Growth of “Boltzmann entropy” and chaos in a large assembly of weakly interacting systems

Lamberto Rondoni – Politecnico di Torino

with: Falcioni, Palatella, Pigolotti, Vulpiani (Roma, Sapienza)
Physica A **385**, 170 (2007)

Bejing 16 March 2012

http://www.rarenoise.lnl.infn.it/

Outline

Boltzmann entropy S_B, defined in μ-space, obeys H-theorem, in accord with 2nd Law of Thermodynamics.
Gibbs entropy S_G, defined in Γ-space, say $\mathcal{M}$, does not grow for hamiltonian evolution, but coarse grained version S_{cg}, obtained partitioning in fixed (time-independent) cells Γ-space, does.

- What distinguishes S_B and S_G, μ- and Γ-space descriptions?
- Interactions and chaos play different roles;
- Model: symplectic maps relaxing to equilibrium;
- Regime: initial nonequilibrium stage (final stage is trivial);
- Characteristic graining scale in μ-space, due to interaction strength, absent in $\Gamma-$space;
- Initial growth of coarse grained entropies due to chaos.

Each microstate $\mathbf{X} \in \mathcal{M}$ represents an N-particle system ($N \geq 1$).

Geometric point $\mathbf{X}$ does not interact with any other $\mathbf{Y} \in \mathcal{M}$: system in microstate $\mathbf{X}$ not affected by system in microstate $\mathbf{Y}$: no coupling between equations of motion of particles with initial condition $\mathbf{X}$ and particles with initial condition $\mathbf{Y}$, even for $\mathbf{X}$ very close to $\mathbf{Y}$.

Macrostate of system of microstate $\mathbf{X}$ determined by values of phase functions of interest $\mathcal{O}(\mathbf{X}), \mathcal{P}(\mathbf{X}), \ldots$, with some tolerance, $\delta_{\mathcal{O}}, \delta_{\mathcal{P}}, \ldots$ negligible with respect to macroscopic measurements: e.g. number density n_i/N of particles in subregion C_i, $i = 1, \ldots, L$, of spatial volume V of system.

Particles tipically interact: equations of motion of j-th particle coupled to those of nearby l-th particle; interactions determine particles' "size": particles are not geometric points.

If $\mathcal{O}$ takes values in $(\overline{\mathcal{O}} - \delta_{\mathcal{O}}, \overline{\mathcal{O}} + \delta_{\mathcal{O}})$ one identifies subset (shell) of $\mathcal{M}$ correspondig to that macrostate:

$$U_{\mathcal{O}}^{\overline{\mathcal{O}},\delta_{\mathcal{O}}} = \{\Gamma \in \mathcal{M} : \mathcal{O}(\Gamma) \in (\overline{\mathcal{O}} - \delta_{\mathcal{O}}, \overline{\mathcal{O}} + \delta_{\mathcal{O}})\} \subset \mathcal{M}$$

Set of shells yields (non-local) partition of $\mathcal{M}$; thickness of shells corresponds to resolution of microstates due to accuracy $\delta_{\mathcal{O}}$ of measurement.

If more quantities are measured, partition of $\mathcal{M}$ given by intersection of corresponding shells.

Shells and their intersection not localized around phase points: e.g. for $\mathcal{O}$ = number density, $\mathcal{P}$ = internal energy, points in opposite regions of velocity space belong to same partition element.

$6N$-dimensional hypercube of small side around point $\mathbf{X}$ does not identify macrostate, far away points are missing.
Physically relevant only if one observes microscopic variables.

Phase space entropies and ensembles

At time t, $\mathcal{M}$ may be endowed with probability density ρ_t.
If dynamics preserve probabilities, ρ_t obeys Liouville Equation.
For Hamiltonian dynamics, Gibbs entropy is constant of motion:

$$S_G = -k_B \int \rho_t(\mathbf{X}) \ln \rho_t(\mathbf{X}) \mathrm{d}\mathbf{X}$$

Attributing relative weights to points of $\mathcal{M}$ representing independent systems, *per se*, ρ_t, differs from any quantity of thermodynamic interest: these express properties of a single system. But the average of its log over equilbrium ensembles equals thermodynamic S.

Because equilibrium does not evolve, microstates have time to explore $\mathcal{M}$ with given frequencies: ρ could be dynamically justified.

Clearly a very special situation for very special ρ. No surprise that in e.g. evolving states, S_G does not conform to S. Why should it? For instance, no time to justify statistics and ρ_t not even a sum observable as required by Khinchin.

Introduce fixed grid on $\mathcal{M}$ made of cells C_i of volume V_i centered in points X_i, and integrate ρ_t to obtain cell probabilities $p_{t,cg}(i)$. The coarse grained entropy,

$$S_{G,cg}(t) = -k_{\scriptscriptstyle B} \sum_i p_{t,cg}(i) \ln p_{t,cg}(i)$$

evolves even for Hamiltonian dynamics.
As $V_i \to 0$, $S_{G,cg} \to S_G$, apart from constant related to size of V_i. Not only arbitrary 0 of entropy, but also arbitrary relaxation times: fine, changing V_i changes observable; single particle never relaxes. Different from evolution of observables, in μ-space, which implies time dependent partitions:

$$U_{\mathcal{O}}^{\overline{\mathcal{O}},\delta_{\mathcal{O}}}(t) = \{\Gamma \in \mathcal{M} : \mathcal{O}(\Gamma) \in (\overline{\mathcal{O}}_t - \delta_{\mathcal{O}}, \overline{\mathcal{O}}_t + \delta_{\mathcal{O}})\}$$

Jaynes: *"since the variation of S_{cg} is due only to the artificial coarse-graining operation and it cannot therefore have any physical significance..."*

Mackey: *"Experimentally, if entropy increases to a maximum only because we have reversible mixing dynamics and coarse graining due to measurement imprecision, then the rate of convergence of the entropy (and all other thermodynamic variables) to equilibrium should become slower as measurement techniques improve. Such phenomena have not been observed."*

Chaotic systems with ρ_0 supported on small region of linear size σ larger than linear size of phase space cells Δ:

$$S_{G,cg}(t) - S_{G,cg}(0) \simeq \begin{cases} 0 & t < t_\lambda \\ h_{KS}(t - t_\lambda) & t_\lambda < t < t_e \end{cases}$$

h_{KS} = Kolmogorov-Sinai entropy

$$t_\lambda \sim \frac{1}{\lambda_1} \ln\left(\frac{\sigma}{\Delta}\right) ,$$

λ_1 = largest Lyapunov exponent.

$S_{G,cg}$ behaves like S_G until phase space structures reach scale Δ in contracting directions, because up to that stage, resolution suffices.

Scenario limited to not too long times (before saturation); not always true (e.g. intermittency must be negligible).

Boltzmann entropy: $S_B = k_B \log \Delta\Gamma$

$\mu = V \times \boldsymbol{R}^3 =$ 1-particle space.

Single, $N \gg 1$, **interacting**, **dilute** particle system.

Fix volumes $v_i \subset \mu$, size Δ, with $n_i \gg 1$ particles ($N \ggg \Delta^{-2d}$).

$f_\Delta(i;t) = n_i/N =$ 1-particle density for given macrostate;
itself a macroscopic observable.

It is not merely a probability density, it is a density of **matter**: particles in 3 dimensions are very different from points of the abstract $6N$-dimensional phase space.

It evolves according to Boltzmann not Liouville Equation;

Boltzmann Eq. requires molecular chaos, Liouville Eq. does not.

A macrostate $U_f^{f_\Delta(t)} = \left\{ \mathbf{X} \in \mathcal{M} : \text{density given by } \{f_\Delta(i;t)\}_{i=1}^{M_{\rm cells}} \right\}$ occupies a volume $\Delta\Gamma(t)$ in $\mathcal{M}$, and all $U_f^{f_\Delta(t)}$ partition $\mathcal{M}$, but not a naive partition of $\mathcal{M}$.

Neglecting Δ and N dependent corrections, one has:

$$S_B(t) = k_{_B} \log \Delta\Gamma(t) \approx -Nk_{_B} \sum_i f_\Delta(i;t)) \log f_\Delta(i;t) = S_{B,\Delta}(t)$$

Then, for $N \to \infty$, $\Delta \to 0$, with $\Delta \gg (1/N)^{1/2d}$ and constant total cross section, one has:

$$S_B(t) = -Nk_{_B} \int f(\mathbf{q},\mathbf{p},t) \ln f(\mathbf{q},\mathbf{p},t) \mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p}$$

Boltzmann's H-theorem

$$\frac{dS_B}{dt} \geq 0.$$

- If particles don't interact, $\rho_t = \otimes \rho_t^{(i)}$, where factors $\rho_t^{(i)}$ represent phase space densities of 1-particle systems.
  Only in this case, do they also represent 1-particle projections of an N particle system, i.e. f, which now obeys "Liouville thm" as the $\rho_t^{(i)}$ do. Γ and μ descriptions and corresponding entropies turn equivalent: S_B does not evolve!
  Indeed: projection of non-interacting hamiltonian system is hamiltonian.
- In general, however, S_G concerns large ensembles of whatever (large or small, dense or rarefied, etc.) independent systems, while S_B concerns large single systems in rarefied conditions, and there is no equivalence.

Can we see this difference in practice?

A discrete time model

N coupled 2-D symplectic volume preserving maps
(one “coordinate” and one “momentum”)

$$\mathbf{X} = (\mathbf{Q}, \mathbf{P}),\ \mathbf{Q} = (q_1 \dots q_n),\ \mathbf{P} = (p_1 \dots p_n), \qquad q_i, p_i \in [0, 1].$$

Each “particle” interacts with M mates; interaction strength ϵ.

$N_S =$ fixed “obstacles” positioned in Y_j, “scatter” with strength k.

$$q_i' = \quad q_i + p_i \mod 1$$

$$p_i' = \quad p_i + k \sum_{j=0}^{N_S} \sin[2\pi\,(q_i' - Y_j)] + \epsilon \sum_{n=-\frac{M}{2}}^{\frac{M}{2}} \sin[2\pi\,(q_i' - q_{i+n}')] \mod 1$$

Without interactions ($\epsilon = 0$): chaotic single-particle dynamics.

Numerical results

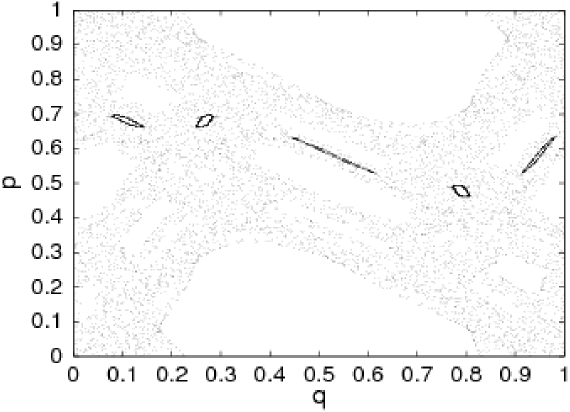
Compute $f_\Delta(q,p,t)$ for given ϵ and Δ, and vary ϵ and Δ. The "Boltzmann entropy"

$$\eta(t,\Delta) = -\sum_{j,k} f_\Delta(q^{(j)}, p^{(k)}, t) \log f_\Delta(q^{(j)}, p^{(k)}, t)$$

is valid if the "potential energy" is a small part of the total, and f_Δ is a good approximation of $f(q,p,t)$ if $n_i \gg 1/\Delta^2$.

$$\delta S(t,\Delta) = \eta(t,\Delta) - \eta(0,\Delta)$$

Points normally distributed, $\sigma = 0.01$, centred at $(q,p) = (1/4, 1/2)$. Obstacles positioned at random.

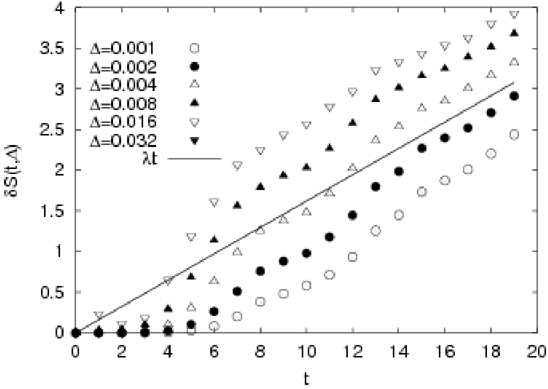


$N_S = 10^3$
$N = 10^7$
$k = 0.017$

Then, λ_1 of single particle dynamics is not too large, but there are no KAM tori as barriers for transport. Trajectory generated by 10^4 iterations in μ-space, with $\epsilon = 0$.

Non-interacting case

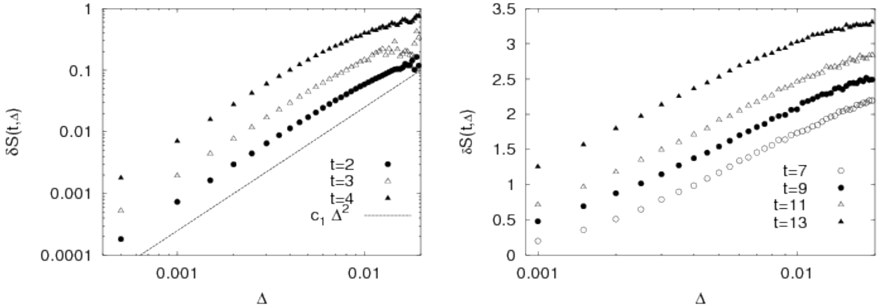
Begin with $\epsilon = 0$.



Slope of straight line equals λ_1

Growth only due to discretization: dynamics concerning $f(q, p, t)$ obeys "Liouville theorem" i.e. Boltzmann Eq. with no collision integral

η constant of motion for $\Delta \to 0$



Extrapolate: $\Delta \to 0$: small times and for Δ not too large

$$\delta S(t,\Delta) \propto \Delta^2 \qquad \text{(No fine-grained evlution!)}$$

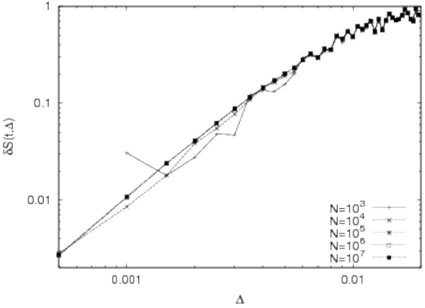
Relevant parameter is cell area. For $t > t_\lambda$,

$$\delta S(t,\Delta) = a \log(\Delta) + b.$$

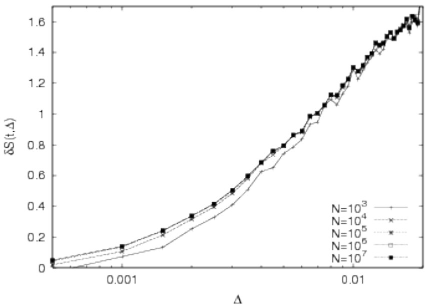
S_B behaves like S_G for $\epsilon = 0$.

Coarse-graining allows η to grow. However, that does not happen if S_B computed with $N \to \infty$, $\Delta \to 0$, $\Delta \gg l_c$, and $l_c \sim N^{-1/2}$: bad statistics are required.

$t = 3$ (small)



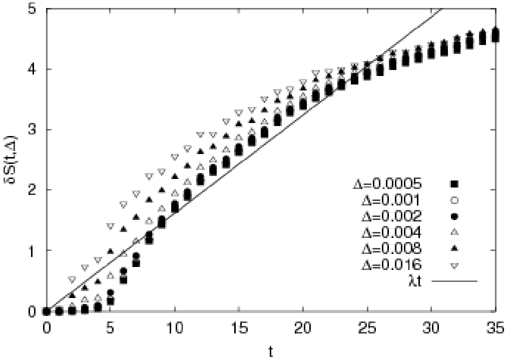
$t = 9$ (large)



Curves tending to 0 collapse for large N at fixed t, Δ: if cells occupied by many particles, S_B does not evolve in time.

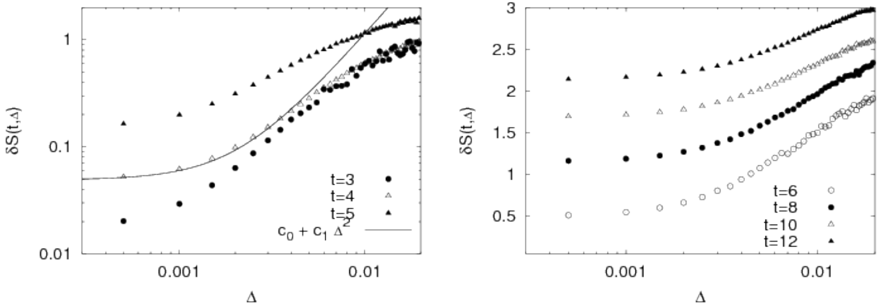
Interacting case

Consider $\epsilon = 10^{-4}$.
After a characteristic time depending on ϵ, $t_*(\epsilon, \lambda_1)$, δS has log dependence on Δ and extrapolates to finite value for $\Delta \to 0$.



Objective value for the entropy!

straight line slope equals λ_1



For small fixed times (left):

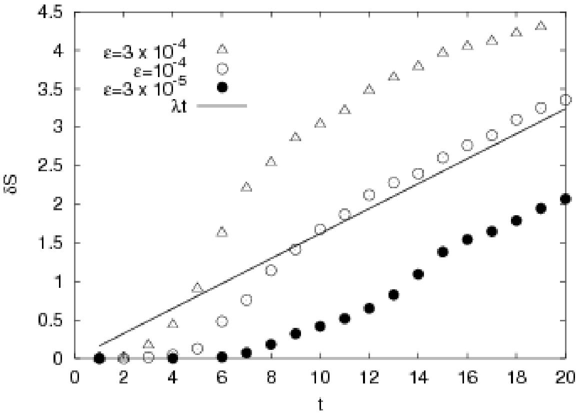
$$\delta S(t,\Delta) \approx c_0(t) + c_1(t)\Delta^2. \qquad \text{(Fine-grained evolution)}$$

Large t (right), $\delta S(t,\Delta)$ also shows weak dependence on Δ for $\Delta \to 0$.

Characteristic size $\Delta_*(\epsilon, \lambda_1)$:

below Δ_*, entropy does not depend on graining (if $n_i \gg 1$).

Extrapolation for $\epsilon \to 0$ of the curves $\delta S(t, \Delta)$ as a function of t.



Mimic interactions with noise

$$p_i(t+1) = p_i(t) + k \sum_j \sin\left[2\pi(q_i(t+1) - Y_j)\right] + \sqrt{2D}\xi_i(t) \quad \mathrm{mod} 1$$

$$\langle \xi_i(t) \rangle = 0, \quad \langle \xi_i(t)\xi_j(t') \rangle = \delta_{t,t'}\delta_{i,j} \ , \qquad D = \frac{M\epsilon^2}{4}$$

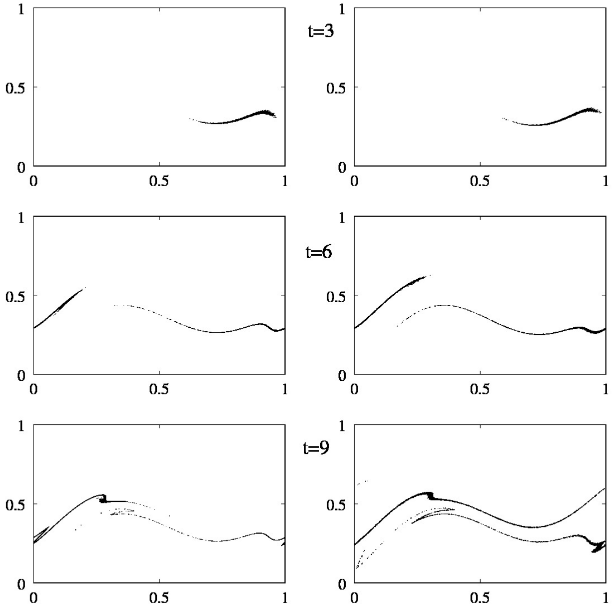
$\delta S(t, \Delta)$ practically constant with M and ϵ, if $M\epsilon^2$ constant.

Let t_c be time for scale of noise induced diffusion to equal scale generated by chaotic dynamics: it should coincide with $t_*(\epsilon, \lambda)$.

As scales of noise and chaos go as $\sqrt{M\epsilon^2 t/2}$ and $\sigma \exp(-\lambda t)$,

$$\epsilon\sqrt{M t_c/2} = \sigma \exp(-\lambda t_c) \ .$$

Numerically confirmed.



Snapshots of evolution of single-particle distribution with $\Delta > \Delta_*$.

Non-interacting case (left) interacting case (right) with $\epsilon = 10^{-4}$ $M = 100$.

Concluding remarks

a) $\epsilon = 0$: $\mu \sim \Gamma$, $S_B \sim S_G$. δS **and** t_λ depend on Δ.

b) small ϵ: characteristic scales Δ_* and t_* at which diffusion smoothes fractal structures (intrinsic properties). Smaller ϵ implies smaller Δ_* and larger t_*.
Below Δ_*, well defined time evolution: δS independent of Δ.

c) small ϵ: time evolution of $f(q, p, t)$ differs from $\epsilon = 0$ case only on tiny scales. Coupling necessary for "genuine" growth of S, but has no dramatic effect on $f(q, p, t)$ for $\Delta \gtrsim \Delta_*$.

d) chaos relevant in $\epsilon \to 0$ limit: slope of $\delta S(t, \Delta)$ given by λ_1 for intermediate t; Δ_* and t_* depend on both ϵ and λ_1.

e) S_G and its coarse grained versions not thermodynamic in general, but maybe useful e.g. for small systems: microscopic observations.