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

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Outline

- Differences and similarities between Gibbs and Boltzmann entropies, hence between μ- and Γ-space descriptions;
- Role of interactions and of chaos in evolution of entropy .

Model: high dimensional symplectic map relaxing under no driving.

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 in single particle evolution;
- Equivalence for “coarse” coarse graining.

Strong views

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."

But not quantitave statements.

These views express a truth,
but not the whole truth, as we will see.

Gibbs

Γ space: set of microstates ($\mathbf{X} \in \Gamma$) each representing $N \geq 1$ particle system. Geometric point $\mathbf{X}$ not affected by any $\mathbf{Y} \in \Gamma$ (evolution equation of $\mathbf{X}$ has no coupling to any other $\mathbf{Y}$).

$\rho_t(\mathbf{X})$ = microstates density corresponding to given macrostate; evolves according to Liouville Equation

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

does not change under Hamiltonian evolution.
Fix cells C_i in Γ. Continuum of points in C_i; integrate $\Rightarrow p_{t,cg}(i)$.

$$S_{G,cg}(t) = -k_B \sum_{\text{cells}} p_{t,cg}(i) \ln p_{t,cg}(i)$$

time dependent even for Hamiltonian evolution.

Chaotic systems with ρ_0 supported on small region of linear size σ,

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

h_{KS} = Kolmogorov-Sinai entropy

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

λ_1 = largest Lyapunov exponent.

Volume conservation until structure reaches scale Δ in contracting directions. Then: as if volumes expand.

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

Boltzmann

$\mu = V \times I\!R^3 =$ 1-particle space; **single**, $N \gg 1$, **interacting** dilute particle system. Particle α affected by particles γ, η...

Fix volumes $v_i \subset \mu$, size Δ, $N \gg \Delta^{-2d}$,
containing n_i particles, $1 \ll n_i \in I\!N$.

$f_\Delta(i;t) = n_i/N =$ 1-particle density for given macrostate;
in some limit, evolves according to Boltzmann Equation
(if molecular chaos holds).

Macrostate $\{f_\Delta(i;t)\}_{i=1}^{M_{\text{cells}}}$ corresponds to volume $\Delta\Gamma(t)$ in Γ-space.

$$S_B(t) = k_B \log \Delta\Gamma(t) \approx -N k_B \sum_i f_\Delta(i;t)) \ln f_\Delta(i;t) = S_{B,\Delta}(t)$$

neglecting Δ and N dependent corrections.

For $N \to \infty$, $\Delta \to 0$, $\Delta \gg (1/N)^{1/2d}$, constant total cross section, one can write

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

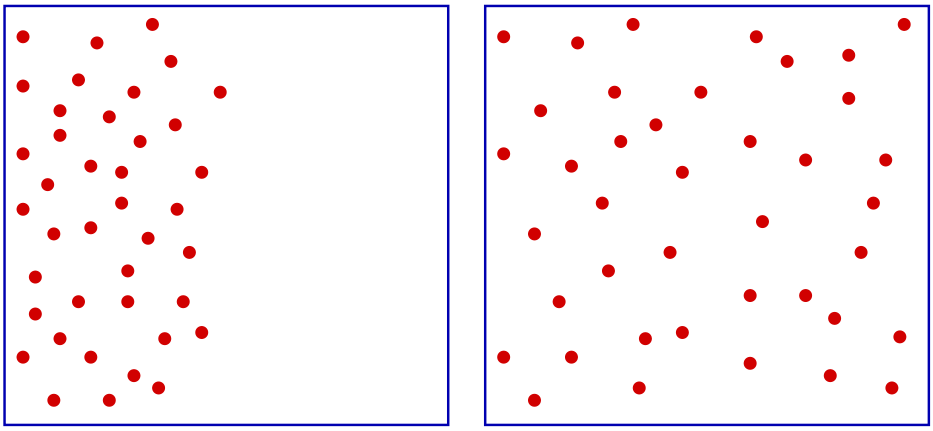
Boltzmann's H-theorem

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

If macrostate $\Delta\Gamma(t)$ of single system specified by more or other observables, similar arguments apply.

S_G and S_B, their coarse grained versions, Γ and μ spaces, appear conceptually different. For instance:

- Both S_B and coarse grained version $S_{B,\Delta}$ vary, if theory applies;
- $S_{G,cg}$ varies because of evolution of $\rho_{t,cg}$, while S_B varies because of evolution of macrostate volume $\Delta\Gamma$



$\Delta\Gamma$ grown by factor 2^N.

Local Equilibrium is essential.

- ρ_t = statistics of collection of possible (independent) systems; f = statistics of (interacting) particles of large single system.

- (Only) if particles don't interact with each other, $\rho_t = \otimes \rho_t^{(i)}$, where equal factors represent phase space densities of 1-particle systems.
  Here, 1-particle projection of large N system, f, obeys Liouville thm like phase space densitities of 1-particle systems $\rho_t^{(i)}$.
  Γ and μ descriptions equivalent.
  Indeed: projection of non-interacting hamiltonian system remains hamiltonian, Liouville thm applies.
  Coarse graining equally needed for growth of S_B and S_G.
- No limitations in Γ space description (N, Δ, interactions...).
- In general, S_G tests large ensembles,
  S_B tests large single systems.

But does this make any difference in practice?
Any computable consequences?

Indeed, at equilibrium, equivalent descriptions.
For a nonequilibrium system, with initial $S_G(0)$ and $S_B(0)$:

a) when do $S_G(t)$ and $S_B(t)$ begin to vary?

b) How do the coarse-grainings in Γ or μ space affect these events?

These times may be measured in a physical system.

We consider only the initial stage; asymptotic stage is trivial.

The discrete time model

N coupled 2-D symplectic (one "coordinate" and one "momentum"), volume preserving, maps

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

Each "particle" interacts with M mates; interaction strength ϵ.

N_S = fixed "obstacles" positioned in Y_j, "scatter" with strength k.

$$\begin{aligned} q_i' &= \ q_i + p_i \bmod 1 \\ p_i' &= \ p_i + k \sum_{j=0}^{N_S} \sin[2\pi\, (q_i' - Y_j)] + \epsilon \sum_{n=-\frac{M}{2}}^{\frac{M}{2}} \sin[2\pi \left(q_i' - q_{i+n}'\right)] \bmod 1 \end{aligned}$$

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

Numerical results

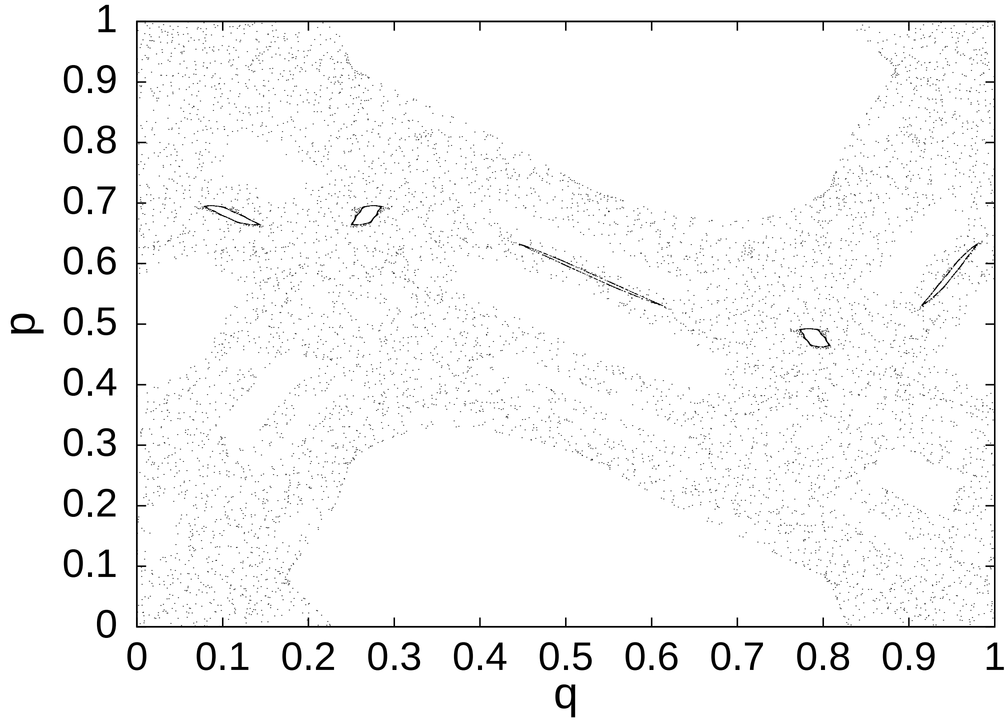
Compute $f_\Delta(q,p,t)$ for given ϵ and Δ, and vary ϵ and Δ. Follow

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

valid if "potential energy" is a small part of total, and f_Δ is agood approximation of $f(q,p,t)$.

This requires $\Delta \gg N^{-1/2d}$.

$N_S = 10^3$ and $k = 0.017$, so that λ_1 of single particle dynamics is not too large, and there are no KAM tori as barriers for transport. Obstacles positioned at random.



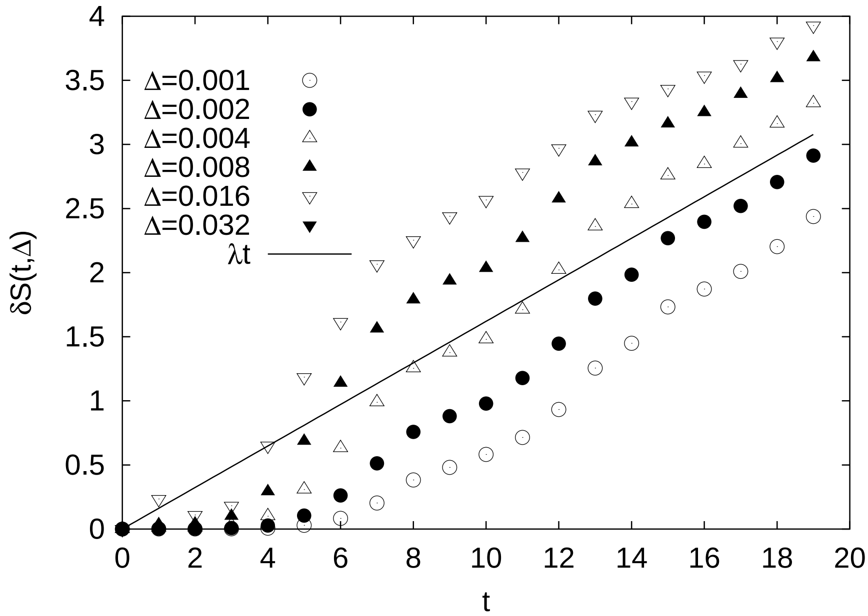
Trajectory generated by 10^4 iterations in μ-space, with $N_S = 10^3$, $k = 0.017$,$\epsilon = 0$, $N = 10^7$, $\lambda_1 \approx 0.162$.

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

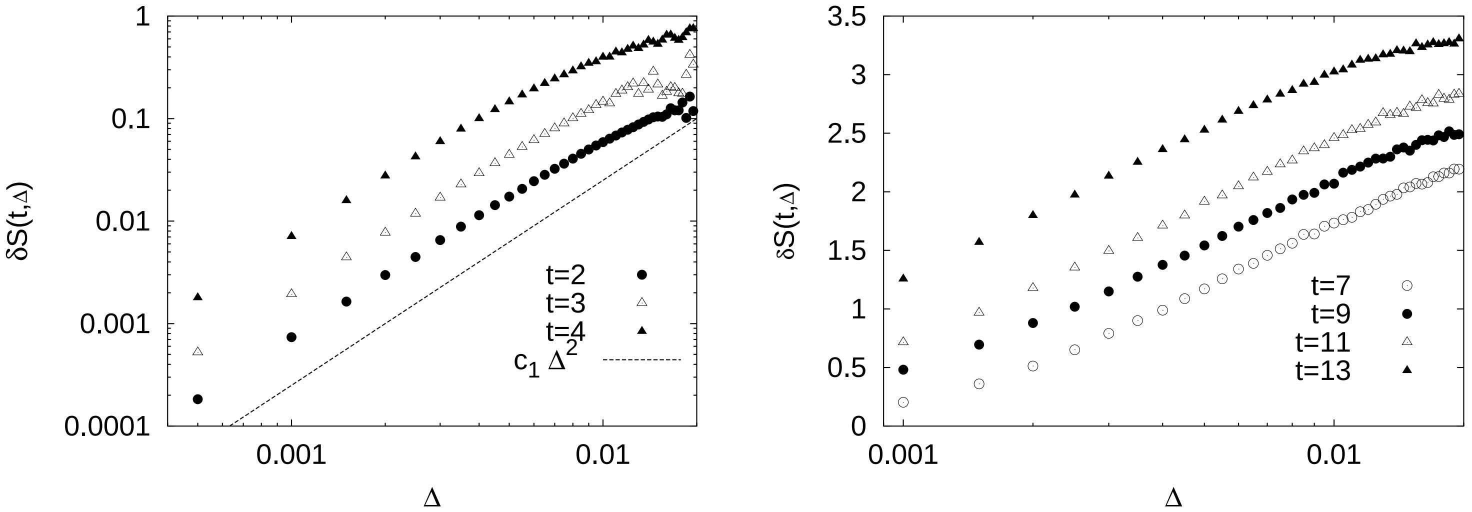
$$\delta S(t,\Delta) = \eta(t,\Delta) - \eta(0,\Delta)$$

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. η constant for $\Delta \to 0$.



Extrapolate: $\Delta \to 0$: far from saturation and for Δ not too large

$$\delta S(t,\Delta) \propto \Delta^2.$$

Relevant parameter is cell area. For $t > t_\lambda$ (reached equilibrium),

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

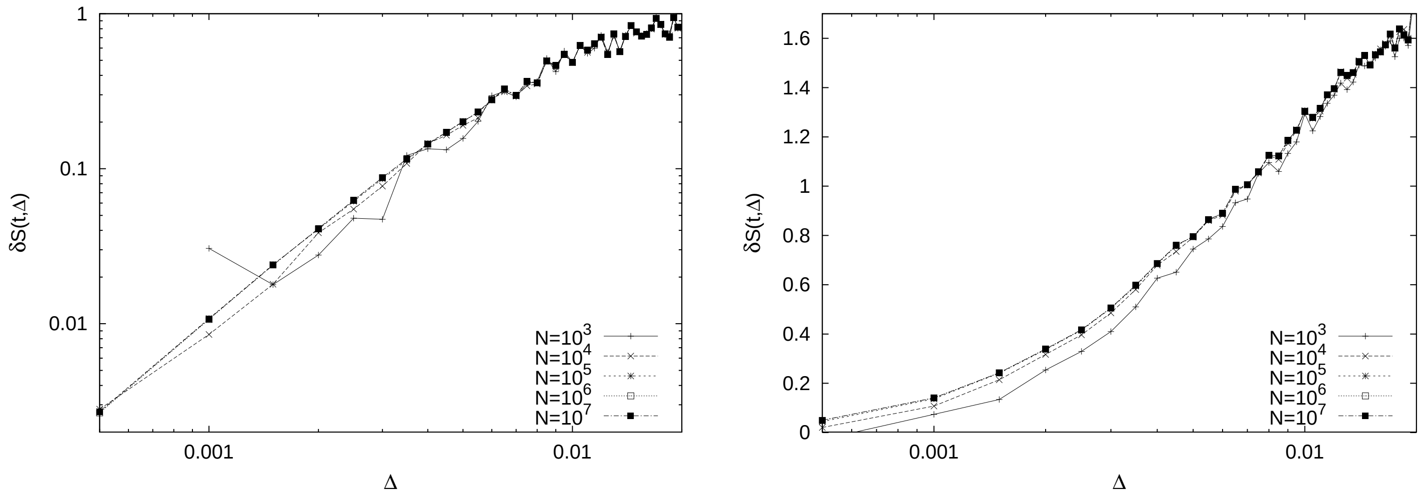
S_B behaves like S_G for $\epsilon = 0$, since f from N particles, is like ρ for ensemble of N single-particle systems (f is 2, ρ is $2N$-dimensional).

Coarse-graining seeems to allow entropy to increase, after some time, in spite of Liouville's theorem.

But requires scales $l_c \sim N^{-1/2}$ in which there is no statistics.

Does not happen if S_B computed with $N \to \infty$, $\Delta \to 0$, $\Delta \gg l_c$.

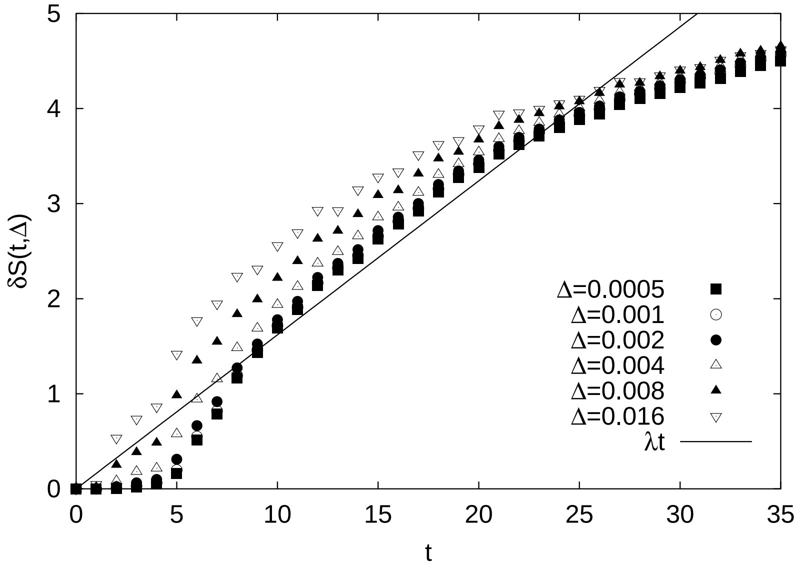
$t = 3$ (small) $\qquad\qquad t = 9$ (large)



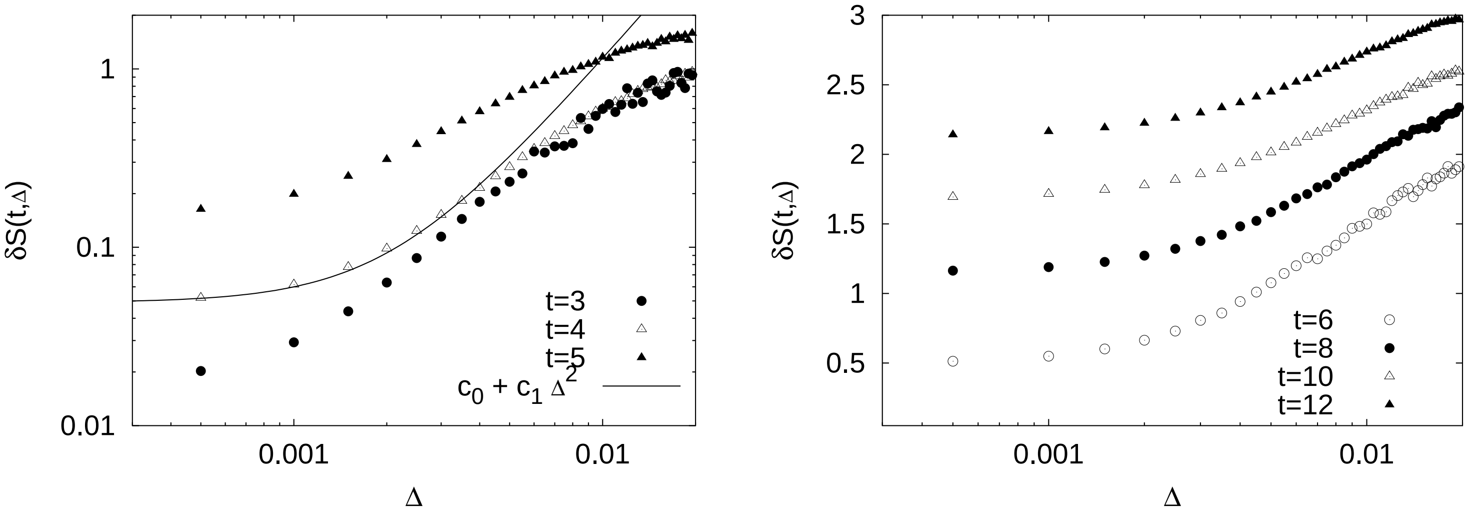
Curves collapse for large N at fixed t, Δ: if cells occupied by many particles, S_B does not evolve in time. We take $N = 10^7$.

"Interacting" case: $\epsilon > 0$.

After a characteristic time depending on ϵ, $t_*(\epsilon, \lambda_1)$, entropy has log dependence on Δ and extrapolates to finite value for $\Delta \to 0$.



$\epsilon = 10^{-4}$; straight line slope equals λ_1.

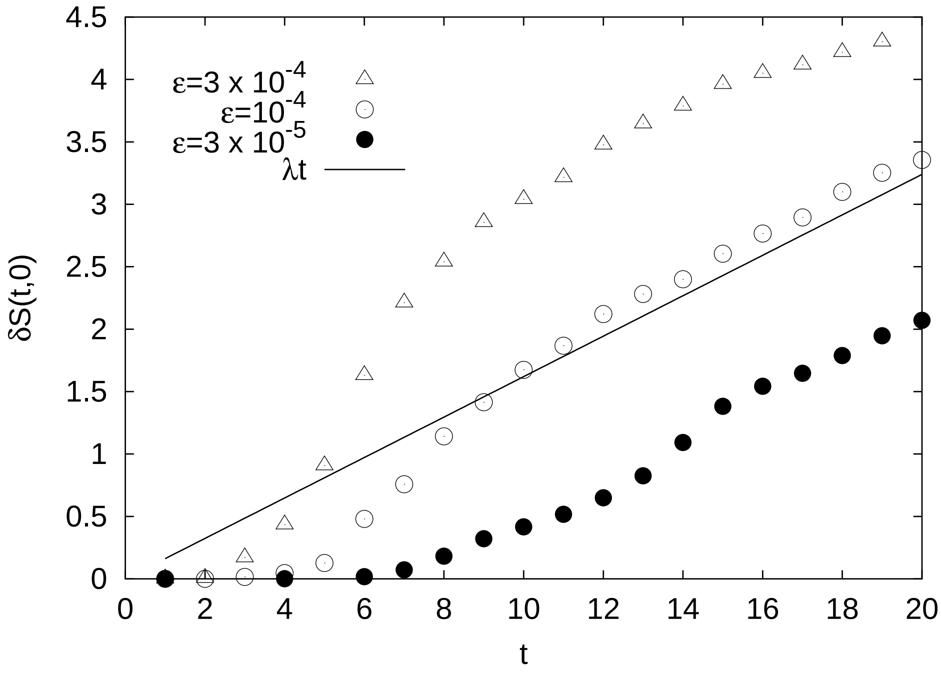


For small (fixed) times:

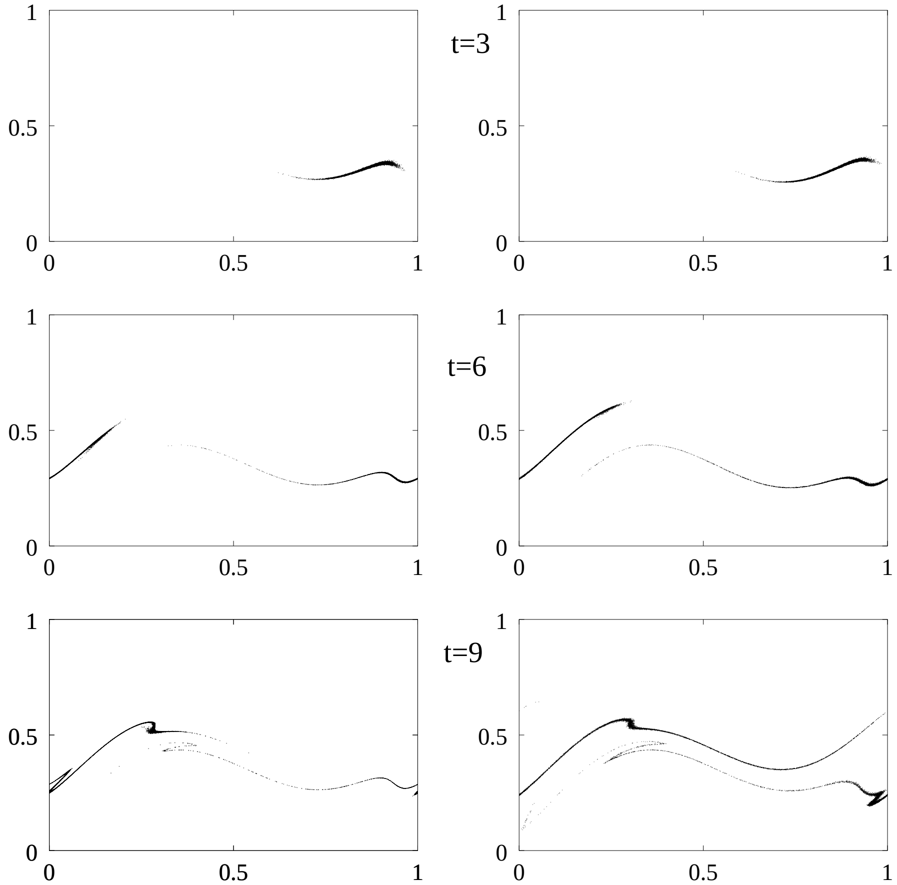
$$\delta S(t,\Delta) \approx c_0 + c_1\Delta^2.$$

Small t (left) and large t (right). In the right panel $\delta S(t,\Delta)$ 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 $\Delta \to 0$ of the curves $\delta S(t, \Delta)$ as a function of t for various values of ϵ.



Snapshots of evolution of single-particle distribution with $\Delta > \Delta_*$. Non-interacting case (left); interacting with $\epsilon = 10^{-4}$ (right). $M = 100$.



Mimic interactions with noise

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

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

$\delta S(t, \Delta)$ 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.

Summary

a) $\epsilon = 0$: $\mu \sim \Gamma$, $\quad S_B \sim S_G$. $\quad \delta S$ **and** t_λ depend on Δ (observation tools). Mackey right on this: delays not observed.

b) small ϵ: characteristic scale $\Delta_*(\epsilon, \lambda_1)$, at which diffusion smoothes fractal structures, and $t_*(\epsilon, \lambda_1)$ (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 $\epsilon \longrightarrow 0$ limit: slope of $\delta S(t, \Delta)$, for intermediate t, given by λ_1; Δ_* and t_* depend on both ϵ and λ_1.

e) S_G tests large ensembles.
S_B tests large, local equilibrium, single systems.
S_G not thermodynamic in general, but less restricitve; maybe useful when thermodynamics does not apply, e.g. small systems.