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Metriplectic Brackets for the Fokker-Planck Equation in Hamiltonian Systems

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In the absence of irreversible processes, the equations of motion governing the evolution of physical systems, such as ideal fluids and plasmas, take the form of a Hamiltonian system:

$$F_t = \{F, H\}. \tag{1}$$

Here, F is an observable, H the Hamiltonian function (the energy of the system), and $\{\circ,\circ\}$ the Poisson bracket. Due to Liouville's theorem, the structure of Hamilton's equations is incompatible with the thermodynamic principle of entropy growth, i.e. it cannot account for irreversible changes in the state of a system.

The metriplectic bracket is an algebraic construction that aims at reconciling Hamiltonian mechanics with thermodynamics by generalizing the Poisson bracket of equation (1) as follows:

$$F_t = (F, H, S) = \{F, H\} + [F, S]. \tag{2}$$

In this notation, $(\circ,\circ,\circ)$ is the metriplectic bracket, S a second generating function representing the entropy of the system, and $[\circ,\circ]$ a dissipative bracket, i.e. a bilinear non-negative symmetric product. The Hamiltonian H and the entropy S are chosen so that the following conditions hold:

$$\{S, H\} = [H, S] = 0. \tag{3}$$

Equation (3) ensures that the first and second laws of thermodynamics are satisfied:

$$H_t = \{H, H\} + [H, S] = 0, \tag{4}$$
$$S_t = \{S, H\} + [S, S] = [S, S] \geq 0.$$

Here, we used the alternativity of the Poisson bracket, $\{H, H\} = 0\ \forall H$, and the non-negativity of the dissipative bracket, $[S, S] \geq 0\ \forall S$.

Aim of the present study is to show that, given a general Hamiltonian system, there exists a Fokker-Planck equation describing the evolution of the associated statistical ensemble with the metriplectic form of equation (2). Our construction starts with a microscopic isolated Hamiltonian system in an n dimensional domain $\Omega \subset \mathbb{R}^n$ with coordinates $(x^1, \dots, x^n)$ and evolving according to

$$\dot{x}^i = \{x^i, h\} = \mathcal{J}^{ij} h_j, \tag{5}$$

with h and $\mathcal{J}^{ij}$ the Hamiltonian function and the Poisson operator respectively, and $h_j = \partial h / \partial x^j$. Then, we consider an ensemble of N elements obeying equation (5), and let them interact. The interaction results in fluctuations δh of the individual energy h, and a dissipative force $\boldsymbol{F} = F_j \nabla x^j$, so that the equation of motion of an element of the statistical ensemble becomes

$$\dot{x}^i = \mathcal{J}^{ij}\left(h_j + \delta h_j - F_j\right). \tag{6}$$

Recalling that $\mathcal{J}$ is a Poisson operator, the associated invariant measure $J dx^1 \dots dx^n$, with J a Jacobian weight, can be obtained by application of the Lie-Darboux theorem: in a sufficiently small neighborhood where the rank of $\mathcal{J}$ is $2r = n - m$, there are local coordinates $(p^1, \dots, p^r, q^1, \dots, q^r, C^1, \dots, C^m)$ such that

$$J dV = dp^1 \dots dp^r dq^1 \dots dq^r dC^1 \dots dC^m. \tag{7}$$

Then, the invariant measure (7) is used to enforce the ergodic hypothesis on the Casimir leaves defined by $\{\boldsymbol{x} \in \Omega :\ C^1 = \text{const.}, \dots,\ C^m = \text{const.}\}$. In particular, energy fluctuations δh are represented by Gaussian white noise processes $\boldsymbol{\Gamma} = \Gamma_j \nabla x^j$ on the Casimir leaves, while the friction force $\boldsymbol{F}$ is assumed proportional to the phase space velocity (5) through a friction coefficient γ:

$$\dot{x}^i = \mathcal{J}^{ij}\left(h_j + D^{1/2}\Gamma_j + \gamma \mathcal{J}^{jk} H_k\right). \tag{8}$$

Here, D is the diffusion coefficient, which is related to γ through the inverse temperature $\beta = 2\gamma / D$. Denoting by $f(x^1, \dots, x^n)$ the distribution function of the ensemble on the invariant measure JdV, we assume that the coordinate system has been chosen so that $J = 1$. Then, in such coordinate system, the stochastic differential equation (8), translates into the following Fokker-Planck equation [1]:

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial x^i} f Z^i, \tag{9}$$

with

$$Z^i = \mathcal{J}^{ij} h_j - \frac{1}{2} D \mathcal{J}^{ik} \mathcal{J}^{jk} \frac{\partial}{\partial x^j}\left(\log f + \beta h\right). \tag{10}$$

It can be shown [2] that equation (9) possesses the metriplectic structure (2) with Poisson bracket

$$\{F, G\} = \int_\Omega f \frac{\partial}{\partial x^i}\left(\frac{\delta F}{\delta f}\right)_\beta \mathcal{J}^{ij} \frac{\partial}{\partial x^j}\left(\frac{\delta G}{\delta f}\right)_\beta dV, \tag{11}$$

and dissipative bracket

$$[F, G] = \int_\Omega f \frac{\partial}{\partial x^i}\left(\frac{\delta F}{\delta f}\right)_\beta \mathcal{J}^{ik} \mathcal{J}^{jk} \frac{\partial}{\partial x^j}\left(\frac{\delta G}{\delta f}\right)_\beta dV. \tag{12}$$

Furthermore, in the limit of thermodynamic equilibrium $t \to \infty$, solutions of (9) converge to

$$\lim_{t \to \infty} f = Z^{-1} \exp\left(-\beta H - \mu_k C^k\right),\ \ Z, \mu_k \in \mathbb{R}. \tag{13}$$

The theory generalizes to infinite dimensional Hamiltonian systems.

References

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