Thermodynamics Based on Time Average and Temporal Extensivity of Entropy

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Invited Talk at the London Mathematical Society, Durham Symposium "Dynamical Systems and Statistical Mechanics", 3-13 July, 2006

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Ⅰ. Introduction

Boltzmann-Gibbs Statistical Mechanics

- **Ergodicity**
  - Molecular Chaos Hypothesis

Dynamical Counterpart of Boltzmann-Gibbs-Shannon Entropy

- **Kolmogorov-Sinai Entropy**
  - Positive Lyapunov Exponent(s)
  - Constant Entropy Production Rate

Thermodynamic Limit

$\updownarrow$

Long-Time Limit

A quantity $A(t)$ is "temporally extensive", if it satisfies

$$\lim_{t\to\infty}\frac{A(t)}{t}=\mathrm{const}$$

e.g.,

The Kolmogorov-Sinai entropy is temporally extensive for chaotic dynamical systems.

N.B.,

Thermodynamic Extensivity of Thermodynamic Entropy

$\Uparrow$

A Basic Premise for Thermodynamics to be Constructible

Complexity at the Edge of Chaos

- The maximum Lyapunov exponent vanishes.

- The Kolmogorov-Sinai entropy fails to be temporally extensive.

Ⅱ. Thermodynamics Based on Time Average

A. Carati, Physica A 348, 110 (2005).

Connection between
"Probabilistic Process in Phase Space"
and
"Thermodynamics"

- Expected to shed new light on temporal extensivity of thermodynamic quantities

Basics of Time-Average Formalism

M: Phase Space

$\phi: M \rightarrow M$ st. $x_{n+1} = \phi(x_n)$ $(x_n \in M)$

$\{x_n\}_{n=0,1,2,\cdots}$: Time Series Generated by the Dynamical Map

Average of a physical quantity A over a fixed long time interval $1 \leq n \leq N$ $(N >> 1)$

$$\overline{A}(x_0) = \frac{1}{N} \sum_{n=1}^{N} A(x_n)$$

↑

still random, depending on the initial data, x_0

"Coarse Graining"

Divide M into cells $L_1, L_2, \cdots, L_K$ $(K >> 1)$

A_i: **representative value of A in L_i**

n_i: **number of times the system visits L_i**

$$\overline{A}(x_0) \cong \sum_{i=1}^{K} A_i \frac{n_i}{N}$$

where

$\{n_i\}_{i=1,2,\cdots,K}$: **random**

Sojourn Time Distribution

Cumulative Probability that L_i is visited $n_i (\leq n)$ times by the system:

$$P(n_i \leq n) \equiv F(n_i)$$

The Average Value of A

$$<\overline{A}> = \frac{1}{N}\sum_{i=1}^{K} A_i <n_i>$$

with

$$<n_i> = \frac{\int \prod_{j=1}^{K} dF(n_j) n_i \delta(N - \sum_j n_j)}{\int \prod_{j=1}^{K} dF(n_j) \delta(N - \sum_j n_j)}$$

Generating Function

$$Z(\lambda)=\int\prod_{j=1}^{K} dF(n_j)\, e^{-\lambda \sum_i A_i n_i}\, \delta(N-\Sigma_i n_i)$$

$$\Downarrow$$

$$<\overline{A}>=-\frac{1}{N}\frac{\partial}{\partial\lambda}\ln Z(\lambda)\bigg|_{\lambda=0}$$

If the constraint is imposed on the energy:

$$U = \frac{1}{N}\sum_{i=1}^{K} \varepsilon_i n_i$$

(ε_i: energy in L_i)

$$\Downarrow$$

$Z(\lambda)$ is replaced by

$$Z_U(\lambda) = \int \prod_{j=1}^{K} dF(n_j) e^{-\lambda \sum_i A_i n_i}$$

$$\times \delta(N - \Sigma_i n_i)\, \delta(U - \Sigma_i \varepsilon_i n_i / N)$$

and accordingly,

$$< \overline{A} >_U = -\frac{1}{N}\frac{\partial}{\partial \lambda} \ln Z_U(\lambda)\Big|_{\lambda=0}$$

Define:

$$\int dF(n)\, e^{-n\zeta} = e^{\chi(\zeta)}$$

Then,

$$Z_U(\lambda) = \frac{N}{(2\pi)^2} \int_{-\infty}^{\infty} dk_1 \int_{-\infty}^{\infty} dk_2$$

$$\times e^{i k_1 U N + i k_2 N + \sum_i \chi(\lambda A_i + i k_1 \varepsilon_i + i k_2)}$$

Large-N Limit

Steepest-Descent Conditions:

$$U = -\frac{1}{N} \sum_{i=1}^{K} \varepsilon_i \chi'(ik_1 \varepsilon_i + ik_2)$$

$$N = -\sum_{i=1}^{K} \chi'(ik_1 \varepsilon_i + ik_2)$$

$$(\chi'(\zeta) = d\chi(\zeta) / d\zeta)$$

in the limit $\lambda \to 0$

Therefore,

$$< \overline{A} >_U = -\frac{1}{N}\sum_{i=1}^{K} A_i \chi'(\theta \varepsilon_i + \alpha)$$

$$= \sum_{i=1}^{K} A_i p_i$$

with the sojourn time probability

$$p_i = -\frac{\chi'(\theta \varepsilon_i + \alpha)}{N}$$

provided that

ik_1 **and** ik_2 **are continued**

to θ **and** α

Boltzmann-Gibbs Statistics

$\Updownarrow$

$F(n)$ is Poissonian!

$$\int dF(n)e^{-n\zeta} := \sum_{n=0}^{\infty} e^{-Np}\frac{(Np)^n}{n!}e^{-n\zeta}$$

$$= e^{Npe^{-\zeta}-Np} \qquad (0<p<1)$$

$$\therefore \quad \chi(\zeta) = Npe^{-\zeta} - Np$$

ζ-dependent relevant part

$$\chi_0(\zeta) = Npe^{-\zeta}$$

(anticipated as the free energy)

The Legendre Transformation

$$s(\nu_i)=\nu_i\,\zeta_i+\chi_0(\zeta_i)$$

$$\nu_i=-\chi'_0(\zeta_i)$$

$$(\zeta_i=\theta\varepsilon_i+\alpha)$$

Then, one finds:

$$\zeta_i=-\ln(p_i/p)$$

$$\nu_i=Np_i$$

$$\Downarrow$$

Boltzmann-Gibbs-Shannon Entropy

$$S=\sum_{i=1}^{K}s(\nu_i)=-N\sum_{i=1}^{K}p_i\ln p_i \quad (p:=1/e)$$

Boltzmann-Gibbs-Shannon Entropy

$$S \propto N$$

i.e.,

Temporally Extensive

"Thermodynamics" Entropy
(Entropy Production Rate)

$$S_{\text{th}} \equiv \frac{S}{N}$$

- $$\frac{\partial S_{\text{th}}}{\partial U} = \theta \equiv \frac{1}{T} := \beta$$

- $$p_i = \frac{e^{-\beta \varepsilon_i}}{Z(\beta)}, \qquad Z(\beta) = \sum_{i=1}^{K} e^{-\beta \varepsilon_i}$$

Ⅲ. Temporal Extensivity of Tsallis Entropy

<u>Two Points</u>:

(i) q-Expectation Value

$$< \overline{A} >_{U,q} = \sum_{i=1}^{K} A_i P_i^{(q)}$$

$$P_i^{(q)} = \frac{(p_i)^q}{\sum_j (p_j)^q}$$ **: Escort Distribution**

$$P_i^{(q)} = -\frac{\chi'(\theta\varepsilon_i + \alpha)}{N}$$

(see p.13)

(ii) Deformation of Poissonian Process

Deformation of Generating Function

$$\chi_0(\zeta) = Npe^{-\zeta} \to \chi_{0,q}(\zeta) = Nr_q e_q(-\zeta)$$

with the q-exponential function

$$e_q(x) = [1 + (1-q)x]_+^{1/(1-q)} \quad \left(\xrightarrow{q \to 1} e^x \right)$$

$$([a]_+ \equiv \max\{0, a\})$$

$$\nu_i = -\chi'_{0,q}(\zeta)\Big|_{\zeta=\zeta_i=\theta\varepsilon_i+\alpha} = N r_q [e_q(-\zeta_i)]^q$$

$$= N P_i^{(q)},$$

$$\zeta_i = -\frac{1}{1-q}\left[\left(\frac{\nu_i}{N r_q}\right)^{1/q-1} - 1\right],$$

$$\chi_{0,q}(\zeta_i) = N r_q \frac{p_i}{(c_q r_q)^{1/q}}$$

$$\left(c_q = \sum_{i=1}^{K} (p_i)^q\right)$$

The corresponding entropy:

$$S_q = \sum_{i=1}^{K} s_q(\nu_i) = \sum_{i=1}^{K} [\nu_i \zeta_i + \chi_{0,q}(\zeta_i)]$$

$$= \frac{N}{1-q}\left[\sum_{i=1}^{K} (p_i)^q - 1\right]$$

∴

The Tsallis Entropy is also Temporally Extensive:

$$S_q \propto N,$$

Whenever Relevant.

N.B., r_q **must be chosen to be**

$$r_q = \left[\frac{q}{(c_q)^{1/q}(2-c_q)} \right]^{q/(1-q)} \quad (\xrightarrow{q \to 1} p = 1/e)$$

Reality Condition:

$$c_q \equiv \sum_{i=1}^{K} (p_i)^q < 2$$

Nonextensive Statistical Mechanics

$$S_{\mathrm{th},\,q} = \frac{S_q}{N}$$

- $$\frac{\partial S_{\mathrm{th},\,q}}{\partial U} = \theta \equiv \frac{1}{T} := \beta$$

- $$p_i = \frac{1}{Z_q(\beta)} e_q(-(\beta \varepsilon_i + \alpha)),$$

$$Z_q(\beta) = \sum_{i=1}^{K} e_q(-(\beta \varepsilon_i + \alpha))$$

Ⅳ. Bound on the Tsallis-Entropy Production Rate

$$c_q \equiv \sum_{i=1}^{K} (p_i)^q < 2$$

(1) $q > 1$ (trivial)

$$0 < c_q < 1$$

$$\Downarrow$$

$$\frac{S_q}{N} = \frac{1}{1-q}\left[\sum_{i=1}^{K} (p_i)^q - 1\right] < \frac{1}{q-1}$$

(2) $0<q<1$ **(nontrivial)**

$$0<c_q<2$$

$$\Downarrow$$

$$\frac{S_q}{N}=\frac{1}{1-q}\left[\sum_{i=1}^{K}(p_i)^q-1\right]<\frac{1}{1-q}$$

$\therefore$

Universal Bound on Tsallis Entropy Production Rate

$$\frac{S_q}{N}<\frac{1}{|1-q|}$$

$$(\forall q>0)$$

Remark:

All known analytical results on nonlinear dynamical systems at the edge of chaos are found to obey this bound.

V. Concluding Remarks

- Temporal Extensivity of Tsallis Entropy

- Complete Derivation of Nonextensive Statistical Mechanics based on Time Average

- Universal Bound on Tsallis Entropy Production Rate

Reference:

S. A. and Y. Nakada, cond-mat/0603550, to appear in Phys. Rev. E