Statistical mechanics of multi-Hamiltonian systems

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Presentation Overview

Problem

We consider the statistical mechanics of multi-Hamiltonian dynamical system in four-dimensional phase space.

We need to...

- ...establish an invariant measure on the phase space based on Poisson geometry.
- ...derive explicit expressions for the partition function and the generalized Gibbs distribution in the special coordinate system.
- ...extend these expressions to the case of an arbitrary coordinate system.

Multi-Hamiltonian systems

Mechanical systems that admit several pairs of Hamiltonians together with their associated Poisson brackets $(H_1, \omega_1), (H_2, \omega_2), \ldots,$ which are not connected by a coordinate transformation yet lead to the same equations of motion, are referred to as multi-Hamiltonian systems (R.L. Fernandes, 1994).

$$\frac{dx^i}{dt} = \underbrace{\omega_1^{jk} \frac{\partial H_1}{\partial x^j} \frac{\partial x^i}{\partial x^k}}_{\{H_1,\, x^i\}_{\omega_1}} = \underbrace{\omega_2^{jk} \frac{\partial H_2}{\partial x^j} \frac{\partial x^i}{\partial x^k}}_{\{H_2,\, x^i\}_{\omega_2}} = \ldots \tag{1}$$

Nambu–Poisson mechanics (Y. Nambu, 1973; L. Takhtajan, 1993)

Consider a phase space N, $\dim N = n$ with local coordinates x^i, together with a set of functionally independent integrals of motion H_k $(k = \overline{1, n-1})$.

In this setting, the dynamics of the system can be expressed within the Nambu–Poisson formalism

$$\frac{dx^i}{dt} = \{H_1, \dots, H_{n-1}, x^i\} = \varepsilon^{i_1 \dots i_{n-1} i_n} \frac{\partial H_1}{\partial x^{i_1}} \dots \frac{\partial H_{n-1}}{\partial x^{i_{n-1}}} \frac{\partial x^i}{\partial x^{i_n}}, \quad i = \overline{1, n}, \tag{2}$$

where $\{H_1, \dots, H_{n-1}, x^i\}$ denotes the generalized Nambu bracket, ε is the completely antisymmetric Levi-Civita tensor.

The Nambu bracket, which generalizes the Poisson bracket, can in turn be reformulated through the Schouten bracket:

$$V^{i}(x) = \{H_1, \dots, H_{n-1}, x^{i}\} = \frac{(-1)^{\frac{n(n-1)}{2}}}{n!}[[\eta, H_1], \dots, H_{n-1}], \tag{3}$$

where $V^{i}(x)$ are the components of the velocity field, and $\eta = \varepsilon^{i_1 \dots i_n}\partial_{i_1} \wedge \cdots \wedge \partial_{i_n}$ is the highest tensor invariant of the system in the sense that $\mathcal{L}_V \eta = 0$.

Schouten bracket

$$[\,.\,,\,.\,] : \mho^{p} \times \mho^{q} \to \mho^{p+q-1}$$

where $\mho^{n}$ is denotes the space of polyvectors of rank n.

This represents a particular case of a multi-Hamiltonian system.

Generalized Gibbs distribution (J. W. Gibbs, 1902)

We consider the canonical ensemble of $\mathcal{N}$ weakly interacting copies of a multi-Hamiltonian system. For such a system, the canonical Gibbs distribution takes the form:

$$f = \frac{1}{z} e^{-\frac{H}{\theta}}, \quad z = \int e^{-\frac{H}{\theta}} d\Gamma, \quad z = \frac{1}{\mathcal{N}!}(Z)^{\mathcal{N}}. \tag{4}$$

Here f denotes the distribution function, Z the partition function per system, $d\Gamma$ the phase space volume element, H the Hamiltonian, and θ the temperature.

A key point is that H is an additive quantity, and in our case we use the form: $H = \alpha_1 H_1 + \alpha_2 H_2 + \cdots + \alpha_{n-1} H_{n-1}$, $\alpha_k \in \mathbb{R}$, $k = \overline{1, n-1}$.

The volume element of a four-dimensional phase space can be expressed as the contraction of a two-form $\Pi \in \Omega^2$ (V. Arnold, Ordinary Differential Equations):

$$d\Gamma = \varepsilon^{ijkl}\Pi_{ij}\Pi_{kl}dx^1dx^2dx^3dx^4\,, \quad \Omega^{ik}\Pi_{kj} = \delta^i_j\,. \tag{5}$$

Here Ω represents a linear combination of the Poisson bivectors $\omega_{1,2,3}$, constructed via equation (3) using the antisymmetry of Schouten bracket. In this setup, however, the bivector Ω is degenerate, which prevents the formulation of a statistical mechanics.

The problem!

The task is to identify a non-degenerate bivector for the multi-Hamiltonian system with a four-dimensional phase space.

Special coordinate system

To address the degeneracy issue, we switch to a special choice of coordinates:

$$\dot{x}^1 = 0\,, \quad \dot{x}^2 = 0\,, \quad \dot{x}^3 = 0\,, \quad \dot{x}^4 = 1\,;$$
$$H_1 = x^1\,, \quad H_2 = x^2\,, \quad H_3 = x^3\,.$$

The original bivector is then modified with the help of its dual bivector:

$$\Omega_{tot} = \Omega + \kappa\tilde{\Omega}\,, \quad \tilde{\Omega}^{ij} = \frac{1}{2}\varepsilon^{ijkl}\Omega_{kl}\,. \tag{6}$$

In this form Ω_{tot} is non-degenerate ($\det \Omega_{tot} \neq 0$), serves as a Poisson bivector ($[\Omega_{tot}, \Omega_{tot}] = 0$), remains invariant ($\mathcal{L}_V \Omega_{tot} = 0$), and preserves the Hamiltonian equations of motion ($\dot{x}^i = \{H, x^i\}_\Omega$). Here κ denotes a real parameter.

In the chosen coordinate system, the bivectors can be conveniently expressed in matrix form:

$$\Omega = \frac{1}{(\alpha_1^2 + \alpha_2^2 + \alpha_3^2)} \begin{pmatrix} 0 & 0 & 0 & -\alpha_1 \\ 0 & 0 & 0 & -\alpha_2 \\ 0 & 0 & 0 & -\alpha_3 \\ \alpha_1 & \alpha_2 & \alpha_3 & 0 \end{pmatrix},$$

$$\tilde{\Omega} = \frac{1}{(\alpha_1^2 + \alpha_2^2 + \alpha_3^2)} \begin{pmatrix} 0 & -\alpha_3 & \alpha_2 & 0 \\ \alpha_3 & 0 & -\alpha_1 & 0 \\ -\alpha_2 & \alpha_1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

It follows immediately that the modified bivector is non-degenerate:

$$\det \Omega_{\text{tot}} = \frac{\kappa^4}{(\alpha_1^2 + \alpha_2^2 + \alpha_3^2)^2} \neq 0$$

Partition function in the special and arbitrary coordinate system

Using equation (5) together with (6) the volume element can be written as:

$$\mathrm{d}\Gamma = \frac{1}{\sqrt{\det \Omega_{\mathrm{tot}}}} \mathrm{dx}^1 \mathrm{dx}^2 \mathrm{dx}^3 \mathrm{dx}^4 = \frac{(\alpha_1^2 + \alpha_2^2 + \alpha_3^2)}{\kappa^2} \mathrm{dx}^1 \mathrm{dx}^2 \mathrm{dx}^3 \mathrm{dx}^4 \,. \tag{7}$$

Upon transition to an arbitrary coordinate system according to formula (4) the partition function of the multi-Hamiltonian system takes the form:

Partition function of multi-Hamiltonian system

$$\mathrm{Z}_\alpha = \int \left| \frac{\partial(\mathrm{H}_1, \mathrm{H}_2, \mathrm{H}_3, \mathrm{x}^4)}{\partial(\mathrm{x}^1, \mathrm{x}^2, \mathrm{x}^3, \mathrm{x}^4)} \left(\frac{\mathrm{dx}^4}{\mathrm{dt}} \right)^{-1} \right| \frac{(\alpha_1^2 + \alpha_2^2 + \alpha_3^2)}{\kappa^2} \mathrm{e}^{-\frac{\alpha_\mathrm{i} \mathrm{H}_\mathrm{i}}{\theta}} \mathrm{dx}^1 \mathrm{dx}^2 \mathrm{dx}^3 \mathrm{dx}^4 \tag{8}$$

In this situation, the partition function and the corresponding distribution depend on the parameters κ and $\alpha_{1,2,3}$. Once these parameters are fixed, a unique energy representative is selected, and the partition function reduces to a function of temperature alone, $(Z = Z(\theta))$. This leads to a well-defined statistical mechanics.

Thermodynamic quantities

- $F = -\theta \ln Z$ – free energy;
- $S = -\dfrac{\partial F}{\partial \theta}$ – entropy;
- $E = -\theta^2 \dfrac{\partial}{\partial \theta}\left(\dfrac{F}{\theta}\right)$ – internal energy;
- $C = \theta \dfrac{\partial S}{\partial \theta}$ – heat capacity.

Example 1: Four-particle Toda lattice system
(Baleanu D., Makhkhaldiani N., 1999)

Equations of motion

$$
\begin{aligned}
\dot{x}^1 &= \gamma_1(e^{x^2} - e^{x^4}), \\
\dot{x}^2 &= \gamma_2(e^{x^3} - e^{x^1}), \\
\dot{x}^3 &= \gamma_3(e^{x^4} - e^{x^2}), \\
\dot{x}^4 &= \gamma_4(e^{x^1} - e^{x^3});
\end{aligned}
$$

Integrals of motion

$$H_1 = \frac{e^{x^1}}{\gamma_1} + \frac{e^{x^2}}{\gamma_2} + \frac{e^{x^3}}{\gamma_3} + \frac{e^{x^4}}{\gamma_4},$$

$$H_2 = \frac{x^1}{\gamma_1} + \frac{x^2}{\gamma_2} + \frac{x^3}{\gamma_3} + \frac{x^4}{\gamma_4},$$

$$H_3 = -\frac{1}{2}\left(\frac{x^1}{\gamma_1} - \frac{x^2}{\gamma_2} + \frac{x^3}{\gamma_3} - \frac{x^4}{\gamma_4}\right),$$

Here γ_a are real parameters, with $a = \overline{1,4}$.

From equation (8), the partition function of the system is given by:

$$Z_\alpha = \frac{(\alpha_1^2 + \alpha_2^2 + \alpha_3^2)}{\kappa^2} \prod_{a=1}^{4} \frac{1}{\gamma_a} \zeta_a^{\xi_a} \Gamma(\xi_a) , \tag{9}$$

where $\Gamma(z) = \int_0^\infty e^{-t} t^{z-1} dt$ $(\mathrm{Re}(z) > 0)$ is the Gamma function and notation used: $\zeta_a = \theta\gamma_a/\alpha_1$, $\xi_a = -\alpha_2/\theta\gamma_a + (-1)^{a-1}\alpha_3/2\theta\gamma_a$, $a = \overline{1,4}$.

Parameter constraints

$$\begin{aligned} &\mathrm{sgn}(\alpha_1) = \mathrm{sgn}(\gamma_a) , \; a = \overline{1,4} , \\ &\alpha_2 < 0, -2|\alpha_2| < \alpha_3 < 2|\alpha_2|, \;\gamma_a > 0 , \\ &\alpha_2 > 0, -2|\alpha_2| < \alpha_3 < 2|\alpha_2|, \;\gamma_a < 0 . \end{aligned} \tag{10}$$

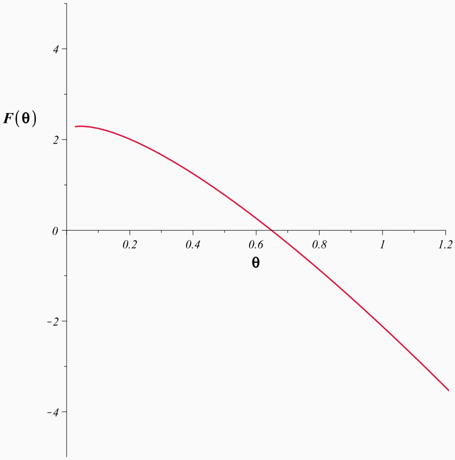

Figure 1 – Free energy F(θ) as a function of temperature θ, with $\alpha_1 = 1$, $\alpha_2 = -2$, $\alpha_3 = -1$, $\kappa = 1$

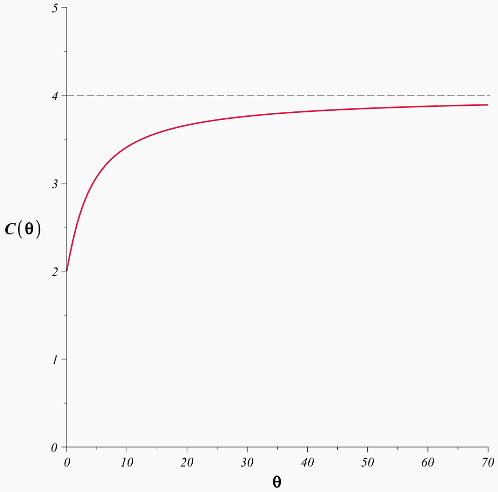

Figure 2 – Heat capacity C(θ) as a function of temperature θ, with $\alpha_1 = 1$, $\alpha_2 = -2$, $\alpha_3 = -1$, $\kappa = 1$

Example 2: The two-dimensional harmonic oscillator

Equations and integrals of motion

$$\dot{p_x} = -x\,, \quad \dot{p_y} = -y\,, \quad \dot{x} = p_x\,, \quad \dot{y} = p_y\,;$$

$$H_1 = \frac{1}{2}(p_x^2 + x^2)\,, \quad H_2 = \frac{1}{2}(p_y^2 + y^2)\,,$$

$$H_3 = xp_x - yp_y\,.$$

From equation (8) the partition function of the system is obtained as:

$$Z_\alpha = \frac{4\pi^2(\alpha_1^2 + \alpha_2^2 + \alpha_3^2)}{\kappa^2(\alpha_1\alpha_2 - \alpha_3^2)^{3/2}}\theta^3\,. \quad (11)$$

Parameter constraints

$$\alpha_1 > 0\,, \quad \alpha_2 > 0\,, \quad \alpha_3^2 - \alpha_1\alpha_2 < 0\,, \quad (12)$$

where $\alpha_3 \equiv \omega \in [0, 1)$ represents the angular velocity.

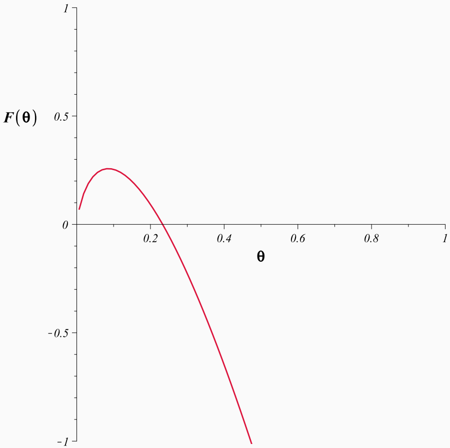

Figure 3 – Free energy F(θ) as a function of temperature θ, with $\alpha_1 = 1$, $\alpha_2 = 1$, $\omega = 0.01$, $\kappa = 1$

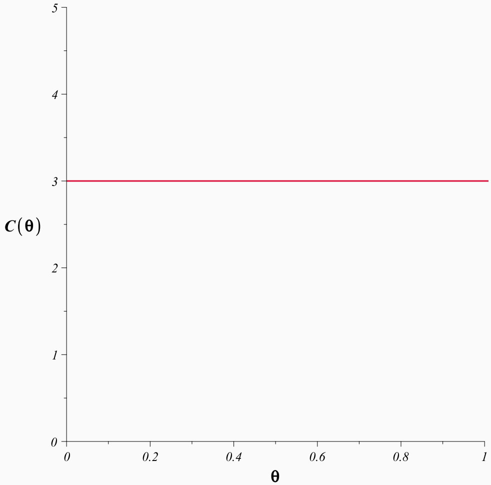

Figure 4 – Heat capacity C(θ) as a function of temperature θ, with $\alpha_1 = 1$, $\alpha_2 = 1$, $\omega = 0.01$, $\kappa = 1$

Algorithm for constructing statistical mechanics

1) Start with $\mathbb{R}^4$, coordinates x^{i}, dynamics $\dot{\mathrm{x}}^{\mathrm{i}} = \mathrm{V}^{\mathrm{i}}(\mathrm{x})$, $\mathrm{i} = \overline{1,4}$ and integrals of motion $\mathrm{H}_1, \mathrm{H}_2, \mathrm{H}_3$.
   The highest tensor invariant is $\eta = \varepsilon^{\mathrm{ijkl}} \partial_{\mathrm{i}} \wedge \partial_{\mathrm{j}} \wedge \partial_{\mathrm{k}} \wedge \partial_{\mathrm{l}}$.
2) Using equation (3) construct the bivectors $\omega_{1,2,3}$, combine them into Ω, $\det \Omega = 0$. To remove degeneracy, introduce the modified bivector:

$$\Omega_{\mathrm{tot}} = \Omega + \kappa \tilde{\Omega}, \quad \det \Omega_{\mathrm{tot}} \neq 0.$$

3) Convert the bivector into a two-form, satisfying $\Omega^{\mathrm{ik}}_{\mathrm{tot}} \Pi_{\mathrm{kj}} = \delta^{\mathrm{i}}_{\mathrm{j}}$.
4) Using equations (4), (5) and (8) construct step by step the volume element $\mathrm{d}\Gamma$, the partition function Z_α and the distribution function f_α.

5*) For fixed parameters $\alpha_{1,2,3}$ compute the thermodynamic quantities F, S, E and C.

Key results:

- We have developed an algorithm for constructing statistical mechanics of multi-Hamiltonian systems with a four-dimensional phase space, based on three specified integrals of motion.
- For the four-particle Toda lattice system and the two-dimensional harmonic oscillator with coincident frequencies, we obtained the partition function, the distribution function, and the main thermodynamic quantities.

Future directions:

- Extension of the present construction to higher-dimensional cases ($\dim N = 6, \dots$).
- Classification of the tensor invariants of the system constructed using the Schouten bracket.
- Analysis of other higher-derivative dynamical systems, in which the well-known problem of energy unboundedness from below arises (M. Pavsic, A. Smilga,…).

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Discover.

Discuss.

Deduce.

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