Generalized Conservative Dynamics in Topologically Constrained Phase Space: Macro-Hierarchy, Entropy Production, and Self-Organization

(トポロジー束縛を受けた位相空間における拡張保存型力学:マクロ階層、エントロピー生成と自己組織化)

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1. Abstract

The dynamics of a microscopic system is naturally written in the language of canonical Hamiltonian mechanics. A macroscopic system emerges when constraints are imposed on the 'flat' phase space of microscopic degrees of freedom. Such topological constraints may destroy the canonical Hamiltonian form. Integrable constraints foliate the phase space and dictate a non-canonical Hamiltonian structure represented by a Poisson operator. Non-integrable constraints impart 'vorticity' to the metric of space and induce an almost Hamiltonian structure with an associated almost Poisson operator. Here, we categorize almost Poisson operators and investigate the statistical properties of ensembles endowed with non-canonical and almost Hamiltonian structures. A proper entropy measure reflecting the geometric properties of space is introduced, the form of the equilibrium probability distribution is calculated, and it is shown that self-organization driven by topological constraints is consistent with the second law of thermodynamics.

2. Introduction

The motion of elementary particles in gravitational and electromagnetic fields is an example of microscopic dynamics. The natural setting of microscopic dynamics is provided by canonical Hamiltonian mechanics [1]. In a canonical Hamiltonian system, motion occurs in a flat space, the symplectic manifold called phase space [2]. A macroscopic description of a physical system can be obtained by removing the redundant degrees of freedom of microscopic dynamics. Such redundant degrees of freedom are mathematically represented by a set of *topological constraints* acting on the phase space of canonical Hamiltonian mechanics. The ideal Euler equations for the motion of a fluid are an example of macroscopic system. Here, the microscopic degrees of freedom of the molecules composing the fluid are reduced to the simplified flow of fluid elements.

The process of reduction may, in general, destroy the canonical Hamiltonian form: the space where the motion of a macroscopic system occurs does not have the properties of canonical phase space. However, if the constraints acting on the system are integrable (in the sense of Frobenius [3]), the reduced space can be locally transformed to the canonical phase space by an appropriate change of coordinates. Systems with this property are called non-canonical Hamiltonian systems and are mathematically represented by a Poisson operator that satisfies the Jacobi identity [4-5]. The ideal Euler equations exhibit a non-canonical Hamiltonian structure.

If the topological constraints cannot be integrated, the resulting dynamics is called almost Hamiltonian and it is described by an almost Poisson operator that fails to satisfy the Jacobi identity [6]. Systems affected by nonholonomic constraints, such as the rolling of a rigid body, fall in this category [7]. We further note that canonical and non-canonical Hamiltonian systems can be regarded as special subclasses of almost Hamiltonian dynamics¹.

Figure 1 shows a schematic view of the radiation belts that surround the Earth. These plasma formations are a prototype of macroscopic self-organization [8-9]. The long-lasting, stable, and heterogeneous structure of a radiation belt seemingly violates the entropy principle dictated by the second law of thermodynamics. Analogous macroscopic and hierarchical structures are observed across different scales (spiral shape of galaxies,

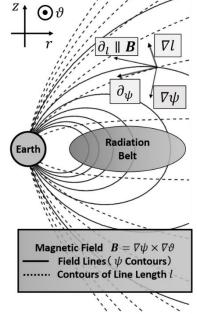


Fig. 1: Schematic view of a radiation belt and magnetic coordinates.

¹ In formulae, an almost Hamiltonian vector field $X = \dot{x}^i \partial_i$ on an *n*-dimensional manifold is represented as: $X = \Im(dH).$

Here, \Im is an antisymmetric operator and H the Hamiltonian (energy) of the system. If X is a canonical Hamiltonian vector field, \Im is the symplectic matrix \mathcal{I}_c . If X is a non-canonical Hamiltonian vector field, \Im satisfies the Jacobi identity $\Im^{im}\Im_m^{jk} + \Im^{jm}\Im_m^{ki} + \Im^{km}\Im_m^{ij} = 0$.

turbulent structures on the surface of gaseous planets) and throughout the physical world (fluid and plasma turbulence, rigid body dynamics, ferromagnetism, and so on).

Aim of the present study is to construct a rigorous theory of the statistical mechanics of macroscopic systems that lack canonical phase space due to the existence of topological constraints. The cornerstone of the standard formulation of statistical mechanics is Liouville's theorem, which states that the phase space volume is preserved by the canonical flow. This theorem justifies the conventional notion of entropy of a probability distribution and the assumption of the ergodic hypothesis [10]. However, we have seen that macroscopic systems are not, in general, canonical. Thereby, none of the above results hold and a new paradigm that takes into account the non-trivial topology of space is needed to understand the statistical and thermodynamic properties of macroscopic systems.

3. Categorization of Almost Poisson Operators, Types of Self-Organization, and Equilibrium

Cardinal part of the present investigation is the classification of almost Poisson operators according to their geometrical properties (see figure 2).

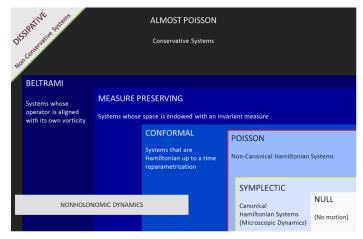


Fig. 2: The hierarchical structure of almost Poisson operators. Each box is named by the corresponding operator. The yellow line indicates transition from microscopic to macroscopic dynamics. The red line indicates transition from Hamiltonian to almost Hamiltonian dynamics, with corresponding loss of phase space. The green line indicates transition from conservative to dissipative dynamics. The latter is not object of the present study.

The symplectic matrix of microscopic dynamics is located at the top of the pyramid. The following category is that of Poisson operators of non-canonical Hamiltonian systems. Beyond Poisson operators, the phase space is lost, and we first encounter conformal operators. Such operators can be transformed to Poisson operators by performing an appropriate time reparametrization. The subsequent class we introduce is that of measure preserving operators. These operators impart an invariant measure to the system for any choice of the Hamiltonian function. Using this property, we prove a theorem on the equilibrium of the probability distribution f on the invariant measure:

$$\lim_{t \to \infty} \Im(d \log f + \beta dH) = 0 \qquad a.e. \tag{1}$$

This theorem, which does not require the existence of the phase space, reduces to the standard Boltzmann distribution $f = ce^{-\beta H}$ when \Im is the symplectic matrix. Here, $c, \beta \in \mathbb{R}_{>0}$ are constants. If, instead, \Im is a Poisson operator, equation (1) becomes:

$$\lim_{t \to \infty} f = c \exp\{-\beta H - \gamma_i C^i\} \qquad a.e.$$
(2)

Here, the functions C^i are the so called Casimir invariants whose gradients span the kernel of the Poisson operator $\Im(dC^i) = 0$. These invariants, which only depend on the properties of \Im , are responsible of the first type of macroscopic self-organization (see figure 3): motion is restricted on the level sets (leaves) of the C^i s.

We further show that, by introducing a new degree of freedom, any *n*-dimensional almost Poisson operator can be extended to an n + 1-dimensional measure preserving operator, and that any measure preserving operator has vanishing

vorticity (i.e. it corresponds to a closed differential form) on the invariant measure. Since operators determine the topological properties of space, we therefore find that, beyond measure preserving operators, the metric of space in endowed with an intrinsic vorticity. This kind of metric induces a second type of self-organization (see figure 3): in this case, a particle will tend to fall toward the center of the metric vortices.

The following category is that of Beltrami operators. These operators are characterized by being completely aligned with their own vorticity and generalize the notion of Beltrami field from 3 to arbitrary dimensions. It is worth to mention that they exhibit peculiar properties from the standpoint of statistical mechanics. Finally, operators that do not fall in any of the previous categories are simply referred to as almost Poisson.

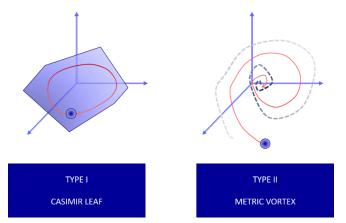


Fig. 3: Types of self-organization. Left: type I self-organization driven by Casimir invariants. Right: type II self-organization driven by metric vorticity.

4. Self-Organization in Non-Canonical Hamiltonian Systems

As a concrete example of self-organization in a non-canonical Hamiltonian system, we examine the mechanism by which radiation belts are created in a dipole magnetic field. Here, the topological constraint affecting the system is the first adiabatic invariant of magnetized particles: the magnetic momentum associated to the cyclotron gyration around the magnetic field.

Exploiting the theory developed so far, we first determine the Poisson operator of the system. The magnetic momentum is found to be a Casimir invariant of the Poisson operator, and dictates a type I self-organization. Then, on the Casimir leaf, the corresponding invariant measure dV_I is obtained, and a diffusion operator is formulated. On this appropriate metric induced by the topology of the magnetic field, the proper entropy measure:

$$\Sigma = -\int f \log f \, dV_I,\tag{3}$$

is maximized, and its entropy production $\sigma = \dot{\Sigma}$ is positive. Here f is the probability distribution on dV_I . The opposite behavior is observed in the laboratory coordinates $dV_L = B^{-1}dV_I$, where the standard (and erroneous) entropy measure:

$$\tilde{S} = -\int f \log f B \, dV_I,\tag{4}$$

is minimized (see figure 4). Here B is the Jacobian of the coordinate change and physically represents the magnetic field strength. Figure 5 shows the numerical simulation of the derived transport equation, where the creation of the radiation belt is manifest. The results of this part, and their generalization to non-canonical Hamiltonian systems, are summarized in [11-14].

5. Self-Organization in Almost Hamiltonian Systems

In this last section we discuss an example of type II selforganization, driven by metric vorticity. For the sake of simplicity, we consider a 3-dimensional system. Then, the equation of motion can be written as:

$$X = \boldsymbol{w} \times \nabla H,\tag{5}$$

Here, the vector w is an almost Poisson operator. Equation (5) may represent the $E \times B$ motion of a charged particle in

an electromagnetic field, the motion of a rigid body, or the evolution equation for the magnetization of a ferromagnet, and so on, depending on the specific choice of w and H. We further assume that:

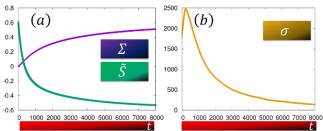
$$\boldsymbol{w}\cdot\nabla\times\boldsymbol{w}\neq\boldsymbol{0},\tag{6.1}$$

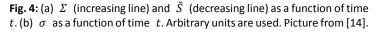
$$\nabla \cdot [\boldsymbol{w} \times (\nabla \times \boldsymbol{w})] \neq 0. \tag{6.2}$$

Equation (6.1) implies the failure of the Jacobi identity (w is not a Poisson operator). Equation (6.2) implies that w is not aligned with its own vorticity $\nabla \times w$, and therefore it is not a Beltrami operator. As energy gradient we consider pure white noise, i.e. we set $\nabla H = \Gamma$. Then, the evolution of the probability distribution f reduces to a purely diffusive equation:

$$\frac{\partial f}{\partial t} = \frac{1}{2} \nabla \cdot [\boldsymbol{w} \times (\nabla \times f \boldsymbol{w})] = \frac{1}{2} (\Delta_{\perp} f + \nabla f \cdot \boldsymbol{b} + f \mathfrak{B}).$$
(7)

In this notation, we introduced the normal Laplacian $\Delta_{\perp} f = \nabla \cdot (\mathbf{w} \times (\nabla f \times \mathbf{w}))$ and set $\mathbf{b} = \mathbf{w} \times (\nabla \times \mathbf{w})$, $\mathfrak{B} = \nabla \cdot \mathbf{b}$. In figure 6 we report the results of the numerical simulation of equation (5) for an ensemble of $8 \cdot 10^6$ particles, when $\mathbf{w} = (1, \sin x + \cos y, \cos x)$. Note that this choice is consistent with (6.1) and (6.2). Regardless of the fact that we are perturbing the system with homogenous fluctuations (the white noise Γ), a complex structure is created.





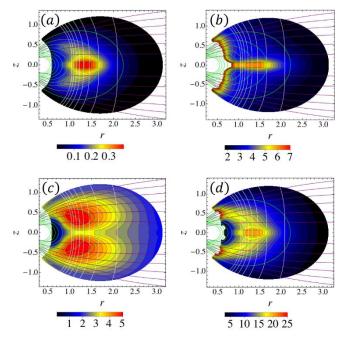
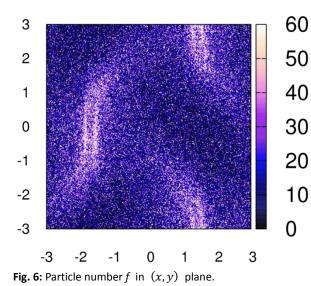


Fig. 5: Self-organized plasma after entropy maximization. (a) Spatial profile of particle density (a.u.). (b) Temperature anisotropy T_{\perp}/T_{\parallel} . (c) Parallel temperature $T_{\parallel}(eV)$. (d) Perpendicular temperature $T_{\perp}(eV)$. White (vertical) lines, green (circular) lines, and purple (spreading from the left to the right) lines represent contours of magnetic field strength *B*, flux function ψ , and field line length *l*. Picture from [14].



From the standpoint of pure mathematics, equation (7) is of special interest since it is a second order non-elliptic partial differential equation. At present, there is no satisfactory theory of non-elliptic partial differential equations [15]. A special case in which an explicit solution to equation (7) with conditions (6.1) and (6.2) can be found occurs when $\hat{w} \times (\nabla \times \hat{w}) = \nabla \zeta$ for some function ζ and with $\hat{w} = w/w$. Then, we prove that in the limit $t \to \infty$ the solution is unique and converges to:

$$\lim_{k \to \infty} f = \frac{c}{w} e^{-\zeta} \qquad a.e.$$
(8)

) In the present work, we further study existence and uniqueness of solution to the normal Laplace equation $\Delta_{\perp} f = \varphi$ by introducing a novel function norm and applying Riesz theorem of representation.

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6. Conclusion

In the present study, we have investigated dynamical properties and statistical behavior of macroscopic ensembles that lack the phase space of canonical Hamiltonian mechanics in virtue of topological constraints. The non-trivial topology is encapsulated in the almost Poisson operator that acts on the energy of the system to generate the dynamics. We have categorized almost Poisson operators, determined the resulting probability distributions, and shown that the creation of macroscopic structures is consistent with the second law of thermodynamics provided that an appropriate metric, reflecting the topology of space, is taken into account. Several examples of both non-canonical and almost Hamiltonian dynamics were discussed.

7. References

[1] L. D. Landau and E. M. Lifshitz, Mechanics, 3rd ed. (Butterworth-Heinenann, Oxford, 1993), pp. 131-3.

[2] V. I. Arnold, Mathematical Methods of Classical Mechanics, 2nd ed. (Springer, New York, 1989), pp. 201-4.

[3] T. Frankel, The Geometry of Physics, An Introduction, 3rd ed. (Cambridge University Press, Cambridge, 2012), pp. 165-78.
[4] P. J. Morrison, Poisson Brackets for Fluids and Plasmas, in Mathematical Methods in Hydrodynamics and Integrability in Dynamical Systems, edited by M. Tabor and Y. Treve, AIP Conference Proceedings No. 88 (AIP, New York, 1982), pp. 13-46.

[5] R. Littlejohn, Singular Poisson Tensors, in Mathematical Methods in Hydrodynamics and Integrability in Dynamical Systems, edited by M. Tabor and Y. Treve, AIP Conference Proceedings No. 88 (AIP, New York, 1982), pp. 47-66.

[6] M. de Léon, Methods of Differential Geometry in Analytical Mechanics, (Elsevier, New York, 1989), p. 234.

[7] A. M. Bloch, J. E. Marsden, and D. V. Zenkov, Nonholonomic Dynamics, Notices of the AMS, 52, pp. 320-9 (2005).

[8] Yoshida_3 Z. Yoshida and S. M. Mahajan, Self-Organization in Foliated Phase Space: Construction of a Scale Hierarchy by Adiabatic Invariants of Magnetized Particles, Prog. Theor. Exp. Phys., 2014, 073J01 (2014).

[9] Z. Yoshida, Self-Organization by Topological Constraints: Hierarchy of Foliated Phase Space, Adv. Phys. X, 1, pp. 2-19 (2016). [10] E. T. Jaynes, Information Theory and Statistical Mechanics, Phys. Rev., 106, 4, pp. 620-30 (1957).

[11] N. Sato and Z. Yoshida, A Stochastic Model of Inward Diffusion in Magnetospheric Plasmas, J. Phys. A: Math. Theor., 48, 205501 (2015).

[12] N. Sato, N. Kasaoka, and Z. Yoshida, Thermal Equilibrium of Non-Neutral Plasma in Dipole Magnetic Field, Phys. Plasmas, 22, 042508 (2015).

[13] N. Sato, Z. Yoshida, and Y. Kawazura, Self-Organization and Heating by Inward Diffusion in Magnetospheric Plasmas, 11, 2401009 (2016).

[14] N. Sato and Z. Yoshida, Up-Hill Diffusion, Creation of Density Gradients: Entropy Measure for Systems with Topological Constraints, Phys. Rev. E, 93, 062140 (2016).

[15] D. Gilbarg and N. S. Trudinger, Elliptic Partial Differential Equations of Second Order, (Springer, 2001).