Classical Dynamics of Fullerenes

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Abstract. The classical mechanics of large molecules and fullerenes is studied. The approach is based on the model of collective motion of these objects. The mixed Lagrangian (material) and Eulerian (space) description of motion is used. In particular, the Green and Cauchy deformation tensors are geometrically defined. The important issue is the group-theoretical approach to describing the affine deformations of the body. The Hamiltonian description of motion based on the Poisson brackets methodology is used. The Lagrange and Hamilton approaches allow us to formulate the mechanics in the canonical form. The method of discretization in analytical continuum theory and in classical dynamics of large molecules and fullerenes enable us to formulate their dynamics in terms of the polynomial expansions of configurations. Another approach is based on the theory of analytical functions and on their approximations by finite-order polynomials. We concentrate on the extremely simplified model of affine deformations or on their higher-order polynomial perturbations.

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1. Introduction

In this paper, the classical motion of large molecules will be studied. As an example of such molecules, the fullerenes are taken into considerations [59]. As a typical and the most suggestive example, the molecule $C_{60}$ is considered (see Fig. 1). The distribution of carbon atoms in this fullerene is maximally compatible with our general assumption about the almost spherical (isotropic) equilibrium positions on the spherical surface. Let us also mention that this is true not only in the case of fullerenes but also in any approximately spherical shapes of molecules, e.g., $P_4$, bacterium cocci (which can be arranged in chains called streptococci), or rotaviruses.

Let us mention that the model of an anisotropic elastic shell was studied by Novikov [28]. However, although the body was there close to a sphere, the topic and results were rather different from our ones. In our approach, the object subjects to affine constraints, or exceptionally, to some higher-order polynomial constraints. Later on, some qualitative consequences are discussed. Then, some Maupertuis-like modifications, namely models where the potential energy is included into the kinetic energy expression, are considered too. This opens the perspective of using the group-theoretical models of the configuration space, with potential energy hidden into the kinetic form, and which based on special functions may be formulated and in some situations explicitly solved.

It is important to mention also that some aspects of our discussion may be applicable in apparently quite different branches of physics, like the theory of collective vibrations of atomic nuclei (nuclear fluids) and even in certain astrophysical problems. Nevertheless, the main application of our approach is the theory of molecular vibrations [11, 34, 43, 48, 49].

In what follows the our earlier developed method of collective motions based on polynomial and of other type functional expansions of configurations will be used. The atoms in fullerenes create a
discrete skeleton of some material shell. More precisely, this shell is obtained by smearing out the discrete atomic structure of the molecule (so to say as the result of the ‘continuumization’ process). It can be deformed as a continuum, and finally one returns to the discrete description by expanding the continuum configurations with respect to the basic monomials of material variables, or equivalently with respect to spherical functions

\[ x^i(t, a) = \sum_{l=0}^{L} q^i_{lm}(t) \|a\|^{l} Y^{lm}\left(\frac{a}{\|a\|}\right). \]  

(1.1)

Here \( a^k \) are the Lagrange coordinates, with \( \|a\| = \left( \sum_k (a^k)^2 \right)^{1/2} \), and \( x^i(t, a) \) are the Euler coordinates of the generic material point. The coefficients \( q^i_{lm} \) are the amplitudes of the vibrations of the \( \|a\|^{l} Y^{lm}\left(\frac{a}{\|a\|}\right) \)-mode appearing in the configuration \( x^i(t, a) \). Obviously, in the general discretization techniques it can be admitted the infinite series in (1.1), i.e., \( L = \infty \). However in our case of a system with the finite number of degrees of freedom, such a generalization would be non-justified and essentially wrong. The reason is that in spite of a finite number of degrees of freedom in a molecule one would then artificially introduce the infinite number of generalized coordinates. Translating the formula (1.1) onto the polynomial language, the expansion of \( x^i(t, a) \) should be rewritten as follows:

\[ x^i(t, a) = \sum_{l=0}^{L} q^i(t)_{A_1 \ldots A_l} a^{A_1} \ldots a^{A_l}. \]  

(1.2)

Like as in the previous formula (1.1) in the discretization of continuum, one can put \( L = \infty \), i.e., represent \( x^i(t, a) \) as an analytical function of \( a^k \)-s. However, in our fullerene problems in the case when the total number of degrees of freedom is finite, this would be just also wrong. The reason is that in a consequence of the symmetry of tensors \( t q^i_{A_1 \ldots A_l} \) those quantities fail to be independent coordinates. In this respect formula (1.1) is better, although also the caution is necessary because \( q^i_{lm} = \overline{q^i_{lm}} \). Let us also mention that even for finite \( L \) the coefficients \( q^i_{A_1 \ldots A_l} \) are not usual generalized coordinates because of the symmetry of tensors \( q^i_{A_1 \ldots A_l} \). The spherical functions \( Y^{lm} \) describe vibrational excitations with \( l \) excited waves. The corresponding wave lengths equal

\[ \lambda = \frac{2\pi R}{l}, \]  

(1.3)

with \( R \) denoting the radius of the smallest sphere approximating the fullerene. Incidentally, let us remember that the motion of an approximately spherical body was discussed by Novikow [28]. However, our approach is quite different. Namely, we consider the motion under the influence of elastic forces, discuss the Maupertuis-like model with potential somehow included into kinetic energy. Our treatment of affine

![Fig. 1. Ideal and the deformed C_{60} fullerenes cells (https://en.wikipedia.org/wiki/Fullerene)](https://en.wikipedia.org/wiki/Fullerene)
motion is not restricted to small vibrations. Nevertheless, it is true that in the model of higher-order polynomial deformations one often assumes that polynomial contributions of the higher order than one are treated as small.

The finite expansions (1.1) and (1.2) are to be substituted to the general multi-particle equations of motion. This is interpreted either as a change of continuum variables $x^i(t, a)$ or as imposing constraints restricting the multi-particle or continuum dynamics to the discrete one in either $q_{lm}^i$ or $q_{A_1...A_l}$-variables. Then, applying the d’Alembert principle, the finite system of equations of motion in terms of the generalized coordinates $q_{lm}^i$ or $q_{A_1...A_l}$ is obtained [56].

The expression with respect to the trigonometric polynomials, i.e., the spherical functions (1.1), or equivalently the polynomial representation (1.2), is physically interpreted as expansions with respect to the lengths of the excited waves. As it was mentioned for the systems with a finite number of degrees of freedom, like fullerenes, those expansions are finite. No doubt, from the mathematical point of view the leading terms correspond to the values $l = 0$ and $l = 1$, i.e., to the model of affinely rigid body (pseudo-rigid body) [3,9,35,36,47]. In this oversimplified model, the body is subjected to translations, rotations and homogeneous deformations. The central cross sections of the fullerenes are in general ellipses, and the total shape of the deformed fullerenes is ellipsoidal.

The Green and Cauchy deformation tensors are constant in the material and the physical spaces. The most beautiful mathematical property of the model is its group structure, or rather homogeneous space of degrees of freedom. The mentioned group is the affine group or simply the linear group when the translational motion of the center of mass is neglected [2–5,8,32,35,36,39].

We start reviewing in short dynamics of affinely rigid bodies. Its lowest order approximation is rather rough. Nevertheless, in the case of fullerenes and, more in general, big molecules, it is the optimal first step toward the rigorous polynomial description. Unfortunately, the degrees of freedom with $l > 1$ cannot be described within the group-theoretical scheme; nevertheless, it seems very natural to consider them as small perturbations to the dynamics of affinely rigid body. It is well known that mappings given by polynomials of the order $1 < l < \infty$ do not form a Lie group [47]. Later on, it will be shown how this perturbation procedure works and how the first step, i.e., the affine dynamics, simplifies the general polynomial method.

### 2. Dynamics of affinely rigid bodies

Let us denote the material and physical spaces by $N$ and $M$, respectively. They are $n$-dimensional affine spaces with linear spaces of translations $U$ and $V$. Of course, physically $n = 3$, but it is convenient to admit the general dimension $n$ at least during the primary discussion.

The corresponding radius vector operations from $N \times N$ onto $U$ and from $M \times M$ onto $V$ are described by $XY \in U$ and $x\bar{y} \in V$ for $X,Y \in N$ and $x,y \in M$. Obviously, the arrow operations satisfy the usual affine axioms [21,47–49]

$$\bar{ab} + \bar{bc} + \bar{ca} = 0.$$  \hspace{1cm} (2.1)

For any point $p$ of the affine space, the operation $q \mapsto \bar{pq}$ is a bijection onto the translational space. Affine mappings $\phi : N \rightarrow M$ are defined as those for which there exists unique linear mapping $L[\phi] : U \rightarrow V$ such that for any $X \in N$ and $Y \in N$ the following formula holds

$$\phi(p)\phi(q) = L[\phi] \bar{pq}.$$  \hspace{1cm} (2.2)

The set of affine mappings will be denoted by $\text{Aff}(N,M)$. If $N = M$, the symbol $\text{Aff}(N)$ will be used. The subset of affine bijections is a Lie group and is denoted by $\text{GAff}(N)$. Similarly, the set of linear mappings will be denoted by $L(U,V)$ or simply $L(U)$ if $V = U$. The group of linear bijections (isomorphisms) of $U$ onto itself will be denoted by $GL(U)$. If $L[\varphi] = \text{Id}_U$ for $\varphi \in \text{GAff}(N)$, then we say that $\varphi$ is a pure translation. Any affine mapping $\phi \in \text{Aff}(\mathbb{R}^n)$ may be written as
The manifolds of the affine isomorphisms of \( N \) onto \( M \) will be denoted by \( \text{Aff}(N,M) \). In representations, (2.3) and (2.4) are denoted by the \(( X, \varphi )\) pairs with nonvanishing determinants of matrices \([ \varphi^i_j ]\) and \([ \varphi^i_A ]\). In other words, \( L[\varphi] \) in (2.2) will be the linear isomorphisms.

Affine structures of \( N, M \) are sufficient for defining affine degrees of freedom of extended bodies or of their structural elements [58]. Situation is more complicated in the case of dynamics. Indeed, metric tensors in \( N, M \) are in principle useful for defining the kinetic energy and the formulas for work and power. It is thought possible to define metric-free and thus affinely invariant models of the kinetic energy. However, they are the relatively exotic. Namely, they fail to be positively definite. On the other hand, their negative contributions may be interpreted as a strange negative ‘centrifugal attraction’ between deformation invariants. This may be interpreted as a partial inclusion of the dynamics into kinetic energy, in a sense resembling the Maupertuis variational principle. Such a model would be useful for describing bounded elastic vibrations without using any attractive potential [47]. The invariance of such a ‘geodetic’ dynamics with respect to the full linear group is a desirable feature because it opens the perspective of solving dynamical equations in terms of relatively well-investigated special functions on Lie groups. Nevertheless, the affine model of a body seems to be relatively strange, except perhaps some problems in nuclear dynamics and elementary particle physics. So, at least temporarily, let us introduce the metrical concepts to our purely affine framework.

Let \( g \in V^* \otimes V^* \), \( \eta \in U^* \otimes U^* \) be, respectively, the spatial and material metric tensors; they are by definition symmetric and are analytically represented by symmetric matrices \( g_{ij}, \eta_{AB} \). The corresponding Cauchy and Green deformation tensors \( C \in V^* \otimes V^* \), \( G \in U^* \otimes U^* \) are given by [12, 18, 46–48]

\[
G = \varphi^* \cdot g, \quad C = (\varphi^{-1})^* \cdot \eta,
\]

i.e., in components:

\[
G_{AB} = g_{ij} \varphi^i_A \varphi^j_B, \quad C_{ij} = \eta_{AB} (\varphi^{-1})^A_i (\varphi^{-1})^B_j.
\]

Their contravariant inverses \( G^{-1} \in U^* \otimes U^* \) and \( C^{-1} \in V^* \otimes V^* \) are analytically represented as:

\[
G^{-1AB} = (\varphi^{-1})^A_i (\varphi^{-1})^B_j g^{ij}, \quad C^{-1ij} = \varphi^i_A \varphi^j_B \eta^{AB}.
\]

The measures of deformation, which vanish in the non-deformed state, are given by [13, 18]

\[
E := \frac{1}{2} (G - \eta), \quad e := \frac{1}{2} (g - C).
\]

Fixing metrics \( \eta \) and \( g \) gives rise to the Euclidean subgroups \( \mathcal{E}(N, \eta) \) and \( \mathcal{E}(M, g) \) of the affine groups \( \text{GAff}(N) \) and \( \text{GAff}(M) \), respectively. Their linear parts are the orthogonal subgroups \( \mathcal{O}(U, \eta) \) and \( \mathcal{O}(V, g) \) preserving, respectively, the metric tensors \( \eta \) and \( g \).

Let us quote the transformation rules for deformation tensors \( G \) and \( C \). They are invariant of transformations in \( N \) and \( M \). More complicated situation is with the transformation properties under the linear parts of \( L[\varphi] \). Let us observe that the most convenient choice of material (Lagrange) coordinates is the one in which the Lagrange coordinates of the center of mass are such that \( a^K = 0 \). Then \( \text{Aff}(N, M) \) and \( \text{GAff}(N, M) \) may be identified, respectively, with \( M \times L(U, V) \) and \( M \times GL(U, V) \). Here the first
component \( r \in M \) is the current (Eulerian) position of the center of mass, and \( \varphi \in GL(U,V) \) is the internal configuration in the relative motion.

Linear mappings \( A \in GL(V) \) and \( B \in GL(U) \) act on the internal configuration as follows:

\[
\varphi \mapsto A\varphi = L_A(\varphi), \quad \varphi \mapsto \varphi B = R_B(\varphi),
\]

where the symbols \( L, R \) refer, respectively, to the left and right actions. If \( A \in \mathcal{O}(V,g) \), \( B \in \mathcal{O}(U,\eta) \), the deformations are invariant under those actions:

\[
G[A\varphi] = G[\varphi], \quad C[\varphi B] = C[\varphi].
\]

The inverse transformation rules, i.e., the right one for internal configuration in the relative motion.

Let us observe that those rules are valid for the general \( B \in GL(U) \), \( A \in GL(V) \) look, respectively, as follows

\[
G[\varphi B]_{KL} = G[\varphi]_{CD}B^C_{\phantom{C}K}B^D_{\phantom{D}L}, \quad C[\varphi B]_{ij} = C[\varphi]_{ab}(A^{-1})^a_i(A^{-1})^b_j.
\]

Let us observe that those rules are valid for the general \( B \in GL(U) \), \( A \in GL(V) \). Unlike this there is no concise formula for \( G[A\varphi] \), \( C[\varphi B] \) if \( A, B \) are not isometries, i.e., if they are not members of \( \mathcal{O}(V,g) \), \( \mathcal{O}(U,\eta) \).

The next very important concept is deformation invariants. By definition, they are scalar functions \( f \) such that for any \( A \in \mathcal{O}(V,g) \), \( B \in \mathcal{O}(U,\eta) \) the following holds

\[
f(A\varphi B) = f(\varphi).
\]

In other words, they are functions on the manifolds of double cosets of \( LI(U,V) \) with respect to the transformation group \((2.10)\) with isometric \( A, B \). In \( n \)-dimensional spaces, there are \( n \) functional independent deformation invariants. They may be chosen in various ways, for example, as

\[
Tr(\hat{G}^k), \quad Tr(\hat{C}^k), \quad Tr(\hat{E}^k), \quad Tr(\hat{e}^k), \quad k = 1, \ldots, n,
\]

where \( \hat{G}, \hat{C}, \hat{E}, \hat{e} \) are defined as mixed tensors:

\[
\hat{G}^A_{\phantom{A}B} = \eta^{AC}G_{CB}, \quad \hat{C}^i_{\phantom{i}j} = g^{ik}C_{kj}, \quad \hat{E}^A_{\phantom{A}B} = \eta^{AC}E_{CB}, \quad \hat{e}^i_{\phantom{i}j} = g^{ik}e_{kj}.
\]

Any element in the list \((2.14)\) may be used as a set of basic deformation invariants. Invariants of any particular system are expressible by functions of any other system. The particular choice depends on the convenience in any particular problem.

Another often used choice of invariants is based on the following eigenequations:

\[
\det[\hat{G}^A_{\phantom{A}B} - \lambda\delta^A_{\phantom{A}B}] = 0, \quad \det[\hat{C}^i_{\phantom{i}j} - \lambda\delta^i_{\phantom{i}j}] = 0,
\]

\[
\det[\hat{E}^A_{\phantom{A}B} - \lambda\delta^A_{\phantom{A}B}] = 0, \quad \det[\hat{e}^i_{\phantom{i}j} - \lambda\delta^i_{\phantom{i}j}] = 0.
\]

Solutions of any of these equations with respect to \( \lambda \) give us another system of basic invariants.

The transformation groups \((2.10)\) give rise to certain non-holonomic velocities and momenta, which are very convenient in theoretical and computational motion of the affine body. These quantities are affine velocities and co-moving spins in the spatial and co-moving representations.

Let the affine motion be described by the following function \([39,40]\):

\[
x^i(t,a) = x^i(t) + \varphi^i_K(t)a^K,
\]

where \( x^i(t) \) denotes the instantaneous position of the center of mass in \( M \), and the linear mapping \( \varphi \in LI(U,V) \) with coordinate \( \varphi^i_K(t) \) is the instantaneous internal configuration.

One can easily show that the Euler velocity field in \( M \) is given by

\[
V^i(t,y) = \frac{dx^i}{dt} + \Omega^i_j(y^j - x^j),
\]

where

\[
\Omega^i_j = \frac{d\varphi^i_K}{dt} \varphi^{-1}K_j.
\]
This quantity was introduced by A.C. Eringen in his theory of micromorphic continua and was called ‘gyration’ by him [12]. It is easy to see that it is a group-theoretic non-holonomic velocity corresponding to the transitive, effective and free action of $GL(V)$ on $LI(U, V)$. This is a left-hand action. Geometrically, it is a tensorial geometric object of valence $T^1_1$ on the manifold $M$ roughly speaking, a spatial or Eulerian one. Its material representation in $N$ is given by

$$\hat{\Omega}^A_B = \varphi^{-1}A_i \frac{d \varphi^i_B}{dt} = \varphi^{-1}A_i \Omega^i_j \varphi^j_B, \quad \tag{2.20}$$

and corresponds to the right-hand side action of $GL(U)$ on $LI(U, V)$. In the case when one puts $V = U = \mathbb{R}^n$ the situation simplifies: $(\Omega^i_j)$ are simply right-invariant and $(\hat{\Omega}^A_B)$ left-invariant objects on $GL(n, \mathbb{R})$. Their transformation rules under the group $GL(V)$ and $GL(U)$ acting on the left and right on $LI(U, V)$ are as follows:

$$A \in GL(V) : \Omega \mapsto A \Omega A^{-1}, \quad \hat{\Omega} \mapsto \hat{\Omega}, \quad \tag{2.21}$$
$$B \in GL(U) : \hat{\Omega} \mapsto B^{-1} \hat{\Omega} B, \quad \Omega \mapsto \Omega. \quad \tag{2.22}$$

Similarly, when using the Hamiltonian language, one can introduce the canonical momenta $P^A_i$ conjugate to velocities $V^i_A$ and their spatial and material non-holonomic representations $\Sigma^i_j$ and $\hat{\Sigma}^A_B$ conjugate to the affine velocities

$$\Sigma^i_j = \varphi^i_A P^A_j, \quad \hat{\Sigma}^A_B = P^A_i \varphi^i_B = \varphi^{-1}A_i \Sigma^i_j \varphi^j_B. \quad \tag{2.23}$$

We stress that $\Omega, \hat{\Omega}$ are non-holonomic velocities, and there are no generalized coordinates $x^i_j, \hat{x}^A_B$ which might have given rise to $\Omega^i_j, \hat{\Omega}^A_B$ by differentiation

$$\Omega^i_j \neq \frac{dx^i_j}{dt}, \quad \hat{\Omega}^A_B \neq \frac{d \hat{x}^A_B}{dt}. \quad \tag{2.24}$$

Similarly, $\Sigma^i_j, \hat{\Sigma}^A_B$ are not canonical momenta conjugated to any generalized coordinates $x^i_j, \hat{x}^A_B$, but in a sense they are canonically conjugated to $\Omega^i_j$ as follows: $\hat{\Omega}^A_B$:

$$\langle \Sigma, \Omega \rangle = \langle \hat{\Sigma}, \hat{\Omega} \rangle = Tr(\Sigma \Omega) = Tr(\hat{\Sigma} \hat{\Omega}) = P^A_i V^i_A. \quad \tag{2.25}$$

The quantities $\Sigma^i_j$ and $\hat{\Sigma}^A_B$ are Hamiltonian generators of the left and right actions of $GL(V)$ and $GL(U)$ on $LI(U, V)$ [1,39,40]. Let us note that their doubled $g$- and $\eta$-skew-symmetric parts, i.e., spin and vorticity

$$S^i_j = \Sigma^i_j - g^{ik} g_{jm} \Sigma^m_k, \quad V^A_B = \hat{\Sigma}^A_B - \eta^{AC} \eta_{BD} \hat{\Sigma}^D_C, \quad \tag{2.26}$$

generate the left and right actions of the orthogonal subgroups $O(V, g)$ and $O(U, \eta)$ on $LI(U, V)$ [1,39,40]. It has to be stressed that $V^A_B$ are co-moving components of $S^i_j$ only when we impose the constraints of isometry onto $\varphi \in LI(U, V)$, but in general

$$S^i_j \neq \varphi^{-1}A_i V^A_B (\varphi^{-1})^B_j. \quad \tag{2.27}$$

We do not use the factor $\frac{1}{2}$ in (2.26) because the Poisson brackets are now more elegant. Also the translational velocity and linear momentum may be represented in co-moving terms, just like $\Omega^i_j$ and $\Sigma^i_j$, and namely as

$$\hat{v}^A = (\varphi^{-1})^A_i \hat{v}^i, \quad \hat{p}_A = p_i \varphi^i_A. \quad \tag{2.28}$$

Transformation properties of $\Sigma$ and $\hat{\Sigma}$ under the mappings $A \in GL(V)$ and $B \in GL(U)$ are analogous to those for $\Omega$ and $\hat{\Omega}$:

$$A \in GL(V) : \Sigma \mapsto A \Sigma A^{-1}, \quad \hat{\Sigma} \mapsto \hat{\Sigma}, \quad \tag{2.29}$$
$$B \in GL(U) : \hat{\Sigma} \mapsto B^{-1} \hat{\Sigma} B, \quad \Sigma \mapsto \Sigma.$$
there exist the orbital and total affine counterparts of the angular momentum. The translational, i.e.,
orbital affine momentum $\Lambda$ with respect to some spatial origin $O \in M$ is defined as follows:

$$\Lambda(O)_j^i = x^i p_j.$$  \hfill (2.30)

Here as usual $x^i$ are the coordinates of the instantaneous position of the center of mass in $M$ related to
the fixed origin $O \in M$. Of course, unlike $\Sigma^i_j$ which is an objective quantity, $\Lambda(O)$ depends explicitly
on the choice of $O$. The total affine momentum with respect to $O$ is obviously defined as the sum:

$$I(O)_j^i := \Lambda(O)_j^i + \Sigma^i_j.$$  \hfill (2.31)

There is a complete analogy between those objects and the translational, internal and total angular
momenta. The angular momenta equal the doubled skew-symmetric parts of the affine momenta \([6,25,39–46,48,49]\).

Let us now quote the fundamental Poisson brackets between the quantities like $\Sigma^i_j$, $\hat{\Sigma}^A_B$ and the
coordinates. They may be either obtained by the direct computation based on the brackets $x^i$, $p_i$, $\varphi^i_A$, $p^A_i$ or just guessed from the structure constants of the linear and affine groups. The first method is based
on the following primary brackets definition between $x^i$, $p_j$, $\varphi^i_A$, $P^B_m$:

$$\{x^i,p_j\} = \delta^i_j, \quad \{\varphi^i_A,p^B_m\} = \delta^B_A \delta^i_m.$$  \hfill (2.32)

The brackets between other pairs vanish. One must use the standard properties of Poisson brackets like
their skew-symmetry, Jacobi identity and the following additional property only:

$$\{F,H(G_1,\ldots,G_k)\} = \sum_{p=1}^k H_p(G_1,\ldots,G_k) \{F,G_p\}.$$  \hfill (2.33)

The Poisson brackets between affine spin components follow also directly from the structure constants of
the linear group, when their property to be Hamiltonian generators is used. One can easily show that

$$\{\Sigma^A_B, \Sigma^C_D\} = \delta^C_B \Sigma^A_D - \delta^A_D \Sigma^C_B,$n\{\Sigma^i_j, \hat{\Sigma}^A_B\} = 0,$n\{\Sigma^i_j, \Sigma^k_l\} = \delta^i_l \Sigma^k_j - \delta^k_j \Sigma^i_l,$  \hfill (2.34)

and similarly

$$\{\Lambda^i_j, \Lambda^k_l\} = \delta^i_l \Lambda^k_j - \delta^k_j \Lambda^i_l,$n\{I^i_j, I^k_l\} = \delta^i_l I^k_j - \delta^k_j I^i_l,$n\{\Lambda^i_j, \Sigma^k_l\} = 0.$$  \hfill (2.35)

Besides, following $GAff(N)$-, $GAff(M)$-brackets exist:

$$\{\hat{\Sigma}^A_B, \hat{P}_C\} = \delta^A_C \hat{P}_B,$n\{\hat{I}^i_j, \hat{p}_k\} = \{\Lambda^i_j, p_k\} = \delta^i_k p_j.$$  \hfill (2.36)

The last subsystem of brackets, which is of relevance for deriving the equations of motion, is that of affine
momenta with functions depending on configuration variables only:

$$\{F, \Sigma^i_j\} = \varphi^i_A \frac{\partial F}{\partial \varphi^j_A},$$n$$\{F, \Lambda^i_j\} = x^i \frac{\partial F}{\partial x^j},$$n$$\{F, \hat{\Sigma}^A_B\} = \varphi^i_B \frac{\partial F}{\partial \varphi^i_A}.$$  \hfill (2.37)

Inertia of the affine body is described by the mass translational motion and by the second-order moment of inertia, roughly speaking the quadrupole moment of the mass distribution.
Let the constant (time-independent) measure $\mu$ on $N$ describe the co-moving (Lagrangian) mass distribution. The total mass and the second-order moment of inertia are the constant quantities $m \in \mathbb{R}$, $\mathcal{J} \in U \otimes U$ given by definition by the integrals:

$$m := \int_N d\mu(a), \quad \mathcal{J}^{KL} := \int_N a^K a^L d\mu(a). \quad (2.38)$$

It is assumed that in the material coordinates of the center of mass the first-order momentum vanishes

$$\mathcal{J}^K = \int_N a^K d\mu(a) = 0. \quad (2.39)$$

The higher-order moments, e.g.,

$$\mathcal{J}^{K_1 \ldots K_m} := \int_N a^{K_1} \ldots a^{K_m} d\mu(a), \quad (2.40)$$

can be useful but only if the affine-rigidity constraints and the higher-order polynomials or spherical functions expansions are admitted. In the mechanics of the homogeneously deformable body, they are not needed. We notice that all $\mathcal{J}^{K_1 \ldots K_m}$-quantities are constant and uniquely characterize the inertial properties of the polynomially deformable body.

In certain problems, the Euler representation of inertial quantities, e.g.,

$$\mathcal{J}[\varphi]^{kl} = \varphi^k A \varphi^l B \mathcal{J}^{AB}. \quad (2.41)$$

will be necessary. Nevertheless, just as in the case of the usual, i.e., metrically rigid body, they depend explicitly on the configuration $\varphi$, so they are not the intrinsic characteristics of inertia.

If $\Phi(t): N \rightarrow M$ is the configuration of the body, then the general formula for the kinetic energy is given by:

$$T = \frac{1}{2} g_{ij} \frac{d\Phi^i}{dt}(t, a) \frac{d\Phi^j}{dt}(t, a) d\mu(a), \quad (2.42)$$

and in the case of the affine motion it reduces to:

$$T = \frac{m}{2} g_{ij} \frac{dx^i}{dt} \frac{dx^j}{dt} + \frac{1}{2} g_{ij} \frac{d\varphi^i_A}{dt} \frac{d\varphi^j_B}{dt} J^{AB} = T_{tr} + T_{int}. \quad (2.43)$$

This is a sum of the translational and the internal (relative motion) kinetic energies. It is seen that $\mathcal{J}^{AB}$ and $m$ of all internal parameters (2.40) enter this formula only. If motion admits higher-order polynomial corrections $Y^{lm}$ with $l > 1$ in (1.1), then also higher-degree inertial moments occur in the internal part of the kinetic energy $T_{int}$. This situation will be discussed in the next part of the paper.

Let us assume that the system is subjected to the potential forces derived from the potential energy function $V(x, \varphi)$ only. Lagrangian of the system is then given by

$$L = T - V(x, \varphi). \quad (2.44)$$

The Lagrange transformation has the form:

$$p_i = \frac{\partial T}{\partial \dot{x}^i} = mg_{ij} \frac{dx^j}{dt}, \quad P^A_i = g_{ij} \frac{d\varphi^i_A}{dt} J^{BA}, \quad (2.45)$$

and the resulting Hamiltonian is given by the expression

$$H = T + V(x, \varphi) = \frac{1}{2m} g^{ij} P_i P_j + \frac{1}{2} g^{ij} J^{-1}_{AB} P^A_i P^B_j + V(x, \varphi), \quad (2.46)$$

where $J^{-1} \in U^* \otimes U^*$ is the twice covariant inverse of $J$, and

$$J^{-1AC} J_{CB} = \delta^A_B. \quad (2.47)$$
So, roughly speaking, \( J^{AB} \) and \( J_{AB}^{-1} \) are related to each other as \( g^{ij} \) and \( g_{ij} \). The symbol \( J^{-1} \) will be used in what follows explicitly just to avoid the impression that the components \( J_{AB}^{-1} \) are related to \( J^{AB} \) via the \( \eta \)-shift of indices. Indeed, in general

\[
J^{-1}_{AB} \neq \eta_{AC} \eta_{BD} J^{CD}.
\] (2.48)

For the metric tensors \( g, \eta \) the same symbol for the original tensors and their contravariant inverses will be used only.

We observe that in the case of non-affine configurations the (Eulerian) spatial and Lagrangian (material) centers of mass, \( o[\varphi] \), \( O[\varphi] \) are not related by the simple formula like in affine situation. Namely, the proper definition of the spatial center of mass \( o[\varphi] \in M \) reads:

\[
\int \overrightarrow{o[\varphi]} p \, d\mu(\varphi)(p) = 0,
\] (2.49)

where the spatial distribution of mass in \( M \) is given by

\[
\mu_{\varphi}(A) = \mu(\varphi^{-1}(A \cap \varphi(N))).
\] (2.50)

In the special case when \( \varphi \) is a bijection of the affine material space \( N \) onto the total \( M \), this expression is given by

\[
\int f \, d\mu_{\varphi} = \int f \circ \varphi \, d\mu.
\] (2.51)

It can be shown that if \( \varphi \) is described in terms of the analytical expansion

\[
\varphi^{i} = \sum_{m=0}^{\infty} m^{\varphi^{i}_{A_{1}...A_{m}} a^{A_{1}}...a^{A_{m}}},
\] (2.52)

and the velocity, i.e., the time derivative of (2.52) by:

\[
\xi^{i} = \sum_{m=0}^{\infty} m^{\xi^{i}_{A_{1}...A_{m}} a^{A_{1}}...a^{A_{m}}},
\] (2.53)

where

\[
m^{\xi^{i}_{A_{1}...A_{m}}} = \sum_{m=0}^{\infty} \frac{d}{dt} m^{\varphi^{i}_{A_{1}...A_{m}} a^{A_{1}}...a^{A_{m}}}.
\] (2.54)

Then, we get

\[
\overrightarrow{o[\varphi]}(O)^{i} = \sum_{m=0}^{\infty} m^{\varphi^{i}_{A_{1}...A_{m}}} \left(a^{A_{1}}...a^{A_{m}} - \frac{1}{M} J_{m A_{1}...A_{m}}\right),
\] (2.55)

Here \( M \) denotes the total mass of the body. The inertial moments \( J_{m} \) are given by the formula

\[
J_{m A_{1}...A_{m}} = \int a^{A_{1}}...a^{A_{m}} \, d\mu(a).
\] (2.56)

It is clear that the quantities (2.55) deal exclusively with internal degrees of freedom (degrees of freedom of the relative motion), because they are independent on \( o[\varphi] \), which describes the translational motion in \( M \) and is dependent on the choice of the origin \( O \) in \( M \).

One can show that the kinetic energy is then given by the formula

\[
T = \frac{1}{2} g_{ij} \sum_{m=0}^{\infty} \sum_{k=0}^{\infty} m^{\xi^{i}_{A_{1}...A_{m}}} J_{m+k A_{1}...A_{m} B_{1}...B_{k}} \xi^{j}_{B_{1}...B_{k}},
\] (2.57)

which is obtained from the direct substitution of (2.53) into the general expression (2.43) for \( T \). It is also clear that the \( i \)-th component of the Euler coordinates of the center of mass is given by

\[
x^{i} = \frac{1}{M} \sum_{m=0}^{\infty} J_{m A_{1}...A_{m}} m^{\varphi^{i}_{A_{1}...A_{m}}} = o^{i} \varphi^{i} + \frac{1}{M} J_{2 A B} 2 \varphi_{AB}^{i} + \ldots,
\] (2.58)
and therefore one has also
\[ v^i = \frac{1}{M} \sum_{m=0}^{\infty} J_m A_1...A_m m \xi_{A_1}...A_m = 0 \xi^i + \frac{1}{M} J_2 A^B 2 \xi_{AB}^i + \ldots \] (2.59)

Here \( M \) denotes the total mass of the body. But there is no need to introduce new symbol, because it is clear that there is confusion with the manifold symbol \( M \). In the case of bodies like fullerenes with a finite number of degrees of freedom, the summation in the formulas (2.52)–(2.55), (2.57)–(2.59) is extended to the range \( \{0, 1\} \).

The kinetic energy in (2.57) may be written in the form:
\[ T(v, \ldots, m \xi, \ldots) = \frac{M}{2} \langle g, v \otimes v \rangle + \frac{1}{2} \sum_{m,l=1}^{\infty} \langle g, (m \xi \otimes l \xi) J_{m,l} \rangle, \] (2.60)
or writing this analytically in terms of the tensor components
\[ T(v, \ldots, m \xi, \ldots) = \frac{M}{2} g_{ij} v^i v^j + \frac{1}{2} \sum_{m,l=1}^{\infty} m \xi_{A_1}...A_m J_{m,l} \xi_{B_1}...B_l. \] (2.61)

In the case of systems with configurations restricted to \( k \)-th order polynomials of material variables, the above infinite series are restricted to \( k \)-th order polynomials, i.e., the summation is restricted to \((k + 1)\) terms. The internal quantities \( J_{m,l} \) are given by:
\[ J_{m,l} = J_{m+l} - \frac{1}{M} J_m \otimes J_1. \] (2.62)

It is easy to see that
\[ J_0 = M, \quad J_{m,1} = J_{1,m} = J_{m+1}, \quad J_{1,1} = J_2. \] (2.63)

In the case of affine bodies, it is sufficient to use \( J_2 = J_{1,1} \) only. The main geometric peculiarity of that case is that the ellipsoids and spheres are transformed into ellipsoids. The more fundamental feature is that the configuration space of affine body may be identified with the affine group \( GAff(n, \mathbb{R}) \), obviously first of all the special cases \( n = 3, n = 2 \) are practically important.

Let us go back to the mechanics of the affine motion. Equations of the affine constraints may be written down either in the parametric, just explicitly solved form, i.e. (2.3) or (2.4), or alternatively, in the following implicit form of equation for the twice differentiable mapping \( \Phi : N \rightarrow M \)
\[ \frac{\partial^2 \Phi}{\partial a^K \partial a^L} = 0. \] (2.64)

Let us remind that the parametric description of affine constraints is given by:
\[ y^i = \Phi^i(t, a) = x^i(t) + \varphi^i_K(t) a^K. \] (2.65)

Therefore, the field of velocities is given by:
\[ \frac{\partial y^i}{\partial t} = \frac{dx^i}{dt}(t) + \frac{d\varphi^i_K}{dt}(t) a^K. \] (2.66)

Of course these constraints cannot be algebraically substituted to the non-constrained equations of motion. More precisely, one can do that, but for the price of introducing to non-constrained law of motion additional forces, namely reactions \( \Psi_R \) responsible for keeping them together. It is assumed that \( \Psi_R \) are forces per unit mass and as usual their power on motions compatible with (2.64) or (2.65) does vanish. Therefore, they satisfy the d’Alembert conditions.
\[ g_{ij} \int (v^i + V_K a^K) \Psi_R \ d\mu(a) = g_{ij} \int \left( \frac{dx^i}{dt} + \frac{d\varphi^i_K}{dt} a^K \right) \Psi_R \ d\mu(a) = 0, \] (2.67)
for any virtual motion $\mathbb{R} \ni t \mapsto (x(t), \varphi(t))$ compatible with the imposed affine conditions. But this means that for any such motion the formula below holds:

$$g_{ij} \int \frac{dx^i}{dt} \Psi^j_R \, d\mu(a) + g_{ij} \int \frac{d\varphi^i}{dt} a^K \Psi^j_R \, d\mu(a) = 0, \quad (2.68)$$

and that for any constraints-compatible virtual motion the following formula for the power $\mathcal{P}$ of $\Psi_R$ is satisfied:

$$\mathcal{P} = g_{ij} F^i_R \frac{dx^j}{dt} + g_{ij} \mathcal{N}^{Kj}_R \frac{d\varphi^j}{dt} = 0. \quad (2.69)$$

Here $F^i_R, \mathcal{N}_R$ denote the monopole and dipole moments of the distribution of $\Psi_R$ in $N$,

$$F^i_R = \int \mathcal{N}^i_R \, d\mu(a), \quad \mathcal{N}^{Kj}_R = \int a^K \Psi^j_R \, d\mu(a). \quad (2.70)$$

So, reactions themselves do not vanish, but their monopole and dipole moments have to vanish. Therefore, the following equations are satisfied:

$$F^i_R = 0, \quad \mathcal{N}^{Kj}_R = 0. \quad (2.71)$$

One can rewrite them as follows:

$$F^i_R = 0, \quad N^{ij}_R = \varphi^i_K \mathcal{N}^{Kj}_R = 0. \quad (2.72)$$

Therefore, the effective reactions-free equations of motion are obtained as the monopole moments of the original equations of motion without affine constraint. On their right-hand sides, it is only the monopole and dipole moments of given forces:

$$F^i = \int \Psi^i \, d\mu(a), \quad \mathcal{N}^{Ki}_R = \int a^K \Psi^i \, d\mu(a), \quad (2.73)$$

that survive the d’Alembert procedure. Reactions are canceled as it is seen from Eqs. (2.70), (2.71), and (2.72).

The left-hand sides are based in a similar way on the monopole and dipole moments of the distribution of linear momentum within the body. They are, respectively, the total translational momentum and the total dipole momentum given by:

$$\mathcal{M}^i_0 = p^i = M v^i, \quad \mathcal{M}^{Ai}_1 = J^{AB} \frac{d\varphi^B}{dt}. \quad (2.74)$$

The total system of equations of motion has the form:

$$M \frac{dv^i}{dt} = \frac{dp^i}{dt} = F^i, \quad J^{AB} \frac{d^2 \varphi^B}{dt^2} = \mathcal{N}^{Ai}. \quad (2.75)$$

This is a system of $n(n + 1)$ ordinary equations imposed on the time dependence of $n(n + 1)$ variables $(x^i, \varphi^i_A)$. The quantities $F^i, \mathcal{N}^{Ai}$ on the right-hand sides are functions of the state variables $(x^i, \varphi^i_A; \dot{x}^i, \dot{\varphi}^i_A)$. When physically $n = 3$, this is a dynamical system with 12 degrees of freedom and 24-dimensional phase space. As it was mentioned, it is more convenient to use as dynamical force variables the quantities

$$N^{ij} = \varphi^i_j \mathcal{N}^{Aj}, \quad \check{N}^{AB} = \varphi^{-1}_i \varphi^{-1}_j \mathcal{N}^{ij}. \quad (2.76)$$

Just as it was for $M$, the very structure of formulas implies that there is no need to introduce a new symbol for $N$ as a generalized force. An alternative way of deriving equations of motion is to begin with the phase space description and representation of equations of motion in terms of Poisson brackets given by Eqs. (2.32)/(2.37). Legendre transformations enable one to identify the quantities $p^i, \check{p}_A, \Sigma^{ij}, \check{\Sigma}^{AB}$ with $K^{ij}, \check{K}^{AB}$, etc. Equations of motion in terms of Poisson brackets have the form:

$$\frac{dF}{dt} = \{F, H\}, \quad (2.77)$$
and become then:

\[ \frac{dp}{dt} = F, \quad \frac{dK}{dt} = (\xi \otimes \xi)J + N, \]  
(2.78)

or in terms of coordinates:

\[ \frac{dp_i}{dt} = F_i, \quad \frac{dK^{ij}}{dt} = \xi^i \xi^j B J^{AB} + N^{ij}. \]  
(2.79)

Expressing the generalized velocities by affine objects, the following Lagrangian objects can be eliminated:

\[ \frac{dp_i}{dt} = F_i, \quad \frac{dK^{ij}}{dt} = \Omega^i_m K^{mj} + N^{ij}. \]  
(2.80)

Let us observe that even in the interaction-free case, when there are no forces and affine moments, \( K^{ij} \) is not conserved. The reason is that the kinetic energy depends explicitly on the metric tensor.

Equations of motion in the mixed Euler–Lagrange form (2.75) are not very well adapted for applications. Unlike this, as it was seen, the Euler form is both useful in calculations and also physically and geometrically interpretable. Also, the purely Lagrangian form is convenient:

\[ \frac{dp^A}{dt} = -\varphi^B J^{-1}_{BC} K^{CA} + \hat{F}^A, \quad \frac{d\hat{K}^{AB}}{dt} = -\hat{K}^{AC} J^{-1}_{CD} \hat{K}^{DB} + \hat{N}^{AB}. \]  
(2.82)

Expressing \( \hat{p}, \hat{K} \) in terms of velocities \( \hat{v}, \hat{\Omega} \) the following system of equations is obtained:

\[ M \frac{d\hat{v}^A}{dt} = -M \hat{\Omega}^A_B \hat{v}^B + \hat{F}^A, \quad \frac{d\hat{\Omega}^B_C}{dt} J^{CA} = -\hat{\Omega}^B_D \hat{\Omega}^D_C J^{CA} + \hat{N}^{AB}. \]  
(2.83)

These equations have homogeneous structure. On their left-hand sides one has the time derivatives of \( \hat{v}^A, \hat{\Omega}^A_B \) and on the right-hand sides there are dynamical quantities \( \hat{F}^A, \hat{N}^{AB} \) and algebraic second-order expressions of co-moving components of the affine velocities.

Rewriting equations (2.78) explicitly in terms of the generalized coordinates \((x^i, \varphi^i_A)\), we obtain

\[ M \frac{d^2 x^i}{dt^2} = F^i(x^j, \frac{dx^j}{dt}; \varphi^j_A, \frac{d\varphi^j_A}{dt}; t), \quad \frac{d^2 \varphi^i_A}{dt^2} J^{AB} = N^{ij}(x^k, \frac{dx^k}{dt}; \varphi^k_C, \frac{d\varphi^k_C}{dt}; t). \]  
(2.84)

It is seen that the left-hand side of this system of equations is not explicitly expressed as the generalized accelerations. Obviously, it may be made so by multiplying the second of equations (2.84) by \( \varphi^{-1} \).

However, this would be only an apparent simplification. The forms (2.79), (2.84) turn out to be much more convenient both from the fundamental-geometric and from computational points of view. The point is that the Legendre transformation identifies \( K^{AB} \) with \( \hat{\Sigma}^{AB} = \hat{\Sigma}^{AC} \eta^{CB} \), i.e., with the Hamiltonian generator of the group of right-acting regular translations in \( Q_{int} = LI(U, V) \). And similarly, \( K^{ij} \) are Legendre-identified with \( \Sigma^{ij} = \Sigma^i_k g^{kj} \), i.e., with the generator of left-acting regular translations in \( Q_{int} \).

Because of these equations of the affine motion with the additional constraints, e.g., metrically rigid, isochoric, non-holonomic rotation-less constraints are almost automatically obtained from Eqs. (2.77), (2.79), e.g., as their \( g \)-skew-symmetric, \( g \)-traceless or \( g \)-symmetric parts.
If one assumes that the equations of motion are self-adjoint, i.e., derivable from the variational model with the potential-type Lagrangian \( L = T - V \), then the equations of motion are given by (2.79) with
\[
N^{ij} = -\varphi^i_A \frac{\partial V}{\partial \varphi^k_A} g^{kj}, \quad \dot{N}^{ij} = -\varphi^i_A \frac{\partial V}{\partial \varphi^j_A}.
\] (2.85)

It can be easily shown that the expression for the power of applied forces may be reduced to
\[
P = g_{ij} F^i v^j + g_{kj} N^{ik} \Omega^j_i = F^i v^i + N^{ij} \Omega^j_i.
\] (2.86)

As usual \( g \) is the symmetric positively defined metric tensor of the physical space. This expression may be transformed to the Lagrangian, i.e., material terms. However, some difficulties appear then, namely the configuration-dependent Green deformation tensor \( G_{AB} \) instead the constant metric tensor \( g_{ij} \) would have to be used:
\[
P = G_{AB} \dot{\varphi}^A \dot{\varphi}^B + G_{CB} \dot{\varphi}^A \dot{\varphi}^B.
\] (2.87)

The \( g \)-skew-symmetric part of (2.84), i.e., the balance of spin, is given by
\[
\frac{dS^{ij}}{dt} = \frac{d}{dt}(K^{ij} - K^{ji}) = N^{ij} - N^{ji} = \Omega^{ij},
\] (2.88)

where the doubled skew-symmetric part of the balance for \( S^{ij} \) may be written as
\[
\varphi_A^i \frac{d^2 \varphi^j_B}{dt^2} - \varphi_A^j \frac{d^2 \varphi^i_B}{dt^2} = N^{ij}.
\] (2.89)

The condition of the isometry for \( [\varphi_A^i] \), i.e.,
\[
g_{ij} \varphi_A^i \varphi_A^j = \eta_{AB},
\] (2.90)

may be here automatically substituted. This would be forbidden when dealing with (2.84), because doing so the d’Alembert principle would be violated.

Similarly, the material Lagrange description is given by
\[
\frac{d\Omega^B_C}{dt} \mathcal{J}^{CA} - \frac{d\Omega^A_C}{dt} \mathcal{J}^{CB} = \dot{\Omega}^A_D \dot{\Omega}^D_C \mathcal{J}^{CB} - \dot{\Omega}^B_D \dot{\Omega}^D_C \mathcal{J}^{CA} + \dot{N}^{AB}.
\] (2.91)

For the isotropic inertia, when
\[
\mathcal{J}^{AB} = \frac{\mu}{2} \eta^{AB},
\] (2.92)

this reduces to the usual balance law
\[
\mu \frac{d\Omega^A}{dt} = \dot{N}^{AB}.
\] (2.93)

Similarly, for the superposition of metrically rigid and dilatational motions the d’Alembert principle leads to equations:
\[
\frac{dS^{ij}}{dt} = N^{ij} = N^{ij} - N^{ji}, \quad \frac{d}{dt}(g_{ij} K^{ij}) = g_{ij} \xi^i_A \xi^j_B \mathcal{J}^{AB} + g_{ij} N^{ij}.
\] (2.94)

The last equation may be written as:
\[
\frac{dK^{ii}}{dt} = 2T + N^i_i.
\] (2.95)

In the explicit form, expressed in terms of the generalized coordinates, those equations of motion become
\[
\varphi_A^i \frac{d^2 \varphi^j_B}{dt^2} \mathcal{J}^{AB} - \varphi_A^j \frac{d^2 \varphi^i_B}{dt^2} \mathcal{J}^{AB} = N^{ij} = N^{ij} - N^{ji},
\] (2.96)

\[
g_{ij} \varphi_A^i \frac{d^2 \varphi^j_B}{dt^2} \mathcal{J}^{AB} = g_{ij} N^{ij},
\]

with the directly distributed constraints:
\[
g_{ij} \varphi_A^i \varphi_A^j = \lambda \eta_{AB},
\] (2.97)
where $\lambda$—an arbitrary parameter. Just as previously, this substitution is forbidden in original constraints-free equations (2.84).

For the isochoric, i.e., incompressible motion, when $\det[\varphi^i_j] = \text{const.}$, and $\text{Tr} \Omega = 0$, $\text{Tr} \hat{\Omega} = 0$, the d’Alembert principle says that the power $P_R$ of reaction forces satisfies the condition:

$$P_R = N_R^{i_j} \Omega^j_i,$$

for the all traceless $\Omega$. Therefore,

$$N_R^{i_j} = \lambda \delta^i_j, \quad N_R^{i_j} = \lambda \delta^i_j.$$  

This implies that the effective reactions-free equations of motion are given by the traceless part of (2.100)

$$\frac{dK}{dt} = \Omega^i_m K^m_j + N^{i_j} + \lambda \delta^i_j,$$  

i.e., by

$$\frac{d}{dt} \left( K^i_j - \frac{1}{n} K^m_m \delta^i_j \right) = \left( \Omega^i_m K^m_j - \frac{1}{n} \Omega^p_m K^m_p \delta^i_j \right) + \left( N^i_j - \frac{1}{n} N^m_m \delta^i_j \right).$$

In the final form:

$$\varphi^i_A \frac{d^2 \varphi^j_B}{dt^2} J^{AB} - \frac{1}{n} g_{ab} \varphi^a_A \frac{d^2 \varphi^b_B}{dt^2} J^{AB} g^{ij} = N^{ij} - \frac{1}{n} g_{ab} N^{ab} g^{ij}. $$

(2.102)

This is a system of $n^2$ equations subject to one linear condition of the trace vanishing. Therefore, it is equivalent to the system of $(n^2 - 1)$ independent equations imposed on $(n^2 - 1)$ degrees of freedom of incompressible affinely rigid body. But ‘esthetically’, in general considerations it is more convenient to use the above system of independent $n^2$ equations. And it is again true that elimination of the reaction forces is easier if the form (2.84) of equations of motion of affinely rigid body is used.

The above constraints may be formulated both in terms of coordinates and virtual displacements, and in terms of conditions imposed on the affine velocities. For example, the constraints of rigid motion may be given in terms of pseudoholonomic conditions of the skew-symmetry of $\Omega$-s, i.e.,

$$\Omega^i_j + \Omega^j_i = 0, \quad \text{or} \quad \hat{\Omega}^A_B + \hat{\Omega}^B_A = 0.$$  

(2.103)

It is interesting to discuss the question concerning the rotation-less motion. In contrast to certain views, it would be incorrect to base them on the conjecture that the placement variable $[\varphi^i_K]$ is symmetric. First of all this would be mathematically incorrect because the indices $i$ and $K$ refer to different spaces, the physical ones $x^i \in M$ (Euler variables) and the material ones $a^K \in N$ (Lagrange variables). Because of this the artificial symmetry of $[\varphi^i_K]$ in $i$, $K$ is completely non-geometric and non-physical. If the configuration $I$ is in this sense rotation-less with respect to the configuration $I$, and the configuration $III$ is rotation-less with respect to the configuration $II$, then nevertheless, the configuration $III$ in general fails to be rotation-less with respect to the configuration $I$. Therefore, such a concept of rotation-less relationship is not transitive. It may be applied only in the absence of rotation with respect to the some fixed configuration. The main obstacle is that symmetric matrices do not form a Lie group, and there is nothing like the integration of the above skew-symmetry of angular velocity to the finite gyroscopic constraints. But there exists some velocity-based concept of rotation-less behavior, just something analogous to the skew-symmetry of angular velocity but formulated as the symmetry of $\Omega^i_j$ or $\hat{\Omega}^A_B$,

$$\Omega^i_j - \Omega^j_i = \Omega^i_j - g_{jk} g^{im} \Omega^m_k = 0, \quad \hat{\Omega}^A_B - \hat{\Omega}^B_A = \hat{\Omega}^A_B - \eta_{BC} \eta^{AD} \hat{\Omega}^C_D = 0.$$  

(2.104)

This is really something dual, inverse with respect to the skew-symmetry of angular velocities; therefore, we suppose that the above equations describe the rotation-less motion. Let us notice however that now the last two conditions are not equivalent to each other. There are two concepts of the rotation-less motion: the Eulerian(spatial) rotation-free motion $(\Omega^i_j - \Omega^j_i = 0)$ and the Lagrangian (material) rotation-free

behavior. Let us stress strongly the fact that both of the above constraints are essentially non-holonomic, just because of the fact that the symmetric matrices do not form Lie algebras or Lie groups. Using the same arguments like previously, it can be easily found that according to the d’Alembert principle the reaction-free equations of motion are given in the case of spatially rotation-free motion are given in the case of spatially rotation-free by the symmetric part of the balance for $K^{ij}$. When written explicitly in terms of the generalized coordinates, they are given by

$$
\frac{d^2 \varphi^j_B}{dt^2} J^{AB} + \frac{d^2 \varphi^j_B}{dt^2} J^{AB} = N^{ij} + N^{ji},
$$

(2.105)
together with equations

$$
\Omega^i_j - \Omega^i_j = 0.
$$

(2.106)

Similarly, in the case of the materially rotation-free equations we find

$$
\frac{d^2 \varphi^b_B}{dt^2} J^{AB} g_{bc} C^{cj} + \frac{d^2 \varphi^b_B}{dt^2} J^{AB} g_{bc} C^{ci} = N^{ib} g_{bc} C^{cj} + N^{jb} g_{bc} C^{ci},
$$

(2.107)
together with equations

$$
\hat{\Omega}^A_B - \hat{\Omega}^B_A = 0,
$$

(2.108)
where, as usual, $C$ denotes the Cauchy deformation tensor:

$$
C^{ij} = \varphi^i_A \varphi^j_B \eta^{AB}.
$$

(2.109)

Summarizing: There is no well-defined concept of the rotation-free configuration, but there is a good concept of rotation-free motion. Namely, in the spatially non-rotating motion infinitesimally, $\varphi(t)$ and $\varphi(t + dt)$ are for any $t$ mutually connected as follows:

$$
\varphi(t + dt) = A(t)\varphi(t)dt,
$$

(2.110)
where $A(t)$ is $g$-symmetric, $A(t)^i_j - A(t)^i_j = 0$. This is a well-defined procedure; however, in consequence of non-holonomy it does not integrate from the infinitesimal $dt$ to the finite one $\Delta t$.

Let us stress: the motion itself is finite, not infinitesimal. But for any infinitesimal time segment $(t, t + dt)$ the configurations $\varphi(t)$, $\varphi(t + dt)$ are related to each other by same equation (2.110) with a $g$-symmetric $A(t)$.

### 3. Toward affinely invariant dynamics

Let us now introduce the concept of the two-polar and the polar decompositions of $\varphi \in LI(U, V)$. Namely, the Green and Cauchy deformations tensors $G[\varphi]$, $C[\varphi]$ give rise to their eigenaxes with respect to the metric tensors $\eta$, $g$. The corresponding orthonormal bases $\{F_a[\varphi]\} \subset U$, $\{f_a[\varphi]\} \subset V$ satisfy

$$
\eta(F_a[\varphi], F_b[\varphi]) = \delta_{ab}, \quad g(f_a[\varphi], f_b[\varphi]) = \delta_{ab}.
$$

(3.1)
Their dual bases in $U^*$, $V^*$ will be denoted by $\{F^a[\varphi]\} \subset U^*$, $\{f^a[\varphi]\} \subset V^*$. Then $G[\varphi]$, $C[\varphi]$ may be expressed as:

$$
G[\varphi] = \sum_a \lambda_a[\varphi] F^a[\varphi] \otimes F^a[\varphi], \quad C[\varphi] = \sum_a \frac{1}{\lambda_a[\varphi]} f^a[\varphi] \otimes f^a[\varphi].
$$

(3.2)

Geometrically speaking, Eq. (3.2) is an expansion of deformation tensors with respect to the main axes.

Therefore, the degrees of freedom of the affine body split in the following way:

Green gyroscope: $\frac{1}{2} n(n - 1)$ degrees of freedom,

Cauchy gyroscope: $\frac{1}{2} n(n - 1)$ degrees of freedom,

Deformation invariants: $n$ degrees of freedom $\lambda_a[\varphi]$.

Altogether, there are $n^2$ degrees of freedom, just as it should be. So finally, the following description of the affine degrees of freedom are given: two gyroscopes (Green and Cauchy deformation tensors, or rather
their $\eta$- and $\varphi$-internal axes) and the $n$ one-dimensional fictitious material points (deformation invariants). The Cauchy tensor is invariant with respect to material (Lagrange) rotations. And conversely, the Euler (spatial) isometries rotate the Cauchy tensor, but the Green deformation tensor is invariant under them. The Green and Cauchy tensors describe how the eigenaxes of deformations are oriented with respect to the physical and material spaces. Deformation invariants contain the information about the scalar magnitude of deformations. In certain problems, it is convenient to use the exponential representations:

$$Q^a = \exp(q^a) = \sqrt{\lambda_a}.$$  \hspace{1cm} (3.3)

The diagonal matrix $D = \text{diag}(Q_1, \ldots, Q^n)$ is identified with the linear mapping

$$D : \mathbb{R}^n \to \mathbb{R}^n.$$ \hspace{1cm} (3.4)

Therefore,

$$\hat{G}R_a = \lambda_a R_a = \exp(2q^a)R_a, \quad \hat{C}L_a = \lambda_a^{-1}L_a = \exp(-2q^a)L_a.$$ \hspace{1cm} (3.5)

It is important to stress two facts: the linear bases $R^a[\varphi], L^a[\varphi], a = 1, \ldots, n$ may be identified, respectively, with some isometric isomorphisms of $\mathbb{R}^n$ onto $U, V$ and namely $R[\varphi] : \mathbb{R}^n \to U$, and $L[\varphi] : \mathbb{R}^n \to V$. And similarly, the dual co-frames $\hat{R}[\varphi], \hat{L}[\varphi]$ are canonically identified with the following linear isometries $R[\varphi]^{-1} : U \to \mathbb{R}^n$, $L[\varphi]^{-1} : V \to \mathbb{R}^n$.

Obviously, when speaking about isometries we have in mind the natural Kronecker metric in $\mathbb{R}^n$. Therefore, $\varphi$ may be expressed as

$$\varphi = L[\varphi]D[\varphi]R[\varphi]^{-1},$$ \hspace{1cm} (3.6)

or writing this in a simplified matrix-based form:

$$\varphi = LDR^{-1},$$ \hspace{1cm} (3.7)

where $L[\varphi] \in SO(V, g), R[\varphi] \in SO(U, \eta)$ and $D$ is a real-diagonal matrix. This simplification is convenient in the simple practical calculations, but in more complicated problems one can really commit the serious mistakes if the natural tensorial identification of objects $L[\varphi], R[\varphi]$ and $D[\varphi]$ is forgotten.

This two-polar decomposition is not unique; however, this is not embarrassing in simple problems when the corresponding procedures are obeyed, just like it is with the polar representation in $\mathbb{R}^n$ which is also not unique.

The left- and right-acting isometry subgroups $SO(V, g), SO(U, \eta)$ act, respectively, on the left and the right factors of the two-polar representations only. Namely, the actions of $SO(V, g), SO(U, \eta)$ are given by:

$$A \in SO(V, g), B \in SO(U, \eta) : \varphi \mapsto AL[\varphi]D[\varphi](BR[\varphi])^{-1},$$ \hspace{1cm} (3.8)

i.e.,

$$L[\varphi] \mapsto AL[\varphi], R[\varphi] \mapsto BR[\varphi], D[\varphi] \text{ - invariant.}$$ \hspace{1cm} (3.9)

It should be stressed that here $V, U$ are both interpreted as the physical spaces. And the both material spaces are identified with $\mathbb{R}^n$. The co-moving and current representations of the angular velocity of the $L[\varphi]$-gyroscope are given by the following elements of the Lie algebras $SO(n, \mathbb{R})', SO(V, g)'$

$$\dot{X}^a_b := \left< L^a, \frac{dL_b}{dt} \right> = L^a_i \frac{dL^i_b}{dt},$$ \hspace{1cm} (3.10)

$$\dot{X}^i_j := \frac{dL^i_a}{dt} L^a_j,$$ \hspace{1cm} (3.11)

i.e.,

$$\dot{X} = \dot{X}^a_b L_a \otimes L^b.$$ \hspace{1cm} (3.12)
Such objects for the \( R[\varphi] \)-gyroscope are expressed as

\[
\dot{\varphi}^a_{\ b} = \left\langle R^a, \frac{dR_b}{dt} \right\rangle = R^a_K \frac{dR^K_b}{dt},
\]

(3.13)

and

\[
\mathcal{V}^K_L := \frac{dR^K_a}{dt} R^a_L,
\]

(3.14)

i.e.,

\[
\mathcal{V} = \dot{\varphi}^a b R_a \otimes R_b,
\]

(3.15)

with the above conventions concerning indices and other symbols.

In a similar way, the non-holonomic conjugate momenta \( p_\varphi, \varphi \), \( \dot{q}_a, \dot{q}^a \), and \( p_a, g^j, \tau^A B \) may be used. Here again \( \dot{q}, \varphi \in SO(n, \mathbb{R})', \varphi \in SO(V, g)' \), \( \varphi \in SO(U, \eta)' \) where the dual pairing between them and the above angular velocities may be used:

\[
\left\langle (\varphi, \tau, p), (\chi, \varphi, \varphi) \right\rangle = \left\langle (\dot{q}, \dot{\varphi}, \dot{\dot{q}}), (\dot{\chi}, \dot{\varphi}, \dot{\varphi}) \right\rangle = p_a \dot{q}^a + \frac{1}{2} \text{Tr}(\varphi \chi) + \frac{1}{2} \text{Tr}(\dot{\varphi} \dot{\chi}) + \frac{1}{2} \text{Tr}(\dot{\dot{\varphi}}). \tag{3.16}
\]

Obviously, \( \varphi, \tau \) coincide, respectively, with spin and minus vorticity, i.e.,

\[
\varphi = \hat{\varphi}, \quad \tau = -\mathcal{V}. \tag{3.17}
\]

The point is that \( L^a[\varphi], R^a[\varphi] \) are the Hamiltonian generators of transformations:

\[
(A, B) \in SO(V, g) \times SO(U, \eta) : \varphi \mapsto A\varphi, \quad \varphi \mapsto \varphi B^{-1}. \tag{3.18}
\]

The quantities \( \hat{\varphi}, \dot{\varphi} \) are obviously Hamiltonian generators of the following right-acting transformations:

\[
L \mapsto LA, \quad R \mapsto RB, \quad A, B \in SO(n, \mathbb{R}), \tag{3.19}
\]

i.e., explicitly

\[
\varphi = L[\varphi] D[\varphi] R[\varphi]^{-1} \mapsto L[\varphi] A D[\varphi] B^{-1} R[\varphi]^{-1}. \tag{3.20}
\]

Unlike the former actions of \((A, B) \in SO(V, g), SO(U, \eta)\) this action of \((A, B) \in SO(n, \mathbb{R}) \times SO(n, \mathbb{R})\) cannot be expressed as a direct action of \((A, B)\) on the total \( \varphi \). And in general they are not conserved quantities even if one uses rather academic, but formally interesting affinely invariant kinetic energy and geodetic dynamical model (one with the vanishing potential energy).

Let us introduce also the polar decomposition of \( \varphi \). It is not very interesting in fullerene—and large molecule—dynamics, but it has the advantage of being unique. There exists namely a unique isometry \( U[\varphi] : U \mapsto V \) which relates the orthonormal bases \( \{ R_a[\varphi] \}, \{ L_a[\varphi] \} \) to each other:

\[
U[\varphi] R_a[\varphi] = L_a[\varphi], \quad a = 1, \ldots, n. \tag{3.21}
\]

Its isometry means that \( \eta = U[\varphi]^* \cdot g \), i.e., in analytical terms:

\[
\eta_{AB} = g_{ij} U[\varphi]^i A U[\varphi]^j B. \tag{3.22}
\]

Finally, we obtain:

\[
\varphi = U[\varphi] A[\varphi] = B[\varphi] U[\varphi], \tag{3.23}
\]

where the linear mappings \( A[\varphi] \in GL(U), B[\varphi] \in GL(V) \) are symmetric with respect to the metrics \( \eta \) and \( g \), i.e.,

\[
\eta(A[\varphi] u, v) = \eta(u, A[\varphi] v), \quad g(B[\varphi] z, w) = g(z, B[\varphi] w). \tag{3.24}
\]

Besides, \( A, B \) are assumed to be positive

\[
\eta(A[\varphi] u, u) > 0, \quad g(B[\varphi] z, z) > 0, \tag{3.25}
\]

if \( u \neq 0, z \neq 0 \). All objects \( U[\varphi], A[\varphi], B[\varphi] \) are uniquely defined. The relationship between them reads:

\[
B[\varphi] = U[\varphi] A[\varphi] U[\varphi]^{-1}. \tag{3.26}
\]
Equations of free (geodetic) gyroscopic motion are always right-invariant. They are also left-invariant in the special case of the spherical rigid body when $J^{AB} = \mu \eta^{AB}$. This follows from the properties of the kinetic energy. But it is no longer the case for the metric tensors affinely rigid body. The reason is that its kinetic energy is neither left- nor right-invariant, because it is explicitly based on the tensors $g \in V^* \otimes V^*$, $J \in U^* \otimes U^*$ which explicitly restrict its symmetry groups to $SO(V, g)$, $SO(U, J)$. Nevertheless, the natural temptation appears to modify the metric tensor on $L J(U, V)$ in such a way as to make it independent on any fixed metrics in $V$, $U$. The resulting kinetic energy will be affinely invariant; therefore, the corresponding classical and quantum equations of motion may be solvable in terms of special functions on the linear and affine groups. Besides, the oscillatory regime of work may be encoded in the form of the kinetic energy, without using any extra potential term. In a sense, this resembles the Maupertuis principle in mechanics [14–17, 39–46, 48, 49, 54, 55].

The kinetic energy affinely invariant on the left may be postulated as

$$ T_{tr} = \frac{m}{2} C_{ij} \frac{dx^i}{dt} \frac{dx^j}{dt} = \frac{m}{2} \eta^{AB} \hat{v}^A \hat{v}^B, $$

$$ T_{int} = \frac{1}{2} L^B_A D_C \hat{\Omega}^A_B \hat{\Omega}^C_D. $$

The coefficients $L^B_A D_C$ are constant and satisfy the following symmetry condition:

$$ L^B_A D_C = L^D_C B_A. $$

The resulting equations of motion are

$$ \frac{dp_i}{dt} = Q_i, \quad \frac{d\Sigma^i_j}{dt} = -\frac{1}{m} (C^{-1})^{ik} p_k p_j + Q^i_j. $$

Here the covariant linear momentum $p_i$ is expressed as the following function of the translational velocity and the Cauchy deformation tensor:

$$ p_i = C^i_{ij} \frac{dx^j}{dt}. $$

Generalized forces $Q_i$, $Q^i_j$ in the case of the potential motion are given by:

$$ Q_i = -\frac{\partial V}{\partial x^i}, \quad Q^i_j = -\hat{\varphi}^i_A \frac{\partial V}{\partial \hat{\varphi}^j_A}. $$

The second, i.e., the internal, equation of motion may be rewritten in the following more compact way:

$$ \frac{dp_i}{dt} = Q_i, \quad \frac{dI(O)^i_j}{dt} = Q_{tot}(O)^i_j, $$

where

$$ I(O)^i_j = \Lambda(O)^i_j + \Sigma^i_j = x^i p_j + \Sigma^i_j, $$

$$ Q_{tot}(O)^i_j = Q_{tr}(O)^i_j + Q^i_j = x^i Q_j + Q^i_j. $$

When the dissipative forces are present, $Q_i$, $Q^i_j$ also depend on the generalized velocities. Equations of motion are the balance laws for the linear momentum and the total affine momentum. The kinetic energy affinely invariant on the right may be postulated as $T = T_{tr} + T_{int}$, where

$$ T_{tr} = \frac{m}{2} g_{ij} \hat{v}^i \hat{v}^j = \frac{m}{2} G_{AB} \hat{v}^A \hat{v}^B, $$

$$ T_{int} = \frac{1}{2} \mathcal{R}^i_j k \Omega^i_j \Omega^k_l. $$

(3.35)
The resulting equations of motion are:
\[
\frac{d\hat{p}_A}{dt} = \dot{Q}_A = Q_i \varphi^i_A, \quad \text{i.e.,} \quad \frac{dp_i}{dt} = Q_i, \tag{3.36}
\]
\[
\frac{d\hat{\Sigma}^A_B}{dt} = \dot{Q}^A_B = (\varphi^{-1})^A_i Q^i_j \varphi^j_B, \tag{3.37}
\]
i.e., the balance laws for \( \hat{p}_A \) and \( \hat{\Sigma}^A_B \).

The full affine group is non-semisimple, and its homogeneous (linear) part has an Abelian dilatational divisor. Because of this, there is no two-sides invariant energy. The highest possible two-side invariant kinetic energy is one affinely invariant on the left (right) and at the same time isometrically invariant on the right (left). Let us notice, however, that when translational degrees of freedom are frozen, there exist kinetic energies, i.e., metric tensors on \( LI(U, V) \), simultaneously left- and right-invariant. They are given by
\[
T_{\text{int}} = \frac{A}{2} \Omega^i_j \Omega^i_j + \frac{B}{2} \Omega^i_i \Omega^i_j = \frac{A}{2} \hat{\Omega}^K_L \hat{\Omega}^L_K + \frac{B}{2} \hat{\Omega}^K_K \hat{\Omega}^L_L, \tag{3.38}
\]
or writing this in a more symbolic form:
\[
T_{\text{int}} = \frac{A}{2} \text{Tr} \Omega^2 + \frac{B}{2} (\text{Tr} \Omega)^2 = \frac{A}{2} \text{Tr} \hat{\Omega}^2 + \frac{B}{2} (\text{Tr} \hat{\Omega})^2. \tag{3.39}
\]
This metric is not positively semi-definite, but this circumstance does not disqualify it. On the contrary, the negative contribution may be physically interpreted as a kind of ‘centrifugal attraction’ which together with the usual ‘centrifugal repulsion’ gives rise to the effective potential of the ‘intermolecular’ shape. It is attractive at large distances in the space of deformation invariants and repulsive at small distances. Because of this, it is possible to describe the oscillatory behavior on the purely geodetic model, without any use of potential energy.

Joining the above expressions with the affinely invariant in the physical space and isometrically invariant in the material space and conversely isometrically invariant in space and affinely invariant in the body standard terms, we obtain the following formulas:
\[
T^{\text{aff-metr}} = \frac{m}{2} \eta_{KL} \hat{v}^K \hat{v}^L + \frac{I}{2} \eta_{KL} \hat{\Omega}^K_M \hat{\Omega}^L_N \eta^{MN} + \frac{A}{2} \hat{\Omega}^K_L \hat{\Omega}^L_K + \frac{B}{2} \hat{\Omega}^K_K \hat{\Omega}^L_L, \tag{3.40}
\]
\[
T^{\text{metr-aff}} = \frac{m}{2} g_{ij} v^i v^j + \frac{I}{2} g_{ij} \Omega^i_k \Omega^j_l g^{kl} + \frac{A}{2} \Omega^i_j \Omega^j_i + \frac{B}{2} \Omega^i_i \Omega^j_j. \tag{3.41}
\]
In the first expression, the Cauchy tensor \( C[\varphi] \) is used as the metric tensor of \( M \), because
\[
\frac{m}{2} \eta_{KL} \hat{v}^K \hat{v}^L = \frac{m}{2} C_{ij} [\varphi] v^i v^j. \tag{3.42}
\]
Therefore, the translational linear momentum is given by
\[
p_i = C_{ij} [\varphi] \frac{dx^j}{dt}. \tag{3.43}
\]

It is clear that it is different from \( g_{ij} \frac{dx^j}{dt} \). When translational forces do not act, \( p_i \) is a constant of motion. But due to the non-constant coefficients \( C_{ij} [\varphi] \), the translational velocity \( \frac{dx^i}{dt} \) is not constant; there appears some kind of the ‘drunk missile effect’ \([22, 47]\). This phenomenon does not appear if we use \( T^{\text{metr-aff}} \) as the kinetic energy. Let us mention that \( T^{\text{metr-aff}} \), or rather its restriction to the volume-preserving motions may be interpreted as a final-dimensional version of the Arnold description of the isochoric ideal fluid.
One can show that the Legendre transformation maps the above models of kinetic energy into the following geodetic Hamiltonians:

\[ T^\text{aff-metr}_{\text{int}} = \frac{1}{2\alpha} \text{Tr} (\hat{\Sigma}^2) + \frac{1}{2\beta} (\text{Tr} \hat{\Sigma})^2 - \frac{1}{4\mu} \text{Tr} (V^2), \]
\[ T^\text{metr-aff}_{\text{int}} = \frac{1}{2\alpha} \text{Tr} (\Sigma^2) + \frac{1}{2\beta} (\text{Tr} \Sigma)^2 - \frac{1}{4\mu} \text{Tr} (S^2), \]

(3.44)

where the new inertial constants \( \alpha, \beta, \mu \) are given by:

\[ \alpha = I + A, \quad \beta = -\frac{1}{B} (I + A)(I + A + nB), \quad \mu = \frac{1}{I} (I^2 - A^2), \]

(3.45)

where \( n = \dim V = \dim U \), usually it is 3 or 2.

Expressing this by the Casimir invariants \( C(1), C(2), ||V||, ||S|| \), where

\[ C(k) = \text{Tr} (\hat{\Sigma}^k) = \text{Tr} (\Sigma^k), \]
\[ ||V||^2 = \frac{1}{2} \text{Tr} (V^2), \quad ||S||^2 = \frac{1}{2} \text{Tr} (S^2), \]

(3.46)

we obtain

\[ T^\text{aff-metr} = \frac{1}{2\alpha} C(2) + \frac{1}{2\beta} C(1)^2 + \frac{1}{2\mu} ||V||^2, \]
\[ T^\text{metr-aff} = \frac{1}{2\alpha} C(2) + \frac{1}{2\beta} C(1)^2 + \frac{1}{2\mu} ||S||^2. \]

(3.47)

It is supposed that the most general form of the kinetic energy simultaneously invariant under the left- and right-acting isometry groups is the following one:

\[ T = \frac{1}{2} (m_1 G_{AB} + m_2 \eta_{AB}) \hat{v}^A \hat{v}^B + \frac{1}{2} (I_1 G_{KL} G^{MN} + I_2 \eta_{KL} \eta^{MN} + I_3 G_{KL} \eta^{MN} + I_4 \eta_{KL} G^{MN}) \hat{\Omega}^K_M \hat{\Omega}^L_N \]
\[ + \frac{A}{2} \hat{\Omega}^I J \hat{\Omega}^J I + \frac{B}{2} \hat{\Omega}^I I \hat{\Omega}^J J. \]

(3.48)

It may be also written as:

\[ T = \frac{1}{2} (m_1 g_{ij} + m_2 C_{ij}) v^i v^j + \frac{1}{2} (I_1 g_{kl} g^{mn} + I_2 C_{kl} C_{mn} + I_3 g_{kl} C_{mn} + I_4 C_{kl} g^{mn}) \Omega^k_m \Omega^l_n \]
\[ + \frac{A}{2} \Omega^i_j \Omega^j_i + \frac{B}{2} \Omega^i_i \Omega^j_j. \]

(3.49)

When translational degrees of freedom are taken into account, the simultaneous left- and right-invariance of this \( T \) is impossible.

This is explicitly seen from the formulas (3.48), (3.49). Indeed, (3.48) is explicitly dependent on the material metric and (3.49) depends on the spatial metric tensors. This excludes possibility of invariance under, respectively, material and spatial non-isometric affine groups. The only possibility of the simultaneous spatial and material affine invariance is to give up the idea of translational invariance and restrict ourselves to the \( A,B \)-model, i.e., to the simultaneous spatial and material linear invariance. The \( A,B \)-model is given by the superposition of two terms—the second-order Casimir invariant and the squared first-order Casimir for \( GL(n, \mathbb{R}) \).

However, it is admissible when they are not admitted, i.e., when \( m_1 = 0, m_2 = 0 \) and in addition \( I_1 = 0, I_2 = 0, I_3 = 0, I_4 = 0 \). Then, the metric tensor on \( Q_{\text{int}} \) is affinely invariant both on the left (in space) and on the right (in the material). It is spatially affine-invariant when \( m_1 = 0, I_1 = 0, I_3 = 0, I_4 = 0 \). The metric is materially affine-invariant when \( m_2 = 0, I_2 = 0, I_3 = 0, I_4 = 0 \). And for any choice
of constants except of $m_2 = 0$, $I_1 = 0$, $I_2 = 0$, $I_4 = 0$, $A = 0$, $B = 0$ the above general metric (kinetic energy) is curved, i.e., Riemannian. In the mentioned exceptional situation, the metric becomes (2.43) with the special substitution $J^{AB} = I \eta^{AB}$. It is seen that the above form of the left- and right-isotropic kinetic energy is rather interesting, especially because of the fact that fullerenes and large molecules have approximately spherical structure in the reference configurations.

The formulas (3.48), (3.49) are very interesting because they unify in a natural way the terms rotationally and affinely invariant. Therefore, one can try to avoid the use of potential energy terms, and instead the purely geodetic models based on the Lagrangians given by ‘kinetic energy’ (3.48) (or equivalently (3.49)) are used. This resembles the Maupertuis procedure in analytical mechanics, where the interaction term is hidden in the ‘kinetic energy,’ i.e., in the appropriately modified metric of the configuration space. This opens the possibility of using more geometric procedure based on special functions. At the end of this article, it will be shown that in some class of such models the rigorous solutions describing stable vibrations may be found.

At this moment, it would be difficult to answer the question if this is possible for the general form (3.48) or (3.49). One will try to answer this question in a subsequent paper. The peculiarity and difficulty of models (3.48), (3.49) in comparison with (3.40), (3.41) consist in greater number of terms, i.e., of the combination constants. This brings about some complications in inverting the formulas for Legendre transformations based on (3.48), (3.49), i.e.,

$$\hat{p}_A = \frac{\partial T}{\partial \hat{v}^A}, \quad \hat{\Sigma}^A_B = \frac{\partial T}{\partial \hat{\Omega}^{BA}},$$

or equivalently

$$p_i = \frac{\partial T}{\partial v^i}, \quad \Sigma^i_j = \frac{\partial T}{\partial \Omega^{ij}}.$$

One can reasonably expect that the formulas for functions

$$\hat{v}^A = \hat{v}^A(\hat{p}_K, \hat{\Sigma}^L_M), \quad \hat{\Omega}^A_B = \hat{\Omega}^A_B(\hat{p}_K, \hat{\Sigma}^L_M),$$

will have a similar structure to expressions for

$$\hat{p}_A = \hat{p}_A(\hat{v}^K, \hat{\Omega}^L_M), \quad \hat{\Sigma}^A_B = \hat{\Sigma}^A_B(\hat{v}^K, \hat{\Omega}^L_M).$$

But nevertheless, in a consequence of the relatively large number of functions, the relationship between combination coefficients in $(\hat{p}_A, \hat{\Sigma}^A_B)$ and $(\hat{v}^A, \hat{\Omega}^A_B)$ may be quite complicated and not very simple to the explicit calculations. Exactly the same is true for the relationship between the functional form of dependencies

$$v^i = v^i(p_k, \Sigma^l_m), \quad \Omega^i_j = \Omega^i_j(p_k, \Sigma^l_m),$$

$$p_i = p_i(v^k, \Omega^l_m), \quad \Sigma^i_j = \Sigma^i_j(v^k, \Omega^l_m).$$

It is observed that the corresponding expressions for (3.44) are also a priori not obvious; on the contrary, the corresponding calculations are relatively embarrassing.

In order to see what would be the structure of the corresponding kinetic and the total energy, the following auxiliary quantities are introduced:

$$q = \frac{1}{n}(q^1 + \ldots + q^n), \quad (3.50)$$

and

$$p = (p_1 + \ldots + p_n). \quad (3.51)$$

Here $q$ is the ‘center of mass’ of the logarithmic deformation invariants and $p$ is the dual quantity, the corresponding canonical momentum conjugate to $q$,

$$\{q, p\} = 1. \quad (3.52)$$
The following quantities which are responsible for some ‘almost diagonalization’ of the kinetic energy form can be introduced now:

\[ M^{a}_{b} = -\tilde{\theta}^{a}_{b} - \tilde{\tau}^{a}_{b}, \quad N^{a}_{b} = \tilde{\theta}^{a}_{b} - \tilde{\tau}^{a}_{b}. \]  

(3.53)

**Proposition 3.1.** The second-order Casimir invariant is then given by:

\[ C(2) = \sum_{a} p_{a}^{2} + \frac{1}{16} \sum_{a,b} \frac{(M^{a}_{b})^{2}}{\sinh^{2} \frac{q^{a} - q^{b}}{2}} - \frac{1}{16} \sum_{a,b} \frac{(N^{a}_{b})^{2}}{\cosh^{2} \frac{q^{a} - q^{b}}{2}}. \]  

(3.54)

**Proof.** We use the definition (3.46) of \( C(2) \) and use as kinetic energy (3.38) with \( A = 1, B = 0 \). Then, performing the Legendre transformation with substituted (3.16) we obtain after rather trivial but involved and large-volume computations (3.54), obviously after using (3.53). \( \square \)

**Proposition 3.2.** The total kinetic energy may be written in the following form, separating the shear and dilatational degrees of freedom:

\[
T^{\text{aff-aff}}_{\text{int}} = \frac{1}{44n} \sum_{a,b} (p_{a} - p_{b})^2 + \frac{1}{2n(A + nB)} p^2 \\
+ \frac{1}{32A} \sum_{a,b} \frac{(M^{a}_{b})^{2}}{\sinh^{2} \frac{q^{a} - q^{b}}{2}} - \frac{1}{32A} \sum_{a,b} \frac{(N^{a}_{b})^{2}}{\cosh^{2} \frac{q^{a} - q^{b}}{2}}.
\]  

(3.55)

**Proposition 3.3.** The corresponding expressions for the spatially affine and materially isotropic kinetic energy, and conversely for the spatially isotropic and materially affine kinetic energies are given by the following formulas:

\[
T^{\text{aff-metr}}_{\text{int}} = \frac{1}{4n(I + A)} \sum_{a,b} (p_{a} - p_{b})^2 + \frac{1}{2n(I + A + nB)} p^2 \\
+ \frac{1}{32(I + A)} \sum_{a,b} \frac{(M^{a}_{b})^{2}}{\sinh^{2} \frac{q^{a} - q^{b}}{2}} - \frac{1}{32(I + A)} \sum_{a,b} \frac{(N^{a}_{b})^{2}}{\cosh^{2} \frac{q^{a} - q^{b}}{2}} \\
+ \frac{1}{2(I^2 - A^2)} ||V||^2,
\]  

(3.56)

\[
T^{\text{metr-aff}}_{\text{int}} = \frac{1}{4n(I + A)} \sum_{a,b} (p_{a} - p_{b})^2 + \frac{1}{2n(I + A + nB)} p^2 \\
+ \frac{1}{32(I + A)} \sum_{a,b} \frac{(M^{a}_{b})^{2}}{\sinh^{2} \frac{q^{a} - q^{b}}{2}} - \frac{1}{32(I + A)} \sum_{a,b} \frac{(N^{a}_{b})^{2}}{\cosh^{2} \frac{q^{a} - q^{b}}{2}} \\
+ \frac{1}{2(I^2 - A^2)} ||S||^2.
\]  

(3.57)

It is seen that the last two formulas, for \( T^{\text{aff-metr}}_{\text{int}} \) and \( T^{\text{metr-aff}}_{\text{int}} \), differ in the last term only. In spite of this, they differ in an essential way in their invariance properties. From the quantized point of view, in molecular theory, the term proportional to \( ||S||^2 \) refers to the magnitude of spin, and the \( ||V||^2 \)-term resembles something similar to the isospin. We shall return to this question in the quantum molecular part of the paper.

Identically let us notice that the affine model may be replaced also by the following expression where \( ||V||, ||S|| \) occur essentially in a symmetric way:

\[
T_{\text{int}} = \frac{1}{2\alpha} C(2) + \frac{1}{2\beta} C(1)^2 + \frac{1}{2\mu} ||V||^2 + \frac{1}{2\nu} ||S||^2.
\]  

(3.58)

Here \( \alpha, \beta, \mu, \nu \) are constants. Let us mention that the formulas (3.48), (3.49) are the special cases of (3.58). It seems that (3.48), (3.49) are promising models. They are not based on the usual d’Alembert
prescription, nevertheless, just like the affine models (3.55)–(3.57) or their submodels corresponding to some special choices of constants, may be considered in the spirit of Maupertuis. The main advantage of them is that they may be used to formulate the effectively working geodetic mechanics of elastic vibrations even without any use of potential energy. The attraction of deformation invariants results from the ‘negative centrifugal’ terms in the kinetic energy.

**Proposition 3.4.** Let us remind also the trigonometric Sutherland formula

\[
T_{\text{int}} = \frac{1}{2A} \sum_a p_a^2 - \frac{B}{2A(A+nB)} p_a^2 + \frac{1}{32A} \sum_{a,b} \frac{(M^a_b)^2}{\sin^2 \frac{q^a-q^b}{2}} + \frac{1}{32A} \sum_{a,b} \sum_{a,b} \frac{(N^a_b)^2}{\cos^2 \frac{q^a-q^b}{2}}.
\] (3.59)

There are only the ‘plus signs’ at expressions \((M^a_b)^2\) and \((N^a_b)^2\), however now in a consequence of the compactness of the circle there is no repulsive action of the term proportional to \((M^a_b)^2\). Indeed, the topology of the circle is compact, because \(D_a = e^{i\alpha_a}\). Therefore, there is no distinction between ‘plus’ and ‘minus’ signs at \((M^a_b)^2\) and \((N^a_b)^2\). Because of this, the trigonometric model is viable without any extra potential, just like hyperbolic one. Unlike this, the isotropic d’Alembert kinetic energy cannot be used as a Hamiltonian.

**Proposition 3.5.** Indeed, kinetic energy is then given by

\[
T_{\text{int}} = \frac{1}{2I} \sum_a P_a^2 + \frac{1}{2I} \sum a,b (M^a_b)^2 (Q^a - Q^b)^2 + \frac{1}{2I} \sum a,b (N^a_b)^2 (Q^a + Q^b)^2.
\] (3.60)

Here \(I^{AB} = J^{AB}\) is the isotropic momentum of inertia, and \(P_a\) is given by

\[
P_a = e^{-q^a} p_a, \quad \text{and} \quad p_a = e^{q^a} P_a.
\] (3.61)

Obviously, no summation convention is used in these formulas. And there are no vibrating solutions. Because of this practically all solutions are non-bounded if no potential energy is used. But if one uses it, the system is not solvable in terms of the special functions on the linear or affine Lie group, so there is no profit from using the group as a configuration space. But the all geodetic models (3.55)–(3.57) may be used and predict the oscillatory and also non-bounded behavior.

The affinely invariant models of the kinetic energy may co-work with the potential energy; however, this is not necessary. When some potential energy is included, then the Hamiltonian in the special case of two-dimensional systems may be written in the form

\[
H_{M,N}^{\text{eff}} = \frac{1}{2m} \left( p_1^2 + p_2^2 \right) + U_{M,N}^{\text{centr}} + V(q^1, q^2).
\] (3.62)

Then the reduced form of the potential is given by

\[
U_{M,N}^{\text{eff}} = \frac{M^2}{16m \sinh^2 \frac{q^1-q^2}{2}} - \frac{N^2}{16m \cosh^2 \frac{q^1-q^2}{2}} + V(q^1, q^2).
\] (3.63)

Here \(M\) and \(N\) are the constants of motion if \(n = 2\), and the extra introduced potential \(V\) is symmetric in logarithmic deformation invariants, i.e.,

\[
V(q^1, q^2) = V(q^2, q^1).
\] (3.64)

It is convenient to use some auxiliary variables

\[
x = q_2 - q_1, \quad q = \frac{1}{2} (q^1 + q^2),
\]

\[
N = N^1_2, \quad M = M^1_2, \quad p = \frac{1}{2} (p_2 - p_1), \quad p = p_1 + p_2.
\] (3.65)
Thus, it was finally found that
\[ T^{\text{aff-aff}}_{\text{int}} = T^{\text{aff-aff}}_{\text{int}}(x) + U^{\text{centr}}_{M,N}(x) = \]
\[ = \frac{p^2}{A} + \frac{M^2}{16A \sinh^2 \frac{x}{2}} - \frac{N^2}{16A \cosh^2 \frac{x}{2}} + \frac{p^2}{4(A + 2B)}. \]  
(3.66)

The linear combination of the second and the third terms equals \( U^{\text{centr}}_{M,N} \), where obviously \( M, N \) are fixed values of the constants of motion, i.e., the spin and the vorticity. It should be noticed that \( M, N \) are constants of motion in the two-dimensional case \((n = 2)\) only. Nevertheless, even for \( n > 2 \), \( M^a_b, N^a_b \), i.e., \( \hat{\rho}^a_b, \hat{\tau}^a_b \) are constants during any motion. In this more general case, there are also some vibrating stationary solutions. And then the time dependence of angular velocities may be found from the solutions of the obviously non-autonomous following differential equations:
\[ \frac{dL}{dt} = L \hat{\chi}, \quad \frac{dR}{dt} = R \hat{\theta}. \]  
(3.67)

There exist also non-periodic, so-to-speak 'abovethreshold' trajectories. When \( n = 2 \), the singularity of \( q^1 - q^2 \) is strongly repulsive, but at large distances in deformation invariants, when \(|q^1 - q^2| \gg 0\), the second attractive term of (3.63) prevails and makes the collapse of the deformation invariants impossible. This is a characteristic behavior of multi-particle potential strongly repulsive at \( q^1 - q^2 = 0 \) but attractive for the large values of \(|q^1 - q^2|\) and making the infinite escaping of invariants and their coincidence impossible.

It follows from the above considerations that in the zeroth order of approximation the large molecules, e.g., fullerenes, are homogeneously deformable and their vibrations are described by equations like: (2.78), (2.82), (2.83), (2.84), (3.36). But as it was said, it is an approximation only. The finite number of degrees of freedom suggests us to replace the affinely rigid behavior by polynomials of a finite order, or by any other finite discretization. But unfortunately the group structure is then lost. The polynomials are the best approximation, in particular due to the fact that the first-order approximation is most convenient and, what is very important, the group structure (affine or linear one) are then saved. And moreover, this approximation is very convenient because we can search our solutions as special functions on the group, both on the classical and quantum levels. The space of special functions is a Hilbert space in the sense of the following scalar product:
\[ \langle \varphi | \psi \rangle = \int \varphi(a) \psi(a) \, d\mu(a), \]  
(3.68)
where the measure \( \mu \) describes the material (Lagrangian) mass distribution. The complex language is used here again to apply the description in terms of spherical functions \( Y^{lm} \). The scalar product in the Hilbert space of the vector-valued functions is given by the obvious generalization:
\[ G[f, g] = g_{ij} \langle f^i | g^j \rangle = g_{ij} \int \overline{f^i(a)} g^j(a) \, d\mu(a). \]  
(3.69)

Denoting the power of forces by \( P \) and the kinetic energy by \( T \), we have the following formulas:
\[ P \left[ \frac{\partial x}{\partial t}(t, \cdot) \right] = \frac{1}{2} G \left[ \frac{\partial x}{\partial t}(t, \cdot), \Phi \left[ x(t, \cdot), \frac{\partial x}{\partial t}(t, \cdot), t, \cdot \right] \right], \]  
(3.70)
\[ T \left[ \frac{\partial x}{\partial t}(t, \cdot) \right] = G \left[ \frac{\partial x}{\partial t}(t, \cdot), \frac{\partial x}{\partial t}(t, \cdot) \right]. \]  
(3.71)

Here, as usual in this paper \( x(t, \cdot) : N \to M \) denotes the configuration, i.e., the mapping of \( N \) onto \( M \) and \( \Phi \) denotes the field of forces. The system of fields \( \Phi \) is an abbreviation for the field of forces. In the proposed approach, one deals with a finite-dimensional subspace of \( L^2(\mu) \) spanned on functions \( H^r \), \( r = 0, 1, 2, \ldots \). It is also assumed that the constant function \( H^0 = 1 \) is an element of this system. The remaining functions \( H^r \) will be denoted by \( H^g \), where \( g = 1, 2, \ldots \). The moments of equations of motions with respect to the system of base functions are denoted by \( M^r_i, N^r_i \), where
\[ M^{ri} = \left\langle H^{r}, \frac{\partial x^{i}}{\partial t} \right\rangle, \quad N^{ri} = \langle H^{r}, \Phi^{i} \rangle. \] (3.72)

So, the following discrete system of the representation of equations of motion was obtained
\[
\frac{d}{dt} M^{ri} = N^{ri}, \quad \text{where } i = 1, 2, 3, \ r = 0, 1, 2, \ldots
\] (3.73)

It is obvious that
\[
M^{0i} = P^{i}, \quad N^{0i} = F^{i},
\] (3.74)
i.e., they are equal to the total linear momentum and the total force which acts on it. This was the main reason for using the constant function \( H^{0} = 1 \) as an element of the complete system \( H^{r} \).

A closed dynamical system describing the problem is obtained by substituting the expansion
\[
x^{i}(t, a) = \sum_{r} q^{i}_{r}(t) H_{r}(a),
\] (3.75)
to the system (3.73). One obtains then the following equations of motion:
\[
\sum_{s} Q^{rs} \frac{d^{2}}{dt^{2}} q^{i}_{s} = N^{ri} \left( q, \frac{dq}{dt}, t \right).
\] (3.76)

Here \( Q^{rs} \) are the quadrupole moments (in the sense of \( H^{r} \)) of the mass distribution in the molecule:
\[
Q^{rs} = \left\langle H^{r} | H^{s} \right\rangle = \int H^{r}(a) H^{s}(a) d\mu(a).
\] (3.77)

Let us observe that in \( Q^{rs} \) the external and internal inertias are mixed. To avoid this, we introduce the new inertial parameters and generalized coordinates:
\[
q^{i} = \frac{1}{M} Q^{r} q^{i}_{r} = q^{i}_{0} + \frac{1}{M} Q^{q} q^{i}_{q}, \quad q = 1, 2, \ldots,
\] (3.78)
\[
Q^{r} = \int H^{r}(a) d\mu(a), \quad Q^{0} = M, \quad Q^{00} = M, \quad Q^{q0} = Q^{q}.
\] (3.79)

Internal inertia is described by the following constant parameters:
\[
Q_{\text{int}}^{q\sigma} = Q^{q\sigma} - \frac{1}{M} Q^{q} Q^{\sigma}.
\] (3.80)

Then, our system of equations of motion splits into two subsystems describing translational and internal motion:
\[
M \frac{d^{2} q^{i}}{dt^{2}} = F^{i}, \quad Q_{\text{int}}^{q\sigma} \frac{d^{2}}{dt^{2}} q^{i}_{\sigma} = N^{ei} - \frac{1}{M} Q^{e} F^{i},
\] (3.81)

where \( i = 1, 2, 3, \ q = 1, 2, \ldots, \sigma = 1, 2, \ldots \).

They may be rewritten as the following balance laws for the translational momentum and the system of internal moments:
\[
\frac{dp^{i}}{dt} = F^{i}, \quad \frac{d}{dt} M_{\text{int}}^{ei} = N^{ei} - \frac{1}{M} Q^{e} F^{i} = N_{\text{int}}^{ei}.
\] (3.82)

Rewriting the kinetic energy and power of forces, we obtain
\[
T = \frac{1}{2} g_{ij} \frac{dq^{j}_{r}}{dt} \frac{dq^{j}_{s}}{dt} = \frac{M}{2} g_{ij} \frac{dq^{j}}{dt} \frac{dq^{j}}{dt} + \frac{1}{2} g_{ij} \frac{dq^{j}_{q}}{dt} \frac{dq^{j}_{q}}{dt} Q_{\text{int}}^{q\sigma},
\] (3.83)
\[
\mathcal{P} = g_{ij} \frac{dq^{j}_{r}}{dt} N^{jr} = g_{ij} \frac{dq^{j}}{dt} F^{j} + g_{ij} \frac{dq^{j}_{q}}{dt} N^{qj}.
\] (3.84)

Let us now assume that the motion is restricted to such situations that
\[
V = \sum_{r=0}^{N} V_{r} H^{r}.
\] (3.85)
Those constraints force us to introduce additional reactions to equations of motion, and those reactions result in the reduction of the kinetic energy to the form

\[ T = \frac{1}{2} g_{ij} \frac{d}{dt} \frac{dq^i_A}{dt} \frac{dq^j_B}{dt} Q^{AB} \]

and with the removed (putting equal zero) all velocities \( \frac{dq^j_A}{dt} = 0 \) with \( \Lambda > n \).

At this point, some interesting question should be mentioned. The above procedure was based on the discretization procedure assuming the linear dependence of Euler coordinates on the discretization parameters \( q^r \). This is not necessary. Namely, one can admit the finite discretization based on arbitrary, not necessarily coinciding linear methods. Let the variable \( a \) runs a differentiable manifold, not necessarily coinciding with a linear space. Let us consider the dependence of the trajectory on the function \( t \mapsto x_t = f(q(t), \cdot) \). The power is given by:

\[ P = g_{ij} \int \frac{\partial f^i(q, a)}{\partial q^B} \frac{dq^B}{dt} \Phi^j \left[ f(q(t), a), \frac{\partial}{\partial t} f(q(t), a); t, a \right] d\mu(a). \]  

So, more rigorously, we have to calculate the above moments with functions \( a \mapsto \frac{\partial f^i}{\partial q^B}(q, a) \). The moments are meant in the sense of our scalar product. We obtain then the following equations:

\[ Q_{AB} \frac{d^2 q^B}{dt^2} + [ABC] \frac{dq^B}{dt} \frac{dq^C}{dt} = N_A, \]

or equivalently

\[ \frac{d^2 q^A}{dt^2} + \left\{ \begin{array}{c} A \\ BC \end{array} \right\} \frac{dq^B}{dt} \frac{dq^C}{dt} = Q^{AB} N_B, \]

where

\[ Q_{AB} = G \left[ \frac{\partial f}{\partial q^A}, \frac{\partial f}{\partial q^B} \right]. \]

The metric tensor is a quantity obtained from the Hilbert space \( L^2(\mu) \) with the help of the metric tensor obtained via \( f \), and \( \left\{ \begin{array}{c} A \\ BC \end{array} \right\} \) is the corresponding Christoffel symbol

\[ \left\{ \begin{array}{c} A \\ BC \end{array} \right\} = \frac{1}{2} Q^{AD} (Q_{DB,C} + Q_{DC,B} - Q_{BC,D}) = Q[DBC]. \]  

The generalized forces \( N_A \) are induced by \((f, \phi)\):

\[ N_A = G \left[ \frac{\partial f}{\partial q^A}, \phi \right]. \]

It may be obtained by using the covariant differentiation \( \frac{d}{dt} \) along the curves in \( Q \):

\[ \frac{d^2 q^A}{dt^2} = Q^{AB} N_B. \]

It may be also constructed by using the balance equation

\[ \frac{dM_A}{dt} = N_A. \]

Here \( M_A \) are moments of the distribution of momentum

\[ M_A = G \left[ \frac{\partial f}{\partial q^A}, \frac{\partial x}{\partial t} \right] = Q^{AB} \frac{dq^B}{dt}. \]
4. Multi-pole moments and virial coefficients

As it was mentioned above, the most convenient method of discretization and using analytical continuum theory and in classical dynamics of large molecules like fullerenes consists in using the polynomial expansion or analytical functions theory.

The idea is to use first of all the expansion of the displacement field in terms of the monomials, i.e., the functions
\[ \{1, A^k, A^K A^L, \ldots, A^K_1 \ldots A^K_n\} \] (4.1)

or spherical harmonics \( Y^{lm} \) multiplied by \(|a|^l\).

Our inertial constants are then
\[
k_Q A_1 \ldots A_k = \int a^{A_1} \ldots a^{A_k} \, d\mu(a),
\] (4.2)

or, if we use their expansions into the translational and the internal parts
\[
Q_{int} = Q_{m,k} A_1 \ldots A_m B_1 \ldots B_k - \frac{1}{M} Q_{m} A_1 \ldots A_m Q_k B_1 \ldots B_k.
\] (4.3)

Let us repeat once more that now \( q^i \) is not the spatial position of the center of mass. The center of mass \( Q^i \) is given by the quoted expression:
\[
q^i = 0q^i + \frac{1}{M} \sum_{m=1}^{N} m q^i A_1 \ldots A_m Q A_1 \ldots A_m.
\] (4.4)

Kinetic moments of linear momentum are given by:
\[
l_M A_1 \ldots A_l i = l_M \, A_1 \ldots A_l i + l_M^{int} A_1 \ldots A_l i,
\] (4.5)

where
\[
l_M \, A_1 \ldots A_l i = l_Q A_1 \ldots A_l dq^i dt,
\]
\[
l_M^{int} A_1 \ldots A_l i = \sum_{m=1}^{N} Q_{l,m} A_1 \ldots A_l B_1 \ldots B_m \frac{d}{dt} m q^j B_1 \ldots B_m.
\]

Similarly, the multi-poles of forces are given by
\[
l_N^{A_1 \ldots A_l i} = l_N A_1 \ldots A_l i - \frac{1}{M} l_Q A_1 \ldots A_l F^i,
\] (4.6)
\[
l_N^{int} A_1 \ldots A_l i = \frac{1}{M} l_Q A_1 \ldots A_l F^i.
\] (4.7)

The kinetic energy splits as follows into translational and internal parts:
\[
T = \frac{1}{2} g_{ij} \frac{dq^j}{dt} \frac{dq^i}{dt} + \frac{1}{2} g_{ij} \sum_{m,l=1}^{N} \frac{d}{dt} m q^i A_1 \ldots A_m Q_{m,l} A_1 \ldots A_m B_1 \ldots B_l \frac{d}{dt} m q^j B_1 \ldots B_l.
\] (4.8)

The corresponding equations of motion are:
\[
M \frac{d^2 q^l}{dt^2} = F^l, \quad \frac{d}{dt} l_M A_1 \ldots A_l i = l_N A_1 \ldots A_l i.
\] (4.9)

To those equations, we can directly substitute constraints:
\[ p q = 0 \quad \text{for} \quad p > N. \]
Let us observe one essentially important circumstance. Our equations of motion may be alternatively written as follows:

\[ \frac{dP^i}{dt} = F^i, \]

\[ \frac{d}{dt} m_{ij}^{\text{int}} = n_{ij}^{\text{int}} + \sum_{r,s=1}^{N} \frac{d}{dt} r q^j_{A_1 \ldots A_r} Q_{r,s}^{A_1 \ldots A_r B_1 \ldots B_s} \frac{d}{dt} s q^i_{B_1 \ldots B_s}, \quad (4.10) \]

\[ \frac{d}{dt} M_{\text{int}}^{A_1 \ldots A_l j} = l N_{\text{int}}^{A_1 \ldots A_l j}, \quad l = 2, 3, \ldots, N. \]

Let us rewrite those equations in terms of the generalized coordinates:

\[ M \frac{d^2 q^i}{dt^2} = F^i, \]

\[ \sum_{r,s=1}^{N} r q^j_{A_1 \ldots A_r} Q_{r,s}^{A_1 \ldots A_r B_1 \ldots B_s} \frac{d^2}{dt^2} s q^i_{B_1 \ldots B_s} = n_{ij}^{\text{int}}, \quad (4.11) \]

\[ \sum_{r=1}^{N} Q_{r,s}^{A_1 \ldots A_r B_1 \ldots B_s} \frac{d^2}{dt^2} s q^i_{B_1 \ldots B_s} = r N_{\text{int}}^{A_1 \ldots A_r i}, \quad r = 2, 3, \ldots, N. \]

This last form is very useful because the second equation is based on the Euler representations terms of spatial tensors, and at the same time, it is written in the shape free of reactions responsible for the constraints. Unfortunately, the third subsystem, although also free of the constraints reactions, is written in the mixed spatial-material form. Because of this, not all quantities used there are directly interpretable in terms of spatial tensors. Writing the the third subsystem in purely spatial terms is non-effective because such equations are dependent on a priory unknown constraints reactions.

Nevertheless, the last form of the total system of equations of motion is maximally satisfactory in spite of its mixed spatial-material structure. Namely, the last, the third subsystem, although partially material, may be in many problems treated as a small perturbation to the background established by the first two subsystems based on the purely spatial and reactions-free description.

5. Polynomially deformed body as a model of fullerenes

Let us stress an important fact that in many molecular and fullerene problems the background motion is in a good approximation qualitatively described in affine terms. The non-affine modes of motion, although important, do not play an essential role. Rather, it is reasonable to analyze equations of motion in terms of the following procedure:

1. To begin with the assumption of the affine motion when the molecule is assumed to undergo only spatial translations, rotations and homogeneous deformations. One can try to solve equations of the affine motion either with the classical d'Alembert model of the kinetic energy or with admitting in the mentioned affinely invariant terms.

2. When some rigorous or approximated solutions of the stage 1. are found, one can try to admit some small higher-order polynomial corrections to them. In general, some linear approximations to these corrections will be satisfactory.

Let us also mention some other approach to the non-affine corrections \( m q^j_{A_1 \ldots A_m}, m > 1 \). Namely, one can describe them in the thermodynamical fashion. Let us remind that there were some attempts to describe even nuclear phenomena with their finite and rather small number of degrees of freedom in terms of the thermodynamical concepts, including temperature and entropy. This thermodynamical approach
is well suited to the interpretation of the non-affine modes as a small, chaotic perturbations of the affine dynamics.

Let us describe the fullerene degrees of freedom in the language (approximation) of a continuous medium. The Piola–Kirchhoff stress tensor $T^{Ai}$ (expressed for simplicity in the Cartesian coordinates) enables one to express the multiple moments of forces in the terms of the following integral formulas:

$$mN^{A_1...A_m} = \int a^{A_1} ... a^{A_m} \frac{\partial}{\partial a^A}(T^{Ai}). \quad (5.1)$$

For simplicity the symbols of the integration variables the material Cartesian coordinates $a$ are omitted. Obviously, $T^{Ai}$ are the components of the mixed spatial—material (Eulerian–Lagrangian) stress $T$. As a matter of fact, $T$ is also the mixed tensor density. However, due to the using the Euclidean variables one cannot some relatively troublesome expressions like roots of the determinant of the metric tensors.

Performing the integration by parts, one obtains the following expression for $mN^{A_1...A_m}$:

$$mN^{A_1...A_m} = \int N \frac{\partial}{\partial a^A}(a^{A_1} ... a^{A_m} T^{Ai}) \rightleftharpoons m \sum_{p=1}^{m} \int N a^{A_1} ... a^{A_{p-1}} a^{A_{p+1}} ... a^{A_m} T^{A_p}. \quad (5.2)$$

The Gauss theorem enables us to replace the first term by the surface integral over the infinitely removed closed submanifold. In the physical case of the finite-size body, this term vanishes. Therefore, one finely obtains the following expression:

$$mN^{A_1...A_m} = \int N \frac{\partial}{\partial a^A}(a^{A_1} ... a^{A_{p-1}} a^{A_{p+1}} ... a^{A_m} T^{A_p}). \quad (5.3)$$

This is simply application of the Leibniz rule. Let us rewrite this expression in the spatial, i.e., Eulerian representation. It turns out that the Cauchy representation of the stress tensor $\sigma: M \rightarrow V \otimes V$ gives rise to the following Euler representation of the generalized forces:

$$m n^{i_1...i_m} = \int M x^{i_1} ... x^{i_{p-1}} \sigma^{i_p j} x^{i_{p+1}} ... x^{i_m}. \quad (5.4)$$

These time integration variables are the spatial Euclidean coordinates in $M$. Particularly interesting and geometrically distinguished are moments of the two lowest order degrees, i.e., the monopole (the total force on the center of mass) and the dipole:

$$1N^{A_i} = -\int N T^{Ai}, \quad 1n^{ij} = -\int m \sigma^{ij}. \quad (5.5)$$

Let us remind that these moments are particularly important because of the role they are playing in the affine rigid special case (first-order polynomials). It is very interesting that the dipole moments are proportional to the mean values of the corresponding stress tensors. Let us observe that $1n^{ij} = 0$. These results in the conservation law of angular momentum for the nonpolar body are free of external interactions.

The dependence of the stress tensors $\sigma^{ij}, T^{Ai}$ on the deformation variables and on the thermodynamical parameters is given by the constitutive laws. Substituting them into the formulas for the polynomial constraints, one can in principle express $m n$ and $m N$ in terms of the state variables $p q^{i A_1...A_p}$, $p v^{i A_1...A_p}$ denoted also briefly as $p q_i, p v, p = 0, 1, \ldots, N$. Let us remind that the polynomial
model is applicable mainly to the elastic and pseudo-elastic bodies. When dealing with fullerenes and their continuous approximations of the Kirchhoff tensor

$$T^{Ai} = T^{AB} \frac{\partial q^i}{\partial a^B}. \quad (5.6)$$

The Green deformation tensor

$$G_{AB} = g_{ij} \frac{\partial q^i}{\partial a^A} \frac{\partial q^j}{\partial a^B}. \quad (5.7)$$
gives rise to the following expression for the deformation rate:

$$\frac{d}{dt} G_{AB} = 2d_{ij} \frac{\partial q^i}{\partial a^A} \frac{\partial q^j}{\partial a^B} = 2D_{AB}. \quad (5.8)$$

The material Kirchhoff tensor $T_{ABij}$ is a function of material variables like $G_{AB}$, $D_{AB}$ and of the absolute temperature $T$ (we hope that no ambiguity results from using the same symbol $T$ as the Kirchhoff tensor and the scalar absolute temperature),

$$T_{AB} = T_{AB}(G_{KL}, D_{KL}, T). \quad (5.9)$$

In purely mechanical models, the temperature $T$ is not a dynamical variable. The deformation tensors $\sigma^{kl}$ and $T^{AB}$ depend on the configuration $\rho^{lq}$ and the generalized velocity $\nu^{pv}$ only. However, in general, some thermal phenomena also occur and are coupled to the mechanical processes. The mechanical tensors $m_{nN}$ depend on both the mechanical state ($\ldots, \rho^{lq}, \ldots, \nu^{pv}, \ldots$) and the temperature $T$. Differential equations for the time dependence of $\rho^{lq}$ and $T$ are mutually coupled. Let us denote by $u$ the internal energy per unit of mass, the reference (Lagrange) density of mass by $\varrho_0$ and the produced heat by $q$. The material time derivative will be denoted by $\frac{d}{Dt}$.

The thermal evolution equation may then be written as the balance of internal energy [18]

$$\frac{Du}{Dt} = \frac{1}{2\varrho_0} T^{AB} \frac{DG_{AB}}{Dt} + q = \frac{1}{\varrho_0} T^{AB} D_{AB} + q. \quad (5.10)$$

In the case of the macroscopic body, molecule and fullerene, it is reasonable to assume that $T^{AB}$ splits additively into elastic and dissipative parts:

$$T^{AB} \left( G, \frac{dG}{Dt}, T \right) = T_{el}^{AB}(G, T) + T_{diss}^{AB} \left( G, \frac{dG}{Dt}, T \right). \quad (5.11)$$

The dissipative part vanishes for the body at rest, thus

$$T_{diss}^{AB}(G, 0, T) = 0. \quad (5.12)$$

However, this condition is not sufficient for the correct definition of $T_{diss}^{AB}$. Indeed, for example the tensor describing the magnetic interaction satisfies this condition, but it describes evidently non-dissipative forces. To be correct, one should assume the following form of $T_{diss}^{AB}$:

$$T_{diss}^{AB} = \frac{1}{2} \nu^{ABCD} \left( G, \frac{DG}{Dt}, T \right) \frac{DG_{CD}}{Dt}, \quad (5.13)$$

where $\nu^{ABCD}$ are smooth functions satisfying the following symmetry conditions:

$$\nu^{ABCD} = \nu^{BACD} = \nu^{ABDC}, \quad \text{and} \quad \nu^{ABCD} = \nu^{CDAB}. \quad (5.14)$$

These symmetry assumptions exclude the possibility of interpreting the evidently Hamiltonian term responsible for the magnetic interactions as a kind of dissipative forces. In infinitesimal problems and for small values of $\frac{DG}{Dt}$, it is sufficient to assume that the tensor $\nu^{ABCD}$ is independent on $\frac{DG}{Dt}$. Then, the above symmetry conditions are responsible for the non-variational, dissipative character of $T_{diss}^{AB}$. 


The second principle of thermodynamics results in the entropy $S$ and the following equations:

$$\frac{1}{2\varrho_0}T_{\text{diss}}^2 \frac{DG_{AB}}{dt} + q = T \frac{DS}{dt}.$$  \hfill (5.15)

This formula implies that the internal energy per unit of mass is independent on the generalized velocity $p^v$. Making use of Eq. (5.15) one obtains

$$2\varrho_0 \frac{\partial u}{\partial G_{AB}} = -T \frac{\partial T_{\text{el}}}{\partial T} + T_{\text{el}}^2.$$  \hfill (5.16)

Denoting the specific heat of a body in the conditions of the constant deformation by

$$C^G = \left( \frac{\partial u}{\partial T} \right)_G = C^E, \quad E_{AB} = G_{AB} - \eta_{AB},$$

one can express the former equation in terms of the following quantities:

$$C^E \frac{DT}{dt} - 2\varrho_0 \frac{\partial T_{\text{el}}}{\partial T} \frac{DE_{AB}}{dt} - 2\varrho_0 T_{\text{diss}} \frac{DE_{AB}}{dt} = q.$$  \hfill (5.18)

In continuous models, one puts usually:

$$q = h^A_{,A},$$

$$h^A = \kappa^{AB} \frac{\partial T}{\partial a^B}.$$  \hfill (5.19, 5.20)

In the isotropic case, one puts

$$\kappa^{AB} = \kappa \eta^{AB}.$$  \hfill (5.21)

So finally, our system of equations consisting of (4.10) and (4.11) is closed and may be (at least in principle) solved. The non-affine degrees of freedom $r_q^{i_{A_1..A_r}}$, $r > 1, T$. $T$ may be treated as small corrections to affine motion $q^i_{A}$, $1q^i_A$ and various approximation procedures may be applied to solve the total system of equations. The non-affine variables are used to express a more or less perturbative character of corrections $q, T$. $T$ may be treated as small corrections to affine motion $q^i_{A}$, $1q^i_A$.

In applications, it is quite natural to use the model of polynomially deformable bodies (large molecules or fullerenes) based on the homogenously deformable background (affinely rigid body) perturbed by the above-defined effectively finite-dimensional thermal corrections. In this way, one obtains the approach isomorphic with the one described above.

In general, the system of the thermomechanical equations is rather complicated and non-effective. However, in certain practical problems, e.g., when some empirical constants are small, one can use various approximations, especially in the affine case. For example, let us assume that the matrix of $q$ is given by

$$q = I + \alpha, \quad e = \frac{1}{2} \left( q + q^T \right), \quad r = \frac{1}{2} \left( q - q^T \right),$$

were, roughly speaking $\alpha$ is the linear approximation to the placement and $e$, $r$ are, respectively, its deformatitive (symmetric) rotational (skew-symmetric) parts (of course one remember that the symmetric and skew-symmetric parts are the coordinate-dependent concepts because $q$ is a mixed spatial-material tensor quantity. When using these matrix symbols, the mechanical equation of the affine motion has the form:

$$\frac{d^2r}{dt^2} = V_\mu (J^{-1}e - eJ^{-1}) + V_\eta \left( J^{-1} \frac{de}{dt} - \frac{de}{dt} J^{-1} \right),$$

$$\frac{d^2e}{dt^2} = -V_\mu (J^{-1}e - eJ^{-1}) + V_\eta \left( J^{-1} \frac{de}{dt} - \frac{de}{dt} J^{-1} \right)$$

$$-V \left( K(1 - \frac{\lambda^2}{\varrho_0} \frac{c_E}{c_E} - \frac{2\mu}{n}) \right) \text{Tr} (eJ) - V \left( \frac{2\eta}{n} \right) \frac{d\text{Tr}(e)}{dt} J^{-1}.$$
Here $V$ denotes the volume of the body, $K$, $\mu$ are elastic modules, $\eta$, $\zeta$ are viscosity coefficients, and $\lambda$ is the thermal expansion coefficient. $T_0$ is the reference temperature, and obviously one has

$$\Theta = T - T_0 = \frac{T_0 \lambda K}{\varrho_0 C_E} \text{Tr}(e) = \frac{T_0 \lambda K}{\varrho_0 C_E} \text{Tr}(q).$$

(5.25)

Here $\varrho_0$ is the density of mass in the reference configuration.

This is an alternative approach to the polynomial dynamics. Namely, instead of using the polynomial description of configurations, one has used the mixed description, where the first-order approximation of the fullerene/large molecules is assumed to behave in the affinely rigid way, but additional degrees of freedom, neglected in this approximation, are described in ‘thermodynamical’ fashion. Let us remind that there are successful attempts to describe molecular and nuclear vibrations just in this way by using thermodynamical concepts for describing relatively small (in degrees of freedom) microscopic and nano-physical concepts. Of course, this approach does not disqualify the literal polynomial description. Namely, in certain problems it may lead to more direct description. In any case, both the polynomial and ‘thermodynamical’ descriptions seem to be maximally suited to describe vibrations of large molecules and fullerenes. And they are in general maximally suited to the collective description of vibrations of systems with a finite but not very large number of degrees of freedom.

6. Conclusions

In the paper, the complete classical theory of macromolecular motion, applying it to fullerenes, was proposed. The group-theoretical approach enabled the discussion of molecular affine transformations (translations, rotations and homogeneous strain). The continuum theory of large molecules was applied, and next the discretization procedure using the polynomial expansions or analytical functions theory was executed.

The full theory of the fullerenes needs to take into considerations the quantum effects, and it will be the subject of our next paper.

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