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Energy balance invariance for interacting particle systems

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Abstract. This paper studies the principle of invariance of balance of energy and its consequences for a system of interacting particles under groups of transformations. Balance of energy and its invariance is first examined in Euclidean space. Unlike the case of continuous media, it is shown that conservation and balance laws do *not* follow from the assumption of invariance of balance of energy under time-dependent isometries of the ambient space. However, the postulate of invariance of balance of energy under arbitrary diffeomorphisms of the ambient (Euclidean) space, *does* yield the correct conservation and balance laws.

These ideas are then extended to the case when the ambient space is a Riemannian manifold. Pairwise interactions in the case of geodesically complete Riemannian ambient manifolds are defined by assuming that the interaction potential explicitly depends on the pairwise distances of particles. Postulating balance of energy and its invariance under arbitrary time-dependent spatial diffeomorphisms yields balance of linear momentum. It is seen that pairwise forces are directed along tangents to geodesics at their end points. One also obtains a discrete version of the Doyle–Ericksen formula, which relates the magnitude of internal forces to the rate of change of the interatomic energy with respect to a discrete metric that is related to the background metric.

Keywords. Continuum mechanics, particle mechanics, energy balance, covariance.

1. Introduction

This paper is concerned with balance of energy for a system of interacting particles and finds a connection between discrete balance laws and invariance, something that has been studied thoroughly in the setting of continuum mechanics (see [4, 9, 16] and references therein).

Particle mechanics is normally formulated in $\mathbb{R}^3$ via balance laws such as balance of momentum; however, the linear structure of $\mathbb{R}^3$ can sometimes obscure important geometric information; for example, balance of linear momentum is not a *covariant* notion in that it looks rather different in curvilinear coordinates; see [9, 16]. Of course one way to overcome this is to make use of generalized

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coordinates and Lagrangian mechanics. However, another interesting alternative approach, that is also used in geometric continuum mechanics, is to make use of invariance properties of balance of energy. A major goal of this paper is to revisit this issue to bring the theory more into line with what one does in geometric continuum mechanics.

In geometric continuum mechanics, one usually works with two configurations—a reference configuration and a current configuration. The configuration space is the manifold of maps between these two configurations [9]. The current configuration has a clear physical interpretation; it is what one can see in the laboratory. Equilibria of the current configuration in the setting of continuum mechanics correspond to local minima of the corresponding particle system in the case of quasi-static deformations. In the corresponding particle system the resultant force on each particle is balanced by its internal forces. In geometric continuum mechanics, the current configuration evolves in a Riemanninan manifold $(\mathcal{S}, \mathbf{g})$ [9, 16]. The reference configuration on the other hand has a less clear physical interpretation. In the traditional treatments of elasticity it is usually assumed that there is a well-defined stress-free reference configuration. This is not always true as was noticed by Eckart a few decades ago [1, 11]. For an elastic body, in general, one can have a set of natural configurations. So, a stress-free reference configuration could be any of these natural configurations. In the corresponding atomic system a natural configuration would be a local minimum of the energy (or free energy) in the absence of external forces. It should be noted that reference configuration is in some sense arbitrary and one can choose different reference configurations for the same problem (see [17] for some discussions on this).

We should emphasize that we are not criticizing the existing treatments of particle mechanics in Euclidean space. As a matter of fact, this would be the natural way of formulating, for example, molecular systems that are embedded in Euclidean space. However, one should note that even for the simple example for the classical rigid body in rotation about its center of mass, the configuration space is a manifold, i.e. $SO(3)$ and the kinetic energy metric is non-Euclidean. The other thing to note is that studying mechanical systems geometrically can give nontrivial insight into mechanics of particles in Euclidean space. A good example of this is the reduction procedure for studying the dynamics of the *shape space* of a molecule; that is, the space obtained when one eliminates translations and rotations. When this is done, one obtains dynamics on a non-Euclidean space and geometric methods are critical when undertaking such a study. There are many examples of this in the literature in the works of, for example, Littlejohn and Iwai. For a concrete example applied to the analysis of conformation changes in Argon-6, see [15] and references therein.

This paper is structured as follows. In §2 we briefly review the classical theorem of Green, Naghdi and Rivlin and the covariance ideas in elasticity. In §3 we start with balance of energy for a system of interacting particles embedded in Euclidean space and study the consequences of postulating its invariance under different groups of transformations of the ambient space. §4 studies these issues when the ambient space is a Riemannian manifold. Consequences of covariance of energy balance are investigated in detail. Conclusions are given in §5.

2. Energy balance, the Green–Naghdi–Rivlin theorem and covariance in elasticity

In every mechanical system there are balance laws and some associated conserved quantities. For example, in elasticity, one has balance of linear and angular momenta and conservation of mass. One can build a continuum theory by postulating the relevant balance laws. However, one can always question the significance of each balance law and whether they have any intrinsic meanings. Most engineering theories, including the theory of elasticity, are traditionally built with the implicit assumption that the ambient spaces are Euclidean. It turns out that the structure of Euclidean space can obscure the covariance of balance laws since these balance laws look rather different in curvilinear coordinates. A more natural way of building field theories is to assume that the ambient spaces are manifolds. This way, for example, one naturally obtains a covariant theory and, in addition, one can more easily separate the metric dependent and independent relations.

It has long been known that there is a deep connection between balance laws and symmetries (see, for instance, [10]). Noether's theorem, for example, identifies a conserved quantity for each local symmetry of the underlying Lagrangian density. In the case of global symmetries in continuum mechanics Green and Rivlin [4] showed that postulating balance of energy and its invariance under spatial isometries of the Euclidean ambient space, one can obtain conservation of mass and balances of linear and angular momenta.

Motivated by this observation and the fact that balance of energy can always be intrinsically defined Marsden and Hughes [9] developed a covariant theory of elasticity by postulating balance of energy and its spatial covariance. This assumption results in conservation of mass, balance of linear and angular momenta and the Doyle–Ericksen formula. Simo and Marsden [14] derived a material version of Doyle–Ericksen formula in terms of the rotated stress tensor. Recently Yavari et al. [16] studied the covariance concepts in elasticity in some detail, possibility of material covariance of energy balance and the connection between covariance and Noether's theorem. In the case of linearized elasticity, recently it was shown that covariance of a linearized energy balance can give all the field equations of linearized elasticity [19]. See also [18] for a connection between energy balance of a discretized solid and its balance laws.

To the best of our knowledge, there is no systematic study of a possible connection between invariance and balance laws for particle systems. In this paper, we first consider the case in which the ambient space is Euclidean and show that there are some subtle differences between continuum elasticity and a system of interacting particles. In particular, we will show that the Green–Naghdi–Rivlin (GNR) Theorem fails for particle systems. We then define pairwise interactions when the ambient space is a Riemannian manifold and study the consequences of spatial covariance of energy balance. We will also obtain a discrete version of the Doyle–Ericksen formula.

3. Balance of energy for particle systems in Euclidean space

We first consider a system of interacting particles in a Euclidean ambient space and show that, unlike classical elasticity, balance laws do not follow from invariance of energy balance under time-dependent isometries of the Euclidean ambient space. In other words, the GNR Theorem fails. We then show that a modified GNR argument using an enlarged group of transformations works and does give the balance laws for the particle system.

The failure of the GNR theorem

Here, we look at balance of energy for an arbitrary collection of atoms $\mathcal{L}$ and make a connection between invariance of balance of energy for a system of particles and the classical Green–Naghdi–Rivlin Theorem for continuous media. For the sake of simplicity, we restrict ourselves to pairwise interactions. Suppose we are given a collection $\mathcal{L}$ of particles which has the configuration $\{\mathbf{x}^i(t)\}_{i\in\mathcal{L}} \subset \mathbb{R}^n$ at time t. Balance of energy for $\mathcal{L}$ can be written as

$$\frac{d}{dt}\frac{1}{2}\sum_{\substack{i,j\in\mathcal{L}\\ j\neq i}} \phi_{ij}(|\mathbf{x}^i - \mathbf{x}^j|) + \frac{d}{dt}\sum_{i\in\mathcal{L}} \frac{1}{2} m_i \dot{\mathbf{x}}^i \cdot \dot{\mathbf{x}}^i = \sum_{i\in\mathcal{L}} \mathbf{F}^i \cdot \dot{\mathbf{x}}^i, \tag{3.1}$$

where "·" is the standard inner product of $\mathbb{R}^n$, m_i is the mass of particle i and $\mathbf{F}^i$ is the external force on particle i. Balance of energy can be simplified to read

$$\frac{1}{2}\sum_{\substack{i,j\in\mathcal{L}\\ j\neq i}} -\mathbf{f}_{ij}\cdot(\mathbf{v}^i - \mathbf{v}^j) + \sum_{i\in\mathcal{L}} m_i \mathbf{v}^i \cdot \mathbf{a}^i = \sum_{i\in\mathcal{L}} \mathbf{F}^i \cdot \mathbf{v}^i, \tag{3.2}$$

where $\mathbf{v}^i = \dot{\mathbf{x}}^i$, $\mathbf{a}^i = \ddot{\mathbf{x}}^i$,

$$\mathbf{f}_{ij} = -\frac{\partial \phi_{ij}\left(|\mathbf{x}^i - \mathbf{x}^j|\right)}{\partial\,|\mathbf{x}^i - \mathbf{x}^j|}\frac{\mathbf{x}^i - \mathbf{x}^j}{|\mathbf{x}^i - \mathbf{x}^j|}, \tag{3.3}$$

and we have used the standard framework of classical mechanics in which the particle masses are assumed to be time independent. Note that for pairwise interactions

$$\mathbf{f}_{ji} = -\mathbf{f}_{ij}. \tag{3.4}$$

Let us now postulate that balance of energy for $\mathcal{L}$ is invariant under a time-dependent rigid translation of the ambient space $\mathcal{S} = \mathbb{R}^3$. Consider $\xi_t : \mathcal{S} \to \mathcal{S}$, where

$$\mathbf{x}'^i = \xi_t(\mathbf{x}^i) = \mathbf{x}^i + (t - t_0)\mathbf{w}, \tag{3.5}$$

for some arbitrary $\mathbf{w} \in \mathbb{R}^3$. This implies that

$$\mathbf{v}'^i = \mathbf{v}^i + \mathbf{w} \qquad \text{for all } \ i \in \mathcal{L}. \tag{3.6}$$

Also at time $t = t_0$ it is assumed that the body forces $\mathbf{F}^i$ transform as follows (see [9]):

$$m'_i\mathbf{a}'^i - \mathbf{F}'^i = m_i\mathbf{a}^i - \mathbf{F}^i \qquad \text{for all } \ i \in \mathcal{L}. \tag{3.7}$$

Invariance of balance of energy means that

$$\frac{d}{dt}\frac{1}{2}\sum_{\substack{i,j\in\mathcal{L}\\ j\neq i}} \phi'(|\mathbf{x}'^i - \mathbf{x}'^j|) + \frac{d}{dt}\sum_{i\in\mathcal{L}} \frac{1}{2}m'_i\mathbf{v}'^i \cdot \mathbf{v}'^i = \sum_{i\in\mathcal{L}} \mathbf{F}'_i \cdot \mathbf{x}'^i, \tag{3.8}$$

where the primed quantities are related to the unprimed ones through Cartan's classical spacetime theory. Simplifying (3.8) and evaluating it at time $t = t_0$, we obtain

$$\frac{1}{2}\sum_{\substack{i,j\in\mathcal{L}\\ j\neq i}} -\mathbf{f}_{ij} \cdot (\mathbf{v}^i - \mathbf{v}^j) + \sum_{i\in\mathcal{L}} m_i(\mathbf{v}^i + \mathbf{w}) \cdot \mathbf{a}^i = \sum_{i\in\mathcal{L}} \mathbf{F}^i \cdot (\mathbf{v}^i + \mathbf{w}). \tag{3.9}$$

Subtracting (3.2) from (3.9) yields

$$\sum_{i\in\mathcal{L}} m_i\mathbf{w} \cdot \mathbf{a}^i = \sum_{i\in\mathcal{L}} \mathbf{F}^i \cdot \mathbf{w}. \tag{3.10}$$

Because $\mathbf{w}$ is arbitrary one can conclude that

$$\sum_{i\in\mathcal{L}} \mathbf{F}^i = \sum_{i\in\mathcal{L}} m_i\mathbf{a}^i. \tag{3.11}$$

Eq. (3.11) is nothing but Newton's second law for the collection of particles. It is seen that the above postulate does *not* give the known governing equations for each particle. Instead, it gives balance of total linear momentum for the whole collection of particles.

Let us now look at (3.1) and try to rewrite it for an arbitrary subset $\mathcal{M} \subset \mathcal{L}$. This is of course not always possible because in the collection $\mathcal{L}$, each particle interacts with all the other particles and balance of energy for a subcollection cannot be written unambiguously, in general. Note also that energy may not even be conserved locally [2]. In other words, for nonlocal systems a localized balance law, in general, involves a so-called "residual" term.

In the case of pairwise interactions, one may be tempted to write the balance of energy for a subcollection $\mathcal{M} \subset \mathcal{L}$ as follows.

$$\frac{d}{dt}\left\{\frac{1}{2}\sum_{\substack{i,j\in\mathcal{M}\\ j\neq i}}\phi_{ij}(|\mathbf{x}^i-\mathbf{x}^j|)+\sum_{i\in\mathcal{M}}\sum_{j\in\mathcal{L}\setminus\mathcal{M}}\frac{1}{2}\phi_{ij}(|\mathbf{x}^i-\mathbf{x}^j|)\right\} + \frac{d}{dt}\sum_{i\in\mathcal{M}}\frac{1}{2}m_i\dot{\mathbf{x}}^i\cdot\dot{\mathbf{x}}^i=\sum_{i\in\mathcal{M}}\mathbf{F}^i\cdot\dot{\mathbf{x}}^i, \quad (3.12)$$

where we have assumed that the energy of the bond between the particles i and j is equally shared by them in the case of pairwise interactions.* Note also that unlike classical continuum mechanics energy density is not a one-point function, i.e., for a given particle energy has contributions from all the other particles in the collection, in general. Balance of energy (3.12) can be simplified to read

$$\frac{1}{2}\sum_{\substack{i,j\in\mathcal{M}\\ j\neq i}}-\mathbf{f}_{ij}\cdot(\mathbf{v}^i-\mathbf{v}^j)+\sum_{i\in\mathcal{M}}\sum_{j\in\mathcal{L}\setminus\mathcal{M}}-\frac{1}{2}\mathbf{f}_{ij}\cdot(\mathbf{v}^i-\mathbf{v}^j)+\sum_{i\in\mathcal{M}}m_i\mathbf{v}^i\cdot\mathbf{a}^i=\sum_{i\in\mathcal{M}}\mathbf{F}^i\cdot\dot{\mathbf{x}}^i. \quad (3.13)$$

Now let us postulate that this balance law is invariant under an arbitrary time-dependent rigid translation of the ambient space, i.e.

$$\frac{1}{2}\sum_{\substack{i,j\in\mathcal{M}\\ j\neq i}}-\mathbf{f}'_{ij}\cdot(\mathbf{v}'^i-\mathbf{v}'^j)+\sum_{i\in\mathcal{M}}\sum_{j\in\mathcal{L}\setminus\mathcal{M}}-\frac{1}{2}\mathbf{f}'_{ij}\cdot(\mathbf{v}'^i-\mathbf{v}'^j)+\sum_{i\in\mathcal{M}}m'_i\mathbf{v}'^i\cdot\mathbf{a}'^i=\sum_{i\in\mathcal{M}}\mathbf{F}'_i\cdot\dot{\mathbf{x}'}^i. \quad (3.14)$$

Subtracting (3.13) from (3.14) evaluated at $t=t_0$ yields

$$\frac{1}{2}\sum_{\substack{i,j\in\mathcal{M}\\ j\neq i}}-\mathbf{f}_{ij}\cdot(\mathbf{w}^i-\mathbf{w}^j)+\sum_{i\in\mathcal{M}}\sum_{j\in\mathcal{L}\setminus\mathcal{M}}-\frac{1}{2}\mathbf{f}_{ij}\cdot(\mathbf{w}^i-\mathbf{w}^j)+\sum_{i\in\mathcal{M}}m_i\mathbf{w}^i\cdot\mathbf{a}^i=\sum_{i\in\mathcal{M}}\mathbf{F}^i\cdot\mathbf{w}^i, \quad (3.15)$$

where $\mathbf{w}^i=\frac{\partial}{\partial t}\xi_t(\mathbf{x}^i)$. Now if ξ_t is a rigid translation, then $\mathbf{w}^i=\mathbf{c}$, for all $i\in\mathcal{L}$ and hence

$$\sum_{i\in\mathcal{M}}m_i\mathbf{c}\cdot\mathbf{a}^i=\sum_{i\in\mathcal{M}}\mathbf{F}^i\cdot\mathbf{c}. \quad (3.16)$$

Because $\mathbf{c}$ is arbitrary, this then implies that

$$\sum_{i\in\mathcal{M}}\mathbf{F}^i=\sum_{i\in\mathcal{M}}m_i\mathbf{a}^i. \quad (3.17)$$

$\mathcal{M}$ is arbitrary so we can choose $\mathcal{M}=\{i\}$ and hence

$$\mathbf{F}^i=m_i\mathbf{a}^i. \quad (3.18)$$

* Note that $\phi_{ij}(|\mathbf{x}^i-\mathbf{x}^j|)$ is the energy of the pair (i,j). There is a factor $\frac{1}{2}$ in the first term of the left-hand side of (3.12) because in the sum both (i,j) and (j,i) are counted. On the other hand, the factor $\frac{1}{2}$ appears in the second term because it is assumed that the energy $\phi_{ij}(|\mathbf{x}^i-\mathbf{x}^j|)$ is shared equally between the atoms i and j.

This means that the interatomic forces are self-equilibrated, i.e.

$$\sum_{\substack{j\in\mathcal{L}\\ j\neq i}} \mathbf{f}_{ij} = \mathbf{0}, \tag{3.19}$$

which is not always true! This shows that the version of "energy balance" given by (3.12) is *not* invariant under time-dependent rigid translations, in general. This goes back to the nonlocal nature of interactions in a particle system and also the presence of self interactions in a given subset. In other words, balance of energy for the whole system should be considered. See [5] and [6] for similar discussions. In summary, the GNR Theorem fails for a particle system.

Remark. In a nonlocal system, one can unambiguously write a global balance of energy, e.g. (3.1) for our particle system, but passage from a global energy balance to a local energy balance or to a balance of energy for an arbitrary material subset may not be unique [2, 3]. In what follows from here on we only write a global balance of energy and study its invariance (covariance) properties.

The success of a modified GNR theorem

Let us now consider a larger group of transformations for energy balance invariance. Instead of considering balance of energy for $\mathcal{M} \subset \mathcal{L}$ and its invariance under rigid translations, let us look at balance of energy for $\mathcal{L}$ and consider an arbitrary C^1 diffeomorphism $\xi_t : \mathcal{S} \to \mathcal{S}$. Thus, instead of (3.10) we have

$$\frac{1}{2}\sum_{\substack{i,j\in\mathcal{L}\\ j\neq i}} -\mathbf{f}_{ij}\cdot(\mathbf{w}^i-\mathbf{w}^j) + \sum_{i\in\mathcal{L}} m_i\mathbf{w}^i\cdot\mathbf{a}^i = \sum_{i\in\mathcal{L}} \mathbf{F}^i\cdot\mathbf{w}^i, \tag{3.20}$$

where

$$\mathbf{w}^i = \frac{\partial}{\partial t}\xi_t(\mathbf{x}^i). \tag{3.21}$$

Note that

$$\frac{1}{2}\sum_{\substack{i,j\in\mathcal{L}\\ j\neq i}} -\mathbf{f}_{ij}\cdot(\mathbf{w}^i-\mathbf{w}^j) = \sum_{i\in\mathcal{L}}\sum_{\substack{j\in\mathcal{L}\\ j\neq i}} -\mathbf{f}_{ij}\cdot\mathbf{w}^i. \tag{3.22}$$

Hence

$$\sum_{i\in\mathcal{L}}\sum_{\substack{j\in\mathcal{L}\\ j\neq i}} -\mathbf{f}_{ij}\cdot\mathbf{w}^i = \sum_{i\in\mathcal{L}}(\mathbf{F}^i - m_i\mathbf{a}^i)\cdot\mathbf{w}^i. \tag{3.23}$$

This can be rewritten as

$$\sum_{i\in\mathcal{L}}\left[-\mathbf{F}^i - \sum_{\substack{j\in\mathcal{L}\\ j\neq i}}\mathbf{f}_{ij} + m_i\mathbf{a}^i\right]\cdot\mathbf{w}^i = 0. \tag{3.24}$$

Now assuming that ξ_t is such that the $\mathbf{w}^j = \mathbf{0},\ j \neq i$, one obtains

$$\mathbf{F}^i + \sum_{\substack{j\in\mathcal{L}\\ j\neq i}} \mathbf{f}_{ij} = m_i \mathbf{a}^i, \tag{3.25}$$

which is what one expects. Let us now consider a time-dependent rigid rotation in the ambient space, i.e.

$$\xi_t(\mathbf{x}^i) = e^{(t-t_0)\boldsymbol{\Omega}}\mathbf{x}^i \tag{3.26}$$

for some skew-symmetric matrix $\boldsymbol{\Omega}$. This means that $\mathbf{w}^i = \boldsymbol{\Omega}\mathbf{x}^i$ for all $i \in \mathcal{L}$. Obviously, postulating invariance under rigid rotations of the ambient space does not give any new balance laws as a rigid rotation is just a special case of diffeomorphisms considered above in (3.20). In other words, balance of angular momentum is trivially satisfied for a collection of interacting particles. In summary, we have proved the following proposition.

Proposition 3.1. *For a collection of particles with pairwise interactions, postulating balance of energy and its invariance under isometries of the ambient Euclidean space is not enough to find all the balance laws (equations of motion). If, however, one postulates balance of energy and its invariance under arbitrary diffeomorphisms of Euclidean space, then these equations are all obtained.*

Remark. In this paper, we do not consider independent rotations, and in general microstructure, for particles. However, the arguments presented here can be extended to more complicated particle systems, e.g. particle systems with anisotropic interactions, etc.

4. Energy balance for particle systems on Riemannian manifolds

To put the previous results in a more general framework and also for the sake of clarity, completeness, and intellectual satisfaction, let us assume that the particles move on a Riemannian manifold. Although this may seem too abstract at first glance, it is natural to ask how the balance laws look when the ambient space is Riemannian. This is also motivated by the previous covariant formulations of continuum elasticity. We should also mention that there have been recent efforts in formulating mechanics on non-Euclidean spaces, e.g. [12, 13].

Suppose the interacting particles lie in a Riemannnian manifold $(\mathcal{S}, \mathbf{g})$, which we assume is geodesically complete. For the sake of simplicity, let us assume that only two-body interactions are present. Consider two particles $i, j \in \mathcal{L}$, which in the current configuration lie in $\mathcal{S}$, i.e., $\mathbf{x}^i, \mathbf{x}^j \in \mathcal{S}$. We assume that the potential energy of these two particles explicitly depends on their relative distance in the Riemanian manifold. Of course, there may be other possibilities but this assumption would be a good starting point.

As a physical system represented by this model, let us consider a finite number of particles lying on a two-manifold $\mathcal{M} \subset \mathbb{R}^3$ connected to each other by some springs that are constrained to lie in $\mathcal{M}$. Energy of this system is obviously an explicit function of lengths of the springs. Given any two particles, energy of the corresponding spring is minimized when the spring coincides with the geodesic connecting the two points on $\mathcal{M}$. What we find covariantly in the following is balance of forces projected on tangent spaces of $\mathcal{M}$ at particle positions.

As another motivation for studying this model, we should mention the recent work by Kotani and Sunada [7]. Kotani and Sunada [7] consider a weighted finite graph $X = (V, E)$, where V and E are the vertex and edge sets, respectively, and consider a piecewise smooth map Φ from X to a Riemannian manifold $(Y, \mathbf{g})$. They denote the restriction of this map to $e \in E$ by $\Phi_e(t),\ t \in [0,1]$. Then, they define energy of this map as

$$E(\Phi) = \frac{1}{2} \sum_{e\in E} m_E(e) \int_0^1 \left\langle\!\!\left\langle \frac{d\Phi_e}{dt}, \frac{d\Phi_e}{dt} \right\rangle\!\!\right\rangle dt, \tag{4.1}$$

where m_E is a weight function defined on E. They show that a map Φ is a critical map for this energy if and only if Φ_e is a geodesic for every $e \in E$. For such a map, energy is an explicit function of geodesic lengths.

Remark. Note that, for a generic Riemannian manifold and two arbitrary points on the manifold, there may be more than one and even infinitely many distance minimizing geodesics connecting the two points. An example would be the north and south pole of a sphere. Here, we assume that in a given configuration of the particle system there are no pairs of particles lying on such a pair of points.

Let us denote the geodesic connecting $\mathbf{x}^i$ and $\mathbf{x}^j$ by $\ell_{\mathbf{g}}^{ij}$, where it is clear from this notation that the geodesic explicitly depends on the metric $\mathbf{g}$. This curve has a parametrization $\ell : [a,b] \to \mathcal{S}$ and its *length* is defined as

$$L_{\mathbf{g}}(\ell_{\mathbf{g}}^{ij}) = \int_a^b \left\langle\!\!\left\langle \frac{d}{ds}\ell_{\mathbf{g}}^{ij}(s), \frac{d}{ds}\ell_{\mathbf{g}}^{ij}(s) \right\rangle\!\!\right\rangle_{\mathbf{g}}^{\frac{1}{2}} ds, \tag{4.2}$$

where $\langle\!\langle .,. \rangle\!\rangle_{\mathbf{g}}$ is the inner product induced from the Riemannian metric $\mathbf{g}$. Therefore, for $\mathbf{x}^i, \mathbf{x}^j \in \mathcal{S}$

$$\phi_{ij} = \phi_{ij}\left(L(\ell_{\mathbf{g}}^{ij})\right). \tag{4.3}$$

The total interaction energy is defined as

$$e\left(\{\mathbf{x}^i\}_{i\in\mathcal{L}}, \mathbf{g}\right) = \frac{1}{2} \sum_{\substack{j\in\mathcal{L}\\ j\neq i}} \phi_{ij}\left(L_{\mathbf{g}}(\ell_{\mathbf{g}}^{ij})\right). \tag{4.4}$$

Note that we can think of $g_{ij} := L_{\mathbf{g}}(\ell_{\mathbf{g}}^{ij})$ as a discrete metric for the collection $\{\mathbf{x}^i\}_{i\in\mathcal{L}} \subset \mathcal{S}$. Of course, this discrete metric is an explicit function of the background Riemannian metric $\mathbf{g}$. Now balance of energy can be written as

$$\frac{d}{dt}\,\frac{1}{2} \sum_{\substack{i,j\in\mathcal{L}\\ j\neq i}} \phi_{ij}\left(L_{\mathbf{g}}(\ell_{\mathbf{g}}^{ij})\right) + \frac{d}{dt}\sum_{i\in\mathcal{L}} \frac{1}{2} m_i \left\langle\!\!\left\langle \dot{\mathbf{x}}^i, \dot{\mathbf{x}}^i \right\rangle\!\!\right\rangle_{\mathbf{g}} = \sum_{i\in\mathcal{L}} \left\langle\!\!\left\langle \mathbf{F}^i, \dot{\mathbf{x}}^i \right\rangle\!\!\right\rangle_{\mathbf{g}}. \tag{4.5}$$

Note that $\mathbf{F}^i \in T_{\mathbf{x}^i}\mathcal{S}$ is the external force on atom i.

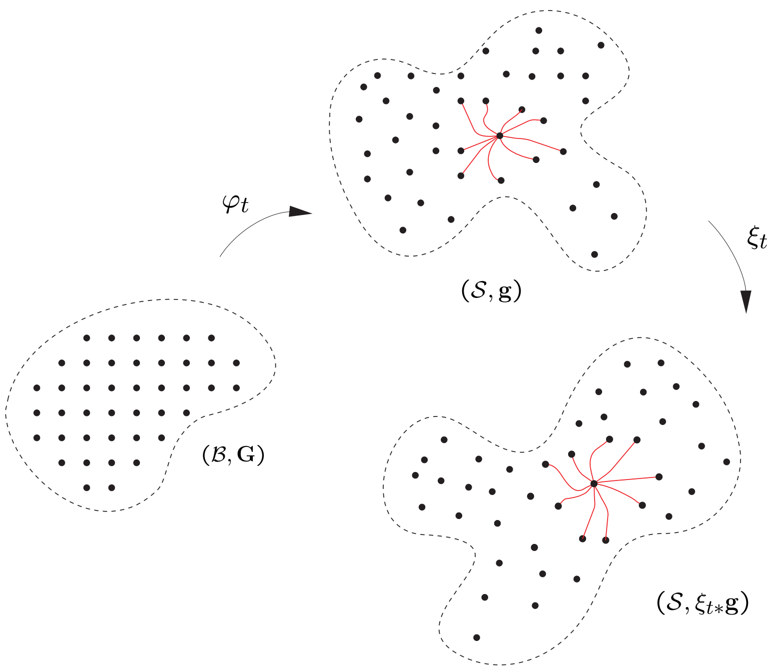

Figure 1. A spatial change of frame for a system of interacting particles.

Let us assume that under a spatial change of frame $\xi_t : \mathcal{S} \to \mathcal{S}$ balance of energy is invariant, i.e.

$$\frac{d}{dt}\,\frac{1}{2}\sum_{\substack{i,j\in\mathcal{L}\\ j\neq i}} \phi'_{ij}\left(L'_{\mathbf{g}'}({\ell'_{\mathbf{g}'}}^{ij})\right) + \frac{d}{dt}\sum_{i\in\mathcal{L}}\frac{1}{2}m'_i\left\langle\!\left\langle \dot{\mathbf{x}}'^i, \dot{\mathbf{x}}'^i\right\rangle\!\right\rangle_{\mathbf{g}'} = \sum_{i\in\mathcal{L}}\left\langle\!\left\langle \mathbf{F}'_i, \dot{\mathbf{x}}'^i\right\rangle\!\right\rangle_{\mathbf{g}'}. \tag{4.6}$$

Note that $\mathbf{g}' = \xi_{t*}\mathbf{g}$ (see Fig. 1). We assume that the pairwise potential transforms tonsorially, i.e.

$$\phi'_{ij}\left(\mathbf{x}'^i, \mathbf{x}'^j, \mathbf{g}\right) = \phi_{ij}\left(\mathbf{x}^i, \mathbf{x}^j, \xi_t^*\mathbf{g}\right). \tag{4.7}$$

Equivalently

$$\phi'_{ij}\left(L_{\mathbf{g}}(\ell^{ij}_{\mathbf{g}})\right) = \phi_{ij}\left(L_{\xi_t^*\mathbf{g}}(\ell^{ij}_{\xi_t^*\mathbf{g}})\right). \tag{4.8}$$

Balance of energy for the new framing at $t = t_0$ reads

$$\sum_{i\in\mathcal{L}} \frac{1}{2} m_i \left\langle\!\left\langle \dot{\mathbf{x}}^i + \mathbf{w}^i, \mathbf{a}^i \right\rangle\!\right\rangle_{\mathbf{g}} + \frac{1}{2} \sum_{\substack{i,j\in\mathcal{L}\\ j\neq i}} \frac{d}{dt}\Big|_{t=t_0} \phi_{ij}\left(L_{\xi_t^*\mathbf{g}}(\ell^{ij}_{\xi_t^*\mathbf{g}})\right) = \sum_{i\in\mathcal{L}} \left\langle\!\left\langle \mathbf{F}^i, \dot{\mathbf{x}}^i + \mathbf{w}^i \right\rangle\!\right\rangle_{\mathbf{g}}, \tag{4.9}$$

where we assumed that $\mathbf{F}'_i - m'_i \mathbf{a}'^i = \xi_{t*}(\mathbf{F}_i - m_i \mathbf{a}^i)$ [9]. Now the nontrivial task is to simplify the second term on the left hand side of Eq. (4.9). Note that given two points in a Riemannian manifold the geodesic and its length both explicitly depend on the metric $\mathbf{g}$. Note also that

$$\frac{d}{dt}\Big|_{t=t_0} \phi_{ij}\left(L_{\xi_t^*\mathbf{g}}(\ell^{ij}_{\xi_t^*\mathbf{g}})\right) = \frac{\partial \phi_{ij}}{\partial g_{ij}} \frac{d}{dt}\Big|_{t=t_0} \left(L_{\xi_t^*\mathbf{g}}(\ell^{ij}_{\xi_t^*\mathbf{g}})\right). \tag{4.10}$$

Before proceeding any further, let us first simplify the balance of energy for the original frame, i.e., the left-hand side of Eq. (4.5)

$$\frac{d}{dt}\frac{1}{2} \sum_{\substack{i,j\in\mathcal{L}\\ j\neq i}} \phi_{ij}\left(L_{\mathbf{g}}(\ell^{ij}_{\mathbf{g}})\right) = \frac{1}{2} \sum_{\substack{i,j\in\mathcal{L}\\ j\neq i}} \frac{\partial \phi_{ij}}{\partial g_{ij}} \frac{d}{dt} L_{\mathbf{g}}(\ell^{ij}_{\mathbf{g}}). \tag{4.11}$$

Consider the geodesic joining the points $\mathbf{x}^i(t), \mathbf{x}^j(t) \in \mathcal{S}$. As these points are time dependent, the geodesic joining them would be time dependent as well, i.e., $\ell = \ell(t,s) := \ell^{ij}_{\mathbf{g}}(t,s)$, where s is the curve parameter and t is time. Note that

$$\frac{d}{dt} L_{\mathbf{g}}(\ell^{ij}_{\mathbf{g}}) = \frac{d}{dt} \int_a^b \langle\!\langle \ell_s, \ell_s \rangle\!\rangle^{\frac{1}{2}} \, ds, \tag{4.12}$$

where $\ell_s = \frac{\partial}{\partial s}\ell(t,s)$ is the velocity of the parameterized geodesic. We assume that the curve ℓ is parameterized by arc length, i.e., it has unit speed everywhere. Thus

$$\frac{d}{dt} \int_a^b \langle\!\langle \ell_s, \ell_s \rangle\!\rangle^{\frac{1}{2}} \, ds = \int_a^b \frac{d}{dt} \langle\!\langle \ell_s, \ell_s \rangle\!\rangle^{\frac{1}{2}} \, ds = \int_a^b \frac{1}{|\ell_s|} \langle\!\langle D_t \ell_s, \ell_s \rangle\!\rangle \, ds, \tag{4.13}$$

where D_t is the covariant derivative along the geodesic and for a vector field along the curve ℓ it is defined as

$$D_t \mathbf{V} = \boldsymbol{\nabla}_{\ell_t} \widetilde{\mathbf{V}}, \tag{4.14}$$

where $\widetilde{\mathbf{V}}$ is an extension of $\mathbf{V}$ to $\mathcal{S}$, $\boldsymbol{\nabla}$ is the Riemannian connection corresponding to the metric $\mathbf{g}$ (see [8] for more details), and $\ell_t = \frac{\partial}{\partial t}\ell(t,s)$. It is easy to show that [8]

$$D_t \ell_s = D_s \ell_t \tag{4.15}$$

as in a local coordinate chart $\{x^a\}$ they both have the following representation

$$D_t \ell_s = D_s \ell_t = \left(\frac{\partial^2 x^c}{\partial s \partial t} + \frac{\partial x^a}{\partial t} \frac{\partial x^b}{\partial s} \gamma^c_{ab} \right) \partial_c, \tag{4.16}$$

where γ_{ab}^c are Christoffel coefficients of the Riemannian connection. Using this property and the fact that $|\ell_s| = 1$ we obtain

$$\frac{d}{dt} L_{\mathbf{g}}(\ell_{\mathbf{g}}^{ij}) = \int_a^b \langle\!\langle D_s \ell_t, \ell_s \rangle\!\rangle \, ds = \int_a^b \left(\frac{d}{ds} \langle\!\langle \ell_t, \ell_s \rangle\!\rangle - \langle\!\langle \ell_t, D_s \ell_s \rangle\!\rangle \right) ds. \tag{4.17}$$

But because ℓ is a geodesic we have $D_s \ell_s = 0$ and hence

$$\frac{d}{dt} L_{\mathbf{g}}(\ell_{\mathbf{g}}^{ij}) = \int_a^b \frac{d}{ds} \langle\!\langle \ell_t, \ell_s \rangle\!\rangle \, ds = \langle\!\langle \ell_t, \ell_s \rangle\!\rangle \Big|_a^b . \tag{4.18}$$

Note that

$$\ell_t(a,t) = \dot{\mathbf{x}}^i, \quad \ell_t(b,t) = \dot{\mathbf{x}}^j \tag{4.19}$$

and let us denote the velocity vectors of the geodesic at points $\mathbf{x}^i$ and $\mathbf{x}^j$ by

$$\ell_s(a,t) = \hat{\mathbf{t}}^{ij} \in T_{\mathbf{x}^i}\mathcal{S}, \quad \ell_s(b,t) = \hat{\mathbf{t}}^{ji} \in T_{\mathbf{x}^j}\mathcal{S}. \tag{4.20}$$

Therefore

$$\frac{d}{dt} L_{\mathbf{g}}(\ell_{\mathbf{g}}^{ij}) = \left\langle\!\left\langle \dot{\mathbf{x}}^j, \hat{\mathbf{t}}^{ji} \right\rangle\!\right\rangle - \left\langle\!\left\langle \dot{\mathbf{x}}^i, \hat{\mathbf{t}}^{ij} \right\rangle\!\right\rangle . \tag{4.21}$$

Now balance of energy can be written as

$$\frac{1}{2} \sum_{\substack{i,j \in \mathcal{L} \\ j \neq i}} \frac{\partial \phi_{ij}}{\partial g_{ij}} \left(\left\langle\!\left\langle \dot{\mathbf{x}}^j, \hat{\mathbf{t}}^{ji} \right\rangle\!\right\rangle - \left\langle\!\left\langle \dot{\mathbf{x}}^i, \hat{\mathbf{t}}^{ij} \right\rangle\!\right\rangle \right) + \sum_{i \in \mathcal{L}} m_i \left\langle\!\left\langle \mathbf{a}^i, \dot{\mathbf{x}}^i \right\rangle\!\right\rangle = \sum_{i \in \mathcal{L}} \left\langle\!\left\langle \mathbf{F}^i, \dot{\mathbf{x}}^i \right\rangle\!\right\rangle . \tag{4.22}$$

Note that the particle acceleration $\mathbf{a}^i$ is the covariant time derivative of $\dot{\mathbf{x}}^i$.

Let us now look at balance of energy for a change of frame $\xi_t : \mathcal{S} \to \mathcal{S}$ such that $\xi_t\big|_{t=t_0} = Id$. Consider a family of geodesics $\widetilde{\ell}(t,s)$ joining the points $\mathbf{x}'^i(t) = \xi_t(\mathbf{x}^i(t)), \mathbf{x}'^j(t) = \xi_t(\mathbf{x}^j(t)) \in \mathcal{S}$. Motivated by (4.8), for a fixed t, $\widetilde{\ell}(t,s)$ is the geodesic with respect to the metric $\mathbf{g}_t = \xi_t^* \mathbf{g}$ joining these two points. Assume that the geodesic $\ell(s) = \widetilde{\ell}(t_0, s)$ is parameterized by arc length, i.e., it has unit speed everywhere. Note that $D_s \widetilde{\ell}_s(t,s) = 0$ is satisfied for each geodesic, where D_s is the covariant derivative along the geodesic $\widetilde{\ell}(t,s)$ with respect to the metric $\mathbf{g}_t$. The time rate of change of the length of this family is simplified to read

$$\frac{d}{dt} L_{\mathbf{g}_t}(\widetilde{\ell}_{\mathbf{g}_t}^{ij}) = \frac{d}{dt} \int_a^b \left\langle\!\!\left\langle \widetilde{\ell}_s, \widetilde{\ell}_s \right\rangle\!\!\right\rangle_t^{\frac{1}{2}} ds = \int_a^b \frac{1}{|\widetilde{\ell}_s(t,s)|} \left\langle\!\!\left\langle D_t \widetilde{\ell}_s, \widetilde{\ell}_s \right\rangle\!\!\right\rangle_t ds, \tag{4.23}$$

where D_t is the covariant time derivative along the curve $\widetilde{\ell}(t,s)$ with respect to the metric $\mathbf{g}_t$. Note that still we have the relation $D_t \widetilde{\ell}_s = D_s \widetilde{\ell}_t$ as in the local representation (4.16) the only difference would be the t-dependance of the Christoffel symbols. Thus

$$\begin{aligned} \frac{d}{dt} L_{\mathbf{g}_t}(\widetilde{\ell}_{\mathbf{g}_t}^{ij}) &= \int_a^b \frac{1}{|\widetilde{\ell}_s(t,s)|} \left\langle\!\!\left\langle D_s \widetilde{\ell}_t, \widetilde{\ell}_s \right\rangle\!\!\right\rangle_t ds \\ &= \int_a^b \frac{1}{|\widetilde{\ell}_s(t,s)|} \left(\frac{d}{ds} \left\langle\!\!\left\langle \widetilde{\ell}_t, \widetilde{\ell}_s \right\rangle\!\!\right\rangle_t - \left\langle\!\!\left\langle \widetilde{\ell}_t, D_s \widetilde{\ell}_s \right\rangle\!\!\right\rangle_t \right) ds. \end{aligned} \tag{4.24}$$

Using the geodesic equation and evaluating the above relation at $t = t_0$, we obtain

$$\frac{d}{dt}\Big|_{t=t_0} L_{\mathbf{g}_t}(\widetilde{\ell}^{ij}_{\mathbf{g}_t}) = \left\langle\!\!\left\langle \widetilde{\ell}_t, \widetilde{\ell}_s \right\rangle\!\!\right\rangle \Big|_a^b. \tag{4.25}$$

Note that

$$\widetilde{\ell}_t(t_0, a) = \dot{\mathbf{x}}^i + \mathbf{w}^i, \quad \widetilde{\ell}_t(t_0, b) = \dot{\mathbf{x}}^j + \mathbf{w}^j, \tag{4.26}$$

where $\mathbf{w} = \frac{d}{dt}\xi_t$. Also

$$\widetilde{\ell}_s(t_0, a) = \hat{\mathfrak{t}}^{ij} \in T_{\mathbf{x}^i}\mathcal{S}, \quad \widetilde{\ell}_s(t_0, b) = \hat{\mathfrak{t}}^{ji} \in T_{\mathbf{x}^j}\mathcal{S}. \tag{4.27}$$

Thus

$$\frac{d}{dt}\Big|_{t=t_0} L_{\mathbf{g}_t}(\widetilde{\ell}^{ij}_{\mathbf{g}_t}) = \left\langle\!\left\langle \dot{\mathbf{x}}^j + \mathbf{w}^j, \hat{\mathfrak{t}}^{ji} \right\rangle\!\right\rangle - \left\langle\!\left\langle \dot{\mathbf{x}}^i + \mathbf{w}^i, \hat{\mathfrak{t}}^{ij} \right\rangle\!\right\rangle. \tag{4.28}$$

Balance of energy for the new framing at time $t = t_0$ reads

$$\frac{1}{2}\sum_{\substack{i,j\in\mathcal{L}\\ j\neq i}} \frac{\partial \phi_{ij}}{\partial g_{ij}} \left(\left\langle\!\left\langle \dot{\mathbf{x}}^j + \mathbf{w}^j, \hat{\mathfrak{t}}^{ji} \right\rangle\!\right\rangle - \left\langle\!\left\langle \dot{\mathbf{x}}^i + \mathbf{w}^i, \hat{\mathfrak{t}}^{ij} \right\rangle\!\right\rangle \right) + \sum_{i\in\mathcal{L}} m_i \left\langle\!\left\langle \mathbf{a}^i, \dot{\mathbf{x}}^i + \mathbf{w}^i \right\rangle\!\right\rangle = \sum_{i\in\mathcal{L}} \left\langle\!\left\langle \mathbf{F}^i, \dot{\mathbf{x}}^i + \mathbf{w}^i \right\rangle\!\right\rangle. \tag{4.29}$$

Subtracting (4.22) from the above balance equation and noting that the vector field $\mathbf{w}$ is arbitrary, we obtain the following balance law

$$\sum_{\substack{j\in\mathcal{L}\\ j\neq i}} \frac{\partial \phi_{ij}}{\partial g_{ij}}\, \hat{\mathfrak{t}}^{ij} + \mathbf{F}^i = m_i \mathbf{a}^i \qquad \text{for all } i \in \mathcal{L}. \tag{4.30}$$

It is seen that assuming that particles are embedded in a Riemannian manifold and postulating energy balance and its invariance under arbitrary spatial diffeomorphisms results in balance of linear momentum. In terms of the number of balance laws, having a Riemannian ambient space does not give us any new relations. However, defining a more general pairwise interaction we see that interaction force at $i \in \mathcal{L}$ due to the particle $j \in \mathcal{L}$ is directed along the tangent to the geodesic joining $\mathbf{x}^i, \mathbf{x}^j \in \mathcal{S}$ at the point $\mathbf{x}^i$ and its magnitude is equal to the rate of change of the potential energy of $i, j \in \mathcal{L}$ with respect to the discrete metric g_{ij}. Thus, we can think of

$$f_{ij} = \frac{\partial \phi_{ij}}{\partial g_{ij}} = \frac{\partial e}{\partial g_{ij}} \tag{4.31}$$

as a *discrete Doyle–Ericksen formula.*

Note that because $\hat{\mathfrak{t}}^{ij}$ and $\hat{\mathfrak{t}}^{ji}$ lie in two different tangent spaces, the relation $\mathbf{f}_{ji} = -\mathbf{f}_{ij}$ is meaningless, in general. However, $f_{ij} = f_{ji}$. In summary, we have proved the following proposition.

Proposition 4.1. *Assuming that balance of energy for a system of pairwisely interacting particles in an ambient Riemannian manifold is spatially covariant is equivalent to balance of linear momentum.*

The proof of converse of this proposition is similar to that of the continuum version [16].

Remarks.

(a) From Eq. (4.30) it is seen that the background metric enters the balance of linear momentum only through the discrete metric g_{ij}.

(b) Note that Eq. (4.30) is the dynamic version of Eq. (12) in [7].

Example. We show in this example that what we just derived for a general Riemannian manifold is reduced to the classical results when the ambient space is Euclidean. In this case the geodesic joining $\mathbf{x}^i, \mathbf{x}^j \in \mathcal{S} = \mathbb{R}^n$ has the following parametrization

$$\ell(s) = \frac{b\mathbf{x}^i - a\mathbf{x}^j}{b-a} + \frac{\mathbf{x}^j - \mathbf{x}^i}{b-a} s \qquad s \in [a, b]. \tag{4.32}$$

Because the curve is parameterized by the arc length we must have $b - a = |\mathbf{x}^j - \mathbf{x}^i|$. Thus

$$\hat{\mathbf{t}}^{ij} = \frac{\mathbf{x}^j - \mathbf{x}^i}{|\mathbf{x}^j - \mathbf{x}^i|}. \tag{4.33}$$

Also in this case $g_{ij} = r_{ij} := |\mathbf{x}^j - \mathbf{x}^i|$. Hence the following classical balance of linear momentum is recovered

$$\sum_{\substack{j \in \mathcal{L} \\ j \neq i}} -\frac{\partial \phi}{\partial r_{ij}} \frac{\mathbf{x}^i - \mathbf{x}^j}{|\mathbf{x}^j - \mathbf{x}^i|} + \mathbf{F}^i = m_i \mathbf{a}^i \qquad \text{for all } i \in \mathcal{L}. \tag{4.34}$$

Note that in this case the relation $\mathbf{f}_{ji} = -\mathbf{f}_{ij}$ holds as tangent space to $\mathbb{R}^n$ at any point can be identified with $\mathbb{R}^n$.

Remark. Balance of linear momentum for a particle system on a Riemannian manifold can of course also be obtained using Hamilton's principle of least action which is another covariant approach via Lagrangian mechanics.

5. Concluding remarks

This paper studied the connection between balance laws and energy balance invariance for a system of interacting particles. It was shown that, unlike classical elasticity, postulating invariance of energy balance under isometries of the (Euclidean) ambient space is not enough to obtain the balance laws. Instead, if one postulates invariance of energy balance under arbitrary diffeomorphisms, then one recovers all the balance laws. This shows a fundamental difference between a continuum and a system of interacting particles and can be associated with the nonlocal nature of interactions in a system of particles.

Balance of energy for a system of particles embedded in a Riemannian manifold was also investigated via a generalized form of pairwise interactions by assuming that the pairwise potential energy of particles explicitly depends on their pairwise distances—the lengths of the geodesics joining them. This definition naturally reduces to the classical notion of pairwise interactions in Euclidean space. Postulating balance of energy and its spatial covariance, shows that one can obtain a geometric version of balance of linear momentum. For a particle $i \in \mathcal{L}$, balance of linear momentum is written in the tangent space of $\mathcal{S}$ at $\mathbf{x}^i \in \mathcal{S}$. It was observed that in this general setting, a relation like $\mathbf{f}_{ji} = -\mathbf{f}_{ij}$ would be meaningless but instead one has the meaningful relation $f_{ji} = f_{ij}$. Defining a discrete metric as the pairwise distances, we showed that

$$f_{ij} = \frac{\partial e}{\partial g_{ij}}, \tag{5.1}$$

which can be thought of as a discrete version of the Doyle–Ericksen formula.

References

[1] Eckart, C., Remarks concerning forces on line defects, *Physical Review* **73** (1948), 373–382.

[2] Edelen, D. G. B. and Laws, N., Thermodynamics of systems with nonlocality, *Archive for Rational Mechanics and Analysis* **43**(1) (1971), 24–35.

[3] Eringen, A. C. and Edelen, D. G. B., Nonlocal elasticity, *International Journal of Engineering Science* **10** (1972), 233–248.

[4] Green, A. E. and Rivlin, R. S., On Cauchy's equations of motion, *ZAMP* **15** (1964), 290–293.

[5] Gurtin, M. E. and Williams, W. O., On the first law of thermodynamics, *Archive for Rational Mechanics and Analysis* **42** (1971), 77–92.

[6] Gurtin, M. E. and Williams, W. O., On continuum thermodynamics with mutual body forces and internal relation, *ZAMP* **22** (1971), 293–298.

[7] Kotani, M. and Sunada, T., Standard realizations of crystal lattices via harmonic maps, *Transactions of the American Mathematical Society* **353** (2000), 1–20.

[8] Lee, J. M., *Riemannian Manifold An Introduction to Curvature*, Springer-Verlag, New York 1997.

[9] Marsden, J. E. and T. J. R. Hughes, *Mathematical Foundations of Elasticity*, Dover, New York 1983.

[10] Marsden, J. E. and T. Ratiu, *Introduction to Mechanics and Symmetry*, Springer, New York 2003.

[11] Rajagopal, K. R. and A. R. Srinivasa, On the thermomechanics of materials that have multiple natural configurations Part II: Twinning and solid to solid phase transformation, *ZAMP* **55**(6) (1984), 1074–1093.

[12] Shchepetilov, A. V., Reduction of the two-body problem with central interaction on simply connected spaces of constant sectional curvature. *Journal of Physics A-Mathematical and General* **31** (1998), 6279–6291.

[13] Shchepetilov, A. V., *Calculus and Mechanics on Two-Point Homogenous Riemannian Spaces (Lecture Notes in Physics)*, Springer, New York 1983.

[14] Simo, J. C. and J. E. Marsden, On the rotated stress tensor and the material version of the Doyle–Ericksen formula, *Archive for Rational Mechanics and Analysis* **86** (1984), 213–231.

[15] Yanao, T., W.-S. Koon, J.E. Marsden, and I. Kevrekidis, Gyration-radius dynamics in structural transitions of atomic clusters, *Journal of Chemical Physics* **126** (2007), 1–17.

[16] Yavari, A., J. E. Marsden and M. Ortiz, On the spatial and material covariant balance laws in elasticity, *Journal of Mathematical Physics* **47** (2006), 85–112.

[17] Yavari, A., M. Ortiz and K. Bhattacharya, A theory of anharmonic lattice statics for analysis of defective crystals, *Journal of Elasticity* **86** (2007), 41–83.
[18] Yavari, A., On geometric discretization of elasticity, *Journal of Mathematical Physics* **49** (2008), 1–36.
[19] Yavari, A. and A. Ozakin, Covariance in linearized elasticity, *Zeitschrift für Angewandte Mathematik und Physik (ZAMP)* (2008), DOI 10.1007/s00033-007-7127-2.

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