Recursive properties of Dirac and metriplectic Dirac brackets with applications

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\textbf{A B S T R A C T}

In this article, we prove that Dirac brackets for Hamiltonian and non-Hamiltonian constrained systems can be derived recursively. We then study the applicability of that formulation in analysis of some interesting physical models. Particular attention is paid to the feasibility of implementation code for Dirac brackets in Computer Algebra System.

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1. Introduction

The fundamental notion in the Hamiltonian formulation of classical dynamics of particles and fields is the canonical Poisson bracket defined over the space of all differentiable functions of the phase space (of even dimension), such that: for each two phase space functions \( f(q, p) \) and \( g(q, p) \) where \( (q, p) = (q_1, \ldots, q_n, p_1, \ldots, p_n) \) denote generalized positions and momenta respectively,

\[
\{ f, g \} = \frac{\partial f}{\partial q} \frac{\partial g}{\partial p} - \frac{\partial f}{\partial p} \frac{\partial g}{\partial q} = \sum_{k=1}^{n} \frac{\partial f}{\partial q_k} \frac{\partial g}{\partial p_k} - \frac{\partial f}{\partial p_k} \frac{\partial g}{\partial q_k}. \tag{1.1}
\]
This bracket is linear in each argument, skew-symmetric: \([f, g] = -[g, f]\), satisfies Leibniz identity: 
\[f, g \cdot h\] = \([f, g] \cdot h + g \cdot [f, h]\), Jacobi identity: 
\([f, [g, h]] + [g, [h, f]] + [h, [f, g]]\] = 0 and is non-degenerate, i.e. \([f, g]\) = 0 for all \(g\), then \(f = \text{const}\). This canonical Poisson bracket equips the phase space with a symplectic structure \([1]\). The Hamiltonian dynamics are then determined by defining the proper Hamiltonian function \(H\). The evolution equation for any phase space function \(f(q, p)\) reads then: 
\[\frac{df}{dt} = \{f, H\}.\]

In applications, one often encounters a situation when the phase space dynamics are subject to certain external restricting conditions on the phase space variables called constraints. Often, the constraints can be written in terms of some phase space functions \(\phi_i(q, p)\) = 0, and we will restrict our analysis to these cases only. The Hamiltonian formalism for such constrained systems requires modifications. These modifications have been first suggested by Dirac \([2]\), and a brief account of the Dirac theory follows.

Let \(\phi_i\) (with \(i = 1, \ldots, L\)) denote all constraints for our Hamiltonian system. Those constraints can be divided into two classes by analyzing the \(L \times L\) skew-symmetric matrix of their mutual Poisson brackets \(A_{ij} = \{\phi_i, \phi_j\}\). Since \(A\) is skew-symmetric, its rank \(K\) must be even. We assume that after relabeling of the \(\phi_i\) and/or redefining the constraints by taking their linear combinations (known as the Dirac separating constraints algorithm), the top left \(K \times K\) submatrix of \(A\), which we denote by \(W\), is regular. The constraint functions \(\phi_{K+1}, \ldots, \phi_L\) are then called first class constraints, and are associated with local gauge symmetries \([2]\), while \(\phi_1, \ldots, \phi_K\) are called second-class. In this work, we will consider second-class constraints only, and for them we can introduce the Dirac bracket \((DB\) \([2]\), of two phase space functions \(f, g\):

\[
[f, g]_D = [f, g] - \sum_{i,j=1}^{K} [f, \phi_i](W^{-1})_{ij}[\phi_j, g].
\]

(1.2)

In the modern language of symplectic geometry, constrained Hamiltonian dynamics can be represented by a triplet \((M, N, \omega)\) where \((M, \omega)\) is a symplectic manifold, namely Phase space, and \(N\) is a constraint submanifold of \(M\). The DB \((1.2)\) is the Poisson bracket on a symplectic submanifold \(\mathcal{N} \subset N\), called second-class constraint manifold \([1,3–5]\).

Symplectic structure requires even dimensional manifolds and non-degenerate Poisson structure. Both these assumptions seem too restrictive and not always applicable. With the appearance of non-canonical Poisson structure (PS) in rigid body dynamics, theory of magnetism, infinite dimensional PS in magneto-hydrodynamics, etc. and issues of geometric quantization, systematic studies of the general Poisson bracket (PB) which is a Lie bracket satisfying the Leibniz identity, has become important.

The fundamental geometric object in the description of any generalized Hamiltonian dynamics is a Poisson manifold. Geometrically, Poisson manifold is a manifold endowed with a bivector field \(\pi\) satisfying \([\pi, \pi] = 0\), where \([-\cdot, -\cdot]\) denotes the Schouten bracket\([6]\) on multivector fields. Algebraically, \(M\) is a Poisson manifold if there is a Poisson bracket on the space of smooth functions defined on \(M\). The Poisson bracket \([\cdot, \cdot]\) and the bivector field \(\pi\) determine each other \([5,7]\) by the formula \([f, g] = \pi(df, dg)\). Both the geometric and algebraic characterization of Poisson manifolds are used in the literature.

In the analysis of the constrained systems dynamics it is of predominant importance to formulate it as a usual Poisson structure on a submanifold of a non-constrained system’s Poisson manifold. The conditions under which the Poisson structure on a submanifold is achievable was investigated in \([8,9]\) and the geometric derivation of the DB formula \((1.2)\) via a procedure called geometric reduction of Poisson tensor was known \([10]\).

In many important physical applications, the systems described are not purely Hamiltonian but also dissipative. The description of such combined dissipative-hamiltonian dynamics can be formulated in various ways, however one of them seems to be particularly elegant and allows to incorporate in it many methods developed in purely sympletic dynamics. This method was introduced first in the phase transformation kinetics in \([11]\) and then independently in \([12,13]\) and called metriplectic. The main point in metriplectic formulation \([13]\) is that a mixed bracket obtained by adding a symmetric bracket to the Poisson bracket can successfully be used for the description of dissipative systems.

In the metriplectic framework, the underlying structure of a dissipative system consists of a Poisson and a symmetric bracket \([13]\), and the obvious generalization of this construction for constrained dissipative system (CDS) must consist of two DB \([14]\): the usual skew-symmetric DB and the symmetric DB, which describe the Hamiltonian and dissipative part respectively. In \([14]\) we have assumed that CDS be geometrically represented by a triplet \((M, N, \omega - g)\), here \(N\) is a submanifold of the symplectic manifold \((M, \omega)\) and \(g\) is a covariant semimetric tensor. A generalized result can be easily obtained by replacing the symplectic 2-form \(\omega\) by a contravariant Poisson tensor \(\pi\), and the covariant metric \((0, 2)\) tensor \(g\) by a contravariant (semi/pseudo)-metric \((2, 0)\) tensor \(G\).

The aim of the article is to give a formal (algebraic) proof of the recursiveness of symmetric and skew-symmetric DB. For the latter, this property probably has been known for years in practical calculations, but no algebraic proof seems to be available in the literature. The proof given in this paper is, to the best of our knowledge, the first one.

The paper is organized as follows. Section 2 presents a rigorous proof for the recursiveness of symmetric and skew-symmetric DB. Section 3 illustrates the constrained metriplectic formalism on two examples, using the computer algebra package Mathematica. Appendix A shows that symbolic/analytical difficulties appeared in the Dirac approach are unavoidable and that they also appear in the Lagrangian approach. Appendix B contains Dirac and the LMM description for a N-pendulum, which serves as our numerical case study.

In this article, we denote a symmetric, skew-symmetric and general bracket by \(\langle\cdot, \cdot\rangle\), \([\cdot, \cdot]\) and \(\eta(\cdot, \cdot)\) respectively.
2. Algebraic formulas for computing Dirac brackets

2.1. Pfaffians and the Tanner’s identities

For any function of two arguments $F$ defined on the set of generators of the commutative algebra $\mathcal{A}$, we introduce the notation

$$F[x_1, x_2, \ldots, x_n, y_1, \ldots, y_n] = \det(F[x_i, y_j]) = \begin{vmatrix} F[x_1, y_1] & \cdots & F[x_1, y_n] \\ \vdots & \ddots & \vdots \\ F[x_n, y_1] & \cdots & F[x_n, y_n] \end{vmatrix}. \quad (2.1)$$

We will use the following identities:

$$F[\alpha, \beta] F[\alpha x, \beta y] = F[\alpha x, \beta y] F[\alpha, \beta t] - F[\alpha, \beta t] F[\alpha x, \beta y] \quad (2.2)$$

$$F[\alpha, \beta] F[\alpha xuv, \beta yst] = F[\alpha, \beta] F[\alpha uv, \beta st] - F[\alpha, \beta s] F[\alpha uv, \beta y] + F[\alpha, \beta t] F[\alpha uv, \beta ys], \quad (2.3)$$

which are a special case of the Tanner identity [15,16]; and they also are known as theorems on bordered determinants [17], pages 46–50. Assuming $F[u, v] = \eta(u, v)$ for $u, v$ from a commutative algebra with the bracket $\eta$, we have

$$F[\phi_1 \cdots \phi_n, \xi_1 \cdots \xi_n] = \begin{vmatrix} \eta(\phi_1, \xi_1) & \cdots & \eta(\phi_1, \xi_n) \\ \vdots & \ddots & \vdots \\ \eta(\phi_n, \xi_1) & \cdots & \eta(\phi_n, \xi_n) \end{vmatrix}. \quad (2.4)$$

2.2. Determinant and recursive formulas

Let $(\mathcal{F}, \cdot)$ be a commutative algebra with the bracket $\eta : \mathcal{F} \times \mathcal{F} \to \mathcal{F}$ and $\{\phi_i\}_{i=1}^n$ be a set of elements from $\mathcal{F}$. Suppose the square matrix $W = (W_{ij})$ with $W_{ij} = \eta(\phi_i, \phi_j)$ is invertible, and let us denote its inverse matrix by $C = [C_{ij}]$. The original DB formula follows:

$$\eta_D(f, g) = \eta(f, g) - \sum_{i,j=1}^n \eta(f, \phi_i) C_{ij} \eta(\phi_i, g), \quad \forall f, g \in \mathcal{F}. \quad (2.5)$$

The new bracket (2.5) is bilinear and it inherits algebraic properties from the original bracket $\eta$. It is easy to check that $\forall f \in \mathcal{F}, \eta_D(\phi_i, f) = 0$, which means that all elements $\phi_i$ are in the algebra center (called Casimir’s elements) of the algebra $(\mathcal{F}, \eta_D)$. For skew-symmetric algebras the number of fixed elements $\phi_i$ must be even, because the skew-symmetric matrix $W$ with odd rank always is singular. Indeed, denoting $\det W$ by $|W|$, for skew-symmetric matrix $W$ we have $|W| = |W^T| = (-1)^n|W|$.

Let $A = (a_{ij})$ be a matrix, then the matrix obtained from $A$ after deleting $i$-th row and $j$-th column will be denoted by $A^{(i,j)}$. Recall the Laplace expansion formula which states that $\det A = |A| = \sum_{j=1}^n (-1)^{i+j} a_{ij} |A^{(i,j)}|$ for any square matrix $A$. Now we can easily prove the following determinant formula for the DB.

**Proposition 1** ([14]). Supposing the matrix $W(\phi_1, \ldots, \phi_n)$ is invertible, the following identity holds

$$\forall f, g \in \mathcal{F} : \eta_D(f, g) = \begin{vmatrix} \eta(\phi_1, \phi_1) & \cdots & \eta(\phi_1, \phi_n) & \eta(\phi_1, g) \\ \vdots & \ddots & \vdots & \vdots \\ \eta(\phi_n, \phi_1) & \cdots & \eta(\phi_n, \phi_n) & \eta(\phi_n, g) \\ \eta(f, \phi_1) & \cdots & \eta(f, \phi_n) & \eta(f, g) \end{vmatrix}. \quad (2.6)$$

Rewriting (2.6) in the notation (2.1) we get

$$\forall f, g \in \mathcal{F} : \eta_D(f, g) = \frac{|W_{f,g}|}{|W|}. \quad (2.7)$$

where $|W| = F[\phi_1 \cdots \phi_n, \phi_1 \cdots \phi_n]$ and $|W_{f,g}| = F[\phi_1 \cdots \phi_n f, \phi_1 \cdots \phi_n g]$. 

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Proof. Apply twice the Laplace formula to the last column and row of the matrix $W_{f,g}$.

**A. Symmetric case:** Now let $(\mathcal{F}, \cdot , \cdot)$ be a commutative algebra with the bracket $\langle \cdot , \cdot \rangle$ and $\{\phi_j\}_{j=1}^n$, be a set of elements from $\mathcal{F}$. We define inductively a family of brackets

$$(f, g)^{(0)} = \langle f, g \rangle.$$ 

$$(f, g)^{(k+1)} = (f, g)^{(k)} - \frac{\langle f, \phi_{k+1} \rangle \langle \phi_{k+1}, g \rangle}{\langle \phi_{k+1}, \phi_{k+1} \rangle}.$$  

(2.8)

Denote the Dirac bracket determined by $k$ constraints $\phi_a$ with $a = 1, \ldots, k$, by $(f, g)^{(k)}_D$, thus

$$(f, g)^{(k)}_D = (f, g) - \sum_{a,b=1}^k \langle f, \phi_a \rangle, C_{ab}^{(k)} \langle \phi_b, g \rangle.$$  

(2.9)

where $C^{(k)}$ is the inverse matrix of $k \times k$ matrix $W^{(k)} = \begin{bmatrix} \eta(\phi_1, \phi_1) & \cdots & \eta(\phi_1, \phi_k) \\ \vdots & \ddots & \vdots \\ \eta(\phi_k, \phi_1) & \cdots & \eta(\phi_k, \phi_k) \end{bmatrix}$.

We prove the following theorem. □

**Theorem 1 (Recursive General Brackets).** Assume that the family of brackets (2.8) is well-defined. Then $\forall f, g \in \mathcal{F}$ and $1 \leq m \leq n$:

$$(f, g)^{(m)} = (f, g)^{(m)}_D.$$  

(2.10)

**Proof.** We prove the formula (2.10) by induction with $m$. For $m = 1$, (2.10) is obviously true. Suppose that it is true for $m = k$, thus

$$\forall f, g : (f, g)^{(k)} = (f, g)^{(k)}_D,$$  

(2.11)

we shall prove that it remains true for $m = k + 1$. The proof is based on the Tanner identity (2.2) and the Proposition 1.

First, let $\alpha = \phi_1 \phi_2 \cdots \phi_k$, using formula (2.7) in the Proposition 1 we have

$$(f, g)^{(k+1)}_D = \frac{F[\alpha \phi_{k+1} \cdot f, \alpha \phi_{k+1} \cdot g]}{F[\alpha \phi_{k+1}, \alpha \phi_{k+1}]}.$$  

(2.12)

Multiplying r.h.s. of (2.12) by $1 = \frac{F[\alpha, \alpha]}{F[\alpha, \alpha]}$ and using (2.2) we get

$$(f, g)^{(k+1)}_D = \frac{F[\alpha f, \alpha g]}{F[\alpha, \alpha]} - \frac{F[\alpha f, \alpha \phi_{k+1}]}{F[\alpha, \alpha]} \frac{F[\alpha \phi_{k+1}, \alpha g]}{F[\alpha, \alpha]}.$$  

(2.13)

Using formula (2.7) again, we show that: the first term in the r.h.s. of Eq. (2.13) is equal $(f, g)^{(k)}_D$ and also equal $(f, g)^{(k)}$ by induction assumption (2.11). Applying a similar argument for the second term in the r.h.s. of Eq. (2.13), we obtain

$$\frac{F[\alpha f, \alpha \phi_{k+1}]}{F[\alpha, \alpha]} = (f, \phi_{k+1})^{(k)} \quad \text{and} \quad \frac{F[\alpha \phi_{k+1}, \alpha g]}{F[\alpha, \alpha]} = (\phi_{k+1}, g)^{(k)}.$$  

In summary, the r.h.s. of Eq. (2.13) is equal

$$(f, g)^{(k+1)} = \frac{(f, \phi_{k+1})^{(k)} \langle \phi_{k+1}, g \rangle^{(k)} - (\phi_{k+1}, \phi_{k+1})^{(k)} (f, g)^{(k)}}{\langle \phi_{k+1}, \phi_{k+1} \rangle^{(k)}}.$$  

(2.14)

It implies that r.h.s. of Eq. (2.13) is equal $(f, g)^{(k+1)}$ which ends the proof. ♠

To apply Theorem 1 we need an existence of the family of brackets (2.8). This condition requires the invertibility of $(\phi_{k+1}, \phi_{k+1})^{(i)}$ for all $i$ with $1 \leq i \leq n$, and therefore it is equivalent to the regularity (or non-degeneracy) of all main minors of $W$. This condition may seem to be too restrictive, however by making new constraints from linear combinations of old constraints, we can go beyond this restriction. The following simple example illustrates the procedure.

**Example 2.1.** Let $x = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$,

$$\langle x_1, x_1 \rangle = \langle x_2, x_2 \rangle = 0, \quad \langle x_1, x_2 \rangle = \langle x_2, x_1 \rangle = a(x),$$

other brackets are whatever, and the constraints are $\phi_1 = x_1 = 0, \phi_2 = x_2 = 0$. 


In the standard approach, after calculating the constraint matrix \( W = a(x) \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \), and its inverse, we easily get the Dirac bracket

\[
\langle f, g \rangle_D = \langle f, g \rangle - \frac{1}{a(x)} \langle f, x_1 \rangle \langle x_2, g \rangle + \langle f, x_2 \rangle \langle x_1, g \rangle.
\]

In this case, direct recursive scheme is inapplicable because of

\[
\langle \phi_1, \phi_1 \rangle = 0 = \langle \phi_2, \phi_2 \rangle,
\]

but by introducing new (equivalent) constraints \( u_1 = x_1 + x_2 = 0 \) and \( u_2 = x_1 - x_2 = 0 \), the recursive scheme may apply as below.

In the first step, we have

\[
\langle f, g \rangle^{(1)} = \langle f, g \rangle - \frac{\langle f, u_1, g \rangle}{\langle u_1, u_1 \rangle}.
\]

Since \( \langle u_1, u_2 \rangle = 0 \) we get \( \langle f, u_2 \rangle = \langle f, u_2 \rangle^{(1)} = \langle u_2, g \rangle^{(1)} = \langle u_2, g \rangle \) and \( \langle u_2, u_2 \rangle^{(1)} = \langle u_2, u_2 \rangle \). Hence,

\[
\langle f, g \rangle^{(2)} = \langle f, g \rangle^{(1)} - \frac{\langle f, u_2, g \rangle^{(1)} - \langle f, u_2, g \rangle}{\langle u_2, u_2 \rangle}
\]

Finally, of returning to the original constraints

\[
\langle f, g \rangle = \langle f, g \rangle - \frac{1}{a(x)} \langle f, x_1 \rangle \langle x_2, g \rangle + \langle f, x_2 \rangle \langle x_1, g \rangle.
\]

We can use Theorem 1 to prove that symmetric DB inherits non-negativity from a semimetric bracket. Precisely,

**Proposition 2.** Suppose \( \mathcal{F} \) be an algebra of real functions with semimetric bracket \( \langle \cdot, \cdot \rangle \), i.e. \( \langle f, f \rangle \) is a non-negative function for every function \( f \in \mathcal{F} \). Let \( \{ \phi_k \}_{k=1}^n \) be a set of elements from \( \mathcal{F} \) such that \( W(\phi_1, \ldots, \phi_n) \) is invertible. Then the Dirac bracket \( \langle \cdot, \cdot \rangle_D \) with respect to \( \{ \phi_k \}_{k=1}^n \) is semimetric.

**Proof.** Since the recursion property of symmetric DB in Theorem 1, it is enough to prove \( \langle f, f \rangle^{(1)} \) is a non-negative function. Indeed, for every real number \( \lambda \), one has

\[
0 \leq \langle f - \lambda \phi_1, f - \lambda \phi_1 \rangle = \langle f, f \rangle - 2\lambda \langle f, \phi_1 \rangle + \lambda^2 \langle \phi_1, \phi_1 \rangle,
\]

which implies that the discriminant \( \Delta = [\langle f, \phi_1 \rangle]^2 - \langle f, f \rangle \langle \phi_1, \phi_1 \rangle \leq 0 \). Thus,

\[
\langle f, f \rangle^{(1)} = \langle f, f \rangle - \frac{\langle f, \phi_1 \rangle^2}{\langle \phi_1, \phi_1 \rangle} \geq 0.
\]

**B. Skew-symmetric case:** Now let \( \langle \cdot, \cdot \rangle \) be a commutative algebra with a skew-symmetric bracket \( \langle \cdot, \cdot \rangle \) and \( \{ \phi_k \}_{k=1}^{2n} \), be a set of elements from \( \mathcal{F} \). We define inductively a family of brackets

\[
\begin{align*}
\langle f, g \rangle^{(0)} &= \langle f, g \rangle \\
\langle f, g \rangle^{(k+1)} &= \langle f, g \rangle^{(k)} - \frac{\langle f, \phi_{2k+2} \rangle^{(k)} \langle \phi_{2k+1}, g \rangle^{(k)} - \langle f, \phi_{2k+1} \rangle^{(k)} \langle \phi_{2k+2}, g \rangle^{(k)}}{\langle \phi_{2k+1}, \phi_{2k+2} \rangle^{(k)}}
\end{align*}
\]

We prove that (2.15) are identical with the Dirac brackets. □

**Theorem 2 (Recursive Skew-Symmetric Brackets).** Suppose that the family of bracket recursively defined by (2.15) is well-defined. Then \( \forall f, g \in \mathcal{F} \) and \( 1 \leq m \leq n \):

\[
\langle f, g \rangle^{(m)} = \langle f, g \rangle^{(2m)}_D,
\]

where the r.h.s. is the Dirac bracket with respect to \( 2m \) constraints

\[
\langle f, g \rangle^{(2m)}_D = \langle f, g \rangle - \sum_{a, b=1}^{2m} \langle f, \phi_a \rangle C_a^{(2m)} \langle \phi_b, g \rangle.
\]
In the above $C^{(2m)}$ in the inverse of the $2m \times 2m$ matrix $W^{(2m)}$

\[
W^{(2m)} = \begin{bmatrix}
\{\phi_1, \phi_1\} & \cdots & \{\phi_1, \phi_{2m}\} \\
\vdots & \ddots & \vdots \\
\{\phi_{2m}, \phi_1\} & \cdots & \{\phi_{2m}, \phi_{2m}\}
\end{bmatrix}.
\]

**Proof.** We prove this theorem by induction with $m$.

It is true for $m = 1$ and suppose that $[f, g]^{(k)} = [f, g]^{(2k)}$ for some $k \geq 1$, we shall prove that $[f, g]^{(k+1)} = [f, g]^{(2k+2)}$. Let denote $\alpha = \phi_1 \cdots \phi_{2k}$, because of (2.7) in the Proposition 1 we have:

\[
[f, g]^{(2k+2)}_D = \frac{F[\alpha \phi_{2k+1} \phi_{2k+2}, \alpha \phi_{2k+1} + \phi_{2k+2}]}{F[\alpha \phi_{2k+1} + \phi_{2k+2}, \alpha \phi_{2k+2}]}.
\] (2.17)

Multiplying the r.h.s. of (2.17) by $1 = \frac{F[\alpha, \alpha]}{F[\alpha, \alpha]}$, using the Tanner identities (2.2) and (2.3) and knowing the determinant of a skew-symmetric matrix of odd size to be zero, $F[\alpha \phi_{2k+1}, \alpha \phi_{2k+1}] = 0$, we get the r.h.s of (2.17)

\[
F[\alpha \phi_{2k+1}, \alpha g] F[\alpha \phi_{2k+1} f, \alpha \phi_{2k+2}] - F[\alpha \phi_{2k+1} f, \alpha \phi_{2k+2}] F[\alpha \phi_{2k+2} f, \alpha \phi_{2k+1} g] + F[\alpha \phi_{2k+2} f, \alpha \phi_{2k+1} g] F[\alpha \phi_{2k+1} \phi_{2k+2}, \alpha \phi_{2k+1} + \phi_{2k+2}].
\]

Again, multiplying by $1 = \frac{F[\alpha, \alpha]}{F[\alpha, \alpha]}$, using the Tanner identities (2.2), the vanishing determinant of a skew-symmetric matrix of odd size, i.e. $F[\alpha \phi_{2k+2}, \alpha \phi_{2k+2}] = 0$, and the recursive assumption $\{u, v\}^{(k)} = \{u, v\}^{(2k)}$ we obtain:

\[
[f, g]^{(2k+2)}_D = \frac{F[\alpha f, \alpha g]}{F[\alpha, \alpha]} + \frac{F[\alpha \phi_{2k+2}, \alpha \phi_{2k+2}]}{F[\alpha \phi_{2k+1}, \alpha \phi_{2k+2}]} \frac{F[\alpha \phi_{2k+1} + \phi_{2k+2}, \alpha \phi_{2k+1} + \phi_{2k+2}]}{F[\alpha \phi_{2k+1} + \phi_{2k+2}, \alpha \phi_{2k+1} + \phi_{2k+2}]} \frac{\phi_{2k+1} \phi_{2k+2}}{\phi_{2k+1} \phi_{2k+2}}.
\]

It implies that the r.h.s. of Eq. (2.17) is equal $[f, g]^{(k+1)}$ which ends the proof. ◇

Theorems 1 and 2 are the main results of this article.

One may use Theorem 2 in proving the Jacobi identity and some other algebraic properties for the Dirac bracket. For example, one can prove the following

**Proposition 3.** Suppose $(F, \cdot, \cdot)$ be skew-symmetric algebra and $\{\phi_k, k = 1, \ldots, 2n\}$ be a set of elements from $F$ such that $W(\phi_1, \ldots, \phi_{2n})$ is invertible. Then $[f, g] \in F$:

\[
[f, g]_D = \frac{|W(\phi_1, \ldots, \phi_{2n}, f, g)|}{|W(\phi_1, \ldots, \phi_{2n})|} = \frac{F[\phi_1 \cdots \phi_{2n} f, \phi_1 \cdots \phi_{2n} g]}{F[\phi_1 \cdots \phi_{2n}, \phi_1 \cdots \phi_{2n}]}.
\] (2.18)

**Proof.** Let $\alpha = \phi_1 \phi_2 \cdots \phi_{2n}$. From the identity (2.2) we have

\[
F[\alpha, \alpha] F[\alpha f g, \alpha f g] = F[\alpha f, \alpha f] F[\alpha g, \alpha g] - F[\alpha f, \alpha g] F[\alpha g, \alpha f] = (F[\alpha f, \alpha g])^2.
\] (2.19)

Dividing both sides of (2.19) by $(F[\alpha, \alpha])^2$ (i.e. $|W(\phi_1, \ldots, \phi_{2n})|^2$) we obtain $\frac{F[\alpha f, \alpha g]}{F[\alpha, \alpha]} = [f, g]_D^2$. □

2.3. Jacobi identity

In [2], Dirac was struggling to prove the Jacobi identity for his bracket formula. He wrote: “I think there ought to be some neat way of proving it, but I haven’t been able to find it”. The Proposition 4 contains what we believe is just that kind of a proof.

**Proposition 4.** Let $(F, \cdot)$ be a commutative algebra with a Lie or Poisson bracket $(\cdot, \cdot)$. Suppose $\{\phi_k, k = 1, \ldots, 2n\}$ be a set of elements from $F$ such that $(\{\phi_1, \phi_2\})$ is invertible. Then $(\cdot, \cdot)_D$ with respect to $\{\phi_k, k = 1, \ldots, 2n\}$ is a Lie or Poisson bracket, respectively.
Only the Jacobi identity is difficult to verify. Using the Theorem 2 and the induction principle, it is enough to show that $\{.,\cdot\}^{(1)}$ satisfies the Jacobi identity. In order to check the Jacobi identity for $\{.,\cdot\}^{(1)}$, it is convenient to introduce the following symbols: $A_i = [f, \phi_i], B_i = [g, \phi_i], C_i = [h, \phi_i]$ with $i = 1, 2$ and $\phi_{12} = \{\phi_1, \phi_2\}$. Since the Jacobi identity holds for $\{.,\cdot\}$ all the following sums vanish
\[
\begin{align*}
I_i &= \{A_i, g\} + \{B_i, h\} + \{\phi_i, [f, g]\}, \\
I_i &= \{A_i, h\} + \{C_i, \phi_i\} + \{\phi_i, [f, h]\}, \\
K_i &= \{C_i, g\} + \{h, B_i\} + \{\phi_i, [g, h]\}, \\
D &= \{\phi_2, A_1\} + \{A_2, \phi_1\} + \{f, \phi_{12}\}, \\
E &= \{\phi_2, B_1\} + \{B_2, \phi_1\} + \{g, \phi_{12}\}, \\
F &= \{\phi_2, C_1\} + \{C_2, \phi_1\} + \{h, \phi_{12}\}. \\
\end{align*}
\] (2.20)

A full expansion of $\text{Jacobi} = [f, [g, h]]_D + [g, [h, f]]_D + [h, [f, g]]_D$ produces 39 non-vanishing terms that can be grouped in a polynomial of the variable $z = (\phi_{12})^{-1}$ as follows:
\[
\begin{align*}
\text{Jacobi} &= \{[f, [g, h]] + [g, [h, f]] + [h, [f, g]]\} \\
&+ \{(A_2K_1 - A_1K_2) + (B_2J_1 - B_1J_2) + (C_1I_2 - C_2I_1)\}z \\
&+ \{(A_1B_2 - A_2B_1)f + (C_1A_2 - C_2A_1)E + (B_1C_2 - B_2C_1)D\}z^2.
\end{align*}
\] (2.21)

Clearly, the r.h.s. of (2.21) is equal to zero since all its coefficients are zero according to (2.20). \qed

3. Applications

One important class of constrained dynamical systems is characterized by $K$ holonomic constraints $\phi_i(q) = 0$, where $i = 1, \ldots, K$. These constraints represent a subclass of time-independent constraints $\phi_i(q, p) = 0$ considered in this article. In the Dirac approach, these dynamical systems are described by a system of $2K$ constraints $\phi_i(q) = 0$ and $\phi_i(q, p) = \{\phi_i, \mathcal{H}\} = 0$.

For holonomic constraints, it is convenient to introduce two $K \times K$ matrices: symmetric $S = (S_{ij})$ with $S_{ij} = \{\phi_i, \phi_j\}$ and skew-symmetric $A = (A_{ij})$ with $A_{ij} = \{\phi_i, \phi_j\}$. The matrix $W$ and its inverse $C$ can then be written as
\[
W = \begin{bmatrix} 0 & S \\ -S^T & A \end{bmatrix}, \quad \text{and} \quad C = W^{-1} = \begin{bmatrix} S^{-1}AS^{-1} & -S^{-1} \\ S^{-1} & 0 \end{bmatrix}. \tag{3.1}
\]

In order to compute $C$ one has to invert one symmetric $K \times K$ matrix and do matrix multiplications twice. Symbolic computation is costly, but numerical computation requires only $\sim K^3$ flops (floating-point operations).

Consider now a constrained model with damping force proportional to the generalized velocity. Such a case is described by a metrical structure:
\[
\begin{align*}
\{x_i, x_j\} &= 0 = \{p_i, p_j\}, \quad \{x_i, p_j\} = \delta_{ij}, \\
\{x_i, x_j\} &= 0, \quad \{p_i, p_j\} = \delta_{ij} \lambda_i(q, p), \quad \text{where} \ \lambda_i \geq 0.
\end{align*}
\]

The dissipative constraint matrix $W^D = (W^D)_{ij}$, where
\[
W^D_{ij} = \langle \phi_i, \phi_j \rangle = \sum_k \frac{\partial \phi_i}{\partial p_k} \frac{\partial \phi_j}{\partial p_k} \lambda_k,
\]

is a symmetric $K \times K$ matrix, and let denote its inverse matrix by $C^D = (W^D)^{-1}$. The metrical Dirac equations for the dynamics governed by $\dot{f} = [f, \mathcal{H}]_D - [f, \mathcal{H}]_D$, take the form:
\[
\begin{align*}
\dot{q}_i &= \frac{\partial \mathcal{H}}{\partial p_i} - \sum_{j,k=1}^{K} (S^{-1})_{jk} \frac{\partial \phi_k}{\partial p_i} \phi_j, \\
\dot{p}_i &= -\frac{\partial \mathcal{H}}{\partial q_i} - \sum_{j,k=1}^{K} (S^{-1})_{jk} \frac{\partial \phi_k}{\partial q_i} \phi_j + \left[ (S^{-1}AS^{-1})_{jk} \frac{\partial \phi_k}{\partial q_i} + (S^{-1})_{jk} \frac{\partial \phi_k}{\partial q_i} \phi_j \right] - \lambda_i \left[ \frac{\partial \mathcal{H}}{\partial p_i} - \sum_{j,k=1}^{K} \frac{\partial \phi_k}{\partial p_j} (C^D)_{jk} \sum_{i=1}^{n} \lambda_i \frac{\partial \phi_k}{\partial p_i} \frac{\partial \mathcal{H}}{\partial p_i} \right].
\end{align*}
\] (3.2)

Recursive symbolic evaluation of explicit equations for a system having $2K$ constraints is realized by $K$ steps. In each step we deal with only two constraints, e.g $\phi_i$ and $\tilde{\phi}_j$ in the $i$-th step. In order to calculate $2n$ explicit equations of motion subject to $2K$ constraints, i.e. $\{x_i, \mathcal{H}\}_{(K)}$ and $\{p_i, \mathcal{H}\}_{(K)}$, we have to compute $(6n + 3)$ brackets determined in the $K - 1$-th step: $\{x_i, \mathcal{H}\}_{(K-1)}, \{p_i, \mathcal{H}\}_{(K-1)}, \{x_i, \phi_k\}_{(K-1)}, \{x_i, \tilde{\phi}_j\}_{(K-1)}, \{x_i, \phi_k\}_{(K-1)}, \{x_i, \tilde{\phi}_j\}_{(K-1)}, \{x_i, \phi_k\}_{(K-1)}, \{p_i, \phi_k\}_{(K-1)}, \{p_i, \tilde{\phi}_j\}_{(K-1)}, \{\phi_k, \mathcal{H}\}_{(K-1)}, \{\tilde{\phi}_j, \mathcal{H}\}_{(K-1)}$ and $\{\phi_k, \tilde{\phi}_j\}_{(K-1)}$.

We illustrate our procedure on the model of a chain molecule often studied in polymer and protein physics, paying particular attention to the implementation of the code for Dirac brackets in a symbolic computer algebra system.
A chain of molecules is a constrained system consisting of \( N \) massive points (or spherical balls) attached by rigid massless bonds having fixed length, in \( d \)-dim space. We are interested in the cases when \( d = 2 \) (planar) or 3. The molecules interact with each other through a pair potential which only on the distance between molecules, e.g the Coulomb interaction and/or the Lennard-Jonnes potential \( V_{ij} = \frac{a_{ij}}{r_{ij}} + e \left[ \left( \frac{r_{ij}}{r_0} \right)^6 - \left( \frac{r_{ij}}{r_0} \right)^{12} \right] \), and with an external field \( \vec{U}(\vec{r}_i) \). In a real application, such a chain is immersed into a fluid matrix, thus each of its molecules is subject to an additional frictional force.

We denote the position of the \( i \)-th molecule as \( \vec{r}_i \) and its momentum as \( \vec{p}_i \). We will lump all the positions into one vector \( \vec{r} = (\vec{r}_1, \ldots, \vec{r}_N) \) and similarly \( p = (p_1, \ldots, p_N) \). It is convenient also to use the following notation: the relative position of \( i \)-th and \( j \)-th molecule \( \vec{r}_{ij} = \vec{r}_j - \vec{r}_i \), the relative position of two consecutive molecules (or shortly link vector) \( \Delta \vec{r}_i = \vec{r}_{i+1} - \vec{r}_i \), the relative velocity of two consecutive molecules \( \Delta \vec{v}_i = \frac{\vec{p}_{i+1}}{m_{i+1}} - \frac{\vec{p}_i}{m_i} \), and the unit vector of the link vector \( \vec{e}_i = \frac{\Delta \vec{r}_i}{|\Delta \vec{r}_i|} \).

The Hamiltonian for our model then reads

\[
\mathcal{H}(\vec{r}, \vec{p}) = \sum_{i=1}^{N} \left[ \frac{\vec{p}_i^2}{2m_i} + \vec{U}(\vec{r}_i) \right] + \sum_{j=i+1}^{N} V_{ij}(\vec{r}_{ij}) = \sum_{i=1}^{N} \left[ \frac{\vec{p}_i^2}{2m_i} + U(\vec{r}_i) \right].
\] (3.3)

Putting \( K = (N - 1) \), the \( 2K \) constraints follow:

\[
\phi_0(\vec{r}) = \frac{1}{2}(|\Delta \vec{r}_i|^2 - \vec{e}_i \cdot \Delta \vec{r}_i) = 0, \quad \phi_k(\vec{r}, \vec{p}) = \Delta \vec{v}_k \cdot \Delta \vec{r}_k = 0.
\] (3.4)

Using this notation, we can easily evaluate matrix coefficients for all the matrices in Eq. (3.2). We found it convenient to collect them in the Table 1 (see Fig. 1), where the \( b_i, c_i, a_i, b^{(D)}_i \) and \( c^{(D)}_i \) (for isotropic friction \( \lambda_i(d-1)+d = \cdots = \lambda_i(d-1)+d = \lambda_i \) which is the frictional coefficient for \( i \)-th molecule) are given as

\[
b_i = \frac{\Delta \vec{r}_i \cdot \Delta \vec{r}_{i+1}}{m_{i+1}}, \quad b^{(D)}_i = \frac{m_i}{m_{i+1}} b_i = \frac{m_i}{m_{i+1}} \frac{l_{i+1}}{m_{i+1}} \cos(\alpha_i), \quad c_i = \frac{(m_i + m_{i+1})}{m_i m_{i+1}} |\Delta \vec{r}_i|^2 = \left( \frac{1}{m_i} + \frac{1}{m_{i+1}} \right) \left( \frac{1}{m_i} \right)^2, \quad a_i = \frac{\Delta \vec{r}_i \cdot \Delta \vec{v}_{i+1} + \Delta \vec{v}_i \cdot \Delta \vec{r}_{i+1}}{m_{i+1}},
\]

\[
c^{(D)}_i = \left( \frac{\lambda_i}{m_i^2} + \frac{\lambda_{i+1}}{m_{i+1}^2} \right) \left( \frac{1}{m_i} \right)^2, \quad b^{(D)}_i = \frac{\lambda_{i+1}}{m_{i+1}^2} \Delta \vec{r}_i \cdot \Delta \vec{r}_{i+1} = \frac{m_{i+1}}{m_i} l_{i+1} \cos(\alpha_i).
\]

Thus, the matrices \( S, A \) and \( S^{(D)} \) are symmetric tridiagonal, while \( A \) is skew-symmetric tridiagonal, shown in the Table 2. For a homogeneous polymer in a homogeneous environment, consisting of identical molecules, \( l_i = l \) and \( m_i = m \), all formulas on elements of \( S, S^{(D)} \) become even simpler:

\[
c_i = \frac{2l^2}{m}, \quad b_i = \frac{l^2}{m} \cos(\alpha_i), \quad \text{and} \quad c^{(D)}_i = \frac{2l^2}{m^2}, \quad b^{(D)}_i = \frac{2l^2}{m^2} \cos(\alpha_i).
\] (3.5)

Though the triadiagonal matrices have been considered numerically for years, the explicit analytic formulas for elements of the inverse matrix of a triadiagonal matrix are known only in some special cases [18]; \( b_i = b \) and \( c_j = c \). Here we propose a general expression for elements of \( S^{-1} \). Details of the derivation of that formula are given in the Appendix A.
Let $S(1, \ldots, i - 1)$ be the top left $(i - 1) \times (i - 1)$ matrix containing rows and columns $\{1, \ldots, i - 1\}$ of $S$ and $S(j + 1, \ldots, K)$ be the bottom right $(K - j) \times (K - j)$ matrix containing rows and columns $\{j + 1, \ldots, K\}$ of $S$, we get the following recursive formula:

\[(S^{-1})_{ij} = (-1)^{i+j} \frac{|S(1, \ldots, i - 1)||S(j + 1, \ldots, K)|}{|S(1 \cdots K)|} b_ib_{i+1} \cdots b_{j-1}, \quad (3.6)\]

for $i \leq j$, and $S^{-1}$ is symmetric. Since both matrices $S$ and $S^{(0)}$ have a similar form, we can use the formula (3.6) in calculating their inverse.

Furthermore, for $K \geq n > l \geq 1$, the $|S(l, \ldots, n)|$ is calculated from the recursive relation: $|S(\emptyset)| = 1$, $|S(l)| = c_l$, $|S(l, \ldots, n)| = c_l|S(l, \ldots, n - 1)| - b_n^2|S(l, \ldots, n - 2)|$.

With the formula (3.6), it is easy to show that the inverse matrix of a symmetric tridiagonal matrix is one-pair matrix. Numerically it can be computed with just $O(N)$ complexity cost, and with modest memory usage. Since the recursion relation (3.6) is rather involved, we can only calculate the Dirac equations via recursion. More technical details are presented in our paper posted on the arxiv page.

**Discussion**

We have implemented our formalism using the package Mathematica version 5.2 and 6.0, the computer algebra system, both for symbolic and numerical calculations, and measured the CPU time needed in computing explicit analytical r.h.s. of (3.2) in two ways: one based on the formula (3.6) and the other based on the recursion relation (2.15). All computation has been done on an ordinary PC (with dual core processor 1.6 GHz and 1GB RAM) running MS Windows XP and Linux FC6 (see Fig. 2).

The symbolic computing time for one pair of equations in 3-dim, after using least square interpolation, seems to grow with the number of constraints proportionally to $0.028 e^{0.49K}$ and as $0.0046 e^{1.06K}$ for the method of inverting triangular matrices and using a recursive formula, respectively. Consequently, the recursive formula is reasonably good only for systems with less than 12 constraints. Since the computing time in both methods grows exponentially in the number of constraints, computing explicit analytical Dirac equations seems to be inapplicable for very long chains. However, a fast algorithm for the numerical inversion of tridiagonal matrices does exist and has a complexity $O(N)$. Thus, Dirac finite difference equations for long chains are computable.

Having explicit equations of motion, one can solve them numerically either by standard explicit/implicit Runger–Kutta algorithm or standard Mathematica’s ODE solver ND Solve.

Another important issue is that alternatively to the system of Eq. (3.2), one can consider the following system:

\[\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad (3.7)\]

\[\dot{p}_i = -\frac{\partial H}{\partial q_i} - \sum_{j,k=1}^{K} (S^{-1})_{jk} \frac{\partial q_j}{\partial q_k} \{q_k, H\} - \lambda_i \left[\frac{\partial H}{\partial p_i} - \sum_{j,k=1}^{K} C_{jk} \frac{\partial \tilde{q}_j}{\partial p_i} \frac{\partial \tilde{q}_k}{\partial p_i}\right]\]

Since constraints are Casimir elements regarding to Dirac bracket, any solution of (3.2) with initial conditions satisfying all constraints, automatically satisfies all constraints for all time. Therefore it must also be a solution of (3.7).

This fact and the uniqueness of solution (locally) implies that two systems (3.2) and (3.7) are equivalent. In our tests, symbolic computation for the latter is 6–7 times faster than for the former. Moreover, for non-dissipative mechanical systems, the latter is exactly the system of equations obtained from the Lagrange Multiplier Method (LMM), Eq. (A.5) in the Appendix A. Though these two systems are mathematically equivalent, they are not equivalent for a numerical algorithms approximating solution, which means that errors grow differently for each of them even if using a common numerical algorithm. Errors in computing an approximate solution of the LMM-like equation (3.7) or (A.5), always grow faster than those of the Dirac-like equation (3.2). We studied the violation of energy and bond length constraints numerically for a particular polymer with one fixed end, e.g., $N$-pendulum described in the Appendix B. These numerical results are presented briefly in the Fig. 3. In summation, standard numerical algorithms seem to work well with Dirac-like equations. To deal numerically with LMM-like equations, we recommend using either constrained algorithms (eg. SHAKE, LINCS) or other advanced symplectic/poisson ones, which have been developed recently.

Although in the simulation, polymers with nearly constant bond length, called stiff bead-spring chains, are more often considered than those with rigid constant length, named bead-rod chains, the matrix $S$ which has been carefully studied here, is closely related to the metric potential $U = \frac{1}{2}kT \log(|S|)$ in the statistical mechanics of Polymers [23].

The application of bracket formalism to the non-linear many-particle models is possible but time-consuming. We have looked at the possibility of using our method to obtain a set of analytical equations and simulate mechanics of the caricatured human body [19]. Instead of models for body dynamics, such as an inverted pendulum [20], or elastic string [21] are used, we used skeletal humanoid consisting of 13 material points, Fig. 4. We found that symbolic calculation each pair of explicit analytical equations for humanoid takes app. 9 min using formula (3.6) for inverting matrix $S$, of uninterrupted Mathematica performance in PC.
Fig. 1. A linear polymer consists of \( N \) molecules interacting with each other.

Fig. 2. CPU time in 2D and 3D computing one pair of equations of motion by the Eqs. (3.6) and (2.15).

(a) Energy calculated from Eqs. (3.2) and (3.7). (b) Energy calculated from Eq. (A.5).

(c) Sum of constraints error calculated from Eq. (3.2). (d) Sum of constraints error calculated from Eq. (A.5).

Fig. 3. Numerical case study: 4-pendulums described by the Hamilton–Dirac equation (3.2), simplified Dirac (3.7) and Lagrange Multiplier Method (A.5) using default numerical algorithm ND Solve. For simplicity we have chosen a system consisting of 4 equal masses which are in the axis \( x \) at the beginning, and whose initial velocities have random values satisfying constraints' equations. (a) Lower and upper curve represent energy calculated from Eqs. (3.2) and (3.7), respectively. (b) Curve represents energy calculated from (A.5). (c) Curve represents the sum of bond length constraints errors calculated from Eq. (3.2). (d) Curve represents the sum of bond length constraints errors calculated from Eq. (A.5).
4. Conclusions

In this article, we have reviewed a geometric construction of Dirac-like brackets and proved the recursive character of such brackets. We showed that computing explicit dynamical equations based on these brackets may be difficult, but it is possible to produce analytical equations, even for systems with many constraints.

We have applied here the Dirac procedure for metriplectic mechanical models with finite degrees of freedom, but in our previous work we have shown its usefulness for continuous models [14], for example incompressible hydrodynamics [22]. Fixman [23] have used a constraints approach in the formulation of statistical mechanics of various polymer models. The fact that constraints can then be visualized as a kind of temperature dependent potential is not unusual. Fixman and others have restricted their procedure to the equilibrium calculations. Our formalism allows us to go beyond the equilibrium application and see the form of the constrained Liouville equations, modifications in the dynamical modes coupling due to the presence of constraints and possible the role of the constraints play in removing the singularities appearing in low dimensional systems statistical mechanics. For example, the fact that the transport coefficients, such as viscosity, thermal conductivity and diffusion coefficient do not exist in \( d = 2 \), can be modified by the presence of the constraints in a fashion analogous to that mentioned in [24].

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Appendix A. Lagrange multiplier method

The purpose of this section is to show that computing explicit analytical equations in the Lagrangian formalism is equally difficult as in the Dirac formalism.

For simplicity, suppose that all constraints of the form: \( \phi_k(q) = 0, \ k = 1, \ldots, K \) and \( q = (q_1, \ldots, q_n) \). Lagrangian of constrained system is a sum of unconstrained Lagrangian and a linear combination of constraints: \( L(q, \dot{q}) = L_0(q, \dot{q}) - \sum_{k=1}^{K} \lambda_k \phi_k(q) \). The Euler–Lagrange equations read

\[
\frac{\partial}{\partial t} \left( \frac{\partial L}{\partial \dot{q}_i} \right) - \frac{\partial L}{\partial q_i} = 0.
\]

Suppose Lagrangian of the form \( L_0 = T(\dot{q}) - V(q) = \frac{1}{2} \dot{q}^T M \dot{q} - V(q) \), with introducing conservative force \( F = -\frac{\partial V}{\partial q} \), the Euler–Lagrange equations become

\[
M \ddot{q} = F - \sum_{k=1}^{K} \lambda_k \frac{\partial \phi_k}{\partial q_i} = F - B \lambda,
\]

where \( B = (B_{ik}) \) is a \( n \times K \) matrix whose elements \( B_{ik} = \frac{\partial \phi_k}{\partial q_i} \). Since \( \phi_k(q) = 0 \), all first and second time derivatives of \( \phi_k \) vanish:

\[
0 = \frac{d \phi_k}{dt} = \sum_{i=1}^{n} \frac{\partial \phi_k}{\partial q_i} \dot{q}_i \quad \text{or} \quad [B^T \dot{q}]_k = 0, \tag{A.2}
\]

\[
0 = \frac{d^2 \phi_k}{d^2 t} = \sum_{i,j=1}^{n} \frac{\partial^2 \phi_k}{\partial q_i \partial q_j} \ddot{q}_i \ddot{q}_j + \sum_{i=1}^{n} \frac{\partial \phi_k}{\partial q_i} \dddot{q}_i = G_k + [B^T \dddot{q}]_k, \tag{A.3}
\]

where \( G_k = \sum_{i,j=1}^{n} \frac{\partial^2 \phi_k}{\partial q_i \partial q_j} \ddot{q}_i \ddot{q}_j \). Substituting for \( \dddot{q} = M^{-1} [F - B \lambda] \), derived from (A.1), in (A.3) we get:

\[
0 = G + B^T M^{-1} [F - B \lambda], \tag{A.4}
\]
Fig. B.1. N-pendulum is a constrained system with N length constraints, which can be viewed as a linear polymer with a fixed end.

here $G = (G_k), \lambda = (\lambda_k)$ are column vectors $K \times 1$ and $F = (F_j)$ is a column vector $n \times 1$. Therefore, $[G + B^T M^{-1} F] = (B^T M^{-1} B) \lambda$ or $\lambda = (B^T M^{-1} B)^{-1} [G + B^T M^{-1} F]$. Substituting this back to (A.1) we get explicit constrained equations:

$$M \ddot{q} = F - B (B^T M^{-1} B)^{-1} [G + B^T M^{-1} F].$$

(A.5)

Thus, for achieving explicit equations in the Lagrangian formalism, it is also necessary to compute analytical inversion of the $K \times K$ matrix $(B^T M^{-1} B)$ which is exactly equal to the matrix $S$ in the Dirac approach where the Hamiltonian obtained from the Legendre transformation: $\mathcal{H} = p \dot{q} - \mathcal{L}$ with $p = \frac{\partial L}{\partial \dot{q}}$.

Appendix B. N-pendulum in d dimensional space

We denote the position of the i-th mass as $\vec{r}_i = (x_{d(i-1)+1}, \ldots, x_{di})$, its momentum as $\vec{p}_i = (p_{d(i-1)+1}, \ldots, p_{di})$, the relative position of i-th and j-th mass $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$, the relative position of two consecutive masses (or shortly link vector) $\Delta \vec{r}_i = \vec{r}_i - \vec{r}_{i+1}$, the relative velocity of two consecutive masses $\Delta \vec{v}_i = \frac{\vec{p}_i}{m_i} - \frac{\vec{p}_{i+1}}{m_{i+1}}$, and the unit vector of the link vector $\vec{e}_i = \frac{\Delta \vec{r}_i}{|\Delta \vec{r}_i|}$ (see Fig. B.1).

B.1. Hamilton–Dirac description for N-pendulum

The Hamiltonian is given by

$$\mathcal{H}(\vec{r}, \vec{p}) = \sum_{i=1}^{N} \left[ \frac{|\vec{p}_i|^2}{2m_i} + g m_i x_{di} \right],$$

and 2N second-class constraints follow:

$$\phi_k(\vec{r}) = \begin{cases} \frac{1}{2} \left( \sum_{j=1}^{d} x_j^2 - l_i^2 \right) = \frac{1}{2} (|\vec{r}_i|^2 - l_i^2) & \text{for } k = 1, \\ \frac{1}{2} (|\Delta \vec{r}_i|^2 - l_k^2) & \text{for } 1 < k \leq N \end{cases}$$

(B.1)

$$\tilde{\phi}_k(\vec{r}, \vec{p}) = \{\phi_k, \mathcal{H}\} = \begin{cases} \vec{r}_i \cdot \vec{v}_i & \text{for } k = 1, \\ \Delta \vec{v}_k \cdot \Delta \vec{r}_k & \text{for } 1 < k \leq N. \end{cases}$$

(B.2)

B.2. Lagrange Multiplier Method for N-pendulum

The Lagrangian is given by

$$\mathcal{L}(\vec{r}, \vec{p}) = \sum_{i=1}^{N} \left[ \frac{|\vec{p}_i|^2}{2m_i} - g m_i x_{di} \right],$$
and $N$ length-constraints follow:

$$\phi_k(\vec{r}) = \begin{cases} 
\frac{1}{2} \left[ \sum_{j=1}^{d} x_j^2 - l_j^2 \right] = \frac{1}{2} \left( |\vec{r}_1|^{2} - l_1^2 \right) & \text{for } k = 1, \\
\frac{1}{2} \left( |\Delta\vec{r}_k|^{2} - l_k^2 \right) & \text{for } 1 < k \leq N.
\end{cases} \tag{B.3}$$

In order to calculate explicit equation (A.5) we need to calculate explicit elements of $S^{-1}$ where $S$ follows:

$$B^TM^{-1}B = S = \begin{bmatrix}
    c_1 & b_1 & 0 & \cdots & \cdots & 0 \\
    b_1 & c_2 & b_2 & 0 & \cdots & \\
    0 & b_2 & c_3 & b_3 & \cdots & \\
    \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\
    \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\
    0 & \cdots & \cdots & 0 & b_{N-1} & b_N
\end{bmatrix}, \tag{B.4}$$

here

$$b_i = \begin{cases}
\frac{\vec{r}_1 \cdot \Delta\vec{r}_1}{m_1} = \frac{l_1 l_2}{m_1} \cos(\alpha_1) & \text{for } i = 1, \\
\frac{-\Delta\vec{r}_{i-1} \cdot \Delta\vec{r}_i}{m_i} = \frac{l_{i} l_{i+1}}{m_i} \cos(\alpha_i) & \text{for } 1 < i \leq N - 1,
\end{cases}$$

$$c_i = \begin{cases}
\frac{1}{m_1} l_1^2 & \text{for } i = 1, \\
\left( \frac{1}{m_{i-1}} + \frac{1}{m_i} \right) \tilde{l}_i^2 & \text{for } 1 < i \leq N.
\end{cases} \tag{B.5}$$

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