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Autoparallel curves and Riemannian geodesics for materially uniform but inhomogeneous bodies

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Abstract
According to the theory of materially uniform but inhomogeneous bodies two geometric structures can be defined on the body manifold when a uniform reference is known. The first is given by the material connection and the second by the intrinsic Riemannian metric. Two important classes of curves related with these structures are the geodesic and the autoparallel curves. The goal of the present contribution is to define and characterize mechanically these kind of curves for materially uniform but inhomogeneous bodies. We propose the use of these curves for constructing the stress-free non-Euclidean material manifold that plays the role of the reference configuration for the dislocated problem. A generic scheme for the construction of this manifold based on geodesics/autoparallel curves is given as well as a discussion related with the field of internal stresses. Attention is then focused on a continuous distribution of edge dislocations. We solve numerically the geodesic equation that corresponds to a solid body with a continuous symmetry group. By using the L_2 norm for the dislocation density tensor we conclude that the higher the dislocation density the greater the deviation from the straight line is. For the same distribution of dislocations, but for a solid body with a discrete symmetry group, we solve analytically the autoparallel curves.

Keywords
Materially uniform, inhomogeneous body, Riemannian metric, material connection, geodesics, autoparallel curves

1. Introduction

The theory of materially uniform but inhomogeneous bodies has been presented by Noll [1] in a seminal paper and expanded by Wang [2]. A recent monograph by Epstein and Elzanowski [3] (see also [4]) describes in a thorough and apt way this theory while giving variable extensions and applications. The starting point is the notion of a material isomorphism which is a linear transformation between tangent spaces that leave the energy invariant.

Based on the notion of a material isomorphism, or the equivalent notion of uniform reference [1], two geometric structures can be defined on the body manifold when a uniform reference is given. The first is given by the material connection and the other by the intrinsic Riemannian metric. The material connection has non-vanishing torsion and zero curvature, while the Riemannian connection has zero torsion but non-vanishing curvature, in general. Related with these structures there are two important classes of curves: geodesics and autoparallel curves.

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In pure mathematics a geodesic is defined as a curve of shortest length between two points of a manifold, while along autoparallel curves vector fields are parallely transported. For a materially uniform body the existence of a material isomorphism between two points give a way to relate these points from the mechanical point of view. In this respect, geodesics and autoparallel curves should be reinterpreted for the mechanical theory in such a way as to incorporate the mechanical part.

The decisive answer to what structure should be used for the body is given by the symmetry group of the material. For a discrete symmetry group the structure induced by the material connection characterizes the body [1]. On the other hand, when the symmetry group is continuous it is the Riemannian structures that characterize the body [1].

The geometric approach to dislocation theory has been also the topic of a very recent paper by Yavari and Goriely [5]. These authors transform the anelastic problem to an elastic problem by putting the dislocated problem in the appropriate material manifold. This manifold is a stress-free non-Euclidean material manifold which is constructed using Cartan's moving frames. It is produced as follows. If one starts with a dislocated body in order to relax the body from the internal stresses he has to cut it into small pieces. By allowing its piece to relax separately the collection of the relaxed pieces do not match in a Euclidean space. However, by assuming that the relaxed pieces lie in a non-Euclidean material manifold they fit together. This configuration is the starting point for these authors. Their analysis is extended to disclinations and thermal effects as well [6, 7]. Within this geometric framework they also evaluate the internal stress field for many interesting cases. The calculation of internal stresses in dislocation theory has been also part of the work of Acharya [5], Zubov [9], Rosakis-Rosakis [10], Sfyris et al. [11].

There is a basic difference between the approach of materially uniform but inhomogeneous bodies [1, 3] and the approach adopted by Yavari and Goriely [5, 6]. The first theory views the curvature tensor as being a characteristic of a body with a continuous symmetry group, while the latter theory attributes the curvature tensor to the existence of disclinations in the body.

Our work follows the theory of materially uniform but inhomogeneous bodies and the major contributions are at two levels: (i) we define geodesics and autoparallel curves for materially uniform but inhomogeneous bodies; (ii) these curves are used to construct the stress-free material manifold which play the role of the reference configuration for the dislocated problem. In particular, we propose an alternative way for constructing this manifold: while Yavari and Goriely [5] utilize the moving frames of Cartan, we use the autoparallel and geodesic lines for the theory of materially uniform and inhomogeneous bodies.

Given a uniform reference and a symmetry group for the material, it is a natural question to ask what kind of energy can support such a body. We present some fundamental examples for the case of a continuous symmetry group for a solid body; isotropic and transversly isotropic. For the discrete case, we work with the triclinic system and the pinacoidal class [12] and give a generic way for finding energies that can support a materially uniform but inhomogeneous body of discrete symmetry. We also give the norm for the space of uniform reference and for the dislocation density tensor as well.

Attention is then focused to a special choice of the uniform reference for a body with a continuous symmetry group that corresponds to a continuous distribution of edge dislocations. We built up the geodesic equations and solve them numerically for two kind of functions describing the defects: linear and tetragonal. They correspond to a constant and linear distribution of dislocations, respectively. As expected, it turns out that the higher the dislocation density, the greater the deviation from the straight line. This way we are able to construct the stress-free manifold that play the role of the reference configuration for this specific dislocated material.

Using the same expression of the uniform reference we set down the system of autoparallel curves. So, we speak about a body with discrete symmetry group. We solve the equations of autoparallel curves analytically for linear and tetragonal functions describing the distribution of the defects. In this way we construct the stress-free material manifold that plays the role of the reference configuration for this body.

The same class of dislocations is studied in [11] where the dislocated body is subjected to antiplane shear. Also, a comparison of this problem with the corresponding elastic problem is given in [13]. Even though the defects are the same, the approach adopted here differs from that of [11, 13] in the sense that the body is not subjected to an elastic deformation. The dislocations are fixed once and for all and we construct the intermediate configuration when viewed as a non-Euclidean manifold. A recent study concerning the role of a continuous symmetry group in the uniqueness of the uniform reference is given in [14].

The paper is organized as follows. Section 2 contains the definition of geodesics and autoparallel curves for materially uniform but inhomogeneous bodies. Section 3 deals with the role played by these curves in constructing the stress-free manifold that play the role of the reference configuration for a dislocated body. It includes also a generic scheme for constructing this manifold as well as a discussion of the role of the internal stresses under the above prism.

Section 4 presents some fundamental examples for the energy that accompany dislocated bodies with continuous and discrete symmetry group. Also, the norm for the space of uniform reference and for the dislocation density tensor is given. The next two sections focus to a specific expression of the uniform reference that correspond to a body with a continuous distribution of edge dislocations. In Section 5 we set down the equations of autoparallel curves and solve them numerically. Section 6 deals with the autoparallel curves which are solved analytically. Section 7 concludes with the main outcomes of the paper.

2. Riemannian geodesics: autoparallel curves

In pure mathematics a geodesic line is a line of shortest length between two different points of a manifold. In mechanics a material point is defined by attaching to every point of the manifold a scalar valued function; the energy, W.[1] So, while for the mathematical theory the arena is simply the manifold, for a mechanical theory to be properly introduced one has to specify the energy function as well. In this respect, geodesics should be reinterpreted for the mechanical theory in such a way as to incorporate the mechanical part.

For a materially uniform body this is feasible starting from the notion of a material isomorphism. A material isomorphism is a non-singular linear mapping from the tangent space of a material point X to the tangent space of a distinct material point Y, such that the energy W remains invariant [1–3]. If, for every point of the body $\mathcal{B}$, there exists a material isomorphism, then the collection of all of these isomorphisms is named material uniformity and defined as

$$\Phi(X, Y) : T_X\mathcal{B} \to T_Y\mathcal{B} \tag{2.1}$$

$$W(F\Phi(X, Y), Y) = W(F, X), \tag{2.2}$$

which should hold for every $X, Y \in \mathcal{B}$. If there exists a material uniformity, then the body is called materially uniform and it is made of the same material at every point.

In formulas (2.1) and (2.2) F stands for the deformation gradient, while $T_X\mathcal{B}$ for the tangent space of an arbitrary material point $X \in \mathcal{B}$. Essentially, a material isomorphism—a particular member of the material uniformity for specific points—is a mapping of a neighborhood of a point to a neighborhood of a different point that leaves the energy invariant. The mathematical characterization stems from the property of being a non-singular linear mapping between vector spaces, while the mechanical significance is revealed by the statement that the energy if left invariant under this mapping.

The existence of a material uniformity in a body gives a way to compare the mechanical response at two different points of the body. When such a mapping can be singled out, geodesics can be defined as the curves of shortest length between two different points $X, Y \in \mathcal{B}$ that leave the energy invariant. The statement that the energy should be invariant introduces the mechanical part of the theory and differentiates it from the pure mathematical one. Stated another way, one may say that a geodesic line is a line of shortest length among all of those lines that leave the energy invariant.

Essentially, the geodesic line is a line in $\mathcal{B}$ when the way of correlating two different points, from the mechanical point of view, is given by the material uniformity. So, one has to differentiate this analysis from the one seeking geodesics in the space of pairs $(X, W), X \in \mathcal{B}, W \in R$, which has the structure of a bundle. One may want to give the notion of a geodesic in this space and not on the body $\mathcal{B}$. In such a case every point of this space is a mechanical state of the body. Thus, a geodesic is a line of shortest length along two different mechanical states of the body. Such models are given in the work of Noll [16], where the idea of a state of a mechanical system is used. In such an analysis along a geodesic the energy should attain its minimum which is not the case here, since the energy remain invariant.

The equations of geodesic are given using a quantity equivalent to the material uniformity; the uniform reference. According to Noll [1] (see also [2, 3]) if there exists a function W_U such that

$$W(\mathbf{F}, \mathbf{X}) = W_U(\mathbf{M}) = W_U(\mathbf{FK}), \tag{2.3}$$

then $\mathbf{K}^{-1}$ is called a uniform reference for the body. One step further, if $\mathbf{K}^{-1}$ can be written as a gradient of a vector field globally on the body, then $\mathcal{B}$ is homogeneous and no dislocations exist. If it cannot be written as a gradient then the dislocation density tensor is defined as (see [17, 18])

$$\hat{\boldsymbol{\alpha}} = \mathrm{Curl}\mathbf{K}^{-1}, \tag{2.4}$$

for its two point expression, while for the full expression in $\mathcal{B}$ one has the true dislocation density tensor

$$\boldsymbol{\alpha} = (\det\mathbf{K})\mathbf{K}^{-1}\hat{\boldsymbol{\alpha}}. \tag{2.5}$$

From the physical point of view, $\mathbf{K}^{-1}$ describes the relaxation process from the internal stresses that the dislocations presence brings about [3, 18, 19].

When a uniform reference is given it induces to the body a Riemannian structure [1,3] defined by the metric

$$\mathbf{G} = \mathbf{K}^{-\mathrm{T}} \cdot \mathbf{K}^{-1}. \tag{2.6}$$

This Riemannian metric is induced in the body by the inner product

$$u * v = (\mathbf{K}^{-1}u) \cdot (\mathbf{K}^{-1}v), \tag{2.7}$$

where u, v belong to the tangent space of the body at a material point. In Equation (2.7) the symbol $\cdot$ denotes the Euclidean inner product. The Riemannian connection corresponding to this metric is given as

$$\Gamma^A_{BC} = \frac{1}{2}G^{-1AD}(-G_{BC,D} + G_{CD,B} + G_{DB,C}), \tag{2.8}$$

where the inverse of $\mathbf{G}$ is denoted by $\mathbf{G}^{-1}$. The connection Γ^A_{BC} has non-zero curvature and zero torsion.

The geodesics related with the above-defined Riemannian connection are given by the following system of ordinary differential equation

$$\frac{d^2X^A}{dt^2} + \Gamma^A_{BC}\frac{dX^B}{dt}\frac{dX^C}{dt} = 0. \tag{2.9}$$

These are curves $X^A(t), t \in (\alpha, \beta)$, that minimize the length between material points in the body $\mathcal{B}$, while keeping the energy invariant. Essentially, the body $\mathcal{B}$ when equipped with the Riemannian connection Γ^A_{BC} becomes a Riemannian manifold. This geometric structure is produced by pulling back the Euclidean structure using the mapping $\mathbf{K}^{-1}$.

When a body is not materially uniform it is not possible to single out a mapping with the properties of material uniformity so there is no way, in general, for someone to relate mechanically the material at different points. Thus, in this case geodesics boil down to the common mathematical geodesics. The mechanical part of the theory does not participate at all. So, if we consider a Cartesian coordinate system and a non materially uniform body the geodesics are going to be straight lines.

Material uniformity, being a means to relate two different material points, gives also a way to characterize two vectors as being materially parallel. Two vectors at (the tangent spaces of) different material points are called materially parallel if it holds [1–3]

$$\vec{c}(X) = \Phi(X, Y)\vec{c}(Y), \tag{2.10}$$

where $\vec{c}(X) \in T_X\mathcal{B}$, $\vec{c}(Y) \in T_Y\mathcal{B}$. So, autoparallel curves for materially uniform bodies are curves along which a vector field is materially parallely transported. The mechanical significance lies in the fact that the notion of parallelity is defined through $\Phi(X, Y)$, that leaves the energy invariant. Thus, we speak about a parallel transporting of vectors that leave the mechanical ingredient – the energy-invariant.

The material connection is

$$\bar{\Gamma}^A_{BC} = K^{-1}{}^{\alpha}_{B,C}K^A_{\alpha} = -K^{-1}{}^{\alpha}_{B}K^A{}_{\alpha,C}. \tag{2.11}$$

It is produced by seeking the mathematical conditions for a smooth vector field to be materially parallel with respect to a given uniformity field (see [3, pp. 16–18] and [5]). It has zero curvature but non-zero torsion tensor defined by

$$T^A_{BC} = \bar{\Gamma}^A_{BC} - \bar{\Gamma}^A_{CB}. \tag{2.12}$$

Autoparallel curves are described by the following system of ordinary differential equations [20]

$$\frac{d^2X^A}{dt^2} + \bar{\Gamma}^A_{BC}\frac{dX^B}{dt}\frac{dX^C}{dt} = 0. \tag{2.13}$$

These are curves $X^A(t), t \in (a,b)$, on $\mathcal{B}$ along which a vector field is materially parallel transported. In contrast, in pure mathematics, these are the curves along which a vector field is parallely transported in the sense of the space where the body is imbedded. The mechanical part does not appear at all in this case and the energy should be omitted. For a Euclidean body that refers to a Cartesian coordinate system the autoparallel curves are straight lines. The body $\mathcal{B}$ equipped with the material connection $\bar{\Gamma}^A_{BC}$ becomes a Weitzenbroeck manifold in the sense of Yavari and Goriely [5].

3. Use of the geodesics and autoparallel curves – internal stresses

The decisive answer to what structure should be used for the body is given by the symmetry group of the material. For a discrete symmetry group the structure induced by the material connection characterizes the body [1]. On the other hand, when the symmetry group is continuous it is the Riemannian structure that characterizes the body [1]. Thus, when geodesics are mentioned tacitly we speak about a body with a continuous symmetry group (isotropic or transversly isotropic). When autoparallel curves are mentioned tacitly we speak about a body with a discrete symmetry group (examples of energies accompanying such bodies are given in the following section).

A question that naturally arises is concerned with the use of these curves in dislocation theory. For explaining this we need some preparatory observations. Suppose that one has a dislocated body. In general, the existence of these defects leads to a field of non-vanishing internal stresses in the body.[2] If one is willing to relax the body from the internal stresses he dissects it into small pieces and allow each one to relax separately. The collection of those small relaxed pieces do not match together to give a connected body when they are assumed to lie in a Euclidean space. However, if we assume that they lie in a non-Riemannian manifold, by appropriately choosing a connection, the collection of the relaxed pieces fit together to give a connected body [18, 19, 21, 22]. This body would then be connected and stress-free since it is relaxed from the internal stresses.

Now suppose that an initially dislocated body has internal stresses and lies in the Euclidean space. So, the geodesics are straight lines. By relaxing this body from the internal stresses we obtain a collection of points ($\mathcal{B}$) equipped with the Riemannian connection Γ^A_{BC}. This $\mathcal{B}$ is the stress-free manifold which is also connected since it is visualized as a non-Euclidean space. The price that we pay for relaxing the stresses is that the stress-free body is curved. The geodesics of this manifold are also curved and provide its shape. So, by juxtaposing the straight geodesics (that correspond to the dislocated body that lies in a Euclidean space) to the curved geodesics (that correspond to the relaxed stress-free non-Euclidean manifold) we are able to see the shape the body obtains after the relaxation. For a geodesically complete body one may construct the whole stress-free body by covering it with a congruence of geodesics. In this respect, geodesics are used for constructing the stress-free non-Euclidean material manifold.

From the mathematical point of view the covering of the body by a congruence of geodesics is done as follows. Say that the three-dimensional body is defined by the components of its points (X^1, X^2, X^3) with respect to a coordinate system. These components take values in subsets of the real line $\mathcal{R}$: (R_1, R_2, R_3). For example, (R_1, R_2, R_3) can be the set $([1.0, 1.8], [1.0, 1.8], [1.0, 1.8])$; so when (X^1, X^2, X^3) vary in this set the body is a cube (this would also be the case for the examples of the last two sections). In order to find the congruence of curves covering the body one has to solve the geodesics equations, (2.9), for the coordinate surfaces, namely for

$$\begin{aligned}
&X^1(t=0) = \text{constant}, && X^2(t=0) = b, && X^3(t=0) = c, \\
&X^1(t=0) = a, && X^2(t=0) = \text{constant}, && X^3(t=0) = c, \\
&X^1(t=0) = a, && X^2(t=0) = b, && X^3(t=0) = \text{constant},
\end{aligned} \tag{3.1}$$

where a, b, c take all possible values of the sets R_1, R_2, R_3, respectively. In this way the totality of geodesics that cover the body can be constructed. For the particular case of the cube mentioned earlier, a, b, c range over the sets $([1.0, 1.8], [1.0, 1.8], [1.0, 1.8])$. So, by solving the geodesic equations with the above conditions one evaluates the geodesics for all faces of the cube. This way the cube is covered by a congruence of geodesic curves.

A different procedure for constructing the same stress-free manifold is given by Yavari and Goriely [5]. They used Cartan's moving frames in order to construct this manifold that play the role of the reference configuration in dislocation theories. It is essentially, the intermediate configuration in elastoplasticity theories.

In an analogous fashion, autoparallel curves are used to construct the non-Euclidean manifold that corresponds to a dislocated body with a discrete symmetry group. In this case the relaxed manifold is the body equipped with the geometric structure induced by the material connection $\bar{\Gamma}^A_{BC}$. So, by using autoparallel curves the stress-free material manifold that play the role of the reference configuration in dislocation theory can be constructed. For covering the body with a congruence of autoparallel curves one has to solve the autoparallel equations, (2.13), with

$$\begin{aligned} &X^1(t=0)=\text{constant}, && X^2(t=0)=b, && X^3(t=0)=c,\\ &X^1(t=0)=a, && X^2(t=0)=\text{constant}, && X^3(t=0)=c,\\ &X^1(t=0)=a, && X^2(t=0)=b, && X^3(t=0)=\text{constant}, \end{aligned} \tag{3.2}$$

where a, b, c range over the sets R_1, R_2, R_3, respectively. As in the previous discussion of geodesics, the sets R_1, R_2, R_3 define the material body based on the components of the material points with respect to a coordinate system.

The space constructed in this way is non-Euclidean according to standard works on the topic [18, 21, 22]. To make this idea more clear in the above framework, imagine the one-dimensional case. The body is assumed to be a straight line. By relaxing the body from the internal stresses, one obtains a curved line. This is the non-Euclidean space: the curved line that corresponds to the relaxed connected body. Nothing is said so far for the space where this object is observed in order to be realizable. One needs a higher-order space in order to realize this one-dimensional non-Euclidean space; a two-dimensional Euclidean space can be used for this purpose.

The same idea may be generalized to higher dimensions as follows. For the two-dimensional case the Euclidean internally stressed body is a plane. By relaxation we obtain a curved surface. This is the connected non-Euclidean space: the points that constitute the curved surface. Nothing has been said so far for the space where this body is embedded in order to be amenable to observation. A three-dimensional Euclidean space can be used since the relaxed space 'goes out' of the two dimensions. The same idea can be generalized to higher dimensions. In general, the non-Euclidean space that is produced by the relaxation has the same dimension as the initial one but it is curved in the about sense. So, in order to be realizable to senses one has to embed it into a higher-order Euclidean space.

Since the stresses the body is relaxed from are the internal stresses, it is natural to examine the role played by these stresses in the above discussion. In this respect one has to remember that the specific expression of the energy, that introduces the constitutive law, has not been introduced yet. The energy interferes up to the existence of a W_U such that $W(F, X) = W_U(M)$ holds. Only the existence of such a function suffices for the construction of the stress-free material manifold using the above-described procedure. Thus, the construction of the stress-free material manifold for materially uniform but inhomogeneous bodies depends on the dislocation distribution and the energy up to the existence of a W_U such that Equation (2.3) hold. The existence of such a W_U allows the introduction of the parallelity through the uniform reference. However, one has to pay attention that a specific form of the strain energy (e.g. neo-Hookean or so) has not been introduced so far.

When this is done the stress field is given as (see, e.g., [5, 11])

$$\mathbf{T} = \frac{\partial W_U}{\partial \mathbf{M}} \mathbf{K}^{\mathrm{T}}, \tag{3.3}$$

with $\mathbf{T}$ being the first Piola–Kirchhoff stress tensor. We obtain the internal stress field by putting $\mathbf{F} = \mathbf{I}$ in the last formula to express the lack of external loading. So, while geodesic and autoparallel curves depend on the dislocation density and are insensitive to the constitutive law (up to the existence of a W_U) internal stresses vary for different materials. Thus, even though geodesics are the same for different materials (with the same distribution of dislocations) internal stresses differ. This is reasonable since the stresses necessary to put the material back to the Euclidean space (these are the internal stresses [23]) should take into account what the material is made of.

4. Energy expressions – norm for the dislocation density

Given a uniform reference it is a natural question as to what kind of energy can accommodate the symmetries of a material. When the body is isotropic the following expressions for the energy may be used

$$W_U = W_U(I_i(\mathbf{M}^{\mathrm{T}}\mathbf{M})), \tag{4.1}$$

where $I_i(\mathbf{M}^T\mathbf{M}),\ i = 1, 2, 3$ are the invariants of the tensor $\mathbf{M}^T\mathbf{M}$. Such expressions for the energy are used in the literature [5, 8, 11]. For transversly isotropic bodies an expression for the energy with the basic invariants may be used as well. For example, an energy of the form

$$W_U = W_U(\mathbf{k} \cdot \mathbf{M}^T\mathbf{M}\mathbf{k}), \tag{4.2}$$

where $\mathbf{k}$ is the vector that defines the axis of symmetry can be used. A complete list of invariants for this case is given in [24], which is a study for the elasticities of a transversly isotropic body with residual-internal stresses. This is also the case here, since the residual stresses stem from the existence of the dislocations.

It is also natural to ask what expression of energy can accommodate a uniform reference when the symmetry group is discrete. As an example we study the case of a triclinic system and the pinacoidal class. The following elements belong to this symmetry group [12]

$$\mathbf{I}, -\mathbf{I}. \tag{4.3}$$

The invariants of a symmetric tensor $\mathbf{N}$ under this class are given by the following integrity basis

$$N_{11}, N_{12}, N_{23}, N_{31}, N_{22}, N_{33}, \tag{4.4}$$

which are the independent components of $\mathbf{N}$. So, for our case if we take any polynomial expression of the following quantities

$$(\mathbf{M}^T\mathbf{M})_{11}, (\mathbf{M}^T\mathbf{M})_{12}, (\mathbf{M}^T\mathbf{M})_{23}, (\mathbf{M}^T\mathbf{M})_{31}, (\mathbf{M}^T\mathbf{M})_{22}, (\mathbf{M}^T\mathbf{M})_{33}, \tag{4.5}$$

it would serve as an invariant under this symmetry group function that fulfils the material isomorphism requirement, Equation (2.3). This is for the case of a discrete symmetry group an energy that can serve for the description of a materially uniform but inhomogeneous body with the pinacoidal class of the triclinic symmetry group, which is discrete. Finding the integrity bases for a symmetric matrix related with a discrete symmetry group and applying it to the matrix $\mathbf{M}^T\mathbf{M}$ of our theory gives, in general, the ingredients of an energy that can accommodate a body with discrete symmetry group.

In order to quantify the dislocation density, when the uniform reference is given, we use a norm, based on the theoretical work of Weyl [25], which has been used by Acharya [8] also. The starting point is the inner product in the space D of a square integrable 3×3 matrix field in $\mathcal{B}$

$$(A, B)_D = \int_{\mathcal{B}} A_{ij}B_{ij}\, dV. \tag{4.6}$$

The linear subspace of D of all of those elements that can be written as a gradient is defined as

$$N_{||}(Curl) = \{W \in D : \int_{\mathcal{B}} W_{rk}e_{kji}Q_{ri,j} = 0, \forall Q \in T\}, \tag{4.7}$$

where T is the set of continuous test functions with vanishing tangential component on the boundary of $\mathcal{B}$ and at least piecewise continuous first derivatives in $\mathcal{B}$. The orthogonal complement of this space is the space where the uniform reference belongs

$$N(Curl) = \{Z \in D : \int_{\mathcal{B}} Z_{ij}Y_{ij} = 0, \forall Y \in N_{||}(Curl)\}. \tag{4.8}$$

Being a linear subspace of the space of square integrable 3×3 matrices the space $N(Curl)$ inherits the inner product as well as the norm, induced by the inner product, which is

$$||\mathbf{K}^{-1}||_2 = \left(\int_{\mathcal{B}} |\mathbf{K}^{-1}|^2\, dV\right)^{1/2}. \tag{4.9}$$

The last relation may be written in components as

$$||\mathbf{K}^{-1}||_2 = \left(\int_{\mathcal{B}} K_{ij}^{-1}K_{ij}^{-1}\, dV\right)^{1/2}. \tag{4.10}$$

For the dislocation density tensor, we use the same norm as follows

$$||\boldsymbol{\alpha}||_2 = \left(\int_{\mathcal{B}} \alpha_{ij}\alpha_{ij}\, dV \right)^{1/2}. \tag{4.11}$$

The last relation gives the norm that we are going to work with in order to measure the dislocation density.

5. Riemannian geodesics

In this section for a specific expressions of the uniform reference we built up and solve the geodesic equations numerically. The body is assumed to be a cube defined with respect to a Cartesian coordinate system by

$$\begin{aligned} 1.0 &\leq X^1 \leq 1.8, \\ 1.0 &\leq X^2 \leq 1.8, \\ 1.0 &\leq X^3 \leq 1.8. \end{aligned} \tag{5.1}$$

The arguments of this section pertain to a material with a continuous symmetry group. Therefore, for a solid body we speak about isotropy or transverse isotropy. Expressions for the energy that can support such a body are given in Equations (4.1), (4.2).

We choose the field $\mathbf{K}^{-1}$ as follows

$$\mathbf{K}^{-1}(X^1) = \begin{pmatrix} 1 & K^{-1}_{12}(X^1) & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{5.2}$$

For this expression the only non-vanishing component of the dislocation density tensor $\boldsymbol{\alpha}$ is the α_{31} and has the form

$$\alpha_{31} = -K^{-1}_{12,1}. \tag{5.3}$$

The component K^{-1}_{12} cannot vanish since this would indicate the absence of dislocations, $\mathbf{K}^{-1} = \mathbf{I}$. Also

$$\alpha_{31} \neq 0 \quad \text{or} \quad -K^{-1}_{12,1} \neq 0. \tag{5.4}$$

If the latter constraint does not hold the tensor $\mathbf{K}^{-1}$ can be written as a gradient. The choice of $\mathbf{K}^{-1}$ in Equation (5.2) corresponds to a continuous distribution of edge dislocations with Burgers vector in the X^1 direction and dislocation line in the X^3 direction.

The non trivial elements of the Riemannian connection for this case are

$$\begin{aligned} \Gamma^1_{11} &= -K^{-1}_{12}K^{-1}_{12,1}, \\ \Gamma^1_{12} &= \Gamma^1_{21} = (K^{-1}_{12})^2 K^{-1}_{12,1}, \\ \Gamma^1_{22} &= -[1 + (K^{-1}_{12})^2](K^{-1}_{12})^2 K^{-1}_{12,1}, \\ \Gamma^2_{11} &= K^{-1}_{12,1}, \\ \Gamma^2_{12} &= \Gamma^2_{21} = K^{-1}_{12}K^{-1}_{12,1}, \\ \Gamma^2_{22} &= (K^{-1}_{12})^2 K^{-1}_{12,1}, \end{aligned} \tag{5.5}$$

which all vanish in the absence of dislocations. Using Equation (2.9) the geodesics related with the Riemannian structure are

$$\begin{aligned} &\frac{d^2X^1}{dt^2} - K^{-1}_{12}K^{-1}_{12,1}(\frac{dX^1}{dt})^2 - 2(K^{-1}_{12})^2K^{-1}_{12,1}\frac{dX^1}{dt}\frac{dX^2}{dt}, \\ &\qquad\qquad - \left[1 + (K^{-1}_{12})^2\right](K^{-1}_{12})^2K^{-1}_{12,1}(\frac{dX^2}{dt})^2 = 0 \\ &\frac{d^2X^2}{dt^2} + K^{-1}_{12,1}(\frac{dX^1}{dt})^2 + 2K^{-1}_{12}K^{-1}_{12,1}\frac{dX^1}{dt}\frac{dX^2}{dt} + (K^{-1}_{12})^2K^{-1}_{12,1}(\frac{dX^2}{dt})^2 = 0, \\ &\frac{d^2X^3}{dt^2} = 0. \end{aligned} \tag{5.6}$$

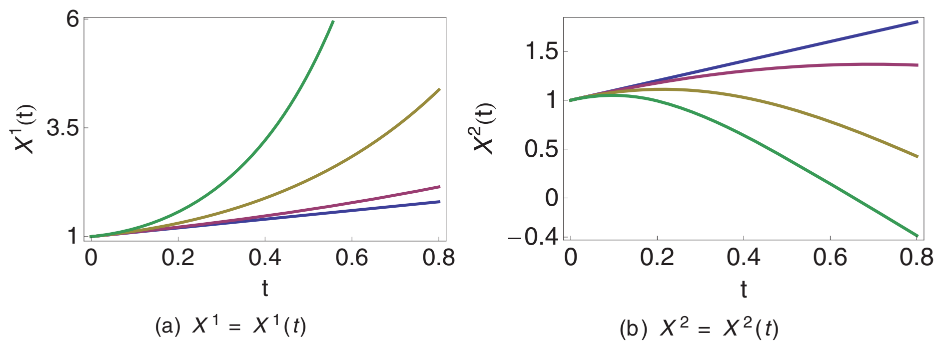

Figure 1. Solution of the components $X^1(t), X^2(t)$ of the geodesic curve for different distribution of constant dislocations. The straight lines correspond to the value $c = 0$ while the curved lines to $c = 0.5, 1.0, 1.5$, respectively.

The third expression of Equation (5.6) may be solved directly to give

$$X^3 = \bar{c}t + \hat{c}, \tag{5.7}$$

where $\bar{c}, \hat{c}$ are arbitrary constants of integration. So, for the problem at hand in the X^3 direction the geodesics are not affected by the defects presence. The dislocation line is along the same direction. When the geodesics are plotted we assume that $X^3 = t + 1$, namely $\bar{c} = 1, \hat{c} = 1$.

We solve numerically the geodesics equations (5.6) by choosing the function K_{12}^{-1} as linear and tetragonal. For the linear choice we make the assumption

$$K_{12}^{-1} = cX^1 \quad \rightarrow \quad \alpha_{31} = -c. \tag{5.8}$$

We have a homogeneous distribution of dislocations, namely at every point the same number of defects. Figure 1(a) and (b) show the numerical solutions for the functions $X^1 = X^1(t)$ and $X^2 = X^2(t)$, respectively, for different values of c. In Figure 1(a) and (b) the straight lines correspond to the case $c = 0$. The lines on its left (right for $X^2 = X^2(t)$) correspond to values $c = 0.5, 1.0, 1.5$, respectively. The dislocation density for these choices is $\alpha_{31} = -0.5, -1.0 - 1.5$, respectively. For the norm we find

$$||\boldsymbol{\alpha}||_2 = \left(\int_1^{1.8} \int_1^{1.8} \int_1^{1.8} \alpha_{31}\alpha_{31}\, dX^1\, dX^2\, dX^3 \right)^{1/2} = \left((0.8)^3 c^2\right)^{1/2}. \tag{5.9}$$

Thus, it turns out, that the higher the dislocation density (greater c) is the greater the deviation from the straight line is.

A three-dimensional plot of the geodesic is given in Figure 2. We plot the straight line for the cube and the geodesic line simultaneously. The straight line correspond to the dislocated body that lies in the Euclidean space. The curved line corresponds to the non-Euclidean stress-free body which is obtained after the relaxation of the internal stresses. Essentially, this body plays the role of the reference configuration for the dislocated problem. By assuming our body to be connected and geodesically complete it can be covered by a congruence of such curves which are no longer straight. The manifold is curved in this sense and represents the non-Euclidean space where the small relaxed pieces are assumed to belong in order to have a connected body.

The curved geodesic depicted in Figure 2 is produced by solving Equations (5.6) with

$$X^1(t = 0) = 1, \quad X^2(t = 0) = 1, \quad X^3(t = 0) = 1. \tag{5.10}$$

In order to cover the stress-free body with a congruence of such curves one has to solve Equations (5.6) for the coordinate surfaces of the body, namely for

$$\begin{aligned} &X^1(t = 0) = \text{constant}, \; X^2(t = 0) = b, \quad\; X^3(t = 0) = c, \\ &X^1(t = 0) = a, \qquad\quad X^2(t = 0) = \text{constant}, \; X^3(t = 0) = c, \\ &X^1(t = 0) = a, \qquad\quad X^2(t = 0) = b, \qquad X^3(t = 0) = \text{constant}, \end{aligned} \tag{5.11}$$

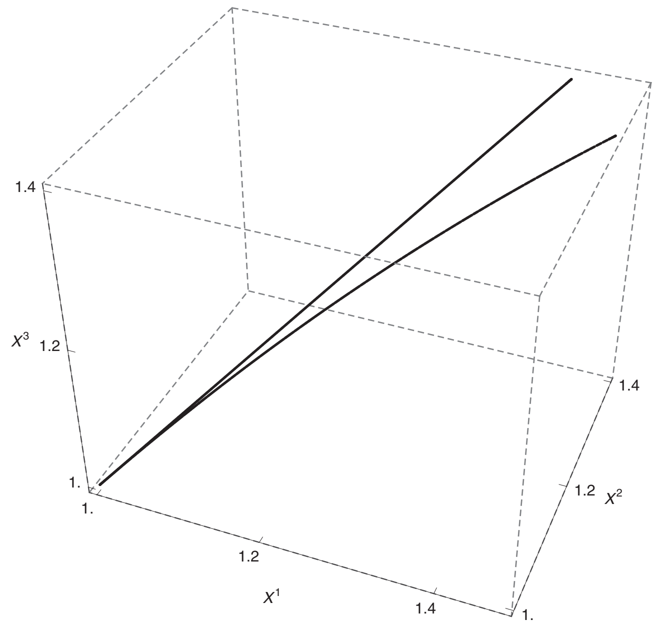

Figure 2. The straight line corresponds to the geodesic of the dislocated body that lie in a Euclidean space. After relaxing the internal stresses in a non-Euclidean space we obtain the curved geodesic. The straight line corresponds to the value $c = 0$, while the curved to the value $c = 0.5$.

with a, b, c taking all possible values in the set $[1.0, 1.8], [1.0, 1.8], [1.0, 1.8]$. The last domain is the one that describes the cube (see Equation (5.1)). So, by solving the geodesic equations for all of the conditions of the above form one obtains the congruence of geodesic curves that cover the body under question, since the geodesics are evaluated for all of the points of the three faces of the cube.

The internal stress field for such a body is calculated in [11] for a neo-Hookean material. As we claimed in the previous section, the shape of the body is insensitive to the specific constitutive law, as far as Equation (2.3) for the energies is valid. The field $\mathbf{K}^{-1}$ plays the important role for this deviation from the straight line and Equation (2.3) allows the introduction of the theory of materially uniform but inhomogeneous bodies. For a different expression of the energy one would result to a different field of internal stresses which is reasonable for the following reason. The internal stresses (at the level of geodesics) are the forces necessary to transform the curved geodesic to a straight line; namely, to put the non-Euclidean body to a Euclidean manifold [23]. These forces should take into account what the material is made of and this is why it is reasonable to have a different internal stress field for different constitutive laws.

For the function K_{12}^{-1} we make a tetragonal assumption as follows

$$K_{12}^{-1} = c(X^1)^2. \tag{5.12}$$

It corresponds to a distribution of dislocations of the form

$$\alpha_{31} = -2cX^1. \tag{5.13}$$

In Figure 3(a) and (b) we plot the numerical solution for $X^1 = X^1(t)$ and $X^2 = X^2(t)$, respectively, for the values $c = 0, 0.3, 0.6, 0.9$. The corresponding dislocation density is $\alpha_{31} = 0, -0.6X^1, -1.2X^1, -1.8X^1$, respectively. For the norm we evaluate

$$||\boldsymbol{\alpha}||_2 = \left(4c^2 \int_1^{1.8} dX^2 \int_1^{1.8} dX^3 \int_1^{1.8} (X^2)^2\, dX^2\right)^{1/2} = 2c\left((0.8)^5/3\right)^{1/2}. \tag{5.14}$$

The straight line correspond to the case $c = 0$. As the distribution of the defects increases we take the lines on the left (right) for $X^1 = X^1(t)$ ($X^2 = X^2(t)$). Thus, the outcome is that the higher the distribution of the defects is, measured by its norm, the greater the deviation from the straight line is for the geodesics in the X^1, X^2 direction.

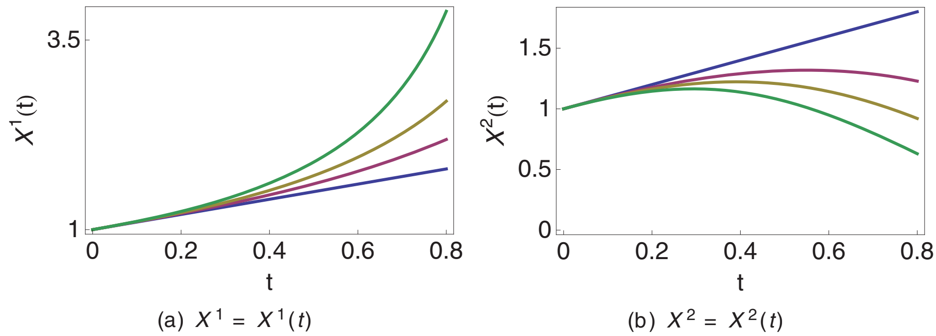

Figure 3. Solution of the functions $X^1(t), X^2(t)$ of the geodesic curve for the choice of a linear distribution of defects. The straight line corresponds to the value $c = 0$, while the curved to values $c = 0.3, 0.6, 0.9$, respectively.

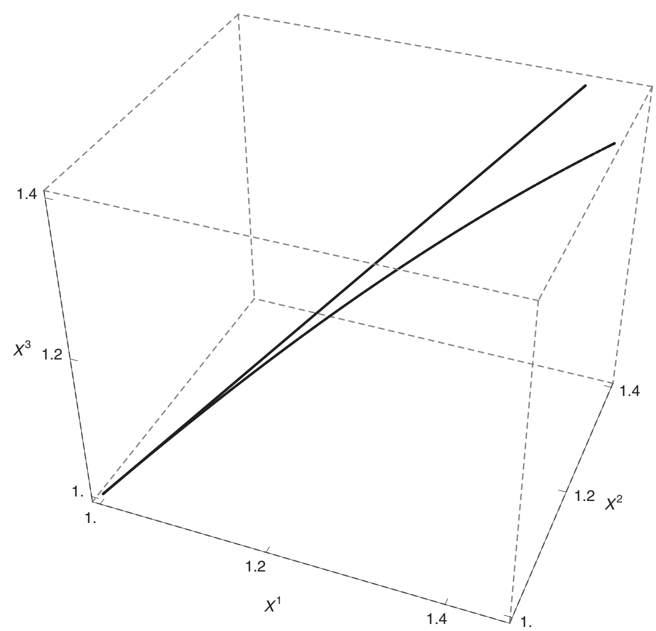

Figure 4. The straight line corresponds to the geodesic of the dislocated body which lie in the Euclidean space. After relaxing the internal stresses in a non-Euclidean space we obtain the curved geodesic. The straight line is for the value $c = 0$, while the curved for the value $c = 0.3$ when we have a linear distribution of defects.

A three-dimensional plot of the geodesics for this case is given in Figure 4. The straight line corresponds to the dislocated body that lies in the Euclidean space. The curved line corresponds to the stress-free body that lies in a non-Euclidean space. By assuming a connected geodesically complete body we can cover it by a congruence of such curves thereby producing the stress-free material manifold.

It should be noted that in all of the above choices the equations are solved for $X^1 = X^1(t), X^2 = X^2(t)$ with the initial conditions $X^1(0) = 1$, $\frac{dX^1}{dt}(0) = 1$, $X^2(0) = 1$, $\frac{dX^2}{dt}(0) = 1$. For the two-dimensional plots we have taken $t \in (0, 0.8)$, while for the three-dimensional plots we have taken $t \in (0, 0.4)$, for a better presentation of the results.

6. Autoparallel curves

In this section for the same expressions of uniform reference we built up and solve analytically the set of autoparallel curves. The body is a cube defined with respect to a Cartesian coordinate system by Equation (5.1). The arguments of this section pertain to a material with a discrete symmetry group. Expressions for the energy that can support such a body are given in Section 3, for the pinacoidal class of a triclinic system. We solve analytically the equations of autoparallel curves and compare them with the straight line. The straight line corresponds to the dislocated body that lies in the Euclidean space. The curved lines that are produced correspond to the stress-free body that is assumed to lie in a non-Euclidean space. This stress-free body is obtained by relaxing the dislocated body from the internal stresses.

For the choice of Equation (5.2) of the uniform reference, the only non-vanishing component of the material connection is

$$\bar{\Gamma}^1_{21} = K^{-1}_{12,1}, \tag{6.1}$$

while the non-trivial component of the torsion tensor associated with this connection acquires the form

$$T^1_{21} = K^{-1}_{12,1}. \tag{6.2}$$

The equations of the autoparallel curves are then (see Equation (2.13))

$$\begin{aligned} &\frac{d^2X^1}{dt^2} + K^{-1}_{12,1}\frac{dX^2}{dt}\frac{dX^1}{dt} = 0,\\ &\frac{d^2X^2}{dt^2} = 0,\\ &\frac{d^2X^3}{dt^2} = 0. \end{aligned} \tag{6.3}$$

The second and the third expressions of Equation (6.3) can be solved directly to give

$$\begin{aligned} X^2(t) &= c_1 t + c_2,\\ X^3(t) &= c_3 t + c_4. \end{aligned} \tag{6.4}$$

With Equations (6.4), the first expression of Equation (6.3) will take the form

$$\frac{d^2X^1}{dt^2} + K^{-1}_{12,1}c_1\frac{dX^1}{dt} = 0. \tag{6.5}$$

In general, this is a nonlinear ordinary differential equation for $X^1(t)$. In order to proceed we make a specific assumption for the function K^{-1}_{12}. We assume that it is a linear and tetragonal function of its argument in order to solve Equation (6.5).

In general, Equation (6.5) belongs to the following class of nonlinear ordinary differential equations of the second order

$$y'' = f(y)y', \tag{6.6}$$

where for us y corresponds to X^1 and the derivative is with respect to t. The generic solution of this class of equations is given as [26]

$$\int \frac{dy}{F(y)+C_1} = C_2 + t, \quad F(y) = \int f(y)\,dy. \tag{6.7}$$

For the linear choice we have

$$K^{-1}_{12} = dX^1 \ \rightarrow\ \alpha_{31} = d, \tag{6.8}$$

namely for a linear choice we have a homogeneous distribution of dislocations; in every point the same amount of dislocations d. With this expression, Equation (6.5) will take the form

$$\frac{d^2X^1}{dt^2} + \bar{d}\frac{dX^1}{dt} = 0, \tag{6.9}$$

where $\bar{d} = dc_1$. So we speak about a linear ordinary differential equation. The solutions of this equation can be found as

$$X^1(t) = c_5\cos(\sqrt{\bar{d}}t) + c_6\sin(\sqrt{\bar{d}}t). \tag{6.10}$$

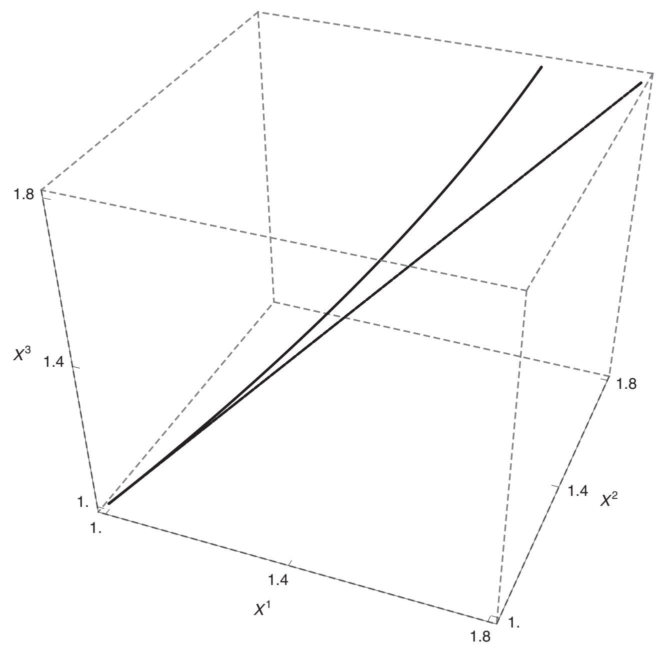

Figure 5. The straight line corresponds to the autoparallel curve of the dislocated body that lies in the Euclidean space. After relaxing the internal stresses in a non-Euclidean space we obtain the curved autoparallel curve. The straight line corresponds to $d = 0$ while the curved to $d = 0.5$.

We plot in Figure 5 the autoparallel curves for $d = 0.5,\ c_1 = 1,\ c_2 = 1,\ c_3 = 1,\ c_4 = 1,\ c_5 = 1,\ c_6 = \frac{1}{\sqrt{0.5}}$. This choice for the constants is taken in order to meet the initial conditions $X^A(t = 0) = 1,\ \frac{dX^A}{dt}|_{t=0} = 1$. With these values the equations of the autoparallel curves are

$$\begin{aligned} X^1(t) &= cos(\sqrt{0.5}t) + \frac{1}{\sqrt{0.5}} sin(\sqrt{0.5}t) \\ X^2(t) &= t + 1, \\ X^3(t) &= t + 1. \end{aligned} \tag{6.11}$$

The straight line is the autoparallel curve of the dislocated body that lies in the Euclidean space, while the curved line is the autoparallel curve of the stress-free body that is assumed to lie in a non-Euclidean space. The internal stresses are the forces the body is relaxed from, or the forces necessary to put the body back to the Euclidean space.

The curved autoparallel depicted in Figure 5 is found by solving Equations (6.3) for the linear choice and for

$$X^1(t = 0) = 1, \quad X^2(t = 0) = 1, \quad X^3(t = 0) = 1. \tag{6.12}$$

In order to construct the congruence of such curves that render the stress-free manifold, one has to solve the equations of the autoparallel Equations (6.3) for the coordinate surfaces of the body, namely for

$$\begin{aligned} &X^1(t = 0) = \text{constant}, && X^2(t = 0) = b, && X^3(t = 0) = c, \\ &X^1(t = 0) = a, && X^2(t = 0) = \text{constant}, && X^3(t = 0) = c, \\ &X^1(t = 0) = a, && X^2(t = 0) = b, && X^3(t = 0) = \text{constant}, \end{aligned} \tag{6.13}$$

where (a, b, c) take values in the domain $[1.0, 1.8], [1.0, 1.8], [1.0, 1.8]$ that defines the body for this case (the cube). So, by solving the autoparallel equations for all of the conditions of the above form one obtains the congruence of curves that covers the body under consideration, since autoparallel curves are evaluated for all of the points of the three faces of the cube.

For the function K^{-1}_{12} we make the following tetragonal assumption

$$K^{-1}_{12} = d(X^1)^2 \ \rightarrow \ \alpha_{31} = 2dX^1. \tag{6.14}$$

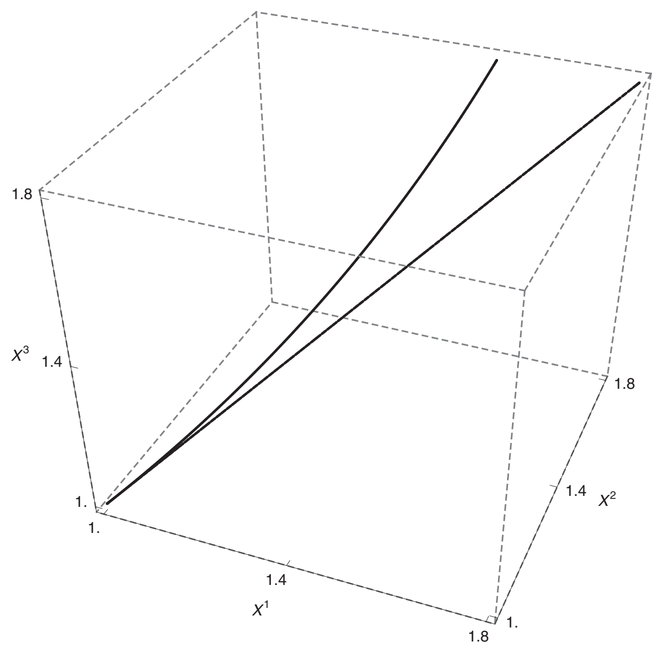

Figure 6. The straight line corresponds to the autoparallel curve of the dislocated body that lies in the Euclidean space. After relaxing the internal stresses in a non-Euclidean space we obtain the curved autoparallel curve. The straight line corresponds to the autoparallel curve of the Euclidean space, while the curved to $d = 0.5$.

With this expression, Equation (6.5) takes the form

$$\frac{d^2X^1}{dt^2} + 2\bar{d}X^1\frac{dX^1}{dt} = 0, \tag{6.15}$$

where $\bar{d} = dc_1$. So we speak about a nonlinear ordinary differential equation. The solution of this equations can be found as

$$X^1(t) = \frac{\sqrt{c_5}}{\sqrt{\bar{d}}}\text{Tanh}\left[\left(\sqrt{\bar{d}}t\sqrt{c_5} + \sqrt{\bar{d}}\sqrt{c_5}\sqrt{c_6}\right)\right] \tag{6.16}$$

For the constant d we assume $d = 0.5$. In order to fulfil the initial conditions $X^A(t = 0) = 1$, $\frac{dX^A(t=0)}{dt} = 1$ for the other constants the following assumptions are made $c_1 = 1,\ c_2 = 1,\ c_3 = 1,\ c_4 = 1,\ c_5 = \frac{3}{2},\ c_6 = ArcSech(\sqrt{\frac{2}{3}})$. With these expressions a three-dimensional plot of the autoparallel curve is given in Figure 6. The straight line is the autoparallel curve for the dislocated body that lies in a Euclidean space. By relaxing the body from the internal stresses the autoparallel is curved. The whole body is therefore curved and represents the non-Euclidean space where the small relaxed pieces are assumed to belong in order to have a connected body.

7. Conclusion

The goal of the present contribution is to highlight the role played by autoparallel and geodesic curves for materially uniform but inhomogeneous bodies. We start by defining such curves for materially uniform but inhomogeneous bodies. We propose their use in order to construct the stress-free non-Euclidean material manifold. This manifold plays the role of the reference configuration for dislocated materials. Essentially, it is the intermediate configuration in plasticity theories. Attention is then focused to the example of a body with a continuous distribution of edge dislocations. Autoparallel equations are solved analytically, while geodesic equations are solved numerically.

Notes

1. Even though a mass density needs to be introduced we suppress its use since it does not result in unpleasant consequences in what follows. However, we should mention that the mass consistency condition of Epstein and Elzanowski [3, p. 11] is assumed to be enforced in order to avoid growth phenomena (for a geometric theory of growth phenomena the interested reader is referred to the work of Yavari [15]). Essentially, this condition guarantees that mass is conserved under the action of the material isomorphism.
2. It is interesting to note that Yavari and Goriely [5] were able to produce some fundamental results of non-trivial dislocation distributions that result to a zero internal stress field.

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Conflict of interest

None declared.

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