REPORT NO.
UCB/SEMM-95/06

STRUCTURAL ENGINEERING
MECHANICS AND MATERIALS

ADVANCES IN DOUBLET MECHANICS: IV. DOUBLET THERMOMECHANICS

BY

K. MON
AND
M. FERRARI

JUNE 1995

DEPARTMENT OF CIVIL ENGINEERING
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA

Advances in Doublet Mechanics: IV. Doublet Thermomechanics

Kevin Mon
Department of Materials Science and Mineral Engineering
University of California
Berkeley, California 94720

Mauro Ferrari
Department of Civil Engineering
Department of Materials Science and Mineral Engineering
University of California
Berkeley, California 94720

Summary

The thermomechanical foundations of the field of doublet mechanics are introduced. The present approach utilizes the concepts of energy and entropy balance to derive thermodynamic restrictions on the governing equations of the theory. The constitutive assumptions of nonlinear elastic doublet mechanics are analyzed. Further restrictions on the material response functions are determined from consideration of superposed rigid body motions. Finally, the equations of the nonlinear elastic case are linearized and presented in simplified form.

1. *Introduction*

It may be said that the field of Continuum Thermomechanics (CT) was established in its contemporary format with the landmark contributions of the late fifties and early sixties (Coleman and Noll 1959, 1963; Gurtin, 1965; Truesdell and Noll, 1965). Disagreement between researchers in CT has not been infrequent (see e.g. Day, 1976; Green and Naghdi 1977; Naghdi 1980; and Kestin 1990), and much it has centered around the Clausius-Duhem Inequality (CDI) as the embodiment of the Second Law of Thermodynamics and its use to derive constitutive restrictions in the manner proposed by Coleman and Noll (1963). Day (1976), using an example of a rigid heat conductor with memory, has shown that the CDI is consistent with nonunique values of entropy. Green and Naghdi (1977) have shown that the CDI predicts, for a class of rigid heat conductors in equilibrium, that if heat is added to the medium, temperature must decrease. Green and Naghdi (1977) proposed use of the Clausius Inequality in conjunction with the concept of an entropy balance law as an alternative to the CDI. The Naghdi-Green formalism has been successfully applied to studies of mixtures of interacting continua (Green and Naghdi 1978) and nonlocal elasticity (Green and Naghdi 1978). For elastic constitutive assumptions, the CDI-based approach of Coleman and Noll (1963) yields identical results to the Naghdi-Green formalism (Naghdi 1980).

Generalized continuum mechanical theories have been proposed, with the objective of modeling continua endowed with a material microstructure (Cosserat 1909; Eringen and Suhubi 1964; Green and Rivlin 1964; Mindlin 1964; Eringen 1966; Stojanovic 1972; Pucci and Saccomandi 1990). These are essentially continuum approaches, in that they are based on the modeling assumption that all continuum points are endowed with additional kinematic variables that are somehow representative of the microstructure contained in the "differential volume element" centered at the point. Literature studies on the thermodynamics of the generalized continua are not as abundant as those in continuum thermomechanics, and are generally based on the CDI as the mathematical embodiment of the Second Law (Stojanovic 1972; Eringen and Suhubi 1964; Eringen 1966). It may be expected that the use of the CDI in this context be subject to the same objections as those mentioned above for conventional continuum mechanics. On this basis, and without entering into the comparative merits of the various approaches to the thermomechanics of media with or without microstructure, in this paper we employ the procedure of Green and Naghdi (1977) to determine the constitutive restrictions that are imposed on a class of microstructured media by the entropy balance law and the Clausius Inequality. The analysis is limited to the thermoelastic range, where the choice of thermomechanical formulations has been shown to be immaterial, not only for the cited case of continuum thermoelasticity, but also for the case of micropolar elasticity (Ferrari, 1985).

The microstructure media to which reference is made in this paper are those that are adequately modeled by the theory of Doublet Mechanics (DM), introduced by Granik and Ferrari (1993). Quite differently from the previously described generalized continuum theories, in the doublet mechanical approach, solids are represented as collections of points or nodes placed at finite distances. DM is "inductive" in the sense that the "differential volume element" of conventional mechanics is supplanted with the concept of a "particle doublet" as the elementary unit on which the theory is built. At each doublet, elongational, torsional, and shear microstrains are evaluated in terms of the two continuous mutually independent vector fields of displacements, $\overline{u}$, and rotations, $\overline{\phi}$. Conjugate to the microstrains are the doublet-level stresses, or microstresses. Equilibrium imposes the relationship by which microstresses are expressed in terms of the microstrains and the microgeometry, providing a noninvertible linkage between the continuum level and its descrete substructure.

The applicability of DM to a wide range of materials, including metals, alloys, unreinforced and steel-fiber reinforced concrete, was demonstrated in the studies by Ferrari and Granik (1994, 1995) on failure and yield envelopes. The theory of doublet viscoelasticity was presented by (Maddalena and Ferrari 1994). In this four paper sequence, we deal with doublet elastodynamics (Granik and Ferrari 1995; Zhang and Ferrari 1995), plane elastostatics (Nadeau, Nashat, and Ferrari 1995), and, in this communication, doublet thermomechanics. A comprehensive review of DM is given in Granik and Ferrari (1995) with which the notation of this communication is standardized.

In analogy with the methods of Green and Naghdi (1977, 1979), in this paper we first identify local energy and entropy balance laws, and make constitutive assumptions as to what variables the functions that appear in these balance laws depend on. Substitution of the constitutive assumption into the balance laws allows simplification of these functional dependencies. Next, an analysis is undertaken to determine what further restrictions are implied by consideration of superposed rigid body motions (Green and Naghdi, 1979). Finally, the results of the analyses are applied to a study of homogeneous linear elastic doublet mechanics.

2. *Balance Laws*

We start from the differential formulation of energy balance:

$$\rho r - \operatorname{div}(\overline{q}) + P - \rho\dot{E} = 0 \tag{2.1}$$

where the superscripted dot ($\dot{E}$) denotes the derivative with respect to time and the overbar ($\overline{q}$) denotes vector quantities. In equation (2.1) r is the volume rate of heat supplied per unit mass, $\overline{q}$

is the heat flux vector, P is the mechanical power, E is the internal energy per unit mass, and ρ is the mass density.

The differential law of entropy balance, introduced by Green and Naghdi (1977), is:

$$\rho\left(\frac{r}{\theta}+\xi\right)-\operatorname{div}\left(\frac{\bar{q}}{\theta}\right)=\rho\dot{\eta} \tag{2.2}$$

where ξ is the internal rate of entropy production per unit mass, η is the entropy per unit mass, and θ is a function of empirical temperature, T, and other constitutive variables such that $\theta \geq 0$ and $\frac{\partial\theta}{\partial T} \geq 0$. The combination of (2.1) and (2.2) yields the relation:

$$\rho r-\operatorname{div}(\bar{q})=\rho\theta\dot{\eta}-\rho\theta\xi-\frac{\bar{q}}{\theta}\cdot\bar{g}=\rho\dot{E}-P \tag{2.3}$$

where $\bar{g}$ is denotes grad(θ). Rewriting (2.3) yields:

$$-\rho(\dot{E}-\theta\dot{\eta})-\frac{\bar{q}}{\theta}\cdot\bar{g}-\rho\xi\theta+P=0 \tag{2.4}$$

or, in terms of the Helmholtz free energy ($\psi = E-\theta\eta$):

$$-\rho\left(\dot{\psi}+\dot{\theta}\eta\right)-\frac{\bar{q}}{\theta}\cdot\bar{g}-\rho\xi\theta+P=0 \tag{2.5}$$

Expressions (2.4) and (2.5) will be referred to as energy/entropy balance equations and must hold for all thermomechanical processes. Definition of a thermomechanical process will be delayed until the mechanical power is discussed further.

The only difference in these equations between Continuum Mechanics (CM) and Doublet Mechanics (DM) lies in how the mechanical power (P) is written. In CM, $P=\tilde{\tau}\cdot\tilde{L}$ where $\tilde{\tau}$ is the stress tensor and the velocity gradient, $\tilde{L}$, is related to the deformation gradient, $\tilde{F}$, by $\tilde{L}=\dot{\tilde{F}}\cdot\tilde{F}^{-1}$. The superscript ~ notation is used to denote tensor quantities. In DM:

$$P = \sum_{\alpha=1}^{n} \left(p_\alpha \dot{\varepsilon}_\alpha + m_\alpha \dot{\mu}_\alpha + \bar{t}_\alpha \cdot \dot{\bar{\gamma}}_\alpha \right) \tag{2.6}$$

where the summation over α ranges from 1 to n, the number of doublets defined at a node. p_α is the elongation microstress conjugate to the elongation microstrain ε_α, m_α is the torsional microstress conjugate to the torsional microstrain μ_α, and $\bar{t}_\alpha$ is the shear microstress vector conjugate to the shear microstrain vector, $\bar{\gamma}_\alpha$. Use has been made of the fact that $\bar{p}_\alpha \cdot \bar{\varepsilon}_\alpha = p_\alpha \varepsilon_\alpha$ and $\bar{m}_\alpha \cdot \bar{\mu}_\alpha = m_\alpha \mu_\alpha$. The microstrains are given by the following relations:

$$\varepsilon_\alpha = \frac{\bar{\tau}^\circ_\alpha \cdot \Delta \bar{u}_\alpha}{\eta_\alpha} \tag{2.7}$$

$$\mu_\alpha = \frac{\bar{\tau}^\circ_\alpha \cdot \Delta \bar{\phi}_\alpha}{\eta_\alpha} \tag{2.8}$$

$$\bar{\gamma}_\alpha = \left(\bar{\phi} + \tfrac{1}{2} \Delta \bar{\phi}_\alpha - \bar{\tau}^\circ_\alpha \times \bar{\tau}_\alpha \right) \times \bar{\tau}^\circ_\alpha \tag{2.9}$$

where η_α is the internodal distance of the α-th particle doublet (*not* entropy density), $\bar{\tau}^\circ_\alpha$ is a unit vector in the undeformed configuration oriented along the α-th doublet axis, and $\Delta \bar{u}_\alpha$ and $\Delta \bar{\phi}_\alpha$ are given by the following relations in Cartesian coordinates:

$$\left. \begin{matrix} \Delta u_{\alpha i}(\bar{X}, t) \\ \Delta \phi_{\alpha i}(\bar{X}, t) \end{matrix} \right\} = \sum_{\kappa=1}^{M} \frac{(\eta_\alpha)^\kappa}{\kappa!} \tau^\circ_{\alpha k_1} \cdots \tau^\circ_{\alpha k_\kappa} \frac{\partial^\kappa}{\partial x_{k_1} \cdots \partial x_{k_\kappa}} \left\{ \begin{matrix} u_i(\bar{X}, t) \\ \phi_i(\bar{X}, t) \end{matrix} \right|_{\bar{X} = \bar{X}_\circ} \tag{2.10}$$

Here, repeated Latin indices (k_j) should be summed over, while repeated Greek indices (α) should not. This equation should be evaluated only at the doublet nodes (when $\bar{X} = \bar{X}_\circ$). The number M refers to the degree of the approximation. The vector fields of translations, $\bar{u}(\bar{X}, t)$, and rotations, $\bar{\phi}(\bar{X}, t)$, are mutually independent and are functions of position, $\bar{X}$, and time, t.

Additionally, the microstresses are required to satisfy the balance of linear momentum:

$$\sum_{\alpha=1}^{n}\sum_{\kappa=1}^{M}(-1)^{\kappa+1}\frac{\eta_{\alpha}^{\kappa-1}}{\kappa!}\overset{\circ}{\tau}_{\alpha k_1}\cdots\overset{\circ}{\tau}_{\alpha k_\kappa}\frac{\partial^{\kappa}(p_{\alpha i}+t_{\alpha i})}{\partial x_{k_1}\cdots\partial x_{k_\kappa}}+b_i=\rho\ddot{u}_i \tag{2.11}$$

and moment of momentum:

$$\sum_{\alpha=1}^{n}\left(\varepsilon_{ijq}\overset{\circ}{\tau}_{\alpha j}t_{\alpha q}+\sum_{\kappa=1}^{M}(-1)^{\kappa+1}\frac{\eta_{\alpha}^{\kappa-1}}{\kappa!}\overset{\circ}{\tau}_{\alpha k_1}\cdots\overset{\circ}{\tau}_{\alpha k_\kappa}\frac{\partial^{\kappa}\left(m_{\alpha i}-\frac{1}{2}\eta_{\alpha}\varepsilon_{ijq}\overset{\circ}{\tau}_{\alpha j}t_{\alpha q}\right)}{\partial x_{k_1}\cdots\partial x_{k_\kappa}}\right)=0 \tag{2.12}$$

where b_i is the volume body force and ε_{ijq} is the permutation tensor.

The independent variables in the above treatment are:

$$\{\bar{u},\ \bar{\phi},\ T\} \tag{2.13}$$

The balance laws (2.2), (2.5), (2.11), and (2.12) contain the fields:

$$\{\psi,\ \theta,\ \eta,\ \xi,\ p_{\alpha},\ m_{\alpha},\ \bar{t}_{\alpha}\ .\ \bar{q}\} \tag{2.14}$$

as well as:

$$\{\bar{b},\ r\} \tag{2.15}$$

We assume that the fields (2.14) depend constitutively on the variables in (2.13) and possibly their space and time derivatives. We assume that:

(1) The balance laws hold for arbitrary choices of the variables in (2.13) and, if constitutive assumptions require, their space and time derivatives;

(2) The fields (2.14) are calculated from their constitutive equations;

(3) The fields (2.15) can then be found from the balance of momentum (2.11) and entropy (2.2);

(4) The energy/entropy balance equation (2.5) may be imposed as an identity for every choice of variables (2.13). This allows restrictions on the constitutive equations to be derived.

A thermomechanical process is defined by specifying the set of variables (2.13) such that the balance laws are satisfied.

3. *Elastic Constitutive Assumptions*

The constitutive assumptions of Doublet Elasticity are:

$$
\begin{aligned}
\psi &= \hat{\psi}\left(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, T, \bar{\nabla} T{:}\bar{X}\right)\\
\xi &= \hat{\xi}\left(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, T, \bar{\nabla} T{:}\bar{X}\right)\\
\theta &= \hat{\theta}\left(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, T, \bar{\nabla} T{:}\bar{X}\right)\\
\eta &= \hat{\eta}\left(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, T, \bar{\nabla} T{:}\bar{X}\right)\\
\bar{q} &= \hat{\bar{q}}\left(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, T, \bar{\nabla} T{:}\bar{X}\right)\\
p_\alpha &= \hat{p}_\alpha\left(\varepsilon_\beta, \mu_\beta, \bar{\gamma}_\beta, T, \bar{\nabla} T{:}\bar{X}\right)\\
m_\alpha &= \hat{m}_\alpha\left(\varepsilon_\beta, \mu_\beta, \bar{\gamma}_\beta, T, \bar{\nabla} T{:}\bar{X}\right)\\
\bar{t}_\alpha &= \hat{\bar{t}}_\alpha\left(\varepsilon_\beta, \mu_\beta, \bar{\gamma}_\beta, T, \bar{\nabla} T{:}\bar{X}\right)
\end{aligned}
\tag{3.1}
$$

where T is the empirical temperature and α and β can vary from 1 to n. The $\bar{X}$ indicates a possible dependence on material inhomogeneity. Expanding these functions into their partial derivatives and substitution, along with equation (2.6), into equation (2.5) yields an equation of the form:

$$
\begin{aligned}
\sum_{\alpha=1}^{n}\Bigg(& A\dot{T} + B_i \frac{\partial \dot{T}}{\partial x_i} + C_{ij}\frac{\partial^2 T}{\partial x_i \partial x_j} + H1_\alpha \dot{\varepsilon}_\alpha + H2_\alpha \dot{\mu}_\alpha + H3_{\alpha i}\dot{\gamma}_{\alpha i} + \cdots \\
& + I1_{\alpha i}\frac{\partial \varepsilon_\alpha}{\partial x_i} + I2_{\alpha i}\frac{\partial \mu_\alpha}{\partial x_i} + I3_{\alpha ij}\frac{\partial \gamma_{\alpha j}}{\partial x_i}\Bigg) + G = 0
\end{aligned}
\tag{3.2}
$$

with coefficients:

$$
A = -\rho\left(\frac{\partial \psi}{\partial T} + \eta\frac{\partial \theta}{\partial T}\right) \qquad B_i = -\rho\left(\partial\psi \Big/ \partial\left(\frac{\partial T}{\partial x_j}\right) + \eta\, \partial\theta \Big/ \partial\left(\frac{\partial T}{\partial x_j}\right)\right)
$$

$$C_{ij} = -\frac{q_i}{\theta}\frac{\partial\theta}{\partial\left(\frac{\partial T}{\partial x_j}\right)} \qquad G = -\frac{q_i}{\theta}\left(\frac{\partial\theta}{\partial T}\frac{\partial T}{\partial x_i} + \frac{\partial\theta}{\partial x_i}\right) - \rho\xi\theta$$

$$H1_\alpha = -\rho\left(\frac{\partial\psi}{\partial\varepsilon_\alpha} + \eta\frac{\partial\theta}{\partial\varepsilon_\alpha}\right) + p_\alpha \qquad I1_{\alpha i} = \frac{-q_i}{\theta}\frac{\partial\theta}{\partial\varepsilon_\alpha}$$

$$H2_\alpha = -\rho\left(\frac{\partial\psi}{\partial\mu_\alpha} + \eta\frac{\partial\theta}{\partial\mu_\alpha}\right) + m_\alpha \qquad I2_{\alpha i} = \frac{-q_i}{\theta}\frac{\partial\theta}{\partial\mu_\alpha}$$

$$H3_{\alpha i} = -\rho\left(\frac{\partial\psi}{\partial\gamma_{\alpha i}} + \eta\frac{\partial\theta}{\partial\gamma_{\alpha i}}\right) + t_{\alpha i} \qquad I3_{\alpha ij} = \frac{q_i}{\theta}\frac{\partial\theta}{\partial\gamma_{\alpha j}}$$

The vectorial subscripts i and j vary from 1 to 3, while the numbering subscript α varies from 1 to n. Equation (3.2) must hold for every thermodynamic process, including arbitrary choices of the functions in the set:

$$\left\{\dot{T}, \frac{\partial\dot{T}}{\partial x_i}, \frac{\partial^2 T}{\partial x_i \partial x_j}, \dot{\varepsilon}_\alpha, \dot{\mu}_\alpha, \dot{\gamma}_{\alpha i}, \frac{\partial\varepsilon_\alpha}{\partial x_i}, \frac{\partial\mu_\alpha}{\partial x_i}, \frac{\partial\gamma_{\alpha j}}{\partial x_i}\right\} \tag{3.3}$$

since these functions do not enter into constitutive assumption (3.1) or the coefficients defined in (3.2). Any functional relationships derived from arbitrary choices of the functions in the set (3.3) must hold for every thermodynamic process. In particular:

a) Taking each member of the set (3.3) to be zero yields $G \equiv 0$.

b) Given that $G = 0$, and taking all of set (3.3) except $\frac{\partial^2 T}{\partial x_i \partial x_j}$ to be zero yields $C_{ij} \equiv 0$. This means that $\theta = \hat{\theta}(T, \varepsilon_\alpha, \mu_\alpha, \gamma_{\alpha i} : \overline{X})$ i.e. θ is not a function of $\overline{\nabla}T$.

c) Given that $C_{ij} = G = 0$ and taking all of the set (3.3) except $\frac{\partial\dot{T}}{\partial x_i}$ to be zero yields $B_i \equiv 0$. This means $\psi = \hat{\psi}(T, \varepsilon_\alpha, \mu_\alpha, \gamma_{\alpha i} : \overline{X})$ i.e. ψ is not a function of $\overline{\nabla}T$.

d) Given that $C_{ij} = G = B_i = 0$ and taking all of the set (3.3) except $\dot{T}$ to be zero yields $A \equiv 0$.

e) Given that $C_{ij} = G = B_i = A = 0$ and taking all of the set (3.3) except $\frac{\partial \varepsilon_\alpha}{\partial x_i}$ to be zero yields $I1_{\alpha i} \equiv 0$. This means θ is not a function of ε_α.

f) Given that $C_{ij} = G = B_i = A = I1_{\alpha i} = 0$ and taking all of the set (3.3) except $\frac{\partial \mu_\alpha}{\partial x_i}$ to be zero yields $I2_{\alpha i} \equiv 0$. This means θ is not a function of μ_α.

g) Given that $C_{ij} = G = B_i = A = I1_{\alpha i} = I2_{\alpha i} = 0$ and taking all of the set (3.3) except $\frac{\partial \gamma_{\alpha j}}{\partial x_i}$ to be zero yields $I3_{\alpha ij} \equiv 0$. This means θ is not a function of $\gamma_{\alpha i}$. At this point $\theta = \hat{\theta}(T{:}\overline{X})$.

h) Given that $C_{ij} = G = B_i = A = I1_{\alpha i} = I2_{\alpha i} = I3_{\alpha ij} = 0$ and taking all of the set (3.3) except $\dot{\varepsilon}_\alpha$ to be zero yields $H1_\alpha \equiv 0$. This means $p_\alpha = \rho\frac{\partial \psi}{\partial \varepsilon_\alpha}$ and, since ψ is not a function of $\overline{\nabla}T$, p_α is not a function of $\overline{\nabla}T$.

i) Given that $C_{ij} = G = B_i = A = I1_{\alpha i} = I2_{\alpha i} = I3_{\alpha ij} = H1_\alpha = 0$ and taking all of the set (3.3) except $\dot{\mu}_\alpha$ to be zero yields $H2_\alpha \equiv 0$. This means $m_\alpha = \rho\frac{\partial \psi}{\partial \mu_\alpha}$ and m_α is not a function of $\overline{\nabla}T$.

j) Given that $C_{ij} = G = B_i = A = I1_{\alpha i} = I2_{\alpha i} = I3_{\alpha ij} = H1_\alpha = H2_\alpha = 0$ and taking all of the set (3.3) except $\dot{\gamma}_{\alpha i}$ to be zero yields $H3_{\alpha i} \equiv 0$. This means $t_{\alpha i} = \rho\frac{\partial \psi}{\partial \gamma_{\alpha i}}$ and $\bar{t}_\alpha$ is not a function of $\overline{\nabla}T$.

Up to this point we have not applied the Second Law of Thermodynamics; nothing has been said of which processes are possible and which are not. In this communication, we retain the viewpoint that different statements of the Second Law are possible, each embodying some aspects of it. In what follows we explore the consequences of the Clausius Inequality (Green and Naghdi, 1977):

$$\oint_I \left(\int_{\partial B_t} \frac{\overline{q}\cdot\overline{n}}{\theta} da - \int_{B_t} \frac{\rho r}{\theta} dv \right) dt \geq 0 \qquad (3.4)$$

which states that the sum of the entropy from heat conduction ($\overline{q}$) through the surface of the body ∂B_t and from radiation (r) in the body B_t, considered over a closed cycle (I), must be greater than or equal to zero. A closed cycle is one in which the entropy, η, is the same before and after the cycle is completed. If the Second Law applies locally to every part of the body, through the use of the divergence theorem and entropy balance (2.2), the Clausius Inequality (3.4) can be reduced to:

$$\oint_I \xi \cdot dt \geq 0 \tag{3.5}$$

If the entropy production rate, ξ, is independent of time, (3.5) implies $\xi \geq 0$.

To incorporate (3.5) into the above analysis, one must reconsider the results of part a) of the application of the constitutive assumptions (3.1) to the energy/entropy balance equation (2.5), particularly:

$$G = -\frac{q_i}{\theta}\left(\frac{\partial\theta}{\partial T}\frac{\partial T}{\partial x_i} + \frac{\partial\theta}{\partial x_i}\right) - \rho\xi\theta = 0 \tag{3.6}$$

Since it is possible to choose the cycle (I) in (3.5) such that $\overline{q}$, T, ∇T, and therefore ξ are independent of time, it must be that $\xi \geq 0$ for all processes. Recalling that $\theta \geq 0$, equation (3.5) is then equivalent to the condition:

$$-q_i\left(\frac{\partial\theta}{\partial T}\frac{\partial T}{\partial x_i} + \frac{\partial\theta}{\partial x_i}\right) \geq 0 \tag{3.7}$$

If we assume Fourier's Law of heat conduction holds i.e. $q_i = K_{ij}\frac{\partial T}{\partial x_j}$ when $\frac{\partial T}{\partial x_j}$ approaches zero, with:

$$\tilde{K} = \hat{\tilde{K}}(\varepsilon_\alpha, \mu_\alpha, \overline{\gamma}_\alpha, T{:}\overline{X}) \tag{3.8}$$

equation (3.7) can be rewritten as:

$$K_{ij}\frac{\partial\theta}{\partial T}\frac{\partial T}{\partial x_i}\frac{\partial T}{\partial x_j}+K_{ij}\frac{\partial\theta}{\partial x_i}\frac{\partial T}{\partial x_j}\leq 0 \tag{3.9}$$

Given that $\tilde{K} \neq 0$, if (3.9) is to hold for arbitrary (near zero) values of $\frac{\partial T}{\partial x_j}$ it must be that

$\frac{\partial\theta}{\partial x_i} = 0$. Thus, θ is not an explicit function of $\overline{X}$. This result, added to the results of parts d) to f) above, show that θ is an explicit function of T only. Given that $\theta \geq 0$ and $\frac{\partial\theta}{\partial T} \geq 0$, $\hat{\theta}(T)$ is an invertible function and θ can replace T as a constitutive variable in all of the foregoing equations and relations.

Armed with this result, conclusion d) above is reinterpreted to be:

$$\frac{\partial\psi}{\partial\theta} = -\eta \tag{3.10}$$

and η is not a function of $\overline{\nabla}\theta$ because ψ is not from part c) above. Also (3.6) can be rewritten as:

$$\rho\xi\theta = -\frac{q_i}{\theta}g_i \tag{3.11}$$

and from (2.3):

$$\rho r - \operatorname{div}(\overline{q}) = \rho\theta\dot{\eta} \tag{3.12}$$

Relations (3.11) and (3.12) are consistent with the results of Coleman and Noll (1963) and Green and Naghdi (1977).

At this point the relations (3.1) can be rewritten as:

$$
\begin{aligned}
\psi &= \hat{\psi}\left(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, \theta{:}\bar{X}\right)\\
\xi &= \hat{\xi}\left(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, \theta, \bar{\nabla}\theta{:}\bar{X}\right)\\
\theta &= \hat{\theta}(T)\\
\bar{q} &= \hat{\bar{q}}\left(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, \theta, \bar{\nabla}\theta{:}\bar{X}\right)\\
\eta &= \hat{\eta}\left(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, \theta{:}\bar{X}\right) = -\frac{\partial\psi}{\partial\theta}\\
p_\alpha &= \hat{p}_\alpha\left(\varepsilon_\beta, \mu_\beta, \bar{\gamma}_\beta, \theta{:}\bar{X}\right) = \frac{\partial\psi}{\partial\varepsilon_\alpha}\\
m_\alpha &= \hat{m}_\alpha\left(\varepsilon_\beta, \mu_\beta, \bar{\gamma}_\beta, \theta{:}\bar{X}\right) = \frac{\partial\psi}{\partial\mu_\alpha}\\
\bar{t}_\alpha &= \hat{\bar{t}}_\alpha\left(\varepsilon_\beta, \mu_\beta, \bar{\gamma}_\beta, \theta{:}\bar{X}\right) = \frac{\partial\psi}{\partial\bar{\gamma}_\alpha}
\end{aligned}
\tag{3.13}
$$

4. *Superposed Rigid Body Motions*

In the various theories of solid mechanics, once a set of measures of the deformation are chosen, these measures are tested against transformations of the deformed configuration that leave them properly invariant. Thus, in finite deformation theories of classical continuum mechanics, the Cauchy-Green tensor $\tilde{C} = \tilde{F}^T\tilde{F}$ is chosen as a strain measure and is determined to be invariant under arbitrary finite rigid motion of the deformed configuration. In geometrically linear continuum theories, $\tilde{\varepsilon} = \text{sym}(\text{grad}(\bar{u}))$ is chosen, and is proven to be invariant under *infinitesimal* rotations of the deformed configuration. As shown by Casey and Naghdi (1981), invariance of $\tilde{\varepsilon}$ under arbitrary finite rotations may be proven, upon choosing to remove the translation and rotation at a "pivot point" in the body from the description of the deformation. This introduces an element of frame specificity to the theory, but allows the linear theory to be deduced as a special subcase of the finite theory.

The set of deformations appropriate to a theory is chosen on the basis of the ability of said measures to quantify those aspects of the deformation that are of interest within the theory itself.

Thus, $\tilde{\varepsilon}$ is an appropriate measure in linear continuum theories in that it contains the desired information on changes in lengths, areas, volumes, and angles. By comparison with this, the variance of $\tilde{\varepsilon}$ under finite rotations has been considered a notion of lesser importance throughout the history of mechanics.

In the present form of doublet mechanics, as presented in the original paper by Granik and Ferrari (1993) and summarized in (Granik and Ferrari 1995), the measures of deformation that are chosen are the elongational strains ε_α, the torsional strains μ_α, and the shear strains $\bar{\gamma}_\alpha$. As discussed above, these deformation measures were chosen for the information which they provide in the chosen reference system. In this section the invariance properties of these measures of deformation are investigated under the transformations:

$$\begin{aligned} u_i &\rightarrow u_i^+ \equiv Q_{ij}(t)u_j + c_i(t) \\ \phi_i &\rightarrow \phi_i^+ \equiv Q_{ij}(t)\phi_j \end{aligned} \qquad (4.1)$$

where $Q_{ij}(t)$ represents a proper orthogonal matrix (a rotation) and $c_i(t)$ represents a rigid translation. Under (4.1), the doublet unit vectors transform as:

$$\tau_{\alpha i}^{o+} = Q_{ij}\tau_{\alpha j}^{o} \qquad (4.2)$$

and the internodal distances remain unaltered, i.e. $\eta_\alpha^+ = \eta_\alpha$.

4.1. *The Microstrains*

Using relations (4.1) and (4.2) and the identities

$$Q_{ij}Q_{ik} = \delta_{jk} \quad \text{and} \quad \frac{\partial v_i^+}{\partial x_j^+} = Q_{im}Q_{jk}\frac{\partial v_m}{\partial x_k} \qquad (4.1.1)$$

it can be deduced from (2.10) that:

$$\Delta u_{\alpha i}^+ = Q_{ij}\Delta u_{\alpha j} \quad \text{and} \quad \Delta\phi_{\alpha i}^+ = Q_{ij}\Delta\phi_{\alpha j} \qquad (4.1.2)$$

and from (2.7), (2.8), (4.1), (4.2), (4.1.1), and (4.1.2) that:

$$\varepsilon^+_\alpha = \varepsilon_\alpha \quad \text{and} \quad \mu^+_\alpha = \mu_\alpha \tag{4.1.3}$$

Relation (2.9) for the microshear strain vector can be rewritten in Cartesian form as:

$$\gamma_{\alpha i} = \left[\left(\phi_j + \tfrac{1}{2}\Delta\phi_{\alpha j}\right)\tau^\circ_{\alpha p}\varepsilon_{ijp} + \left(\frac{\tau^\circ_{\alpha i}\tau^\circ_{\alpha j} - \delta_{ij}}{\eta_\alpha}\right)\Delta u_{\alpha j}\right] \tag{4.1.4}$$

where ε_{ijk} is the permutation tensor. Again using the relations (4.1), (4.2), (4.1.1), and (4.1.2) it is found that:

$$\gamma^+_{\alpha i} = \left[\left(\phi_l + \tfrac{1}{2}\Delta\phi_{\alpha l}\right)Q_{jl}Q_{pq}\tau^\circ_{\alpha q}\varepsilon_{ijp} + \left(\frac{Q_{il}\tau^\circ_{\alpha l}\tau^\circ_{\alpha q} - Q_{iq}}{\eta_\alpha}\right)\Delta u_{\alpha q}\right] \tag{4.1.5}$$

with no further algebraic simplification apparent. We note that:

(1) If the material is torsionless ($\phi = 0$), then transformation $(4.1)_1$ leaves $\bar{\gamma}_\alpha$ unchanged apart from orientation, i.e. $\bar{\gamma}^+_\alpha = \overline{Q}\bar{\gamma}_\alpha$.

(2) From (4.1.4) and (4.1.5), $\bar{\gamma}^+_\alpha = \overline{Q}\bar{\gamma}_\alpha$ if $\overline{Q}$ is such that:

$$Q_{jm}Q_{il}Q_{pq}\varepsilon_{jip} = \varepsilon_{mlq} \tag{4.1.6}$$

(3) If $\overline{Q}$ is an infinitesimal rotation, relation (4.1.6) is satisfied and $\bar{\gamma}^+_\alpha = \overline{Q}\bar{\gamma}_\alpha$.

By (4.1.3) and (4.1.6) it is seen that the axial and torsional microstrains are unaltered under finite rigid rotations, while the shear microstrains are invariant only under infinitesimal rotations.

4.2. *The Microstresses*

It is postulated that the doublet mechanical microstresses are invariant apart from orientation, under the transformations (4.1):

$$p_\alpha^+ = p_\alpha, \quad m_\alpha^+ = m_\alpha, \quad \text{and} \quad t_{\alpha i}^+ = Q_{ij} t_{\alpha j} \tag{4.2.1}$$

Under the constitutive assumptions (3.1), relations (4.2.1) imply that:

$$\begin{aligned} &\hat{p}_\alpha(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha^+, \theta{:}\overline{X}) = \hat{p}_\alpha(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, \theta{:}\overline{X}) \\ &\hat{m}_\alpha(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha^+, \theta{:}\overline{X}) = \hat{m}_\alpha(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, \theta{:}\overline{X}) \\ &\hat{\bar{t}}_\alpha(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha^+, \theta{:}\overline{X}) = \overline{Q} \cdot \hat{\bar{t}}_\alpha(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, \theta{:}\overline{X}) \end{aligned} \tag{4.2.2}$$

where $\bar{\gamma}_\alpha^+$ is given by (4.1.5). Relations (4.2.2) place significant restrictions on the functional forms of the microstresses. No further simplifications through application of Cauchy's representation theorems (Truesdell and Noll, 1965) are possible unless $\overline{Q}$ obeys relation (4.1.6) or the material is torsionless. If $\overline{Q}(t)$ is infinitesimal, then $\bar{\gamma}_\alpha^+ = \overline{Q}\bar{\gamma}_\alpha$ and Cauchy's representation theorems allow (4.2.2) to be rewritten as:

$$\begin{aligned} &p_\alpha = \hat{p}_\alpha(\varepsilon_\alpha, \mu_\alpha, \theta{:}\overline{X}) \\ &m_\alpha = \hat{m}_\alpha(\varepsilon_\alpha, \mu_\alpha, \theta{:}\overline{X}) \\ &\bar{t}_\alpha = \hat{\tilde{I}}_\alpha(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha \cdot \bar{\gamma}_\alpha, \theta{:}\overline{X}) \cdot \bar{\gamma}_\alpha \end{aligned} \tag{4.2.3}$$

where $\tilde{I}_\alpha$ is a second order tensor of material properties.

4.3. *Other Functions*

The other functions in our development also have similar restrictions for finite $\overline{Q}(t)$:

$$\begin{aligned} &\hat{\psi}(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha^+, \theta{:}\overline{X}) = \hat{\psi}(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, \theta{:}\overline{X}) \\ &\hat{\eta}(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha^+, \theta{:}\overline{X}) = \hat{\eta}(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, \theta{:}\overline{X}) \\ &\hat{\xi}(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha^+, \theta, \overline{Q} \cdot \overline{\nabla}\theta{:}\overline{X}) = \hat{\xi}(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, \theta, \overline{\nabla}\theta{:}\overline{X}) \\ &\hat{\bar{q}}(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha^+, \theta, \overline{Q} \cdot \overline{\nabla}\theta{:}\overline{X}) = \overline{Q} \cdot \hat{\bar{q}}(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, \theta, \overline{\nabla}\theta{:}\overline{X}) \end{aligned} \tag{4.3.1}$$

Again, for infinitesimal $\overline{Q}(t)$ Cauchy's representation theorems allow (4.3.1) to be rewritten as:

$$\psi = \hat{\psi}(\varepsilon_\alpha, \mu_\alpha, \theta : \overline{X})$$

$$\eta = \hat{\eta}(\varepsilon_\alpha, \mu_\alpha, \theta : \overline{X}) \qquad (4.3.2)$$

$$\xi = \hat{\xi}(\varepsilon_\alpha, \mu_\alpha, \theta : \overline{X})$$

$$\begin{aligned}\overline{q} = \tilde{K}_\alpha(\varepsilon_\alpha, \mu_\alpha, \overline{\gamma}_\alpha \cdot \overline{\gamma}_\alpha, \theta, \overline{\nabla}\theta \cdot \overline{\nabla}\theta, \overline{\gamma}_\alpha \cdot \overline{\nabla}\theta : \overline{X}) \cdot \overline{\gamma}_\alpha + \cdots \\ + \tilde{L}_\alpha(\varepsilon_\alpha, \mu_\alpha, \overline{\gamma}_\alpha \cdot \overline{\gamma}_\alpha, \theta, \overline{\nabla}\theta \cdot \overline{\nabla}\theta, \overline{\gamma}_\alpha \cdot \overline{\nabla}\theta : \overline{X}) \cdot \overline{\nabla}\theta\end{aligned}$$

5. Linear Elastic Doublet Mechanics

The next step in this analysis is to choose the most general linear elastic form (linearization of (4.2.2)) for the constitutive laws relating the microstrains to the microstresses without restriction to infinitesimal SRBMs. We then explore the effect of finite SRBMs on these relations and compare to the linearized forms obtained from restriction to infinitesimal SRBMs as in (4.2.3). Assuming material homogeneity, the most general linear relation between the microstrains and microstresses takes the form:

$$\hat{p}_\alpha = A_{\alpha\beta}\varepsilon_\beta + B_{\alpha\beta}\mu_\beta + C_{\alpha\beta i}\gamma_{\beta i} + J_\alpha\Theta$$

$$\hat{m}_\alpha = D_{\alpha\beta}\varepsilon_\beta + E_{\alpha\beta}\mu_\beta + F_{\alpha\beta i}\gamma_{\beta i} + K_\alpha\Theta \qquad (5.1)$$

$$\hat{t}_{\alpha i} = G_{\alpha\beta i}\varepsilon_\beta + H_{\alpha\beta i}\mu_\beta + I_{\alpha\beta ij}\gamma_{\beta j} + L_{\alpha i}\Theta$$

where sums are again taken over repeated Latin and Greek indices. $\Theta \equiv \theta - \theta_o$ is an increment of the temperature and θ_o is the temperature of the granular media in an initial state. Using relations (5.1) and (4.1.3), it is seen that:

$$\hat{p}^+_\alpha = A_{\alpha\beta}\varepsilon_\beta + B_{\alpha\beta}\mu_\beta + C_{\alpha\beta i}\gamma^+_{\beta i} + J_\alpha\Theta$$

$$\hat{m}^+_\alpha = D_{\alpha\beta}\varepsilon_\beta + E_{\alpha\beta}\mu_\beta + F_{\alpha\beta i}\gamma^+_{\beta i} + K_\alpha\Theta \qquad (5.2)$$

$$\hat{t}^+_{\alpha i} = G_{\alpha\beta i}\varepsilon_\beta + H_{\alpha\beta i}\mu_\beta + I_{\alpha\beta ij}\gamma^+_{\beta j} + L_{\alpha i}\Theta$$

However, relations (4.2.2) require that $p^+_\alpha = p_\alpha$ and $m^+_\alpha = m_\alpha$. Clearly this can only be true if $\gamma_{\beta i} = \gamma^+_{\beta i}$ or $C_{\alpha\beta i} = 0$ and $F_{\alpha\beta i} = 0$. Consideration of (4.1.4) and (4.1.5) show that generally $\gamma_{\beta i} \neq \gamma^+_{\beta i}$, therefore $C_{\alpha\beta i} = F_{\alpha\beta i} = 0$. In the linear regime, the tensile and torsional microstresses, p_α and m_α, do not depend on the shear microstrain, $\gamma_{\alpha i}$.

Relations (4.2.2) also require that $t^+_{\alpha i} = Q_{ij}t_{\alpha j}$. Substitution of (5.1) and (5.2) into this relation results in conditions:

$$Q_{ij}G_{\alpha\beta j} - G_{\alpha\beta i} = 0$$

$$Q_{ij}H_{\alpha\beta j} - H_{\alpha\beta i} = 0$$

$$Q_{ij}L_{\alpha j} - L_{\alpha i} = 0 \tag{5.3}$$

$$Q_{ij}I_{\alpha\beta jk}\gamma_{\beta k} - I_{\alpha\beta ij}\gamma^+_{\beta j} = 0$$

The first three conditions in (5.3) require that $G_{\alpha\beta i} = H_{\alpha\beta i} = L_{\alpha i} = 0$. In the linear regime, the shear microstress, $\bar{t}_\alpha$, is not a function of ε_α, μ_α, or θ i.e. $\bar{t}_\alpha = \hat{\bar{t}}_\alpha(\bar{\gamma})$. Thermal loads produce no microshear stresses.

Further restrictions on the micromoduli follow from the results of parts h) through j) of the application of the constitutive assumption to the energy/entropy balance equation and the mathematical requirement that partial differentiation be independent of the sequence of differentiation i.e.:

$$\rho\frac{\partial^2\psi}{\partial\varepsilon_\alpha\partial\varepsilon_\beta} = \rho\frac{\partial^2\psi}{\partial\varepsilon_\beta\partial\varepsilon_\alpha} = \frac{\partial p_\alpha}{\partial\varepsilon_\beta} = \frac{\partial p_\beta}{\partial\varepsilon_\alpha} = A_{\alpha\beta} = A_{\beta\alpha} \tag{5.4}$$

Such considerations lead to the conclusions that:

$$A_{\alpha\beta} = A_{\beta\alpha},\ E_{\alpha\beta} = E_{\beta\alpha},\ I_{\alpha\beta ij} = I_{\beta\alpha ji},\ \text{and } B_{\alpha\beta} = D_{\beta\alpha} \tag{5.5}$$

In summary, for a homogeneous linear elastic material subject to finite SRBMs:

$$\hat{p}_\alpha = A_{\alpha\beta}\varepsilon_\beta + B_{\alpha\beta}\mu_\beta + J_\alpha\Theta$$

$$\hat{m}_\alpha = D_{\alpha\beta}\varepsilon_\beta + E_{\alpha\beta}\mu_\beta + K_\alpha\Theta \tag{5.6}$$

$$\hat{t}_{\alpha i} = I_{\alpha\beta ij}\gamma_{\beta j}$$

with the conditions:

$$Q_{ij}I_{\alpha\beta jk}\gamma_{\beta k} - I_{\alpha\beta ij}\gamma^{+}_{\beta j} = 0 \tag{5.7}$$

$$A_{\alpha\beta} = A_{\beta\alpha},\ E_{\alpha\beta} = E_{\beta\alpha},\ I_{\alpha\beta ij} = I_{\beta\alpha ji}, \text{ and } B_{\alpha\beta} = D_{\beta\alpha}. \tag{5.8}$$

It is instructive to compare the above results to the linearized form of relations (4.2.3) which are identical to relations (5.6) and (5.8). Relation (5.7) is not an identity for infinitesimal $\overline{Q}(t)$ but is satisfied to first order (neglecting terms of order ε). This graphically illustrates the exact point where finite proper invariance breaks down for linear elastic assumptions. Relation (5.7) can be used as a measure of departure of the linear theory from proper invariance. In the linear regime, p_α and m_α do not depend on the shear strain, $\bar{\gamma}_\alpha$, or the temperature gradient, $\overline{\nabla}\theta$, and the shear microstress, $\bar{t}_\alpha$, does not depend on anything but the shear microstrain, whether $\overline{Q}(t)$ is infinitesimal or finite.

6. *Conclusion*

From the present thermomechanical analysis it is concluded that:

1. The constitutive functional measure of temperature, θ, must be a function only of empirical temperature, T.
2. The Helmholtz free energy, ψ, is not a function of the temperature gradient, $\bar{g} = \text{grad}(\theta)$.
3. The microstresses and microstrains obey the following relations:

$$p_\alpha = \rho\frac{\partial\psi}{\partial\varepsilon_\alpha},\ m_\alpha = \rho\frac{\partial\psi}{\partial\mu_\alpha},\ t_{\alpha i} = \rho\frac{\partial\psi}{\partial\gamma_{\alpha i}}$$

and thus the microstresses are also independent of grad(θ).

4. The Helmholtz free energy and the entropy, η, are related by:

$$\frac{\partial\psi}{\partial\theta} = -\eta$$

and thus the entropy is also independent of grad(θ).

5. The microstrains ε_α and μ_α are properly invariant under arbitrary finite rotation ($\varepsilon^+_\alpha = \varepsilon_\alpha$, $\mu^+_\alpha = \mu_\alpha$), however the shear microstrain transforms according to:

$$\gamma^+_{\alpha i} = \left[\left(\phi_1 + \tfrac{1}{2}\Delta\phi_{\alpha l}\right)Q_{jl}Q_{pq}\tau^\circ_{\alpha q}\varepsilon_{ijp} + \left(\frac{Q_{il}\tau^\circ_{\alpha l}\tau^\circ_{\alpha q} - Q_{iq}}{\eta_\alpha}\right)\Delta u_{\alpha q}\right]$$

6. The shear microstress, $\bar{\gamma}_\alpha$, satisfies the relation $\bar{\gamma}^+_\alpha = \bar{Q}\bar{\gamma}_\alpha$ if any of the following are true:

   (a) The material is torsionless ($\bar{\phi} = 0$);
   (b) $\bar{Q}(t)$ is such that $Q_{jm}Q_{il}Q_{pq}\varepsilon_{ijp} = \varepsilon_{mlq}$;
   (c) $\bar{Q}(t)$ is infinitesimal.

7. For a homogeneous elastic solid, the functional representations of the microstresses must obey the following relations:

$$\hat{p}_\alpha(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}^+_\alpha, \theta) = \hat{p}_\alpha(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, \theta)$$

$$\hat{m}_\alpha(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}^+_\alpha, \theta) = \hat{m}_\alpha(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, \theta)$$

$$\hat{\bar{t}}_\alpha(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}^+_\alpha, \theta) = \bar{Q}\cdot\hat{\bar{t}}_\alpha(\varepsilon_\alpha, \mu_\alpha, \bar{\gamma}_\alpha, \theta)$$

8. The constitutive laws for a homogeneous linear elastic solid reduce to:

$$\hat{p}_\alpha = A_{\alpha\beta}\varepsilon_\beta + B_{\alpha\beta}\mu_\beta + J_\alpha\Theta$$

$$\hat{m}_\alpha = D_{\alpha\beta}\varepsilon_\beta + E_{\alpha\beta}\mu_\beta + K_\alpha\Theta$$

$$\hat{t}_{\alpha i} = I_{\alpha\beta ij}\gamma_{\beta j}$$

with conditions $Q_{ij} I_{\alpha\beta jk} \gamma_{\beta k} - I_{\alpha\beta ij} \gamma^{+}_{\beta j} = 0$ and
$A_{\alpha\beta} = A_{\beta\alpha}$, $E_{\alpha\beta} = E_{\beta\alpha}$, $I_{\alpha\beta ij} = I_{\beta\alpha ji}$, and $B_{\alpha\beta} = D_{\beta\alpha}$.

The support of the National Science Foundation with MF's National Young Investigator Award is gratefully acknowledged.

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