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Generalized Navier–Stokes Equations and Dynamics of Plane Molecular Media †

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† Dedicated to memory of our friend Rem Gasparov.

Abstract: The first analysis of media with internal structure were done by the Cosserat brothers. Birkhoff noted that the classical Navier–Stokes equation does not fully describe the motion of water. In this article, we propose an approach to the dynamics of media formed by chiral, planar and rigid molecules and propose some kind of Navier–Stokes equations for their description. Examples of such media are water, ozone, carbon dioxide and hydrogen cyanide.

Keywords: Navier–Stokes equations; media with inner structures; plane molecules; water; Levi–Civita connections

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1. Introduction

It was the Cosserat brothers, [1], who first analyzed media formed by "rigid microelements", and G. Birkhoff [2] who noted that the classical Navier–Stokes equations give us uncomplete descriptions of water flows (see also [3]). In papers [4,5] the authors gave a general approach to dynamics of media having some inner structure and proposed some generalizations of the Euler and Navier–Stokes equations.

In this paper, we consider the dynamics of media formed by chiral, planar and rigid molecules (we call them CPR-molecules) molecules and propose some kind of Navier–Stokes equations for their description. Recall that a molecule is called planar if it is formed by atoms lying in the same plane and it is chiral and rigid if its symmetry group belongs to $SO(3)$. Hence, we consider a molecule as a rigid body on an oriented plane, the mechanical properties of which are specified by the tensor of inertia.

2. The Configuration Space of a CPR-Molecule

We will assume that all CPR-molecules under consideration have the trivial point symmetry group. Then a position of such a CPR-molecule is defined, up to rotations, by an oriented plane in the three-dimensional space, passing through of the center of mass of the molecule, or by the unit vector perpendicular to this plane or by a point on the unit sphere S^2.

Such molecules include, for example, molecules of ortho-water, i.e., molecules of water with different spins of hydrogen atoms [6].

Let $a \in S^2$ be a fixed point and let T_aS^2 be the tangent space to the sphere at the point a. The position of a CPR molecule on the oriented plane is uniquely determined by a rotation, and therefore, by a point on the unit circle on the tangent space T_aS^2.

Thus, the configuration space of a planar molecule with a fixed center of mass is the circle bundle of the tangent bundle for the unit two-dimensional sphere. For our goal it is more convenient to use the cotangent bundle $T^*_aS^2$ instead of the tangent one. We denote

the circle bundle of the cotangent bundle by N and it will be the configuration space of the molecule.

Let us introduce local coordinates on the configuration space. The position of a rigid body in the space is determined by the position of its center of mass and angular parameters (the Euler angles) showing its position relative to the center of mass. Let us choose a Cartesian coordinate system x, y, z in the space $\mathbb{R}^3$ so that its axes coincide with the principal axes of inertia tensor of the molecule. The metric tensor has the form $g = dx^2 + dy^2 + dz^2$, and the Lie algebra $\mathfrak{so}(3)$ can be represented by the triple of vector fields on $\mathbb{R}^3$:

$$X = z\frac{\partial}{\partial y} - y\frac{\partial}{\partial z}, \quad Y = x\frac{\partial}{\partial z} - z\frac{\partial}{\partial z}, \quad Z = y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}, \tag{1}$$

corresponding to the rotations around the axes OX, OY, OZ respectively.

In spherical coordinates ϕ, ψ, r in $\mathbb{R}^3$:

$$x = r\cos\psi\sin\phi, \quad y = r\sin\psi\sin\phi, \quad z = r\cos\phi,$$

where

$$\phi = \arccos\left(\frac{z}{r}\right), \quad \psi = \arctan\left(\frac{y}{x}\right), \quad r = \sqrt{x^2 + y^2 + z^2},$$

vector fields (1) will take the following form:

$$R_X = \sin\psi\frac{\partial}{\partial\phi} + \cot\phi\cos\psi\frac{\partial}{\partial\psi}, \quad R_Y = -\cos\psi\frac{\partial}{\partial\phi} + \cot\phi\sin\psi\frac{\partial}{\partial\psi}, \quad R_Z = -\frac{\partial}{\partial\psi}$$

respectively, and the metric tensor takes the form

$$g = r^2\left(d\phi^2 + \sin^2\phi\, d\psi^2\right)$$

in spherical coordinates. The metric g generates the invariant tensor field (the inverse metric)

$$g^{-1} = \frac{1}{r^2}\left(\partial_\phi^2 + \frac{1}{\sin^2\phi}\partial_\psi^2\right).$$

which defines the metric on the cotangent bundle $T_a^*\mathbb{R}^3$. The metric g^{-1} induces the metric

$$g_1^{-1} = \partial_\phi^2 + \frac{1}{\sin^2\phi}\partial_\psi^2$$

on the cotangent bundle $T_a^*S^2$ of a sphere of unit radius $r = 1$.

Let $q_1 = \phi, q_2 = \psi, p_1, p_2$ be the canonical coordinates on the cotangent bundle $T_a^*S^2$, and

$$\Omega = dq_1 \wedge dp_1 + dq_2 \wedge dp_2$$

be the structure differential 2-form that defines the symplectic structure on $T_a^*S^2$.

Then the Hamiltonian, corresponding to the metric g_1^{-1}, has the form

$$H = p_1^2 + \frac{1}{\sin^2 q_1}p_2^2.$$

The Hamiltonians of the vector fields R_X, R_Y, R_Z are

$$H_X = p_1\sin q_2 + p_2\cot q_1\cos q_2, \quad H_Y = -p_1\cos q_2 + p_2\cot q_1\sin q_2, \quad H_Z = -p_2$$

respectively, and therefore, corresponding Hamiltonian vector fields are

$$X_1 = \sin q_2 \frac{\partial}{\partial q_1} + \cot q_1 \cos q_2 \frac{\partial}{\partial q_2} + p_2 \frac{\cos q_2}{\sin^2 q_1} \frac{\partial}{\partial p_1} - (p_1 \cos q_2 - p_2 \cot q_1 \sin q_2) \frac{\partial}{\partial p_2},$$
$$X_2 = -\cos q_2 \frac{\partial}{\partial q_1} + \cot q_1 \sin q_2 \frac{\partial}{\partial q_2} + p_2 \frac{\sin q_2}{\sin^2 q_1} \frac{\partial}{\partial p_1} - (p_1 \sin q_2 + p_2 \cot q_1 \cos q_2) \frac{\partial}{\partial p_2},$$
$$X_3 = -\frac{\partial}{\partial q_2}.$$

Thus, we have the representation of the Lie algebra $\mathfrak{so}(3)$ by Hamiltonian vector fields X_1, X_2, X_3 with the commutation relations:

$$[X_1, X_2] = X_3, \quad [X_1, X_3] = -X_2, \quad [X_2, X_3] = X_1.$$

It is easy to see these fields are tangential to N: $X_1(H) = X_2(H) = X_3(H) = 0$.

Thus the motion of a molecule relative to its center of mass corresponds to the motion of a point on the level surface N. We take q_1, q_2 and

$$q_3 = \arctan\left(\frac{p_2}{p_1 \sin q_1}\right).$$

as local coordinates on the configuration space $N = \{H = 1\}$.

3. Metric and Levi–Civita Connection, Associated with a CPR-Molecule

The restrictions of the vector fields X_1, X_2, X_3 on the level surface N are

$$E_1 = \sin q_2 \frac{\partial}{\partial q_1} + \cot q_1 \cos q_2 \frac{\partial}{\partial q_2} - \frac{\cos q_2}{\sin q_1} \frac{\partial}{\partial q_3},$$
$$E_2 = -\cos q_2 \frac{\partial}{\partial q_1} + \cot q_1 \sin q_2 \frac{\partial}{\partial q_2} - \frac{\sin q_2}{\sin q_1} \frac{\partial}{\partial q_3},$$
$$E_3 = -\frac{\partial}{\partial q_2}$$

respectively.

Any motion of a CPR-molecule around the center of mass occurs along the trajectory of vector fields, which are linear combinations of vector fields E_1, E_2, E_3.

The basis dual to E_1, E_2, E_3 is formed by the differential 1-forms

$$\Omega_1 = \sin q_2 dq_1 - \cos q_2 \sin q_1 dq_3,$$
$$\Omega_2 = -\cos q_2 dq_1 - \sin q_2 \sin q_1 dq_3,$$
$$\Omega_3 = -dq_2 - \cos q_1 dq_3,$$

such that the Maurer–Cartan relations hold:

$$d\Omega_1 = -\Omega_2 \wedge \Omega_3, \quad d\Omega_2 = \Omega_1 \wedge \Omega_3, \quad d\Omega_3 = -\Omega_1 \wedge \Omega_2.$$

The vector fields E_1, E_2, E_3 and the differential 1-forms $\Omega_1, \Omega_2, \Omega_3$ give us the base (over $\mathbb{R}$) in the space of left-invariant vector fields and correspondingly left invariant differential 1-forms on the configuration space. Moreover, any left invariant tensor on N is a linear combination of tensor products of these vector fields and differential 1-forms with constant coefficients.

Let Λ be the inertial tensor of a molecule. It can be consid ered as a positive self adjoint operator acting on the Lie algebra $\mathfrak{so}(3)$. Let positive numbers $\lambda_1, \lambda_2, \lambda_3$ be eigenvalues of Λ. The inertia tensor defines the metric tensor on the Lie algebra $\mathfrak{so}(3)$:

$$g_\lambda = \frac{1}{2}\left(\lambda_1\Omega_1^2 + \lambda_2\Omega_2^2 + \lambda_3\Omega_3^2\right),$$

where Ω_i^2 are the symmetric squares of the 1-forms. The inertia tensor has the following coordinate representation:

$$\begin{aligned} g_\lambda =& (\lambda_1 \sin^2 q_2 + \lambda_2 \cos^2 q_2) dq_1^2 + \lambda_3 dq_2^2 \\ &+ (\lambda_1 \sin^2 q_1 \cos^2 q_2 + \lambda_2 \sin^2 q_1 \sin^2 q_2 + \lambda_3 \cos^2 q_1) dq_3^2 \\ &+ 2(\lambda_2 - \lambda_1) \sin(q_2) \cos q_2 \sin q_1 dq_1 \cdot dq_3 \\ &+ 2\lambda_3 \cos q_1 dq_2 \cdot dq_3. \end{aligned}$$

Here the dot $\cdot$ means the operation of symmetric multiplication.

Let ∇^λ be the Levi–Civita connection [7] associated with the metric g_λ and ∇_i^λ be the covariant derivative along vector field E_i. Then

$$\nabla_i^\lambda(E_j) = \sum_k \Gamma_{ij}^k E_k,$$

where Γ_{ij}^k are the Christoffel symbols. Direct calculations show that

$$\begin{aligned} \Gamma_{12}^3 =& \frac{\lambda - \lambda_1}{\lambda_3}, \quad \Gamma_{21}^3 = -\frac{\lambda - \lambda_2}{\lambda_3}, \\ \Gamma_{23}^1 =& \frac{\lambda - \lambda_2}{\lambda_1}, \quad \Gamma_{32}^1 = -\frac{\lambda - \lambda_3}{\lambda_1}, \\ \Gamma_{31}^2 =& \frac{\lambda - \lambda_3}{\lambda_2}, \quad \Gamma_{13}^2 = -\frac{\lambda - \lambda_1}{\lambda_2}. \end{aligned} \tag{2}$$

where

$$\lambda = \frac{\lambda_1 + \lambda_2 + \lambda_3}{2}.$$

All other Christoffel symbols equal to zero.

4. Metric Associated with the Media

Let $\mathbb{R}^3$ be the 3-dimensional Euclidian space, endowed with the standard metric tensor g. Consider a medium, formed by CPR-molecules filling a region $D \subset \mathbb{R}^3$. The configuration space for this type of media is the $SO(3)$-bundle $\pi : \Phi \longrightarrow D$, where $\Phi = N \times D$.

The group $SO(3)$ acts in the natural way on fibers of the projection π and we will continue to use notation E_1, E_2, E_3 for the induced vertical vector fields on Φ. These fields form the basis in the module of vertical vector fields on Φ, and accordingly differential 1-forms $\Omega_1, \Omega_2, \Omega_3$ define the dual basis in the space of differential forms on N.

The medium is also characterized by a $SO(3)$-connection in the bundle π, (see [4,5]). We call this connection the media connection and denote it by ∇^μ. The media connection allows us to compare molecules at different points of the region D.

The connection ∇^μ depends on the properties of the medium and establishes a relation between the translational motion of the molecule and its motion relative to the center of mass. Such a relation can be caused, for example, by physical inhomogeneity of space or

by the presence of effects on the environment. Let us show how it can be defined (see [5]). The connection form ω we will consider as a matrix

$$\omega = \begin{Vmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{Vmatrix}$$

where $\omega_1, \omega_2, \omega_3$ are differential 1-forms on D. In other words, connection ∇^μ shows that a molecule is subject to rotation along vector $(\omega_1(X)E_1 + \omega_2(X)E_2 + \omega_3(X)E_3)$ on the angle

$$\varphi = \sqrt{\omega_1(X)^2 + \omega_2(X)^2 + \omega_3(X)^2}$$

when we transport it on the vector X in D.

Let (x_1, x_2, x_3) be the standard Euclidian coordinates on D and $(\partial_1, \partial_2, \partial_3)$ and (d_1, d_2, d_3) be the corresponding frame and coframe respectively. Here $\partial_i = \dfrac{\partial}{\partial x_i}$ and $d_i = dx_i$. In these coordinates we have

$$\omega = \begin{Vmatrix} 0 & -\omega_{31} & \omega_{21} \\ \omega_{31} & 0 & -\omega_{11} \\ -\omega_{21} & \omega_{11} & 0 \end{Vmatrix} d_1 + \begin{Vmatrix} 0 & -\omega_{32} & \omega_{22} \\ \omega_{32} & 0 & -\omega_{12} \\ -\omega_{22} & \omega_{12} & 0 \end{Vmatrix} d_2 + \begin{Vmatrix} 0 & -\omega_{33} & \omega_{23} \\ \omega_{33} & 0 & -\omega_{13} \\ -\omega_{23} & \omega_{13} & 0 \end{Vmatrix} d_3.$$

This connection allows us to split tangent spaces $T_b\Phi$ into the direct sum

$$T_b\Phi = V_b \bigoplus H_b,$$

where V_b is the vertical part with basis $E_{1,b}, E_{2,b}, E_{3,b}$, and the horizontal space H_b is generated by the following vector fields:

$$\begin{aligned} &\partial_1 - \omega_{11}E_1 - \omega_{21}E_2 - \omega_{31}E_3, \\ &\partial_2 - \omega_{12}E_1 - \omega_{22}E_2 - \omega_{32}E_3, \\ &\partial_3 - \omega_{13}E_1 - \omega_{23}E_2 - \omega_{33}E_3. \end{aligned}$$

The horizontal distribution

$$H : \Phi \ni b \longrightarrow H_b \subset T_b\Phi$$

could be also defined as the kernel of the following system of differential 1-forms on Φ:

$$\begin{aligned} \theta_1 =& \Omega_1 + \omega_{11}d_1 + \omega_{12}d_2 + \omega_{13}d_3, \\ \theta_2 =& \Omega_2 + \omega_{21}d_1 + \omega_{22}d_2 + \omega_{23}d_3, \\ \theta_3 =& \Omega_3 + \omega_{31}d_1 + \omega_{32}d_2 + \omega_{33}d_3. \end{aligned}$$

Define a metric g^μ on the manifold Φ as a direct sum of the metric g_λ on the vertical space V and the standard metric $g_0 = dx_1^2 + dx_2^2 + dx_3^2$ on the horizontal space H:

$$g^\mu = \frac{1}{2}\sum_{i=1}^{3}\left(\lambda_i\Omega_i^2 + d_i^2\right).$$

Note that the frame $(E_1, E_2, E_3, \partial_1 - \omega(\partial_1), \partial_2 - \omega(\partial_2), \partial_3 - \omega(\partial_3))$ and the coframe $(\Omega_1, \Omega_2, \Omega_3, d_1, d_2, d_3)$ are dual and their elements are pairwise orthogonal with respect to the metric g^μ.

5. Levi–Civita Connection Associated with the Homogeneous Media

A media is said to be homogeneous if components of the connection form ω and the inertia tensor Λ are constants. Below we consider only homogeneous media.

Let ∇ be the Levi–Civita connection on the configuration space Φ associated with the metric g^{μ}.

For basic vector fields E_i and ∂_j, where $i, j = 1, 2, 3$, we have the following commutation relations:

$$[\partial_i, \partial_j] = [\partial_i, E_j] = 0, [E_1, E_2] = E_3, [E_1, E_3] = -E_2, [E_2, E_3] = E_1. \tag{3}$$

Therefore, the Levi–Civita connection ∇ on the configuration space Φ associated with the metric g^{μ} and homogeneous media has the form wherein the non trivial Christoffel symbols are given by Formula (2).

The operator of the covariant differential d_{∇} associated with the Levi–Civita connection acts on the basis vectors as follows:

$$\begin{aligned} d_{\nabla}(\partial_i) =& 0 \quad (i = 1, 2, 3), \\ d_{\nabla}(E_1) =& \Gamma^2_{31} E_2 \otimes \Omega_3 + \Gamma^3_{21} E_3 \otimes \Omega_2, \\ d_{\nabla}(E_2) =& \Gamma^1_{32} E_1 \otimes \Omega_3 + \Gamma^3_{12} E_3 \otimes \Omega_1, \\ d_{\nabla}(E_3) =& \Gamma^1_{23} E_1 \otimes \Omega_2 + \Gamma^2_{13} E_2 \otimes \Omega_1, \end{aligned}$$

and on the basic differential 1-forms:

$$\begin{aligned} d_{\nabla}(d_i) =& 0 \quad (i = 1, 2, 3). \\ d_{\nabla}(\Omega_1) =& -\Gamma^1_{32} \Omega_2 \otimes \Omega_3 - \Gamma^1_{23} \Omega_3 \otimes \Omega_2; \\ d_{\nabla}(\Omega_2) =& -\Gamma^2_{31} \Omega_1 \otimes \Omega_3 - \Gamma^2_{13} \Omega_3 \otimes \Omega_1; \\ d_{\nabla}(\Omega_3) =& -\Gamma^3_{21} \Omega_1 \otimes \Omega_2 - \Gamma^3_{12} \Omega_2 \otimes \Omega_1. \end{aligned}$$

6. Thermodynamic State of Media

The motion of the medium will be described by the trajectories of vector fields on the configuration space, which preserve the bundle $\pi : \Phi \longrightarrow D$,

$$U = \sum_{i=1}^{3} (X_i(t, x)\partial_i + Y_i(t, x, q)E_i).$$

The tensor $\Delta = d_{\nabla}U$ is called the rate of deformation tensor [4]. Following [5,8], this tensor bears an enormous thermodynamic quantity. Using properties of covariant derivative we get:

$$\Delta = \sum_{i,j=1}^{3} \left(\partial_j(X_i)\partial_i \otimes d_j + \partial_j(Y_i)E_i \otimes d_j + E_j(Y_i)E_i \otimes \Omega_j \right) + \sum_{i=1}^{3} Y_i d_{\nabla}(E_i).$$

The matrix corresponding to the tensor Δ has the block structure:

$$\Delta = \begin{Vmatrix} \Delta_H & 0 \\ \Delta_{HV} & \Delta_V \end{Vmatrix}$$

where

$$\Delta_H = \begin{Vmatrix} \partial_1(X_1) & \partial_2(X_1) & \partial_3(X_1) \\ \partial_1(X_2) & \partial_2(X_2) & \partial_3(X_1) \\ \partial_1(X_3) & \partial_2(X_3) & \partial_3(X_1) \end{Vmatrix}, \qquad \Delta_{HV} = \begin{Vmatrix} \partial_1(Y_1) & \partial_2(Y_1) & \partial_3(Y_1) \\ \partial_1(Y_2) & \partial_2(Y_2) & \partial_3(Y_2) \\ \partial_1(Y_3) & \partial_2(Y_3) & \partial_3(Y_3) \end{Vmatrix},$$

$$\Delta_V = \begin{Vmatrix} E_1(Y_1) & E_2(Y_1) + \Gamma^1_{23} Y_3 & E_3(Y_1) + \Gamma^1_{32} Y_2 \\ E_1(Y_2) + \Gamma^2_{13} Y_3 & E_2(Y_2) & E_3(Y_2) + \Gamma^2_{31} Y_1 \\ E_1(Y_3) + \Gamma^3_{12} Y_2 & E_2(Y_3) + \Gamma^3_{21} Y_1 & E_3(Y_3) \end{Vmatrix}.$$

The metric tensor g^μ defines the canonical isomorphism between vector fields and differential 1-forms on Φ: a vector field X on Φ is associated with the differential 1-form $X^\flat$ on Φ and vice versa: with any differential 1-form ω on Φ we can associate the vector field $\omega^\flat$. We have

$$E_i^\flat = \lambda_i \Omega_i, \quad \Omega_i^\flat = \frac{1}{\lambda_i} E_i, \quad \partial_i^\flat = d_i, \quad d_i^\flat = \partial_i \quad i = 1, 2, 3.$$

For fields of endomorphisms we put $(X \otimes \omega)^\flat = \omega^\flat \otimes X^\flat$. Then we have:

$$\Delta^\flat = \sum_{i,j=1}^{3} \left(\partial_j(X_i)\partial_j \otimes d_i + \lambda_i \partial_j(Y_i)\partial_j \otimes \Omega_i + \frac{\lambda_i}{\lambda_j} E_j(Y_i) E_j \otimes \Omega_i \right) + \sum_{i=1}^{3} Y_i d_\nabla^\flat(E_i),$$

where

$$\begin{aligned} d_\nabla^\flat(E_1) =& \frac{\lambda_2}{\lambda_3} \Gamma_{31}^2 E_3 \otimes \Omega_2 + \frac{\lambda_3}{\lambda_2} \Gamma_{21}^3 E_2 \otimes \Omega_3, \\ d_\nabla^\flat(E_2) =& \frac{\lambda_1}{\lambda_3} \Gamma_{32}^1 E_3 \otimes \Omega_1 + \frac{\lambda_3}{\lambda_1} \Gamma_{12}^3 E_1 \otimes \Omega_3, \\ d_\nabla^\flat(E_3) =& \frac{\lambda_1}{\lambda_2} \Gamma_{23}^1 E_2 \otimes \Omega_1 + \frac{\lambda_2}{\lambda_1} \Gamma_{13}^2 E_1 \otimes \Omega_2. \end{aligned}$$

Let σ be a stress tensor which can be considered as a field of endomorphisms on the tangent bundle. Let $\sigma^\flat$ be field of endomorphisms on the tangent bundle $T\Phi$ dual to σ. The following differential 1-form

$$\psi = ds - \frac{1}{T}(d\epsilon - \mathrm{Tr}(\sigma^\flat d\Delta) - \xi d\rho)$$

defines the contact structure on the thermodynamic phase space of medium

$$\Psi = \mathbb{R}^5 \times \mathrm{End}(T^*\Phi) \times \mathrm{End}(T\Phi)$$

with coordinates $s, T, \epsilon, \xi, \rho, \sigma, \Delta$. Here ρ, s, ϵ are the densities of the media, entropy and inner energy respectively, T and ξ are temperature and chemical potential respectively (see [4,9]). Since $\dim \mathrm{End}(T^*\Phi) = \dim \mathrm{End}(T\Phi) = 9$ we get $\dim \Psi = 23$. Legendrian manifolds L we call thermodynamic states of the media, in given case $\dim L = 11$.

Consider only those thermodynamic states for which T, ρ, Δ can be selected as coordinates.

Let $h = \epsilon - Ts$ be the density of Helmholtz free energy. Then we have the following description of the Legendrian manifold:

$$s = h_T, \quad \sigma = h_\Delta, \quad \xi = h_\rho.$$

In this case when the media is Newtonian and satisfies the Hooke law, the Helmholtz free energy is a quadratic function of Δ and has the form [4]:

$$\begin{aligned} h =& \frac{1}{2}\left(a_1 \mathrm{Tr}(\Delta^2) + a_2 \mathrm{Tr}(\Delta\Delta^\flat) + a_3(\mathrm{Tr}\Delta)^2 + a_4(\mathrm{Tr}(\Delta\Pi))^2 + a_5 \mathrm{Tr}(\Delta^\flat \Delta\Pi) + a_6 \mathrm{Tr}(\Delta\Delta^\flat\Pi) \right) \\ &+ b_1 \mathrm{Tr}(\Delta) + b_2 \mathrm{Tr}(\Delta\Pi) + c, \end{aligned}$$

where Π is the projector to the vertical component and $a_1, \ldots, a_6, b_1, b_2, c$ are some functions of ρ, T.

In this case the stress tensor has the form

$$\sigma = a_1\Delta^\flat + a_2\Delta + (a_3\mathrm{Tr}(\Delta) + b_1) + (a_4\mathrm{Tr}(\Delta\Pi) + b_2)\Pi + a_5\Delta\Pi + a_6\Pi\Delta.$$

7. Divergence of Operator Fields

In order to write the momentum conservation law, we need a notation of the divergence of the endomorphism field on Φ (see [4]). The covariant differential of an endomorphism field $A \in T\Phi \otimes T^*\Phi$ is the tensor field $d_\nabla A \in T\Phi \otimes T^*\Phi \otimes T^*\Phi$. Taking the contraction, the first and third indices of this tensor, we get the differential 1-form which is called the divergence of the operator field A:

$$\mathrm{div}A = c_{1,3}(d_\nabla A).$$

For decomposable fields $A = X \otimes \omega$, where X is a vector field and ω is a differential 1-form, the divergence operator can be calculated by the following formula:

$$\mathrm{div}(X \otimes \omega) = (\mathrm{div}X)\omega + \nabla_X(\omega). \tag{4}$$

Note that

$$\mathrm{div}(fX \otimes \omega) = f\mathrm{div}(X \otimes \omega) + X(f)\omega.$$

The following formula gives an explicit form of the divergence operator. If the operator has the form

$$A = \sum_{i,j=1}^{3} \left(a_{ij}\partial_i \otimes d_j + b_{ij}E_i \otimes \Omega_j\right),$$

then

$$\mathrm{div}A = \sum_{i,j=1}^{3} \partial_i(a_{ij})d_j + \sum_{\sigma\in S_3} \left(E_{\sigma(2)}\left(b_{\sigma(2)\sigma(1)}\right) - \Gamma^{\sigma(3)}_{\sigma(2)\sigma(1)}b_{\sigma(2)\sigma(3)}\right)\Omega_{\sigma(1)}. \tag{5}$$

Here a_{ij}, b_{ij} are functions on Φ.

For endomorphisms that are linear combinations of tensors $\partial_i \otimes \Omega_j$ and $E_i \otimes d_j$, the divergence is zero.

8. Conservation Laws

8.1. The Momentum Conservation Law

Let

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \nabla_U$$

be a material derivative; then [4] the momentum conservation law, or Navier–Stocks equation, takes the form

$$\rho\frac{dU}{dt} = (\mathrm{div}\sigma)^\flat + F,$$

or, equivalently,

$$\rho\left(\frac{\partial U}{\partial t} + \nabla_U(U)\right) = (\mathrm{div}\sigma)^\flat + F. \tag{6}$$

Here F is a density of exterior volume forces.

Let us calculate the covariant derivative $\nabla_U(U)$. We have

$$\nabla_U(U) = \sum_{j=1}^{3}\left(X_j\nabla_{\partial_j}(U) + Y_j\nabla_{E_j}(U)\right)$$

and

$$\begin{aligned}
&\nabla_{\partial_i}(\partial_j) = \nabla_{\partial_i}(E_j) = 0,\\
&\nabla_{E_i}(\partial_j) = \nabla_{E_i}(E_i) = 0,\\
&\nabla_{E_1}(E_2) = \Gamma^3_{12}E_3, \quad \nabla_{E_1}(E_3) = \Gamma^2_{13}E_2,\\
&\nabla_{E_2}(E_1) = \Gamma^3_{21}E_3, \quad \nabla_{E_2}(E_3) = \Gamma^1_{23}E_1,\\
&\nabla_{E_3}(E_1) = \Gamma^2_{31}E_2, \quad \nabla_{E_3}(E_2) = \Gamma^1_{32}E_1.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\nabla_{\partial_j}(U) =& \sum_{i=1}^{3} \partial_j(X_i)\partial_i + \partial_j(Y_i)E_i, \quad j = 1,2,3;\\
\nabla_{E_1}(U) =& E_1(Y_1)E_1 + (E_1(Y_2) + \Gamma^2_{13}Y_3)E_2 + (E_1(Y_3) + \Gamma^3_{12}Y_2)E_3\\
\nabla_{E_2}(U) =& (E_2(Y_1) + \Gamma^1_{23}Y_3)E_1 + E_2(Y_2)E_2 + (E_2(Y_3) + \Gamma^3_{21}Y_1)E_3,\\
\nabla_{E_3}(U) =& (E_3(Y_1) + \Gamma^1_{32}Y_2)E_1 + (E_3(Y_2) + \Gamma^2_{31}Y_1)E_2 + E_3(Y_3)E_3,
\end{aligned}$$

and

$$\begin{aligned}
\nabla_U(U) = &\sum_{i,j=1}^{3} \left(X_j\partial_j(X_i)\partial_i + (X_j\partial_j(Y_i) + Y_jE_j(Y_i))E_i\right)\\
&+ (\Gamma^1_{23} + \Gamma^1_{32})Y_2Y_3E_1 + (\Gamma^2_{13} + \Gamma^2_{31})Y_1Y_3E_2 + (\Gamma^3_{12} + \Gamma^3_{21})Y_1Y_2E_3
\end{aligned}$$

Moreover, we have

$$\begin{aligned}
&\nabla_{\partial_i}(d_j) = \nabla_{\partial_i}(\Omega_j) = \nabla_{E_i}(d_j) = \nabla_{E_i}(\Omega_i) = 0 \quad i,j = 1,2,3;\\
&\nabla_{E_1}(\Omega_2) = -\Gamma^2_{13}\Omega_3, \qquad \nabla_{E_1}(\Omega_3) = -\Gamma^3_{12}\Omega_2,\\
&\nabla_{E_2}(\Omega_1) = -\Gamma^1_{23}\Omega_3, \qquad \nabla_{E_2}(\Omega_3) = -\Gamma^3_{21}\Omega_1,\\
&\nabla_{E_3}(\Omega_1) = -\Gamma^1_{32}\Omega_2, \qquad \nabla_{E_3}(\Omega_2) = -\Gamma^2_{31}\Omega_1.
\end{aligned}$$

The momentum conservation law takes the form:

$$\begin{cases}
\rho\left(\partial_t(X_i) + \sum\limits_{j=1}^{3} X_j\partial_j(X_i)\right) = ((\mathrm{div}\sigma)^\flat + F)_{d_i} \qquad i = 1,2,3;\\
\rho\left(\partial_t(Y_1) + \sum\limits_{j=1}^{3} \left(X_j\partial_j(Y_1) + Y_jE_j(Y_1)\right) + (\Gamma^1_{23} + \Gamma^1_{32})Y_2Y_3\right) = ((\mathrm{div}\sigma)^\flat + F)_{\Omega_1};\\
\rho\left(\partial_t(Y_2) + \sum\limits_{j=1}^{3} \left(X_j\partial_j(Y_2) + Y_jE_j(Y_2)\right) + (\Gamma^2_{13} + \Gamma^2_{31})Y_1Y_3\right) = ((\mathrm{div}\sigma)^\flat + F)_{\Omega_2};\\
\rho\left(\partial_t(Y_3) + \sum\limits_{j=1}^{3} \left(X_j\partial_j(Y_3) + Y_jE_j(Y_3)\right) + (\Gamma^3_{12} + \Gamma^3_{21})Y_1Y_2\right) = ((\mathrm{div}\sigma)^\flat + F)_{\Omega_3};
\end{cases} \tag{7}$$

where $((\mathrm{div}\sigma)^\flat + F)_\omega$ is the coefficient of the right-hand side of (6) at the differential 1-form ω. The divergence div can be found by Formula (5). We do not give explicit formulas due to their cumbersomeness.

Equation (7) is the Navier–Stokes equation for the CPR-molecular medium.

8.2. The Mass Conservation Law

The mass conservation law has the form

$$\frac{\partial \rho}{\partial t} + U(\rho) + \rho \operatorname{div} U = 0,$$

where

$$\operatorname{div} U = \operatorname{Tr}(d_{\nabla} U) = \operatorname{Tr} \Delta = \sum_{i=1}^{3} \left(\frac{\partial X_i}{\partial x_i} + E_i(Y_i) \right).$$

The coordinate representation of this equation is as follows:

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^{3} \left(X_i \frac{\partial \rho}{\partial x_i} + Y_i E_i(\rho) \right) + \rho \sum_{i=1}^{3} \left(\frac{\partial X_i}{\partial x_i} + E_i(Y_i) \right) = 0. \tag{8}$$

8.3. The Energy Conservation Law

We suppose that there are no internal energy sources in the media. Then the conservation law of energy has the form (see [5])

$$\frac{\partial \epsilon}{\partial t} + \epsilon \operatorname{div}(U) - \operatorname{div}(\chi \operatorname{grad}(T)) + \operatorname{Tr}(\sigma^{\flat} \Delta) = 0. \tag{9}$$

Here $\chi \in \operatorname{End} T\Phi$ is the thermal conductivity of the medium.
Equations (7)–(9), and the equation of thermodynamic states of the media

$$s = h_T, \quad \sigma = h_{\Delta}, \quad \xi = h_{\rho}$$

describe the motion and thermodynamics of the CPR-molecular medium.

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References

1. Cosserat, E.; Cosserat, F. *Théorie des Corps Déformables*; A. Hermann et Fils: Paris, France, 1909.
2. Birkhoff, G. *Hydrodynamics: A study in Logic, Fact, and Similitude*, 2nd ed.; Princeton University Press: Princeton, NJ, USA, 1960; 184p.
3. Altenbach, H.; Maugin, G.A.; Verichev, N. (Eds.) *Mechanics of Generalized Continua*; Springer: Berlin/Heidelberg, Germany, 2011.
4. Duyunova, A.; Lychagin, V.; Tychkov, S. Continuum mechanics of media with inner structures. *Differ. Geom. Appl.* **2021**, *74*, 101703. [CrossRef]
5. Lychagin, V. Euler equations for Cosserat media. *Glob. Stoch. Anal.* **2020**, *7*, 197–208.
6. Kilaj, A.; Gao, H.; Rösch, D.; Küpper, J.; Willitsch, S. Observation of different reactivities of para and ortho-water towards trapped diazenylium ions. *Nat. Commun.* **2018**, *9*, 2096. [CrossRef] [PubMed]
7. Chern, S.S.; Chen W.H.; Lam, K.S. *Lectures on Differential Geometry*; Series on University Mathematics, 1; World Scientific Publishing Co., Inc.: River Edge, NJ, USA, 1999.
8. Lychagin, V. Contact Geometry, Measurement, and Thermodynamics. In *Nonlinear PDEs, Their Geometry and Applications*; Kycia, R., Schneider, E., Ulan, M., Eds.; Birkhäuser: Cham, Switzerland, 2019; pp. 3–52.
9. Gibbs, J.W. A Method of Geometrical Representation of the Thermodynamic Properties of Substances by Means of Surfaces. *Trans. Connect. Acad.* **1873**, *1*, 382–404.