Generalized Euler equations for linked rigid bodies

Gerald R. Kneller[1] and Konrad Hinsen[2,*]
[1] *Institut für Theoretische Physik A, Rheinisch-Westfälische Technische Hochschule Aachen, Templergraben 55, D-52056 Aachen, Germany*
[2] *Centre Européen de Calcul Atomique et Moléculaire, Bâtiment 506, Université Paris Sud, F-91405 Orsay Cedex, France*
(Received 16 March 1994)

We derive the equations of motion for linked rigid bodies from Lagrange mechanics and from Gauß's principle of least constraint. The rotational motion of the subunits is described in terms of quaternion parameters and angular velocities. Different types of joints can be incorporated via axis constraints for the angular velocities. The resulting equations of motion are generalizations of the Euler equations of motion for a single rotor.

PACS number(s): 03.20.+i, 02.70.Ns

I. INTRODUCTION

During the last three decades a considerable amount of work has been devoted to the study of complex mechanical systems. In this article we are concerned with classical systems consisting of assemblies of point masses. Such systems are used to describe molecules in molecular dynamics simulations, where the point masses represent atoms or small groups of atoms. In such simulations, stiff bonds—corresponding to fast vibrations—are commonly replaced by rigid connections to improve the efficiency of the numerical integration [1]. Basically there are three methods to describe the motion of such constrained systems: (a) the method of constraint forces, (b) a Lagrange formalism in terms of generalized coordinates and velocities, and (c) rigid body dynamics in terms of positions, angles, translational velocities, and angular velocities. It should be noted that (b) does *not* include (c) since the angular velocities cannot be written as time derivatives of angular coordinates, i.e., they are not generalized velocities suitable for the Lagrange formalism. Although Lagrange mechanics seems to be the obvious choice to describe *any* mechanical system with holonomic constraints, it has not been widely used to describe the dynamics of linked rigid bodies. The reason is that the equations of motion can become very bulky and inconvenient to deal with in numerical calculations if the generalized coordinates are not chosen carefully [2,3]. Because of its conceptual simplicity and versatility, the method of constraint forces [4–6] has been most widely used until now. An exception is the treatment of disconnected rigid bodies, which can be conveniently described by the well-known Euler equations of motion for a spinning top [7–10].

The purpose of this paper is to generalize the Euler equations of motion to the case of linked rigid bodies, maintaining the same analytical and numerical advantages. This is achieved by describing angular positions in terms of quaternion parameters and rotations in terms of angular velocities. The equations of motion are derived from Lagrange mechanics and, independently, from Gauß's principle of least constraint.

II. EQUATIONS OF MOTION

A. Orientation and angular velocity

Before deriving the equations of motion for linked rigid bodies, we consider first a simple rotor, consisting of N mass points. The orientation of such a rotor is commonly described by three Euler angles. However, this description has the disadvantage that the equations of motion for the rotor contain terms that become singular for certain orientations. A description that does not lead to singularities can be based on quaternion parameters [8,1]. A comprehensive treatise on quaternions and rotations may be found in [11].

Let $\vec{e}_j$ $(j = 1,\ldots,3)$ be the basis vectors of the laboratory-fixed frame, and $\vec{e}'_i$ $(i = 1,\ldots,3)$ those of the body-fixed frame. The relation between the two sets of basis vectors is given by

$$\vec{e}'_i = D_{ij}(q_\alpha)\vec{e}_j, \tag{1}$$

where D_{ij} is a rotation matrix with $(D_{ij})^{-1} = D_{ji}$. Here and in the following, we assume summation over pairwise like indices. The rotation matrix depends on four quaternion parameters q_α $(\alpha = 0,\ldots,3)$, which are subject to the normalization condition $q_0^2 + q_1^2 + q_2^2 + q_3^2 = 1$. Its explicit form reads [11]

*On leave from Institut für Theoretische Physik A, Rheinisch-Westfälische Technische Hochschule Aachen, Templergraben 55, D-52056 Aachen, Germany.

$$\mathbf{D}(q_\alpha) = \begin{pmatrix} q_0^2+q_1^2-q_2^2-q_3^2 & 2(-q_0q_3+q_1q_2) & 2(q_0q_2+q_1q_3) \\ 2(q_0q_3+q_1q_2) & q_0^2+q_2^2-q_1^2-q_3^2 & 2(-q_0q_1+q_2q_3) \\ 2(-q_0q_2+q_1q_3) & 2(q_0q_1+q_2q_3) & q_0^2+q_3^2-q_1^2-q_2^2 \end{pmatrix}. \tag{2}$$

One can derive linear relations between the components of the angular velocity and the time derivatives of any set of angular variables by using the orthogonality of **D**. For quaternion parameters one obtains ([13], Appendix C)

$$\begin{aligned} \omega_i &= A_{i\beta}(q_\alpha)\dot{q}_\beta, & \omega'_i &= A'_{i\beta}(q_\alpha)\dot{q}_\beta, \\ \dot{q}_\alpha &= B_{\alpha j}(q_\beta)\omega_j, & \dot{q}_\alpha &= B'_{\alpha j}(q_\beta)\omega'_j, \\ & i,j = 1,\ldots,3, \quad \alpha,\beta = 0,\ldots,3, \end{aligned} \tag{3}$$

where ω_i and ω'_i are the components of the angular velocity in the space-fixed and the body-fixed coordinate system, respectively:

$$\omega_i = D_{ij}(q_\alpha)\omega'_j. \tag{4}$$

The matrices **A** and **B** are given by

$$\mathbf{A} = 2\begin{pmatrix} -q_1 & q_0 & -q_3 & q_2 \\ -q_2 & q_3 & q_0 & -q_1 \\ -q_3 & -q_2 & q_1 & q_0 \end{pmatrix}, \qquad \mathbf{B} = \frac{1}{2}\begin{pmatrix} -q_1 & -q_2 & -q_3 \\ q_0 & q_3 & -q_2 \\ -q_3 & q_0 & q_1 \\ q_2 & -q_1 & q_0 \end{pmatrix}. \tag{5}$$

The corresponding matrices **A**′ and **B**′ read

$$\mathbf{A}' = 2\begin{pmatrix} -q_1 & q_0 & q_3 & -q_2 \\ -q_2 & -q_3 & q_0 & q_1 \\ -q_3 & q_2 & -q_1 & q_0 \end{pmatrix}, \qquad \mathbf{B}' = \frac{1}{2}\begin{pmatrix} -q_1 & -q_2 & -q_3 \\ q_0 & -q_3 & q_2 \\ q_3 & q_0 & -q_1 \\ -q_2 & q_1 & q_0 \end{pmatrix}. \tag{6}$$

B. Equations of motion from Lagrange mechanics

To describe the dynamics of a chain of linked rigid subunits with f degrees of freedom, we define a suitable set of generalized coordinates x_α ($\alpha = 1,\ldots,n_c$) and velocities u_i ($i = 1,\ldots,f$), which are in general not the time derivatives $\dot{x}_\alpha$. The x_α are the Cartesian coordinates of an arbitrary reference point, defining the position of the chain as a whole, and quaternion parameters, defining the orientation of each subunit. The use of quaternions necessitates the addition of quadratic normalization conditions

$$X_{J,\alpha\beta}x_\alpha x_\beta = 1, \quad J = 1,\ldots,s, \tag{7}$$

with $X_{J,\alpha\beta} = X_{J,\beta\alpha}$ and $s = n_c - f$. In analogy to Eq. (3) we assume the linear relations

$$u_i = A_{i\beta}(x_\alpha)\dot{x}_\beta, \tag{8}$$

$$\dot{x}_\beta = B_{\beta j}(x_\alpha)u_j \tag{9}$$

to be valid for all x_α that fulfill the normalization condition. By inserting (9) into (8), one can see that $A_{i\alpha}(x_\beta)B_{\alpha j}(x_\gamma) = \delta_{ij}$ for all x_β, x_γ. [One might be tempted to insert (8) into (9) and conclude that also $B_{\alpha i}(x_\gamma)A_{i\beta}(x_\delta) = \delta_{\alpha\beta}$. This is not true, however, since the product $B_{\alpha i}(x_\gamma)A_{i\beta}(x_\delta)$ maps only *normalized* x_β onto themselves.] Inserting (9) into the time derivative of (7), one obtains the condition $X_{J,\beta\gamma}B_{\beta j}(x_\alpha)x_\gamma u_j = 0$. Since the components of the velocities u_j can take any value, it follows that

$$X_{J,\beta\gamma}B_{\beta j}(x_\alpha)x_\gamma = 0, \quad J = 1,\ldots,s, \quad j = 1,\ldots,f. \tag{10}$$

The Cartesian positions of all mass points are functions of the generalized coordinates x_α and a set of reference positions $r'_j = r_j(t=0)$:

$$r_i = r_i(x_\alpha(t); r'_j). \tag{11}$$

The relation between Cartesian and generalized velocities is obtained by differentiating the Cartesian coordinates r_i with respect to time and using (9):

$$\dot{r}_i = C_{ij}(x_\alpha)u_j, \tag{12}$$

where the matrix C_{ij} is given by

$$C_{ij}(x_\alpha) = \frac{\partial r_i}{\partial x_\beta}B_{\beta j}(x_\alpha). \tag{13}$$

In Cartesian coordinates the Lagrangian of the system reads $L = \frac{1}{2}M_{ij}\dot{r}_i\dot{r}_j - V(r_k)$, where $M_{ij} = M_i\delta_{ij}$ is a diagonal mass matrix. In terms of generalized coordinates one obtains

$$\begin{aligned} L = {} & \frac{1}{2}M_{ij}\frac{\partial r_i}{\partial x_\alpha}\dot{x}_\alpha\frac{\partial r_j}{\partial x_\beta}\dot{x}_\beta - V\left[r_k(x_\gamma)\right] \\ & -\frac{1}{2}\lambda_J\left(X_{J,\mu\nu}x_\mu x_\nu - 1\right). \end{aligned} \tag{14}$$

The auxiliary coordinates λ_J have been introduced to account for the normalization conditions. The derivatives of the Lagrangian are

$$\frac{\partial L}{\partial \lambda_K} = \frac{1}{2}(X_{K,\mu\nu}x_\mu x_\nu - 1), \qquad \frac{\partial L}{\partial \dot{\lambda}_K} = 0, \tag{15}$$

$$\frac{\partial L}{\partial x_\mu} = M_{ij}\frac{\partial^2 r_i}{\partial x_\mu \partial x_\alpha}\dot{x}_\alpha \frac{\partial r_j}{\partial x_\beta}\dot{x}_\beta - \frac{\partial V}{\partial r_i}\frac{\partial r_i}{\partial x_\mu} - \lambda_J X_{J,\mu\nu}x_\nu, \tag{16}$$

$$\frac{\partial L}{\partial \dot{x}_\mu} = M_{ij}\frac{\partial r_i}{\partial x_\mu}\frac{\partial r_j}{\partial x_\beta}\dot{x}_\beta. \tag{17}$$

Writing the time derivative of the generalized momentum as

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}_\mu} = M_{ij}\frac{\partial^2 r_i}{\partial x_\mu \partial x_\alpha}\dot{x}_\alpha \frac{\partial r_j}{\partial x_\beta}\dot{x}_\beta + M_{ij}\frac{\partial r_i}{\partial x_\mu}\frac{d}{dt}\left[\frac{\partial r_j}{\partial x_\beta}\dot{x}_\beta\right], \tag{18}$$

and introducing the notation $F_i = -\partial V/\partial r_i$ for the Cartesian forces, we obtain the Lagrange equations of motion

$$M_{ij}\frac{\partial r_i}{\partial x_\mu}\frac{d}{dt}\left[\frac{\partial r_j}{\partial x_\beta}\dot{x}_\beta\right] = F_k\frac{\partial r_k}{\partial x_\mu} - \lambda_J X_{J,\mu\nu}x_\nu, \tag{19}$$

$$X_{J,\mu\nu}x_\mu x_\nu = 1. \tag{20}$$

The equations of motion for the dynamical variables x_α and u_i are found by multiplying Eq. (19) by $B_{\mu k}(x_\alpha)$, summing over μ, and using the definition (13) of the matrix C_{ij}:

$$M_{ij}C_{ik}(x_\alpha)\frac{d}{dt}\left[C_{jl}(x_\beta)u_l\right] = F_m C_{mk}(x_\gamma), \tag{21}$$

$$\dot{x}_\alpha = B_{\alpha i}(x_\beta)u_i. \tag{22}$$

Due to Eq. (10) the terms containing λ_J do not contribute. The normalization conditions (7) are automatically fulfilled by Eq. (22). The time derivative of the matrix $\mathbf{C}$ is given by

$$\dot{C}_{ij} = \frac{d}{dt}\left[\frac{\partial r_i}{\partial x_\alpha}B_{\alpha j}\right] = \Delta_{ijk}u_k, \tag{23}$$

where

$$\Delta_{ijk} := \left[\frac{\partial^2 r_i}{\partial x_\alpha \partial x_\beta}B_{\alpha j} + \frac{\partial r_i}{\partial x_\alpha}\frac{\partial B_{\alpha j}}{\partial x_\beta}\right]B_{\beta k}. \tag{24}$$

To emphasize the similarity to Euler's equations of motion for a single rigid body, Eq. (21) can be cast in the form

$$\frac{d}{dt}\left[\Theta_{ij}(x_\alpha)u_j\right] + \xi_{ijk}(x_\beta)u_j u_k = F_m C_{mk}(x_\gamma), \tag{25}$$

where

$$\Theta_{ij}(x_\alpha) := M_{kl}C_{ki}C_{lj}, \tag{26}$$

$$\xi_{ijk}(x_\beta) := -\Delta_{lij}M_{ln}C_{nk}. \tag{27}$$

The quantity Θ_{ij} can be considered as a generalized tensor of inertia.

C. Equations of motion from Gauß's principle of least constraint

The equations of motion for a system of linked rigid bodies may also be derived from Gauß's principle of least constraint. This principle states that the function

$$g(\ddot{r}_i) := \frac{1}{2}\sum_{i,j} M_{ij}\left(\ddot{r}_i - a_i\right)\left(\ddot{r}_j - a_j\right) \tag{28}$$

is a minimum with respect to the actual accelerations $\ddot{r}_i$ under the given constraints, with $a_i = F_i/M_i$ being the accelerations due to the external forces. Obviously, if no constraints are present, the principle yields Newton's equations of motion, $M_i\ddot{r}_i = F_i$. To include the constraints we write the Cartesian accelerations as time derivatives of the generalized velocities by using Eq. (12):

$$\ddot{r}_i(u_j, \dot{u}_j) = \frac{d}{dt}\left[C_{ij}(x_\beta)u_j\right] = C_{ij}(x_\beta)\dot{u}_j + \dot{C}_{ij}(x_\beta)u_j. \tag{29}$$

The Cartesian accelerations depend on the generalized accelerations $\dot{u}_i$ and the generalized velocities u_i. Inserting (29) into (28) and minimizing $g(\ddot{r}_i(u_j, \dot{u}_j))$ with respect to the *generalized accelerations* $\dot{u}_j$ yields again the equations of motion (21).

Gauß's principle of least constraint allows us to rewrite the equations of motion (21) in a form which is more useful for numerical purposes, where the generalized accelerations must be calculated explicitly as a function of the velocities and coordinates. Using the square root of the mass matrix M_{ij} in (28),

$$\mathbf{M}^{\frac{1}{2}} = \mathrm{diag}(\sqrt{M_i}), \tag{30}$$

Gauß's principle takes the form

$$g(\ddot{\mathbf{r}}) = \frac{1}{2}\left[\mathbf{M}^{\frac{1}{2}}(\ddot{\mathbf{r}} - \mathbf{a})\right]^2 = \text{minimum}. \tag{31}$$

Here $\ddot{\mathbf{r}}$ and $\mathbf{a}$ are the $3N$-dimensional vectors whose components are given by $\ddot{r}_i$ and a_i, respectively. Inserting (29), which in matrix form reads

$$\ddot{\mathbf{r}} = \mathbf{C}(\mathbf{x})\dot{\mathbf{u}} + \dot{\mathbf{C}}(\mathbf{x})\mathbf{u}, \tag{32}$$

yields a quadratic form to be minimized with respect to $\dot{\mathbf{u}}$:

$$\tilde{g}(\dot{\mathbf{u}}) = \frac{1}{2}\left[\mathbf{G}(\mathbf{x})\dot{\mathbf{u}} - \mathbf{b}(\mathbf{x}, \mathbf{u})\right]^2 = \text{minimum}. \tag{33}$$

The matrix $\mathbf{G}$ and the vector $\mathbf{b}$ are given by

$$\mathbf{G}(\mathbf{x}) = \mathbf{M}^{\frac{1}{2}}\mathbf{C}(\mathbf{x}), \quad \mathbf{b}(\mathbf{x}, \mathbf{u}) = \mathbf{M}^{\frac{1}{2}}[\mathbf{a} - \dot{\mathbf{C}}(\mathbf{x})\mathbf{u}]. \tag{34}$$

Equation (33) has a unique solution for $\dot{\mathbf{u}}$ if the columns in $\mathbf{C}$ are linearly independent [12], i.e., if $\mathbf{C}$ has column rank f, with f being the number of degrees of freedom. This is the case if the generalized velocities u_i are independent variables, as it has been assumed. The solution for $\dot{\mathbf{u}}$ can formally be written as

$$\dot{\mathbf{u}} = \mathbf{G}^{+}(\mathbf{x})\mathbf{b}(\mathbf{x},\mathbf{u}), \tag{35}$$

where $\mathbf{G}^{+}$ is the *generalized inverse*, or *Moore-Penrose inverse* of $\mathbf{G}$ [12]. In a numerical integration scheme, (35) can be used to calculate the generalized accelerations explicitly.

The fact that the generalized accelerations $\dot{u}_i$ are the minimum of a quadratic form allows us to use efficient and numerically stable solution procedures which are well established in the field of least-squares problems [12]. The straightforward solution of (33), which is equivalent to writing $\mathbf{G}^{+}$ as

$$\mathbf{G}^{+} = (\mathbf{C}^T\mathbf{M}\mathbf{C})^{-1}\mathbf{C}^T\mathbf{M}^{\frac{1}{2}}, \tag{36}$$

can lead to numerical instabilities if the positive definite matrix $\mathbf{C}^T\mathbf{M}\mathbf{C}$ is ill conditioned. This is indeed the case for large chains, where the size of the eigenvalues varies from the mass of a single mass point to the mass of the whole chain.

III. EXAMPLES

A. Translation and rotation of a single rigid body

If the u_l are Cartesian velocities, the matrix C_{ij} is given by the unit matrix and Eqs. (21) and (22) reduce to Newton's equations of motion:

$$M_{ij}\dot{u}_j = F_i(x_k), \tag{37}$$

$$\dot{x}_k = u_k. \tag{38}$$

In the case of free rotational motion of a rigid body around some reference point, which is assumed to be the origin, we choose the generalized velocities and coordinates to be the components ω_i of the angular velocity and the quaternion parameters q_α, respectively. The Cartesian coordinates of the mass points are given by

$$r_{s,i}(q_\alpha) = D_{ij}(q_\alpha)r'_{s,j}, \quad s = 1,\ldots,N, \quad i,j = 1,\ldots,3, \tag{39}$$

where $r_{s,i}$ are the Cartesian coordinates of mass point s in the laboratory-fixed frame and $r'_{s,j}$ are those in the body-fixed frame. N is the number of mass points in the rigid body, and $D_{ij}(q_\alpha)$ are the coefficients of the rotation matrix (2).

The constraint matrix C_{ij} defined in (13) has the block structure

$$\mathbf{C} = \begin{pmatrix} \mathbf{C}_1 \\ \mathbf{C}_2 \\ \vdots \\ \mathbf{C}_N \end{pmatrix}. \tag{40}$$

The block matrices $C_{s,ij}$ can be derived from (13),

$$C_{s,ij} \equiv \frac{\partial r_{s,i}}{\partial q_\beta}B_{\beta j} = \epsilon_{ijk}D_{kl}r'_{s,l} = \epsilon_{ijk}r_{s,k}, \tag{41}$$

using $r_{s,i}$ and $B_{\beta j}$ from (39) and (5), respectively. By ϵ_{ijk} we denote the completely antisymmetric Levi-Cività tensor. The matrix $\mathbf{C}$ expresses the relation $\frac{d}{dt}\vec{r}_s = \vec{\omega} \times \vec{r}_s$. Inserting $\mathbf{C}$ into the equations of motion (25) yields the familiar form

$$\frac{d}{dt}\left[\Theta_{ij}\omega_j\right] = T_i, \tag{42}$$

with Θ_{ij} being the tensor of inertia and T_i being the torque:

$$\Theta_{ij} = M_{kl}C_{ki}C_{lj} = \sum_{s=1}^{N} M_s\left([r_{s,1}^2 + r_{s,2}^2 + r_{s,3}^2]\delta_{ij} - r_{s,i}r_{s,j}\right), \tag{43}$$

$$T_i = F_jC_{ji} = \sum_{s=1}^{N} -\epsilon_{ijk}r_{s,k}F_{s,j}. \tag{44}$$

$F_{s,k}$ is the force on mass point s. Straightforward calculation shows that the term quadratic in the velocities in (25) vanishes.

Alternatively, one can choose the angular velocities ω'_i in the body-fixed frame as generalized velocities. The matrix C'_{ij} has the same block structure as C_{ij}, where the blocks are now given by

$$C'_{s,ij} = C_{s,ik}D_{jk}. \tag{45}$$

The equations of motion are the Euler equations of motion in the rotating frame:

$$\frac{d}{dt}\left[\Theta'_{ij}\omega'_j\right] + \epsilon_{ikl}\omega'_k\Theta'_{lm}\omega'_m = T'_i. \tag{46}$$

Here $\Theta'_{ij} = M_{kl}C'_{ki}C'_{lj}$ is constant and equal to the tensor of inertia in the body-fixed frame, and $T'_i = F_jC'_{ji}$ is the torque in the body-fixed frame.

B. Linked rigid bodies

1. Constraints for the angular velocity

In the following we consider chains of rigid subunits in which neighboring rigid bodies can only rotate relative to each other. The generalization to links with translational degrees of freedom is straightforward. The connection between two rigid bodies can have two types: a common point (free relative rotation with three degrees of freedom) or a common axis (relative rotation with one degree of freedom). In addition, each rigid body by itself may have three degrees of freedom, or it may be a linear assembly of mass points with only two degrees of freedom. Combining all possibilities, one finds that three types of relative motion must be considered: (a) rotation about a specified axis (one degree of freedom), (b) rotation with an angular velocity perpendicular to the axis of a linear assembly (two degrees of freedom), and (c) free rotation with three degrees of freedom. All three cases can be treated in a similar way by writing the angular velocity of a rigid body relative to its anchor point as

$$\omega_i = N_{ij} u_j, \quad i = 1, \ldots, 3,\ j = 1, \ldots, d \leq 3, \quad (47)$$
$$N_{ik} N_{jk} = \delta_{ij}, \quad (48)$$

where N_{ij} is a matrix whose orthonormal column vectors span the subspace to which the angular velocity is constrained. Note that the generalized velocities are the u_j. In case (a), N_{ij} is a unit vector along the common axis. For (b), N_{ij} has two orthonormal column vectors which are both perpendicular to the axis of the linear rigid body, and in case (c) N_{ij} is simply the unit matrix. It should be noted that the matrix N_{ij} is in general time dependent.

The constraint matrix C_{ij} is constructed as

$$C_{ij} = C_{ik}^{(0)} N_{kj}, \quad (49)$$

where $C_{ik}^{(0)}$ corresponds to *unconstrained* rotation.

2. Constraint matrix for linked rigid bodies

As an illustration we consider a system of four mass points $1, \ldots, 4$ (see Fig. 1), where the subsets $\{1, 2, 3\}$ and $\{2, 3, 4\}$ form rigid subunits. This system has seven degrees of freedom: three degrees of freedom for the translation of the whole system, arbitrarily specified by the translation of mass point 1, three degrees of freedom for the free rotation of subunit $\{1, 2, 3\}$ around mass point 1, and one degree of freedom for the rotation of subunit $\{2, 3, 4\}$ around the axis 2–3. The positions of the mass points are given by [in the following we abbreviate $D_{ij}(x_\alpha(t))$ etc. as $D_{ij}(t)$]

$$\vec{r}_1 = \vec{R}, \quad (50)$$
$$\vec{r}_2 = \vec{r}_1 + \mathbf{D}_1(t)(\vec{r}_2^{\,\prime} - \vec{r}_1^{\,\prime}), \quad (51)$$
$$\vec{r}_3 = \vec{r}_1 + \mathbf{D}_1(t)(\vec{r}_3^{\,\prime} - \vec{r}_1^{\,\prime}), \quad (52)$$
$$\vec{r}_4 = \vec{r}_2 + \mathbf{D}_2(t)(\vec{r}_4^{\,\prime} - \vec{r}_2^{\,\prime}). \quad (53)$$

We define the generalized coordinates to be the Cartesian coordinates (X, Y, Z) of the reference point $\vec{R}$ and two sets of quaternion parameters, $(q_0^1, q_1^1, q_2^1, q_3^1)$ and $(q_0^2, q_1^2, q_2^2, q_3^2)$, specifying the orientation of the subunits. In contrast to the case of rotational motion of a single rigid body, it is convenient to write the equations of motion for linked rigid bodies in the laboratory frame. The velocity variables are then $(\dot{X}, \dot{Y}, \dot{Z})$, $(\omega_x^{(1)}, \omega_y^{(1)}, \omega_z^{(1)})$, and the angular velocity along the 2–3 axis $\omega_{\parallel}^{(2)}$.

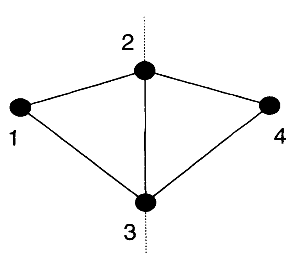

FIG. 1. A chain consisting of two rigid subunits.

The matrix $\mathbf{C}$ has the block structure [compare to (40)]

$$\mathbf{C} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & \mathbf{C}_{12} & 0 \\ 1 & \mathbf{C}_{13} & 0 \\ 1 & \mathbf{C}_{12} & \mathbf{C}_{24} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \mathbf{N}_2 \end{pmatrix} \equiv \mathbf{C}^{(0)} \mathbf{N}, \quad (54)$$

where $\mathbf{C}_{ij}$ and $\mathbf{N}_2$ are given by

$$\mathbf{C}_{ij} = - \begin{pmatrix} 0 & -z_{ij} & y_{ij} \\ z_{ij} & 0 & -x_{ij} \\ -y_{ij} & x_{ij} & 0 \end{pmatrix}, \qquad \mathbf{N}_2 = \begin{pmatrix} n_x^{23} \\ n_y^{23} \\ n_z^{23} \end{pmatrix}, \quad (55)$$

with $x_{ij} = x_j - x_i$ etc., and $\vec{n}_{23}$ being the unit vector along the axis 2–3. The superscript (0) in Eq. (54) refers to unconstrained rotations.

To find an explicit form for the time dependence of the constraint matrix, it is convenient to use a further factorization. It is easy to see that for our example system

$$\mathbf{C}^{(0)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \mathbf{C}_{12} & 0 \\ 0 & \mathbf{C}_{13} & 0 \\ 0 & 0 & \mathbf{C}_{24} \end{pmatrix} \equiv \mathbf{L} \tilde{\mathbf{C}}^{(0)}. \quad (56)$$

The matrix $\tilde{\mathbf{C}}^{(0)}$ relates the generalized velocities $\mathbf{u}$ to the *relative* Cartesian velocities of each mass point with respect to the center of rotation of the respective rigid body, whereas $\mathbf{L}$ reflects the connectivity of the chain. The time dependence of $\tilde{\mathbf{C}}^{(0)}$ can be conveniently expressed as

$$\tilde{\mathbf{C}}^{(0)}(t) = \mathbf{U}(t) \tilde{\mathbf{C}}^{(0)}(0) \mathbf{V}^T(t), \quad (57)$$

where $\mathbf{U}(t)$ and $\mathbf{V}(t)$ read

$$\mathbf{U}(t) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \mathbf{D}_1(t) & 0 & 0 \\ 0 & 0 & \mathbf{D}_1(t) & 0 \\ 0 & 0 & 0 & \mathbf{D}_2(t) \end{pmatrix},$$
$$\mathbf{V}(t) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \mathbf{D}_1(t) & 0 \\ 0 & 0 & \mathbf{D}_2(t) \end{pmatrix}. \quad (58)$$

Similarly the time dependence of $\mathbf{N}$ is given by

$$\mathbf{N}(t) = \mathbf{W}(t) \mathbf{N}(0), \quad (59)$$

with

$$\mathbf{W}(t) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \mathbf{D}_1(t) \end{pmatrix}. \quad (60)$$

With these relations, it is easy to calculate $\mathbf{C}(t)$ and also $\dot{\mathbf{C}}(t)$, since the time dependence is entirely due to the time dependence of the rotation matrices $\mathbf{D}(t)$ [13].

Any open chain of linked rigid bodies can be treated in the way dicussed above, the main difference being the structure of the matrix $\mathbf{L}$, which depends on the topology of the chain. Closed chains require a modified description for two rigid units within each ring.

IV. CONCLUSIONS

We have derived the equations of motion for classical systems of linked rigid bodies using the familiar concept of Lagrange mechanics and Gauß's principle of least constraint. Our approach makes it possible to treat complex molecular systems with constraints using the actual degrees of freedom instead of Cartesian coordinates and constraint forces. Special cases such as linear subunits and rotations around specified body-fixed axes have been considered. For the case of a single rigid body we find again the well-known Euler equations of motion. The choice of quaternions for the description of rotations facilitates the numerical solution of the equations of motion, which we will describe elsewhere. Advantages similar to those for systems of single rotors [9,10] can be expected. We also expect further advantages in comparison with methods based on constraint forces, such as easier parallelization.

[1] M.P. Allen and D.J. Tildesley, *Computer Simulation of Liquids* (Oxford University Press, Oxford, 1987).

[2] A.K. Mazur, V.E. Doroveev, and R.A. Abagyan, J. Comput. Phys. **92**, 261 (1991).

[3] A.K. Mazur and R.A. Abagyan, J. Biomolec. Struct. Dyn. **6**, 815 (1989).

[4] J.-P. Ryckaert, G. Ciccotti, and H.J.C. Berendsen, J. Comput. Phys. **23**, 327 (1977).

[5] G. Ciccotti, M. Ferrario, and J.-P. Ryckaert, Mol. Phys. **47**, 1253 (1982).

[6] R. Edberg, D.J. Evans, and G.P. Morris, J. Chem. Phys. **84**, 6933 (1986).

[7] A. Rahman and F.H. Stillinger, J. Chem. Phys. **55**, 3336 (1971).

[8] D.J. Evans and S. Murad, Mol. Phys. **34**, 327 (1977).

[9] D. Fincham, Mol. Sim. **8**, 165 (1992).

[10] D. Fincham, Mol. Sim. **11**, 79 (1993).

[11] B. Altmann, *Rotations, Quaternions, and Double Groups* (Clarendon Press, Oxford, 1986).

[12] S. Ben-Israel and T.N.E. Greville, *Generalized Inverses: Theory and Application* (John Wiley, New York, 1974).

[13] G. Kneller and A. Geiger, Mol. Sim. **3**, 283 (1989).