Finite-Precision, Periodic Orbits, Boltzmann's Constant, Nonequilibrium Entropy

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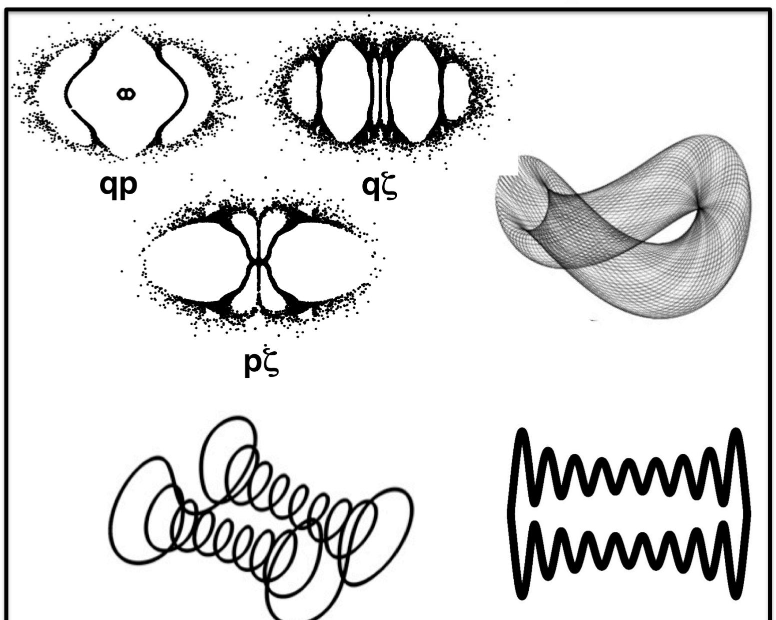
Nosé's idea applied at and away from equilibrium

Consider a harmonic oscillator with temperature control forming a three-dimensional phase space → regular tori and a chaotic sea !

$$\dot{q} = p\ ;\ \ \dot{p} = -q - \zeta p\ ;$$
$$\dot{\zeta} = \Sigma(p^2 - kT)/\tau^2\ .$$

Equilibrium solutions

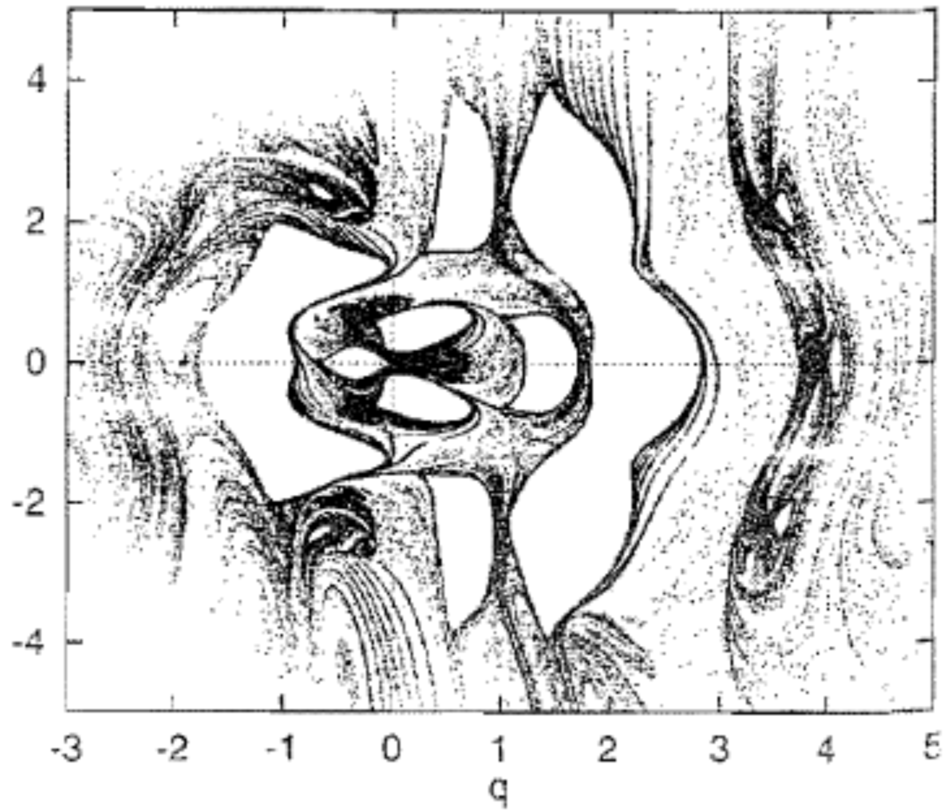


But consider an oscillator with the possibility of heat conduction!

$$1 - \varepsilon < T(q) = 1 + \varepsilon \tanh(q) < 1 + \varepsilon$$

Nonequilibrium steady state solutions are dissipative !

Three-Dimensional Dissipative Nosé-Hoover Oscillator



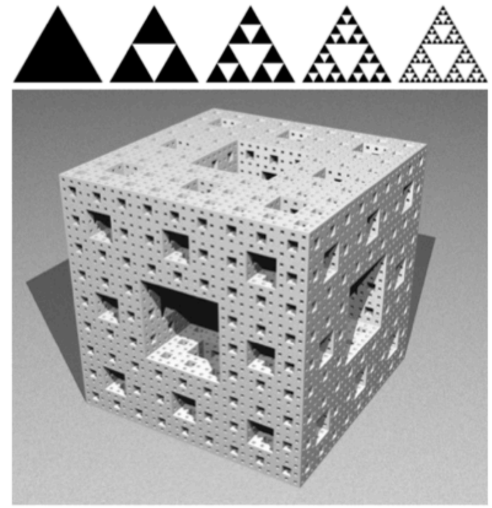
Complicated, with a Kaplan-Yorke Dimension of 2.56 out of 3
Posch and Hoover, Physical Review E, 55 No. 6, (1997).

Notice the many holes in this 3-dimensional case

Fractals have a dimensionality less than that of the embedding space

Sierpinski Carpet D_C =1.58496

Menger Sponge D_C = 2.72683



S_{Gibbs}= kln(Ω)

Correlation Dimension D_c follows from the number of pairs of points within a volume of radius r : number in the embedding space :

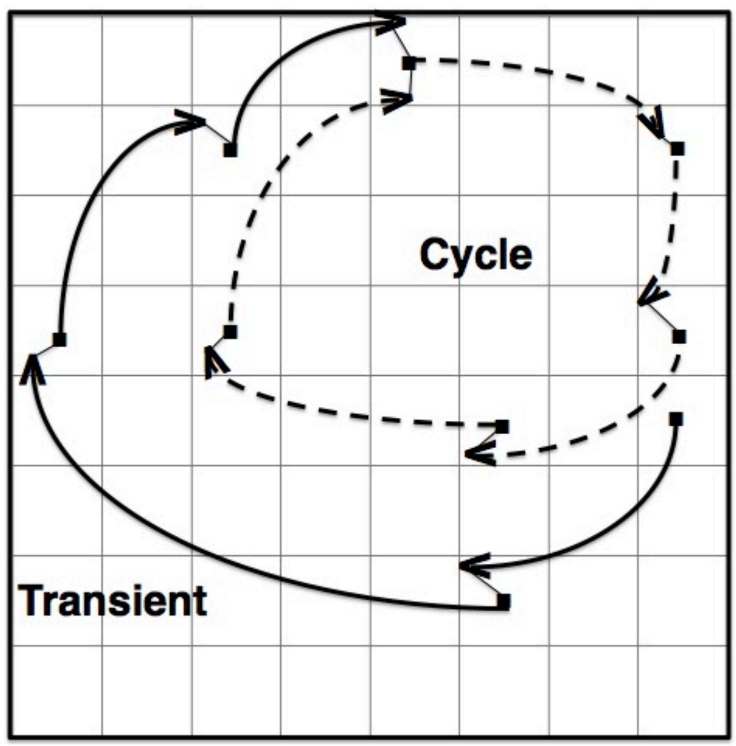
$$N_{pairs} = r^{D_C}$$

Fractal D_C is less than the dimensionality of the embedding space.

Ergodicity and periodic orbits with finite precision

Ergodicity in a bounded phase space implies that a trajectory comes close to all of the available phase-space states.

Finite-precision orbits eventually produce periodic orbits.



Oscillators with two control variables : Hoover – Holian control 2nd and 4th moments

How does ergodicity vary with phase-space dimensionality ?
Consider two oscillators in a four-dimensional space.

$$\dot{q} = p \; ; \; \dot{p} = -q - \zeta p - \xi p^3 \; ;$$

HH oscillator

$$\dot{\zeta} = p^2 - T \; ;$$

$$\dot{\xi} = p^4 - 3p^2 T$$

If ergodic: $f \propto \exp(-q^2/2 - p^2/2 - \zeta^2/2 - \xi^2/2)$

Fractal steady states with a temperature gradient.

$$1 - \varepsilon < T(q) = 1 + \varepsilon \tanh(q) < 1 + \varepsilon$$

Oscillators with two control variables :
Martyna – Klein – Tuckerman Chain Thermostats

$$\dot{q} = p \; ; \; \dot{p} = -q - \zeta p \; ;$$

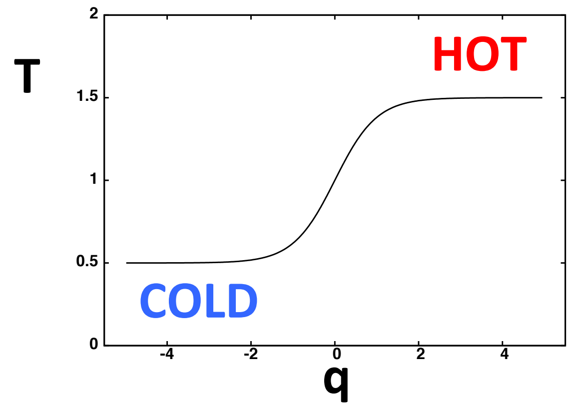
MKT oscillator

$$\dot{\zeta} = (p^2 - T) - \zeta\xi \; ;$$

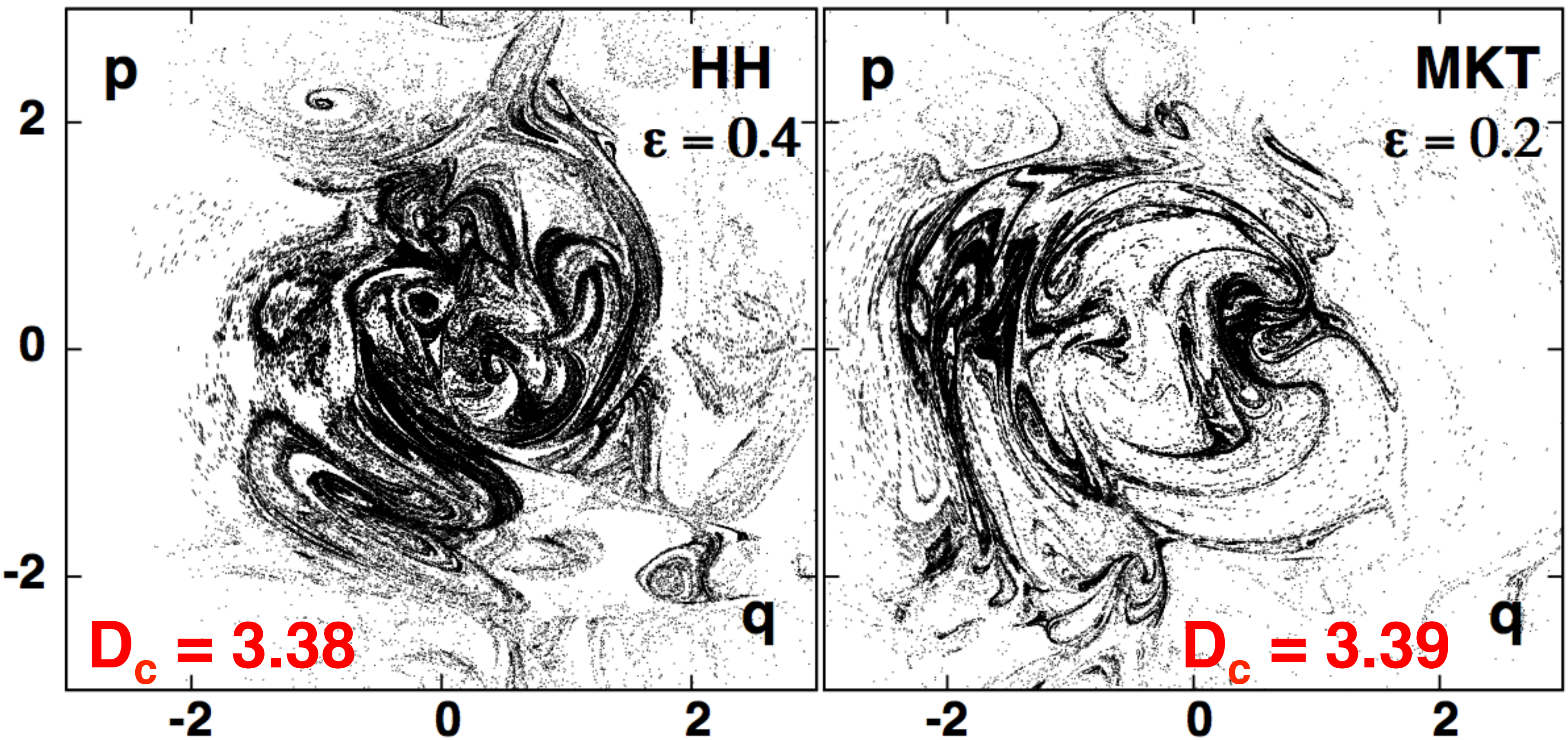
$$\dot{\xi} = \zeta^2 - T$$

If ergodic: $f \propto \exp(-q^2/2 - p^2/2 - \zeta^2/2 - \xi^2/2)$

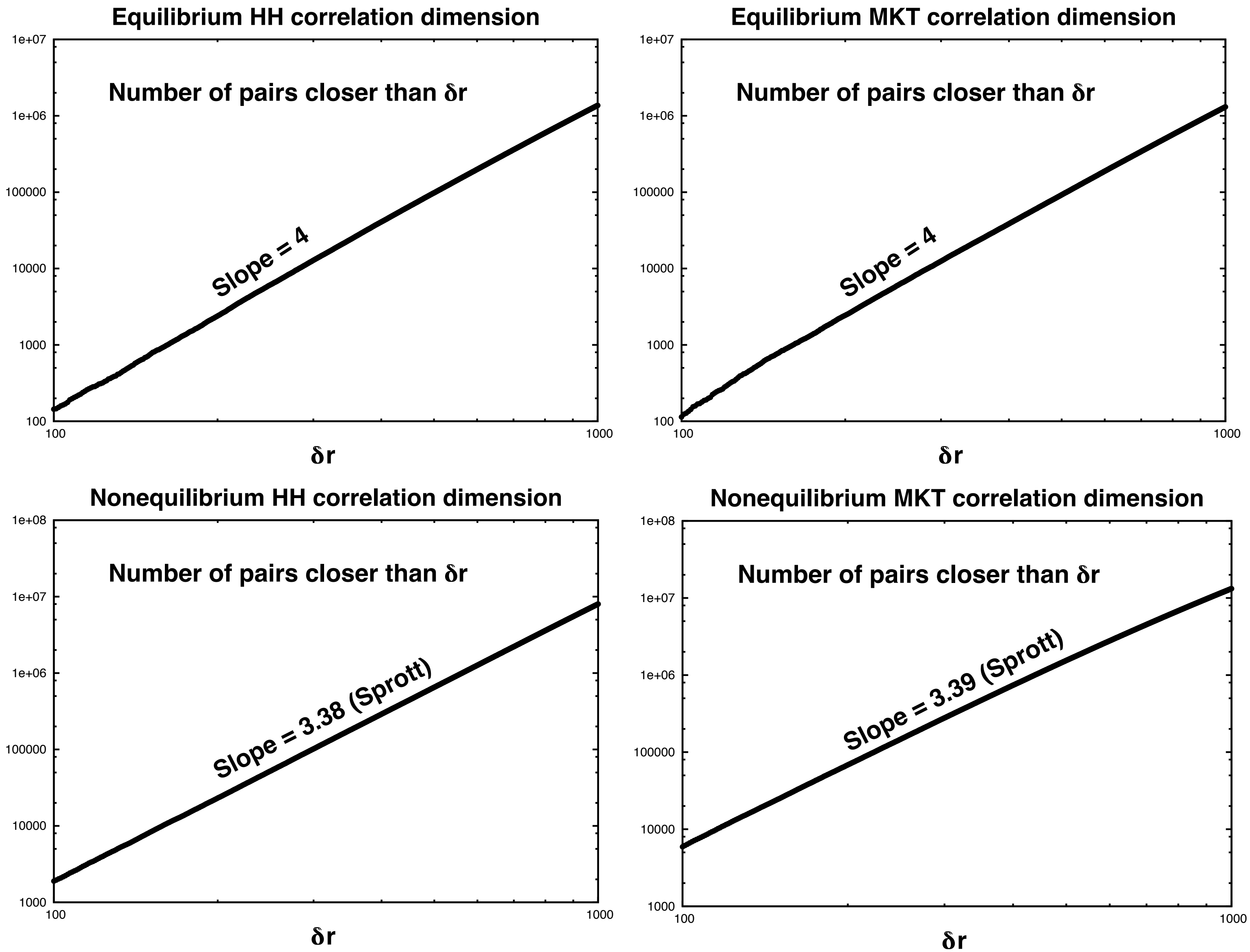
Steady state with a temperature gradient .



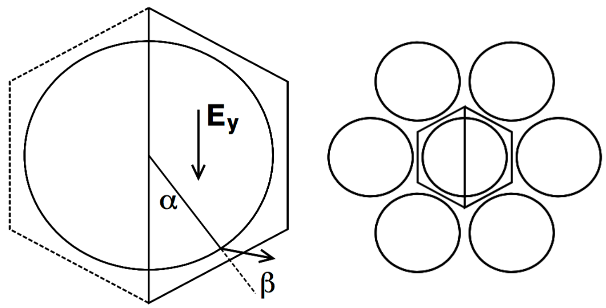
HH and MKT (qp00) for the four-dimensional oscillator with a temperature gradient

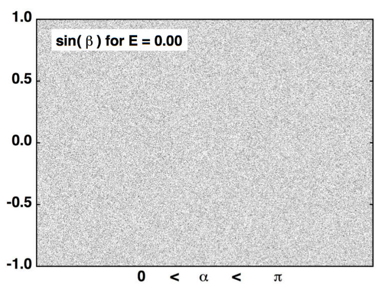


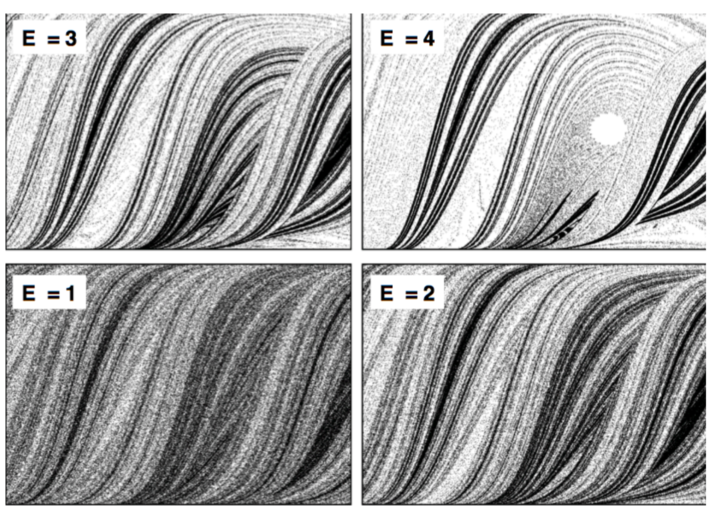
Correlation dimension for equilibrium and nonequilibrium oscillators

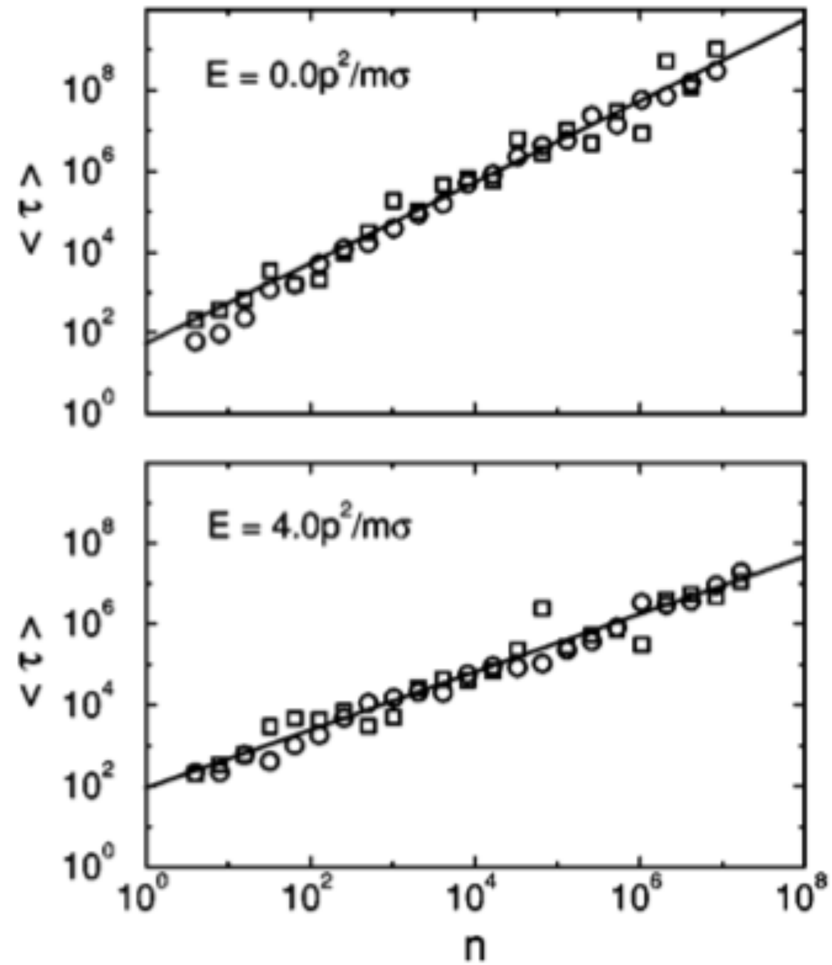


Extensive studies of the Galton Board by Dellago and Hoover for finite-precision states









D_c / 2 = (1.0 and 0.715)

Accessible states, periodic orbits and the Birthday Problem

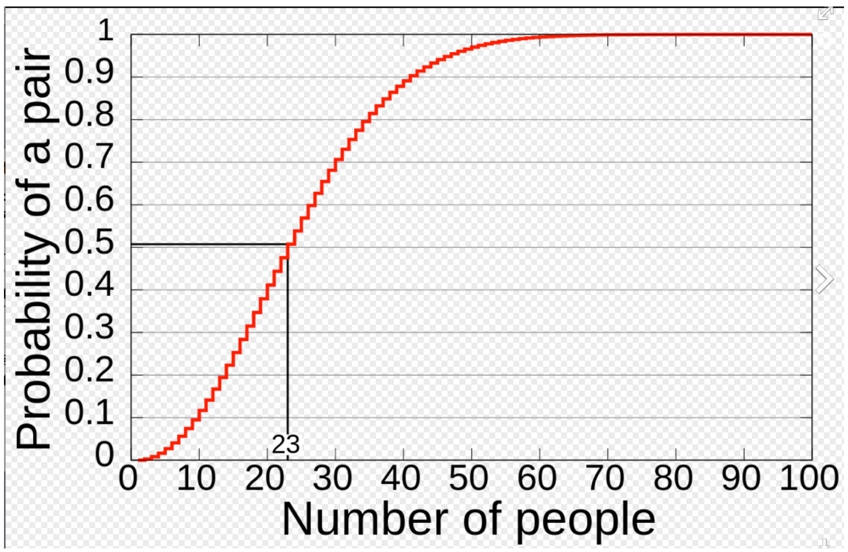
In a set of n randomly selected people, what is the probability that a pair will not have the same birthday?

$$p(n) = 1 \text{x} (1 - \frac{1}{365})(1 - \frac{2}{365}) \; . \; . \; . \; (1 - \frac{n-1}{365})$$

$$= \frac{365 \text{ x } 364 \text{ x } . \; . \; . \; (365 - n + 1)}{365^n} = \frac{365!}{365^n (365 - n)!}$$

$$= \frac{n!}{365^n (365 - n)!} = \frac{{}_{365}P_n}{365^n}$$

$$\Omega_{orbit} = \sqrt{(\pi / 8)\Omega_{total}}$$



Gibbs' entropy *versus* Finite-Precision entropies for periodic orbits

Jumps for recurrence in a space with Ω_{total} states is :

$$\Omega_{total} = \tfrac{1}{2}(\Omega_{orbit})(\Omega_{orbit} - 1)$$

Consider an ensemble of trajectories such that all states in the space are accessed. The density of periodic-orbit states is given by

$$f = \Omega_{orbit} / \Omega_{total} = \sqrt{1 / \Omega_{total}}$$

Following through the usual ensemble averaging and the entropy for periodic orbits is given by :

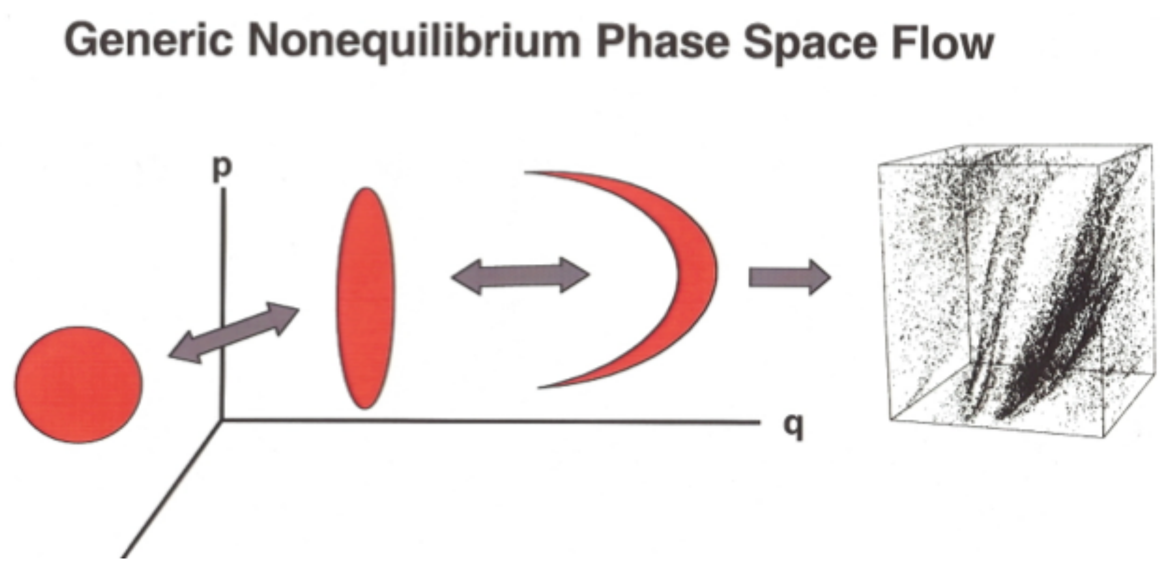
$$S_{orbit} = k\ln(\Omega_{orbit}) = \tfrac{1}{2}k\ln(\Omega_{total}) = \tfrac{1}{2}S_{Gibbs}$$

But in fact entropy does not even exist for fractals !!

Entropy production for Nonequilibrium Oscillators

Follow a 4-dimensional hypersphere in phase-space for the oscillator in a temperature gradient . The volume in phase space grows in some directions and shrinks in others with a net decrease in volume representing the heat extracted by the thermostats to maintain the temperature gradient . The reduction in volume corresponds to the sum of the Lyapunov exponents . Grebogi, Ott, and Yorke pointed out that the correlation dimension describes the length of periodic orbits and is much less than four ! When the sum of the Lyapunov exponents vanishes this gives the dimensionality of the nonequilibrium state .

ΔD is given by $\sum \lambda / \lambda_1$ where the sum is negative !



CONCLUSIONS from our work

[1] The number of states on a typical periodic orbit is proportional to square root of the total number of accessible states .

[2] Adjust Boltzmann's constant by a factor of two and Molecular Dynamics entropy = Monte Carlo entropy .

[3] Gibbs' entropy diverges away from equilibrium .

[4] Ergodicity is enhanced by higher dimensionality .

2014 Ian Snook Prize

Challenge: To what extent are trajectory-based solutions of the equilibrium Martyna-Klein-Tuckerman oscillator ergodic ?

Motivation: To honor the memory of our Australian colleague : Ian Snook

Prize: $500 US awarded in January 2015 to the author(s) of the most convincing solution of the MKT ergodicity challenge .

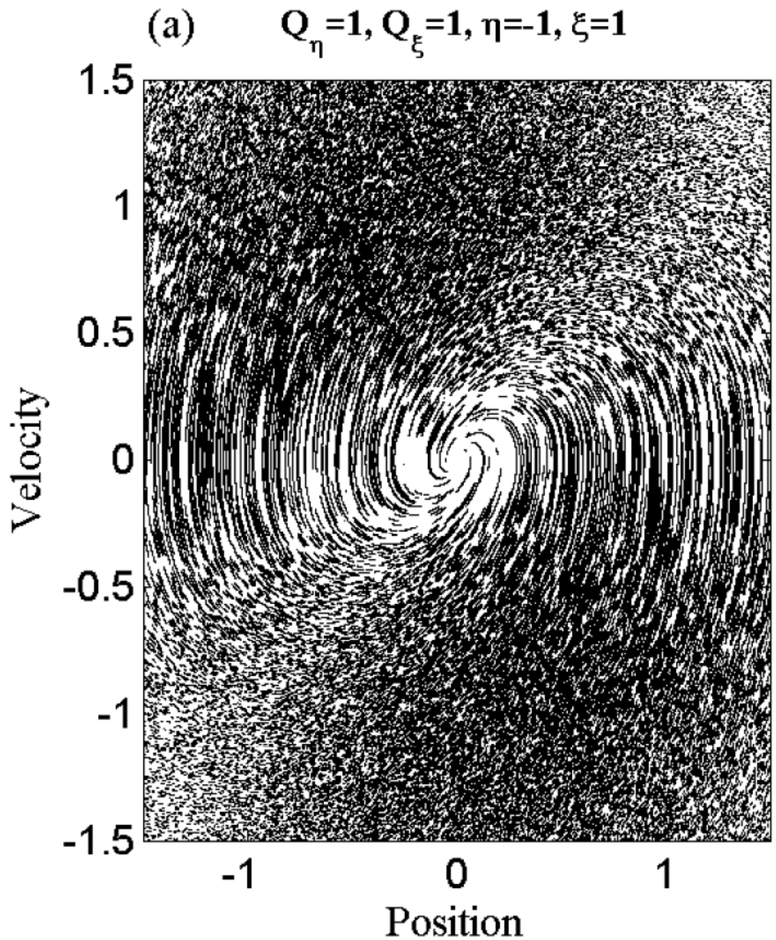
Submission information:

Details of the challenge problem are in an arxiv publication arXiv:1408.0256. Submit solutions to www.arxiv.com before 1 January 2015 or to Computational Methods in Science and Technology . For further details see www.williamhoover.info

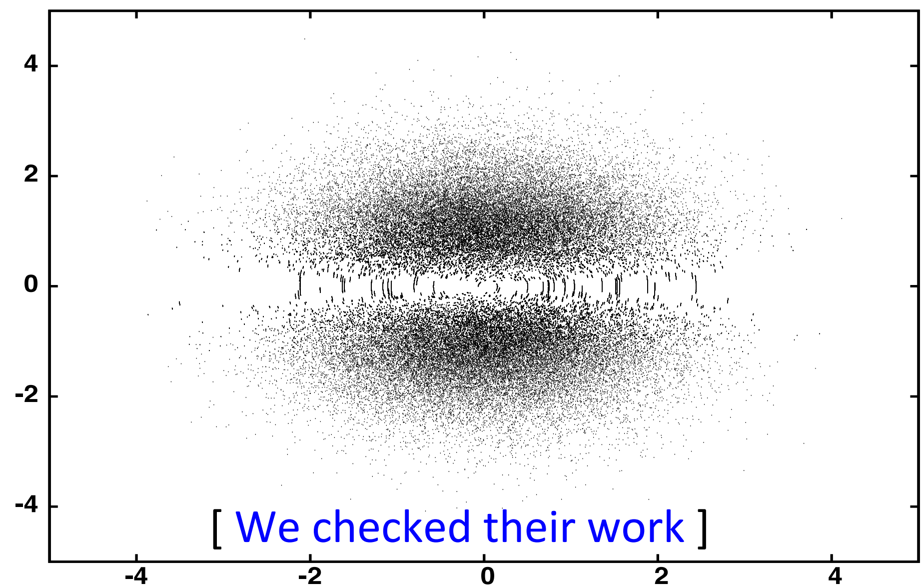
Shuichi Nosé (1951 – 2005)

Ian Snook (1945 – 2013)

Martyna – Klein – Tuckerman Chain Thermostat



(q, p, -1, +1) section



Puneet Kumar Patra and Baidurya Bhattacharya, "Nonergodicity of the Nosé-Hoover Chain Thermostat in Computationally Achievable Time", Physical Review E 90, 043303 (2014)

"The [MKT] thermostat therefore does not generate the canonical distribution or preserve quasi-ergodicity for the Poincaré Section".