PHYSICAL REVIEW E **80**, 025601(R) (2009)

Nonholonomic double-bracket equations and the Gauss thermostat

Alberto G. Rojo*
Department of Physics, Oakland University, Rochester, Michigan 48309, USA

Anthony M. Bloch†
Department of Mathematics, University of Michigan, Ann Arbor, Michigan 48109, USA
(Received 10 May 2009; published 17 August 2009)

In this Rapid Communication we consider certain equations that arise from imposing a constant kinetic-energy constraint on a one-dimensional set of oscillators. This is a nonlinear nonholonomic constraint on these oscillators and the dynamics are consistent with Gauss's law of least constraint. Dynamics of this sort are of interest in nonequilibrium molecular dynamics. We show that under certain choices of external potential these equations give rise to a generalization of the so-called double-bracket equations which are of interest in studying gradient flows and integrable systems such as the Toda lattice. In the case of harmonic potentials the flow is described by a symmetric bracket and periodic solutions are obtained.

DOI: 10.1103/PhysRevE.80.025601 PACS number(s): 45.50.−j, 05.70.Ln

I. INTRODUCTION

This Rapid Communication brings together two area of interest in recent years—the study of systems with nonholonomic constraints and the study of gradient flows, in particular their formulation as double-bracket equations.

Nonholonomic mechanics is the study of systems subject to nonintegrable constraints on their velocities. The classical study of such systems (see, e.g., [1–6]) and references therein) is concerned with constraints that are linear in their velocities. Nonlinear nonholonomic constraints essentially do not arise in classical mechanics but are however of interest in the study of nonequilibrium or constant temperature dynamics which model the interaction of system with a bath (see, e.g., [7–11]). In this setting the dynamics can be derived using the classical Gauss's principle of least constraint. In this Rapid Communication we analyze some simple examples of such systems and show that the dynamics gives rise to a generalization of another very interesting class of dynamical systems, gradient flows, and, in particular, double-bracket flows. Double-bracket flows on matrices (see [12–16]) arise as the gradient flows on orbits of certain Lie groups with respect to the so-called normal metric. It was shown in [13,14] that in the tridiagonal matrix setting the Toda lattice flow (see [17]), an integrable Hamiltonian flow may be written in double-bracket form, thus exhibiting a dual Hamiltonian or gradient structure. This elucidates its dynamics and scattering behavior. Double-bracket flows have also been shown to give a very interesting kind of dissipation in classical mechanical systems (see [18] and also [19]).

In this Rapid Communication we consider certain equations that arise from imposing a constant kinetic-energy constraint on a one-dimensional set of particles. This is a nonlinear nonholonomic constraint on these particles and the dynamics are consistent with Gauss's law of least constraint. We show that under a constant force these equations give rise to a generalization of the double-bracket equations. We show the flow asymptotically approaches the setting where all particles are moving with the same velocity. We note also that in the case of equal masses we obtain equipartition of energy but that this is not the case when the masses differ. In the case of harmonic potentials the flow is described by a symmetric bracket and periodic solutions are obtained.

II. DYNAMICS OF PARTICLES WITH CONSTANT KINETIC-ENERGY CONSTRAINT

A. Nonholonomic constraints

The standard setting for nonholonomic systems (see, e.g., [1]) is the following: one has n coordinates $q_i(t)$ and m (linear in the) velocity-dependent constraints of the form

$$\sum_{i=1}^{n} a_i^{(j)}(\mathbf{q})\dot{q}_i = 0, \quad j = 1, \ldots, m. \tag{1}$$

Let $L(q_i, \dot{q}_i)$ be the system Lagrangian. and suppose the m velocity constraints are represented by the equation $A(q)\dot{q} = 0$, where $A(q)$ is an $m\times n$ matrix and $\dot{q}$ is a column vector. Let λ be a row vector of Lagrange multipliers which are used to define the virtual forces which are necessary to impose the constraints. The equations we obtain are thus

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = \lambda A(q), \quad A(q)\dot{q} = 0. \tag{2}$$

Note that such systems are not variational and the dynamics may not be derived by appending the constraint to the Lagrangian by Lagrange multipliers.

In the current setting we are interested in a nonlinear constraint, the constraint of constant kinetic energy. This again may be implemented using Lagrange multipliers by differentiating the constraint and enforcing the system to lie on the resultant hypersurface defined by this constraint. This is equivalent to Gauss's principle of least constraint.

In the linear setting (see [1]), the system energy is preserved. This is not true in the nonlinear setting as can be seen below. Another feature of nonholonomic systems is that volume may not be preserved in the phase space even in the

*rojo@oakland.edu
†abloch@.umich.edu

absence of external friction [1,20]. In the systems below volume is also not preserved in general.

B. Constraint in the case of equal masses

The simplest setting is the case of N particles with equal mass. In this case the constraint of kinetic energy corresponds to the norm of the velocity being constant under the flow.

Consider an N-dimensional vector $\mathbf{V}=(\dot{x}_1,\ldots,\dot{x}_N)$ and an N-dimensional force $\mathbf{F}=(f_1,\ldots,f_N)$. The constraint of constant kinetic energy is imposed by a "time dependent viscosity" $\eta(t)$

$$\dot{\mathbf{V}} = \mathbf{F} - \eta(t)\mathbf{V}. \tag{3}$$

The crucial ingredient is that the viscosity term can be positive or negative. The condition that the norm of $\mathbf{V}$ is constant (or constant kinetic energy) means

$$\dot{\mathbf{V}} \cdot \mathbf{V} = 0 \Rightarrow \eta(t) = \frac{\mathbf{F}\cdot\mathbf{V}}{\mathbf{V}\cdot\mathbf{V}}. \tag{4}$$

The equation of motion is therefore

$$\dot{\mathbf{V}} = \mathbf{F} - \frac{\mathbf{F}\cdot\mathbf{V}}{\mathbf{V}\cdot\mathbf{V}}\mathbf{V}. \tag{5}$$

III. CORRELATIONS INDUCED BY THE CONSTRAINT IN THE CASE OF CONSTANT FORCE

Consider the case of N particles in one dimension subject to a constant gravitational force $f=mg$ and random initial conditions. In the absence of the constraint the particles move independently and the kinetic energy fluctuates. We now show that the constraint induces correlations and that the long time behavior corresponds to *all* particles moving with the same velocity, regardless of the initial conditions.

The equation of motion of the nth particle is

$$\dot{v}_n = g - \frac{\sum_{m=1}^{N} g v_m}{\mathbf{V}^2} v_n. \tag{6}$$

Of course $\mathbf{V}^2=\sum v_n(t)^2$ is preserved by the dynamics. Define

$$u_q = \frac{1}{N}\sum_n v_n e^{iqn}, \tag{7}$$

with $q=\frac{2\pi}{N}k$, $k=0,1,\ldots,(N-1)$. Also define a (constant) mean quadratic velocity as $v_M^2=\frac{\mathbf{V}^2}{N}$.

Replace these two transformations in Eq. (6) to obtain

$$\dot{u}_q(t) = g\,\delta_{q,0} - \frac{g u_0(t)}{v_M^2} u_q(t). \tag{8}$$

From Eq. (8) the equation of motion for u_0 is

$$\dot{u}_0 = g\left(1 - \frac{u_0^2}{v_M^2}\right), \tag{9}$$

with solution (and long time limit) given by

$$u_0(t) = v_M \tanh(gt/v_M) \to v_M.$$

The solution for $u_q(t)$ for $q>0$ is given by

$$u_q(t) = \frac{u_q(0)}{\cosh(gt/v_m)}.$$

In the long time limit, $u_q(t)\to 0$. Substituting in Eq. (7) we see that the long time solution is

$$v_n(t\to\infty) = v_M.$$

This means that in this particular example, at long times, the constraint enforces all particles to move *with the same velocity* v_M. In the absence of the constraint, the velocities are of course independent, and the total energy is conserved.

In the constrained case the long time behavior for each $x_n(t)$ is a linear increase, meaning that, although the kinetic energy is constant, the potential energy is linearly decreasing: $\dot{U}_n=-mgv_M$.

The extension to nonequal masses is essentially immediate. The main result is that the long time behavior remains the same: regardless of the mass differences, the asymptotic velocities are all the same. This means of course that in that case equipartition does not occur. One can also apply the analysis to the case of equal mass particles with different charges in an electric field. In this case one gets a sorting behavior as in [12,13,15]. These ideas will be discussed in a forthcoming publication [21].

A. Three particles in one dimension and the evolution as a double-bracket equation

Since, for particles of equal mass, the motion is always in a sphere of radius $|\mathbf{V}_0|$, for three particles we can formulate the dynamics as a rotation:

$$\dot{\mathbf{V}} = \vec{\Omega} \times \mathbf{V}, \tag{10}$$

with $\Omega_i=(1/\mathbf{V}_0^2)\epsilon_{ijk}v_j f_k$.

Note that in fact we have

$$\Omega = \frac{1}{\mathbf{V}_0^2}\mathbf{V}\times\mathbf{F}.$$

Hence

$$\dot{\mathbf{V}} = -\frac{1}{\mathbf{V}_0^2}\mathbf{V}\times(\mathbf{V}\times\mathbf{F}). \tag{11}$$

Now use the standard map from three-vectors to matrices in so(3) (see, e.g., [22]), denoted by $\mathbf{V}\to\hat{\mathbf{V}}$. Explicitly this map is given by

$$\hat{\mathbf{V}} \equiv \begin{pmatrix} 0 & -V_3 & V_2 \\ V_3 & 0 & -V_1 \\ -V_2 & V_1 & 0 \end{pmatrix},$$

and implies $[\hat{\mathbf{V}},\hat{\mathbf{F}}]=(\mathbf{V}\hat{\times}\mathbf{F})$. Then Eq. (11) may be rewritten in the form

$$\dot{\mathbf{V}} = -\frac{1}{\mathbf{V}_0^2}[\hat{\mathbf{V}},(\hat{\mathbf{V}},\hat{\mathbf{F}})].$$

This is the classic double-bracket form and links nonlinear nonholonomic mechanics (second order) to double-bracket flows. Note also that this tells us precisely what the equilibria (steady-state solutions) should be when $\hat{\mathbf{V}}$ and $\hat{\mathbf{F}}$ commute.

N-particle case

For N particles in one dimension, the extension of the discussion above is as follows: the dynamics in general is given by the skew matrix $\mathbf{O}$:

$$\dot{\mathbf{V}} = \mathbf{O}\mathbf{V}, \tag{12}$$

with

$$O_{ij} = \frac{f_i v_j - v_i f_j}{\mathbf{V}_0^2}, \tag{13}$$

and formal solution

$$\mathbf{V}(t) = T \exp \int_0^t dt' \mathbf{O}(t') \times \mathbf{V}_0,$$

and T the time ordering operator.

B. Stability and generalized double-bracket form

Note that this equation can be reformulated in the following way:

O_{ij} is the rank two matrix

$$\mathbf{O} = \frac{\mathbf{F}\mathbf{V}^T - \mathbf{V}\mathbf{F}^T}{\mathbf{V}_0^2}.$$

Hence the flow may be written as

$$\dot{\mathbf{V}} = \frac{\mathbf{F}\mathbf{V}^T - \mathbf{V}\mathbf{F}^T}{\mathbf{V}_0^2}\mathbf{V} = \frac{\mathbf{F} \otimes \mathbf{V} - \mathbf{V} \otimes \mathbf{F}}{\mathbf{V}_0^2}\mathbf{V}, \tag{14}$$

where $\otimes$ denotes the tensor product. (Note that this is effectively a generalization of the double-bracket form above to the N-vector setting.)

Now consider the derivative of $\mathbf{V}\cdot\mathbf{F}$ in the case $\mathbf{F}$ is constant. We have

$$\frac{d}{dt}(\mathbf{V}\cdot\mathbf{F}) = \mathbf{F}\cdot\dot{\mathbf{V}} = \mathbf{F}\cdot\mathbf{O}\mathbf{V} = \mathbf{F}\cdot\frac{\mathbf{F}\mathbf{V}^T - \mathbf{V}\mathbf{F}^T}{\mathbf{V}_0^2}\mathbf{V}.$$

But the numerator here just equals $\|\mathbf{V}\|^2\|\mathbf{F}\|^2 - \|\mathbf{V}\cdot\mathbf{F}\|^2$ which is sign definite. Hence $\mathbf{V}\cdot\mathbf{F}$ changes monotonically along the flow.

This is similar to what happens in the double-bracket flow (see [12,14]). Note also that it has the right equilibrium structure: when $\mathbf{V}$ and $\mathbf{F}$ are parallel one gets a dynamic equilibrium (see Fig. 1).

Note these flows are not Hamiltonian and in this setting one expects this kind of asymptotic behavior (see, e.g., [9]).

IV. GENERAL ORBITS FOR HARMONIC FORCES

Now consider harmonic forces for particles of unit mass and call $\mathbf{V}_0$ the constant radius of the n-dimensional sphere in velocity space

$$\dot{\mathbf{V}} = -k\mathbf{X} + \frac{k\mathbf{X}\cdot\mathbf{V}}{\mathbf{V}_0^2}\mathbf{V}. \tag{15}$$

From the calculation for three dimensions, we see that if the n-dimensional vectors $\mathbf{X}$ and $\mathbf{V}$ are collinear, then a constant velocity solution is possible. That is, in this case, if $\mathbf{X}(t) = \hat{\mathbf{u}}|\mathbf{V}_0|t$, with $\hat{\mathbf{u}}$ as an arbitrary constant vector, Eq. (15) is satisfied.

We now discuss the general orbits of the system, a fixed point of which is the perfect circular orbit. Since the force is "central," the constrained force is in the $(\mathbf{X},\mathbf{V})$ plane and therefore the N-dimensional orbit remains in the plane of the initial conditions $(\mathbf{X}_0,\mathbf{V}_0)$. The relevant parameters of the evolution will therefore be the angle α between $\mathbf{X}$ and $\mathbf{V}$ and the magnitude of $\mathbf{X}$. In an interval δt the rotation angle $\delta\theta_{\mathbf{x}}$ for $\mathbf{X}$ and $\delta\theta_{\mathbf{v}}$ for $\mathbf{V}$ is (see Fig. 2)
.

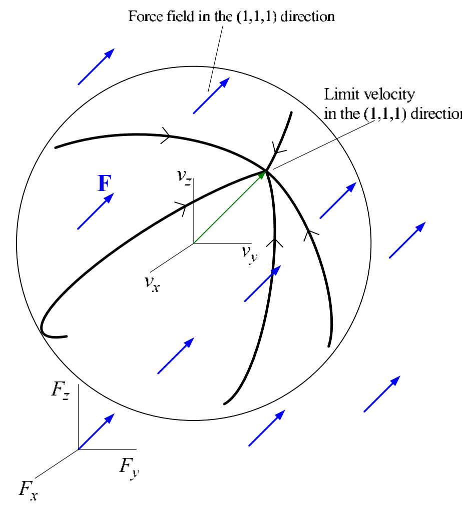

FIG. 1. (Color online) Flow in constant force case.

$$\delta\theta_{\mathbf{x}} = \frac{|\mathbf{V}_0|\sin\alpha}{|\mathbf{X}|}\delta t,$$

$$\delta\theta_{\mathbf{v}} = \frac{k|\mathbf{X}|\sin\alpha}{|\mathbf{V}_0|}\delta t.$$

The time derivative of the angle is therefore

$$\frac{d\alpha}{dt} = \frac{\delta\theta_{\mathbf{x}}}{\delta t} - \frac{\delta\theta_{\mathbf{v}}}{\delta t} = \frac{k|\mathbf{X}|^2 - |\mathbf{V}_0|^2}{|\mathbf{V}_0||\mathbf{X}|}\sin\alpha. \tag{16}$$

At the same time, the variation in the length of $\mathbf{X}$ is

$$\frac{d|\mathbf{X}|}{dt} = |\mathbf{V}_0|\cos\alpha.$$

We will rewrite the above equations using the following dimensionless parameters: $\rho = \sqrt{k}|\mathbf{X}|/|\mathbf{V}_0|$ and $\tau = \sqrt{k}t$.

The flow equations are

$$\frac{d\alpha}{d\tau} = \frac{\rho^2 - 1}{\rho}\sin\alpha,$$

$$\frac{d\rho}{d\tau} = \cos\alpha. \tag{17}$$

The fixed points of the flow are $(\rho_0,\alpha_0) = (\tau,0)$ (a straight line with the force parallel to the velocity) and $(\rho,\alpha) = (1,\pi/2)$ (circular motion). Let us discuss the stability of each of these fixed points. Linearizing around (ρ_0,α_0) it is immediate to see that the linear orbits around this fixed point are periodic. On the other hand, linearizing around the linear fixed point $\rho = \tau + \eta$, $\alpha = \xi$ we can see that those are unstable orbits.

The phase portrait of the oscillator is shown in Fig. 3.

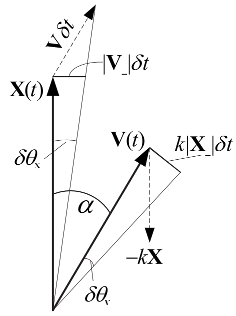

FIG. 2. Instantaneous evolution in the $(\mathbf{X},\mathbf{V})$ plane for harmonic forces with α as the angle between $\mathbf{X}$ and $\mathbf{V}$. The corresponding perpendicular projections are $|\mathbf{X}|_{\perp}=|\mathbf{X}|\sin\alpha$ and $|\mathbf{V}|_{\perp}=|\mathbf{V}_0|\sin\alpha$.

Bracket equation for harmonic forces

We now show that in the harmonic setting the flow may be described by a symmetric bracket. The equation of motion [from Eq. (15)] for $\mathbf{V}$ becomes

$$\dot{\mathbf{V}} = \frac{k}{\mathbf{V}_0^2}[\mathbf{V}\otimes\mathbf{X} - \mathbf{X}\otimes\mathbf{V}]\mathbf{V} \tag{18}$$

or rescaling the time

$$\dot{\mathbf{V}} = [\mathbf{V}\otimes\mathbf{X} - \mathbf{X}\otimes\mathbf{V}]\mathbf{V} \equiv \mathbf{L}\mathbf{V}. \tag{19}$$

Now compute the evolution of the operator $\mathbf{L}$ defined above

$$\dot{\mathbf{L}} = (\mathbf{V}\otimes\mathbf{X})(\mathbf{V}\otimes\mathbf{X}) - (\mathbf{X}\otimes\mathbf{V})(\mathbf{X}\otimes\mathbf{V}), \tag{20}$$

where we have used $[(\mathbf{a}\otimes\mathbf{b})\mathbf{c}]\otimes\mathbf{d}=(\mathbf{a}\otimes\mathbf{b})(\mathbf{c}\otimes\mathbf{d})$ and $\mathbf{a}\otimes[(\mathbf{b}\otimes\mathbf{c})\mathbf{d}]=(\mathbf{a}\otimes\mathbf{c})(\mathbf{d}\otimes\mathbf{b})$.

Now it is immediate to show that, in terms of the operator $\mathbf{B}$ defined as

$$\mathbf{B} = \frac{1}{2}(\mathbf{V}\otimes\mathbf{X} + \mathbf{X}\otimes\mathbf{V}),$$

Eq. (20) can be written as

$$\dot{\mathbf{L}} = \mathbf{B}\mathbf{L} + \mathbf{L}\mathbf{B} \equiv \{\mathbf{B},\mathbf{L}\}. \tag{21}$$

In summary, the equation of motion can be cast into an *anticommutator* form. This is consistent with the type of flow seen, for example, in [19] and also applied to the constant force case (see [21]).

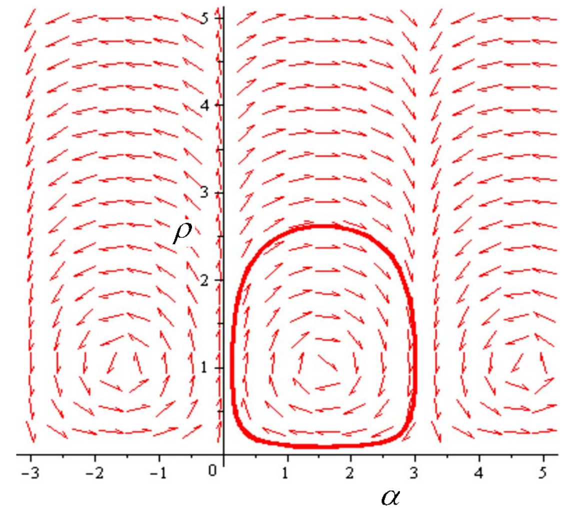

FIG. 3. (Color online) Phase portrait for the flow Eqs. (17) corresponding to N harmonic oscillators. The solid line corresponds to the orbit for initial conditions $\alpha_0=3$ and $\rho_0=1$.

V. CONCLUSION

We have analyzed some nonlinear nonholonomic flows that arise in the nonequilibrium thermodynamics setting and described the structure and solutions of these flows in special cases, yielding double-bracket and symmetric bracket flows. In future work we intend to examine more general flows of this type, their numerics, and their connections with nonlinear nonholonomic mechanics.

ACKNOWLEDGMENTS

A.G.R. was partially supported by the Research Corporation. A.M.B. was partially supported by the National Science Foundation.

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