &= -\oint \Gamma_{pn}^s v^p \,\mathrm{d}x^n = -\int\!\!\int \left[\partial_m \left(\Gamma_{pn}^s v^p\right) - \partial_n \left(\Gamma_{pm}^s v^p\right)\right] \mathrm{d}x^m \wedge \mathrm{d}x^n \\ &= -\int\!\!\int R_{pmn}^s v^p \,\mathrm{d}x^m \wedge \mathrm{d}x^n \end{aligned} \tag{9}$$

where the curvature tensor,

$$R^s_{pmn} = \partial_m \Gamma^s_{pn} - \partial_n \Gamma^s_{pm} + \Gamma^s_{jm}\Gamma^j_{pn} - \Gamma^s_{jn}\Gamma^j_{pm} \tag{10}$$

measures the density of disclinations. Equation (9) is valid for any vector and any arbitrary closed circuit. Thus $R^s_{pmn} = 0$ means distant parallelism or absence of disclinations.

With the pure gauge connection (8), the curvature tensor vanishes. The geometry is flat and the material has distant parallelism.

Here the components s, p of the curvature tensor are given in the actual state of the system. But they could as well be given in the natural state, α, β. Only the contour elements $\mathrm{d}x^m$, $\mathrm{d}x^n$ are always in the actual state of the material.

The nonmetricity tensor or Q-tensor, is defined as the covariant derivative of the metric [13]

$$Q_{qsp} = D_p g_{qs} = \partial_p g_{qs} - \Gamma^t_{qp} g_{ts} - \Gamma^t_{sp} q_{qt}. \tag{11}$$

The corresponding defect is called extra-matter. If the Q-tensor induces strain in the material, it is the scalar density of extra-matter $\rho(x)$ which is the source of the strain field (cf equation (37) below). If $D_p g_{qs} = 0$ (Ricci lemma), the connection is called metric compatible [27].

The pure gauge connection (8) is compatible with the metric (4), $Q = 0$. Here, with the connection (8) and metric (4) defined in terms of the same mapping ϕ^α_n, we have an example illustrating region 1 of figure 1, where two of the three fundamental tensors vanish, $Q = 0$, $R = 0$.

4. Riemannian geometry $T = 0$, $Q = 0$

When the torsion vanishes everywhere, the Lagrange coordinates $\mathrm{d}X^\alpha$ are holonomic. The connection $\Gamma^0_{spn} = g_{st}\Gamma^{0t}_{pn} = \Gamma^0_{snp}$ is symmetric. If one makes the further assumption that $Q_{qsp} = D_p g_{qs} = 0$, then the connection can be given explicitly in terms of the metric, as the Christoffel symbol

$$\Gamma^0_{spn} = \tfrac{1}{2}(\partial_n g_{sp} + \partial_p g_{sn} - \partial_s g_{pn}).$$

This situation is region 3 of figure 1.

5. Differential geometry of topological defects

In this section, we discuss the general case of an elastic continuum with topological defects, disclinations, dislocations and extra-matter, in the formalism of differential geometry.

The metric is defined in terms of the mapping ϕ^α_m between relaxed and deformed states of matter, by equation (4).

Using the notation of differential forms (see [28–31] and the appendix), we can write formally the two-forms R, T and the one-form Q in terms of the connection (Γ) and the soldering (ν) one-forms as

$$R^s_p = \mathrm{d}\Gamma^s_p + \Gamma^s_t \wedge \Gamma^t_p \equiv D\Gamma^s_p \tag{12}$$

$$T^s = \mathrm{d}\nu^s + \Gamma^s_m \wedge \nu^m \equiv D\nu^s \tag{13}$$

$$Q_{qs} = \mathrm{d}g_{qs} - \Gamma^t_q g_{ts} - \Gamma^t_s g_{tq} \equiv D g_{qs} \tag{14}$$

where the operator D is the covariant exterior derivative and

$$R^s_p = \tfrac{1}{2} R^s_{pmn} \mathrm{d}x^m \wedge \mathrm{d}x^n \tag{15}$$

$$T^s = \tfrac{1}{2} T^s_{mn} \mathrm{d}x^m \wedge \mathrm{d}x^n \tag{16}$$

$$Q_{qs} = Q_{qsn}\mathrm{d}x^n \tag{17}$$

$$\Gamma^s_q = \Gamma^s_{qn}\mathrm{d}x^n \tag{18}$$

$$\nu^s = \nu^s_n\mathrm{d}x^n. \tag{19}$$

The metric g_{ts} is a zero-form. The soldering form ν^s is necessary to define the torsion two-form in the presence of extra-matter. Its physical role as an integrating factor will be justified shortly (section 6).

In ordinary tensor notation, the curvature tensor R^s_{pmn} is given by (10)

$$R^s_{pmn} = \partial_m\Gamma^s_{pn} - \partial_n\Gamma^s_{pm} + \Gamma^s_{jm}\Gamma^j_{pn} - \Gamma^s_{jn}\Gamma^j_{pm}.$$

Indeed, from (12) and (15),

$$\begin{aligned}\tfrac{1}{2}R^s_{pmn}\mathrm{d}x^m \wedge \mathrm{d}x^n &= \mathrm{d}\left(\Gamma^s_{pn}\mathrm{d}x^n\right) + \Gamma^s_{jm}\mathrm{d}x^m \wedge \Gamma^j_{pn}\mathrm{d}x^n \\ &= \partial_m\Gamma^s_{pn}\mathrm{d}x^m \wedge \mathrm{d}x^n + \Gamma^s_{jm}\Gamma^j_{pn}\mathrm{d}x^m \wedge \mathrm{d}x^n \\ &= \tfrac{1}{2}\left(\partial_m\Gamma^s_{pn} - \partial_n\Gamma^s_{pm} + \Gamma^s_{jm}\Gamma^j_{pn} - \Gamma^s_{jn}\Gamma^j_{pm}\right)\mathrm{d}x^m \wedge \mathrm{d}x^n.\end{aligned}$$

Similarly, the torsion tensor is

$$T^s_{mn} = \partial_m\nu^s_n - \partial_n\nu^s_m + \Gamma^s_{jm}\nu^j_n - \Gamma^s_{jn}\nu^j_m \tag{20}$$

a generalization of equation (7); when ν^s_n takes uniform values (in the actual state), $\mathrm{d}\nu^s = 0$ and equation (20) is identical to equation (7) up to a global transformation of coordinates.

Indeed, from (13) and (16),

$$\begin{aligned}\tfrac{1}{2}T^s_{mn}\mathrm{d}x^m \wedge \mathrm{d}x^n &= \mathrm{d}\left(\nu^s_n\mathrm{d}x^n\right) + \Gamma^s_{jm}\mathrm{d}x^m \wedge \nu^j_n\mathrm{d}x^n \\ &= \left(\partial_m\nu^s_n\right)\mathrm{d}x^m \wedge \mathrm{d}x^n + \Gamma^s_{jm}\nu^j_n\mathrm{d}x^m \wedge \mathrm{d}x^n \\ &= \tfrac{1}{2}\left(\partial_m\nu^s_n - \partial_n\nu^s_m + \Gamma^s_{jm}\nu^j_n - \Gamma^s_{jn}\nu^j_m\right)\mathrm{d}x^m \wedge \mathrm{d}x^n.\end{aligned}$$

The nonmetricity tensor reads

$$Q_{qsn} = \partial_n g_{qs} - \Gamma^t_{qn}g_{ts} - \Gamma^t_{sn}g_{tq}. \tag{21}$$

Indeed, from (14) and (17),

$$Q_{qsn}\mathrm{d}x^n = \mathrm{d}g_{qs} - \Gamma^t_{qn}\mathrm{d}x^n g_{ts} - \Gamma^t_{sn}\mathrm{d}x^n g_{tq} = \partial_n g_{qs}\mathrm{d}x^n - \Gamma^t_{qn}g_{ts}\mathrm{d}x^n - \Gamma^t_{sn}g_{tq}\mathrm{d}x^n.$$

Conservation laws for the densities of topological defects are expressed in terms of Bianchi's identities. Their derivation is less cumbersome in the formalism of differential forms than in tensor notation.

Conservation of curvature (Bianchi's identity proper) reads [27]

$$DR^s_p = \mathrm{d}R^s_p + \Gamma^s_m \wedge R^m_p - R^s_m \wedge \Gamma^m_p = 0 \tag{22}$$

since from equation (16)

$$\mathrm{d}R^s_p = \mathrm{d}\Gamma^s_t \wedge \Gamma^t_p - \Gamma^s_t \wedge \mathrm{d}\Gamma^t_p = \left(R^s_t - \Gamma^s_n \wedge \Gamma^n_t\right) \wedge \Gamma^t_p - \Gamma^s_t \wedge \left(R^t_p - \Gamma^t_n \wedge \Gamma^n_p\right) \tag{23}$$

thus

$$\mathrm{d}R^s_p - R^s_t \wedge \Gamma^t_p + \Gamma^s_t \wedge R^t_p = 0.$$

Disclination lines form closed loops.

The torsion identity is

$$DT^s = \mathrm{d}T^s + \Gamma^s_m \wedge T^m = R^s_n \wedge \nu^n \tag{24}$$

since from equations (13) and (16)

$$\mathrm{d}T^s = \mathrm{d}\Gamma^s_m \wedge \nu^m - \Gamma^s_m \wedge \mathrm{d}\nu^m = \mathrm{d}\Gamma^s_m \wedge \nu^m - \Gamma^s_m \wedge \left(T^m - \Gamma^m_n \wedge \nu^n\right)$$

thus

$$\mathrm{d}T^s + \Gamma^s_m \wedge T^m = \left(\mathrm{d}\Gamma^s_n + \Gamma^s_m \wedge \Gamma^m_n\right) \wedge \nu^n = R^s_n \wedge \nu^n.$$

Recall that $dd = 0$ (Poincaré's identity). Curvature is the source of torsion and dislocation lines may terminate on disclinations.

The third identity relates Q- and curvature tensors:

$$DQ_{qs} = -R^t_q g_{ts} - R^t_s g_{tq} \tag{25}$$

since from equations (14) and (17),

$$\begin{aligned}-\mathrm{d}Q_{qs} &= \mathrm{d}\left(\Gamma^t_q g_{ts}\right) + \mathrm{d}\left(\Gamma^t_s g_{tq}\right)\\ &= \mathrm{d}\Gamma^t_q g_{ts} - \Gamma^t_q \wedge \mathrm{d}g_{ts} + \mathrm{d}\Gamma^t_s g_{tq} - \Gamma^t_s \wedge \mathrm{d}g_{tq}\\ &= \mathrm{d}\Gamma^t_q g_{ts} - \Gamma^t_q \wedge \left(Q_{ts} + \Gamma^m_t g_{ms} + \Gamma^m_s g_{mt}\right)\\ &\quad + \mathrm{d}\Gamma^t_s g_{tq} - \Gamma^t_s \wedge \left(Q_{tq} + \Gamma^m_t g_{mq} + \Gamma^m_q g_{mt}\right)\end{aligned}$$

thus

$$-\mathrm{d}Q_{qs} + \Gamma^t_q \wedge Q_{ts} + \Gamma^t_s \wedge Q_{tq} = \left(\mathrm{d}\Gamma^t_q - \Gamma^n_q \wedge \Gamma^t_n\right) g_{ts} + \left(\mathrm{d}\Gamma^t_s - \Gamma^n_q \wedge \Gamma^t_n\right) g_{tq}.$$

If the curvature is zero, the three Bianchi identities read simply

$$DR^s_p = 0 \qquad DT^s = 0 \qquad DQ_{qs} = 0.$$

6. Extra-matter only, $R = 0$, $T = 0$

Let us now find the connection in the case $R = 0$, $T = 0$. A material free of disclinations has long-range orientational order and zero curvature. The connection is pure gauge in terms of an *arbitrary* mapping A, that is,

$$\Gamma^s_{qp} = (A^{-1})^s_\alpha \partial_p A^\alpha_q \tag{26}$$

where $(A^{-1})^s_\alpha A^\alpha_q = \delta^s_q$. We shall use the shortened notation $(A^{-1})^s_\alpha = A^s_\alpha$.

For $T = 0$, it is sufficient that the physical mapping ϕ^α_q is a gradient $\phi^\alpha_q = \partial X^\alpha / \partial x^q$. It remains to relate the physical mapping ϕ^α_q, which defines the metric (equation (4)), to the mapping A^α_q, which defines the connection. This is done through the soldering tensor ν^m_n as

$$\phi^\alpha_n = A^\alpha_m \nu^m_n. \tag{27}$$

Equation (27) is justified by noting that, from equations (20) and (26),

$$\begin{aligned}T^s_{pn} &= \partial_p \nu^s_n - \partial_n \nu^s_p + \Gamma^s_{mp} \nu^m_n - \Gamma^s_{mn} \nu^m_p\\ &= \partial_p \nu^s_n + A^{-1\,s}_{\ \ \alpha} \left(\partial_p A^\alpha_m\right) \nu^m_n - \partial_n \nu^s_p - A^{-1\,s}_{\ \ \alpha} \left(\partial_n A^\alpha_m\right) \nu^m_p\\ &= A^{-1\,s}_{\ \ \alpha} \left[\partial_p \left(A^\alpha_m \nu^m_n\right) - \partial_n \left(A^\alpha_m \nu^m_p\right)\right] = A^{-1\,s}_{\ \ \alpha} T^\alpha_{pn}.\end{aligned} \tag{28}$$

Thus, the torsion tensor is identically zero if the mapping $\phi^\alpha_n = A^\alpha_m \nu^m_n$ is a gradient. Note, however, that it is the connection mapping A, rather than the full mapping ϕ, which transforms the vector-valued torsion $T^\alpha_{mn} = \partial_m \phi^\alpha_n - \partial_n \phi^\alpha_m$ from the natural state (equation (6)) to the actual state (equation (28)). The two mappings are related by a local change of coordinates ν^m_n.

The metric can be written as

$$g_{pq} = \delta_{\alpha\beta} \phi^\alpha_p \phi^\beta_q = \delta_{\alpha\beta} A^\alpha_m \nu^m_p A^\beta_s \nu^s_q = \left[\nu^m_p \nu^s_q\right] g^0_{ms}$$

where $g^0_{ms} = \delta_{\alpha\beta} A^\alpha_m A^\beta_s$ and $D_t g^0_{ms} = 0$. (The pure gauge connection is compatible with its own metric.) But $D_t g_{pq} = D_t\left[\nu^m_p \nu^s_q g^0_{ms}\right] \neq 0$, so that a nonuniform soldering tensor yields a nonvanishing Q-tensor.

Let us now construct the soldering tensor explicitly. The mapping ϕ_q^α from the actual state to the natural state contains two pieces of physical information: the orientation of a local frame and the local scale, or gauge. The orientation is controlled by the map A_q^α, through the choice of a pure gauge connection (26) which implies zero curvature and long-range orientational order.

We set, therefore,

$$\phi_q^\alpha = \frac{A_q^\alpha}{\lambda} \tag{29}$$

where $1/\lambda(x)$ is the local scale, or gauge, and the corresponding soldering tensor is

$$\nu_n^s = \delta_n^s / \lambda. \tag{30}$$

We show that this choice separates the effects of torsion and nonmetricity. From the pure gauge connection (26), we can calculate curvature, torsion and nonmetricity from equations (10), (20) and (21),

$$R^s_{pmn} = 0 \tag{31}$$

$$T^s_{mn} = \frac{1}{\lambda}\left(\phi^s_\alpha \partial_m \phi^\alpha_n - \phi^s_\alpha \partial_n \phi^\alpha_m\right) \tag{32}$$

$$Q_{qsn} = \frac{-2\partial_n \lambda}{\lambda} g_{qs}. \tag{33}$$

The torsion (32) vanishes if the mapping is a gradient: $\phi_m^\alpha = \partial X^\alpha / \partial x^m$; the natural state has holonomic coordinates, the geometry is integrable, there is no plastic deformation.

Equation (33) indicates that the Q-tensor does not vanish if the local gauge or scale $1/\lambda(x)$ is not uniform. From the point of view of Weyl's theory $g_{qs} = \theta(x) g^0_{qs}$, with $Q^0_{qsp} = D_p g^0_{qs} = 0$, then

$$Q_{qsp} = \frac{\partial_p \theta}{\theta} g_{qs}$$

and $\theta(x) = 1/(\lambda(x))^2$. Indeed

$$D_p g_{qs} = \partial_p\left[\theta g^0_{qs}\right] - \Gamma^t_{qp}\theta g^0_{ts} - \Gamma^t_{sp}\theta g^0_{tq} = (\partial_p\theta) g^0_{qs} + \theta D_p g^0_{qs} = (\partial_p \theta) g^0_{qs} = \frac{\partial_p \theta}{\theta} g_{qs}.$$

Moreover, given that $g_{qs} = \delta_{\alpha\beta}\phi^\alpha_q \phi^\beta_s = 1/(\lambda(x))^2 \delta_{\alpha\beta} A^\alpha_q A^\beta_s$, $g^0_{qs} = \delta_{\alpha\beta} A^\alpha_q A^\beta_s$, the mapping A^α_q only serves to set up the pure gauge connection. It does not include the gauge $1/(\lambda(x))^2$ which describes extra-matter. Indeed $D_n g^0_{qs} = \partial_n g^0_{qs} - \Gamma^t_{qn} g^0_{ts} - \Gamma^t_{sn} g^0_{tq} = 0$.

7. Burgers' vector and nonmetricity scalar

Dislocations are topological defects. Like current lines or charges in electromagnetism, they can be detected and measured by constructing a Burgers circuit, a closed contour in the actual state of the material enclosing the dislocation. In the natural state, the image of the Burgers contour does not close, and the missing element is Burgers' vector (5)

$$-b^\alpha = \int\!\!\int T^\alpha_{mn} \mathrm{d}x^m \wedge \mathrm{d}x^n$$

where

$$T^\alpha_{mn} = \partial_m \phi^\alpha_n - \partial_n \phi^\alpha_m = A^\alpha_s T^s_{mn} \tag{34}$$

is the density of dislocations, with values measured in the natural state. This is the correct, invariant expression, since b^α is the measure of the anholonomy (it does not, by definition, include any elastic distortion), in the absence of disclinations.

The above formulation can be extended to extra-matter. First, we define

$$q_m = g^{st} Q_{stm} = \frac{-2\partial_m \lambda}{\lambda} \qquad {}^*q_{ab} = e_{abc}\sqrt{g} q_s g^{sc} \tag{35}$$

where $e_{abc} = e_{[abc]} = 0, \pm 1$, is the fully antisymmetric pseudo-tensor in flat space and $g = \det(g_{ij})$. Then the amount $N = \int\int\int \rho\sqrt{g}\, \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3$ of extra-matter in the volume V is the flux of ${}^*q_{ab}$ across the surface ∂V bounding V, namely,

$$\begin{aligned} N &= \oint \tfrac{1}{2}{}^*q_{ab}\, \mathrm{d}x^a \wedge \mathrm{d}x^b \\ &= \int\int\int \tfrac{1}{2}\partial_c {}^*q_{ab}\, \mathrm{d}x^c \wedge \mathrm{d}x^a \wedge \mathrm{d}x^b \\ &= \int\int\int \tfrac{1}{2}\partial_c \left(e_{abm}\sqrt{g} q_s g^{sm}\right) \mathrm{d}x^c \wedge \mathrm{d}x^a \wedge \mathrm{d}x^b \\ &= \int\int\int \tfrac{1}{2}\partial_c \left(\sqrt{g} q_s g^{sm}\right) e_{abm} e^{abc}\, \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3 \\ &= \int\int\int \partial_c \left(\sqrt{g} q_s g^{sm}\right) \delta^c_m\, \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3 \\ &= \int\int\int -2\partial_m \left(\sqrt{g} g^{ms}\partial_s \ln\lambda\right) \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3 \end{aligned} \tag{36}$$

so that $\rho(x)$, the density of extra-matter, obeys Poisson's equation in curved space

$$\frac{1}{\sqrt{g}}\partial_m\left(\sqrt{g} g^{ms}\partial_s \ln\lambda^{-2}\right) = \Delta_2(\ln\lambda^{-2}) = \rho(x) \tag{37}$$

where Δ_2 is the Laplacian in curved space (Beltrami's operator).

Remark: It is $\rho(x)$, and not the Q-tensor, which is the density of extra-matter, unlike R and T which are the densities of disclinations and dislocations, respectively. If one looks for an analogy with electrostatics, $\ln\lambda^{-2}$ corresponds to the scalar potential, q_m to the electric field and $\rho(x)$ to the density of electric charge; N is the total charge enclosed.

8. Example: conformal crystal, phyllotaxis

The structure of many compound flowers (*compositae*: daisy, sunflower, pinecone, etc) can be described as a two-dimensional, conformal mapping of a strip of a triangular lattice in the complex plane $z = x + \mathrm{i}y$ into an annulus in the complex plane $w = u + \mathrm{i}v$ [32–34]:

$$w = \exp(bz)$$

that is,

$$u = \exp(b_1 x - b_2 y)\cos(b_2 x + b_1 y) \qquad v = \exp(b_1 x - b_2 y)\sin(b_2 x + b_1 y) \tag{38}$$

where w are the coordinates of the actual state of the material, z those of the natural state, the triangular lattice, and $b = b_1 + \mathrm{i}b_2$ is a complex number which describes the inclination of the strip [32, 33] (figure 3). The lattice in w is still triangular but deformed. Notably the lattice lines become spirals, recognizable in sunflowers, etc.

The mapping (Jacobian) matrix ${\phi^{-1}}^p_\alpha = \mathrm{d}w/\mathrm{d}z$ from the natural to the actual states is

$$\begin{aligned} {\phi^{-1}}^1_1 &= \frac{\partial u}{\partial x} = b_1 u - b_2 v = \frac{\partial v}{\partial y} = {\phi^{-1}}^2_2 \\ {\phi^{-1}}^1_2 &= \frac{\partial u}{\partial y} = -b_2 u - b_1 v = -\frac{\partial v}{\partial x} = -{\phi^{-1}}^2_1. \end{aligned} \tag{39}$$

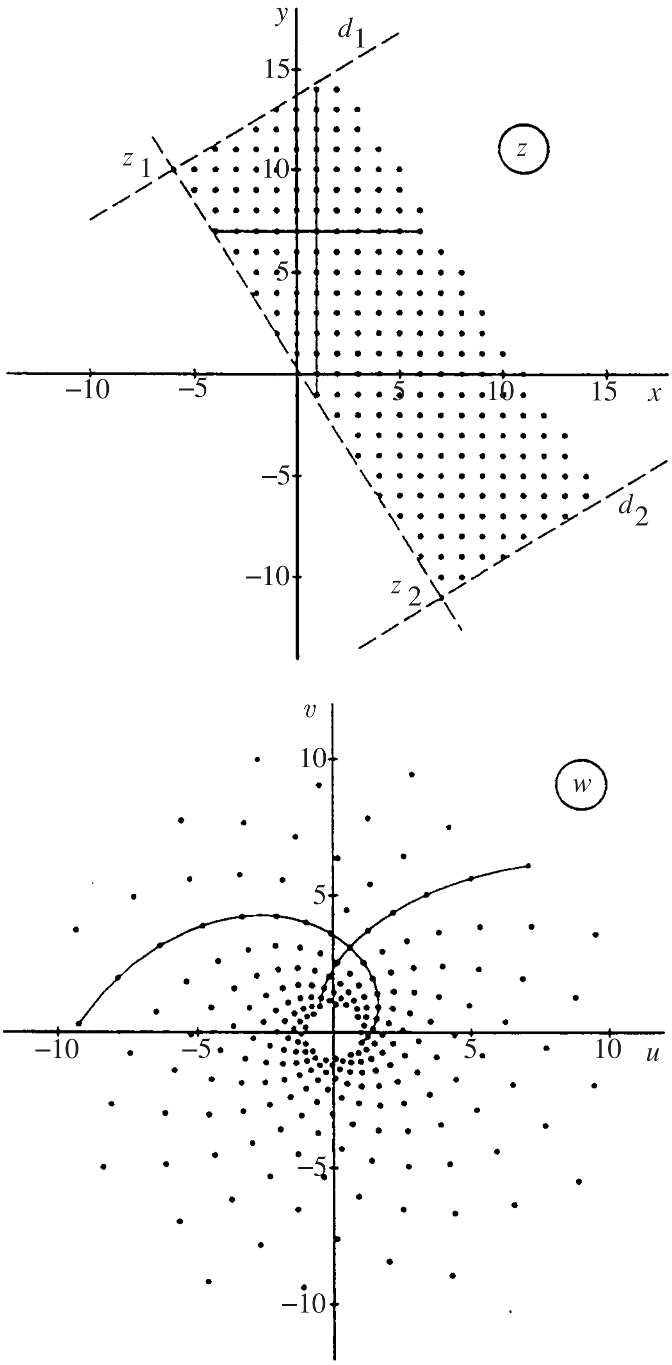

Figure 3. Phyllotaxis: the conformal mapping $w = \exp(bz)$ of a strip in the natural state (here, square lattice in (z) with periodic boundary conditions $d_1 = d_2$) into an annulus in the actual state (w), with $b = 2\pi/(21 + \mathrm{i}13)$. The extra-matter lies inside the inner circle of the annulus (called the meristem), which is the image of the left boundary of the strip in (z). The distortion which it causes is measured by the Q-tensor. The parastichies (images of reticular lines) are equiangular (logarithmic) spirals (from [32], with permission).

The Cauchy–Riemann equations are satisfied. Thus from equation (4),

$$g^{pq} = |b^2 w^2| \delta^{pq} \qquad g_{pq} = \frac{1}{|b^2 w^2|} \delta_{pq}. \tag{40}$$

Since the mapping is conformal, there are neither disclinations nor dislocations (the mapping (39) is a gradient), except on the domain boundaries. However, the density of points in the w plane decreases radially outwards as $1/(|\mathrm{d}w/\mathrm{d}z|^2) = 1/(|bw|^2)$, so that $|bw|$ is a natural length scale, and the size of the floret grows linearly with its distance from the meristem. There is, therefore, a nonvanishing Q-tensor distributed in the w plane (see figure 3 and [33, 34]).

Let us construct the metric tensor $g^0_{qs} = g_{qs}/\theta(w)$ (section 5). We may choose

$$\lambda = |bw|^{1-\sigma} \qquad \theta = \frac{1}{\lambda^2} = |bw|^{-2+2\sigma}$$

with arbitrary σ for now. Then,

$$g^0_{qs} = \lambda^2 g_{qs} = |bw|^{-2\sigma} \delta_{qs} \qquad Q_{qsp} = -2(1-\sigma)\partial_p[\ln(|bw|)] g_{qs}.$$

The natural and physical choice is $\sigma = 0$. Then the gauge $\lambda = |bw|$ is indeed a length scale. $\theta = 1/(|bw|^2)$ is the density of florets (points in the w plane); $g^0_{qs} = \delta_{qs}$ is a metric without length scale, and the mapping A^α_p has determinant 1, so that the connection is also without length scale.

To find the density of extra-matter in two-dimensional space, we define

$$^*q_a = e_{am}\sqrt{g} q_s g^{sm}$$

where $e_{ab} = e_{[ab]} = 0, \pm 1$, is the fully antisymmetric pseudo-tensor in flat two-dimensional space. Then, the amount N of extra-matter in two dimensions is

$$\begin{aligned}
N &= \oint {}^*q_a \, \mathrm{d}x^a \\
&= \oint \left(e_{am}\sqrt{g} q_s g^{sm}\right) \mathrm{d}x^a \\
&= \int\!\!\int \partial_b\left(e_{am}\sqrt{g} q_s g^{sm}\right) \mathrm{d}x^b \wedge \mathrm{d}x^a \\
&= \int\!\!\int \partial_b\left(\sqrt{g} q_s g^{sm}\right) e_{am} e^{ba} \, \mathrm{d}x^1 \wedge \mathrm{d}x^2 \\
&= \int\!\!\int -\partial_m\left(\sqrt{g} q_s g^{sm}\right) \mathrm{d}x^1 \wedge \mathrm{d}x^2 \\
&= \int\!\!\int 2\partial_m\left(\sqrt{g} g^{ms} \partial_s \ln\lambda\right) \mathrm{d}x^1 \wedge \mathrm{d}x^2.
\end{aligned}$$

For our conformal crystal, the amount of extra-matter is

$$\begin{aligned}
N &= \int\!\!\int 2\partial^s \partial_s (\ln\lambda) \, \mathrm{d}u \, \mathrm{d}v \\
&= \int\!\!\int (1-\sigma)\partial^s \partial_s \ln(u^2 + v^2) \, \mathrm{d}u \, \mathrm{d}v \\
&= \int\!\!\int 4\pi(1-\sigma)\delta(u)\delta(v) \, \mathrm{d}u \, \mathrm{d}v \\
&= 4\pi(1-\sigma)
\end{aligned}$$

so the density of extra-matter reads

$$\rho(u, v) = 4\pi(1-\sigma)\delta(u)\delta(v).$$

For $\sigma = 0$, $\rho(u, v) = 4\pi\delta(u)\delta(v)$. In figure 3, the extra-matter is located inside the inner circle of the annulus, the meristem of the flower.

9. Conclusions

We have constructed a field theory of defects, identifying disclinations, dislocations and extra-matter with their fundamental tensors, curvature, torsion and nonmetricity, respectively. We have calculated explicitly the deformations and the connection when there is only extra-matter (the torsion and curvature tensors are explicitly zero), and when there are extra-matter and dislocations (the curvature tensor is explicitly zero).

We showed that extra-matter is a topological defect. Its density is a source of nonmetricity strain (Q-tensor), expressed through a Poisson equation. The amount of extra-matter can be obtained by an integral formula over a closed contour, just like disclinations or dislocations in elasticity, or charges and currents in electromagnetism.

The torsion tensor vanishes, and there are no dislocations, if the physical mapping ϕ_n^α between actual and natural states is a gradient. The curvature tensor vanishes, and there are no disclinations, if the connection, expressed in terms of some arbitrary mapping A_m^α, is pure gauge (equation (26)). If $\phi_n^\alpha = A_n^\alpha$, the Q-tensor vanishes and there is no extra-matter. The extra-matter is given by the soldering tensor ν relating ϕ to A, $\phi_n^\alpha = A_m^\alpha \nu_n^m$. The tensor ν serves as an integrating factor for A if there are no dislocations.

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Appendix. Differential forms

In terms of local coordinates, the set $\{\partial/\partial x^m\}$ with $m = 1, 2, \ldots, n$ forms a basis for the tangent space T of an n-dimensional manifold. The tangent space is a linear, vector space.

The mapping $\omega: T \to \mathbb{R}$ ($\mathbb{R}$ is the set of real numbers) is a linear mapping if $\omega(av + bu) = a\omega(v) + b\omega(u)$ for all $a, b \in \mathbb{R}$ and $u, v \in T$. The set $L(T, \mathbb{R})$ of all linear mappings from T to $\mathbb{R}$ becomes a linear space over $\mathbb{R}$ when addition and scalar multiplication are defined by $(\omega_1 + \omega_2)(u) = \omega_1(u) + \omega_2(u)$ and $(a\omega)(u) = a\omega(u)$. The set $L(T, \mathbb{R})$ is called the dual of tangent space T, or cotangent space, and is denoted by T^*. $\omega(u)$ is often denoted as $\langle \omega, u \rangle$.

The set $\{\mathrm{d}x^m\}$ with $m = 1, 2, \ldots, n$, defined by $\langle \mathrm{d}x^m, \partial/\partial x^n \rangle = \delta_n^m$, is a basis for the cotangent space. A one-form, an arbitrary element of cotangent space, can be written as

$$\omega = a_p \mathrm{d}x^p.$$

Tensors of type (a, b) are constructed by taking a elements from tangent space and b elements from cotangent space. Antisymmetric tensors of type (0, r) are called *r-forms*, and written

$$\omega = T_{m_1,\ldots,m_r} \mathrm{d}x^{m_1} \wedge \cdots \wedge \mathrm{d}x^{m_r}.$$

The symbol $\wedge$ denotes the wedge product and is defined by

$\mathrm{d}x^{m_1} \wedge \cdots \wedge \mathrm{d}x^{m_r} = 0$ if any two basic one-forms $\mathrm{d}x^{m_1}, \ldots, \mathrm{d}x^{m_r}$ are equal;
$\mathrm{d}x^{m_1} \wedge \cdots \wedge \mathrm{d}x^{m_r}$ changes sign if any two $\mathrm{d}x^{m_1}, \ldots, \mathrm{d}x^{m_r}$ are interchanged;
$\mathrm{d}x^{m_1} \wedge \cdots \wedge \mathrm{d}x^{m_r}$ is linear in any basic one-form $\mathrm{d}x^{m_1}, \ldots, \mathrm{d}x^{m_r}$ separately.

Given the r-form $\omega = T_{m_1,\ldots,m_r}\mathrm{d}x^{m_1} \wedge \cdots \wedge \mathrm{d}x^{m_r}$, its exterior derivative is written as $\mathrm{d}\omega$ and is defined as

$$\mathrm{d}\omega = \frac{\partial T_{m_1,\ldots,m_r}}{\partial x^{m_{r+1}}}\mathrm{d}x^{m_{r+1}} \wedge \mathrm{d}x^{m_1} \wedge \cdots \wedge \mathrm{d}x^{m_r}.$$

It follows that, for any form,

$$\mathrm{d}^2\omega = 0. \tag{41}$$

Moreover, for any q-form ξ and r-form ω,

$$\mathrm{d}(\xi \wedge \omega) = \mathrm{d}\xi \wedge \omega + (-1)^q \xi \wedge \mathrm{d}\omega. \tag{42}$$

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