

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

**Carol G. Hoover and Wm G. Hoover
Ruby Valley, Nevada USA**

**Clint Sprott
University of Wisconsin
Madison, Wisconsin USA**

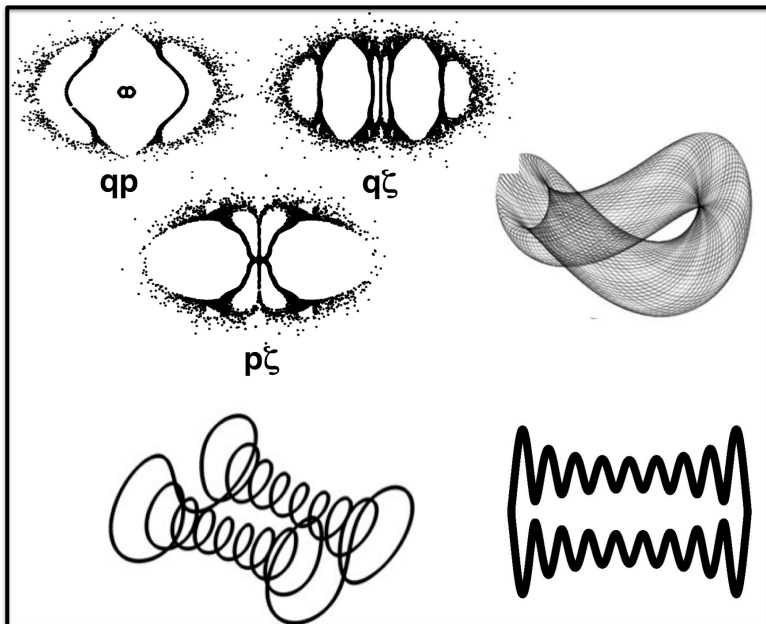
**Keio University
Mita Campus, 10-11 November 2014**

Nosé's idea applied at and away from equilibrium

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

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

Equilibrium solutions

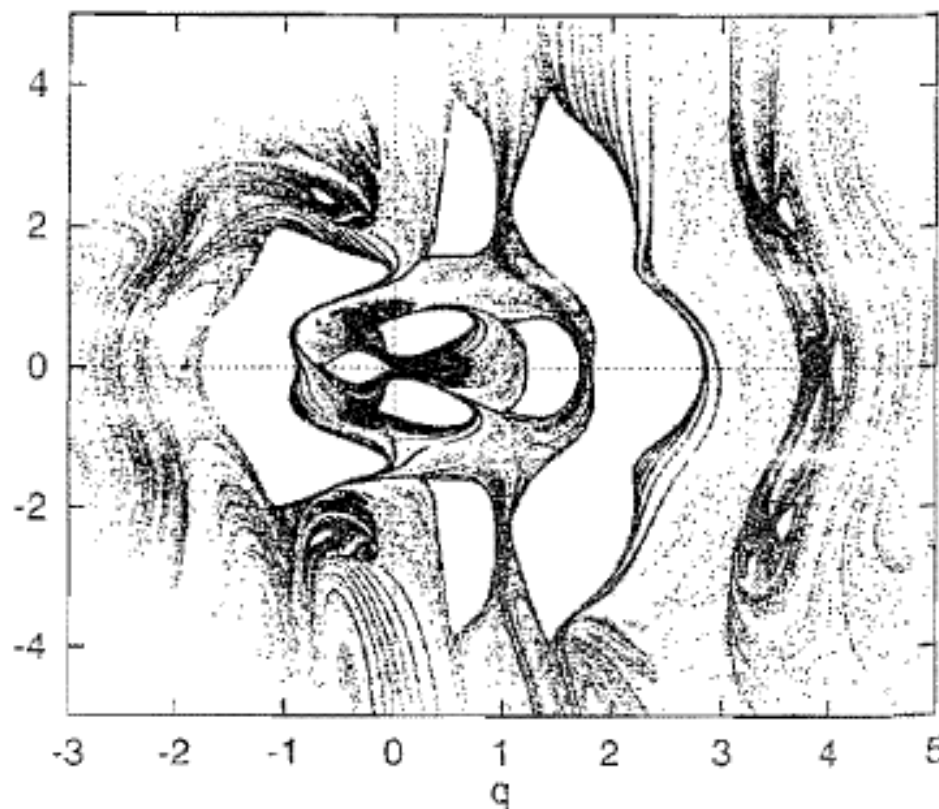


But consider an oscillator with the possibility of **heat conduction!**

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

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).

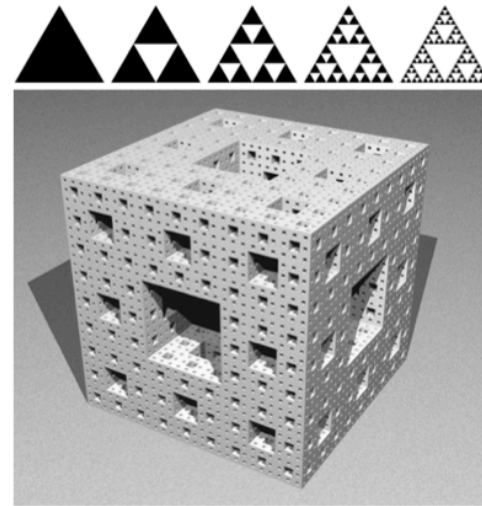
Notice the many holes in this 3-dimensional case

Fractals have a dimensionality less than that of the embedding space

Sierpinski Carpet $D_c = 1.58496$

Menger Sponge $D_c = 2.72683$

$$S_{\text{Gibbs}} = k \ln(\Omega)$$



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

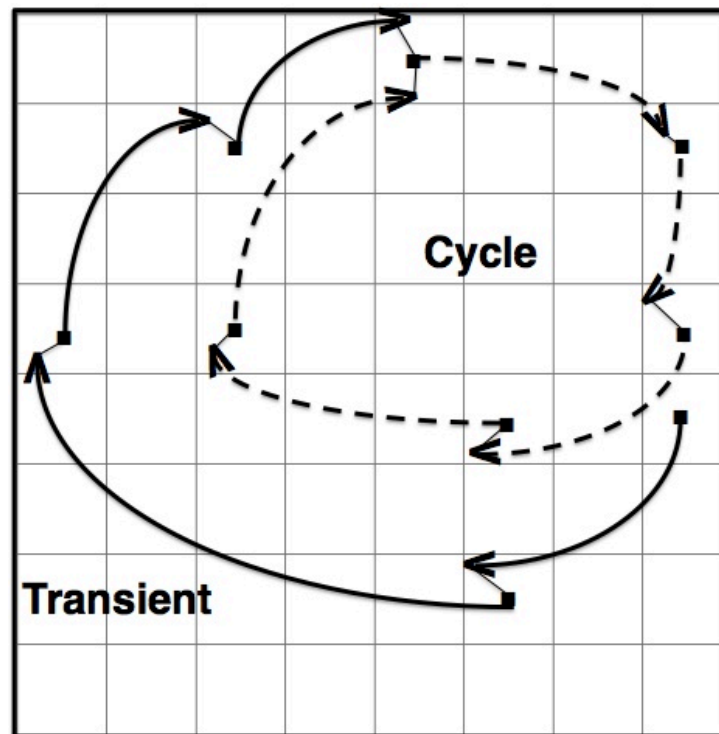
$$N_{\text{pairs}} = r^{D_c}$$

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.

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

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

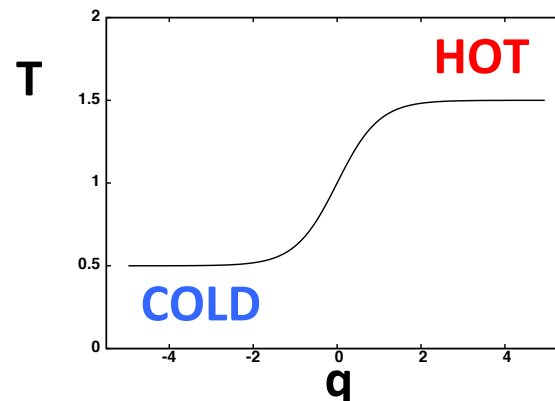
$$\dot{q} = p ; \dot{p} = -q - \zeta p ;$$

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

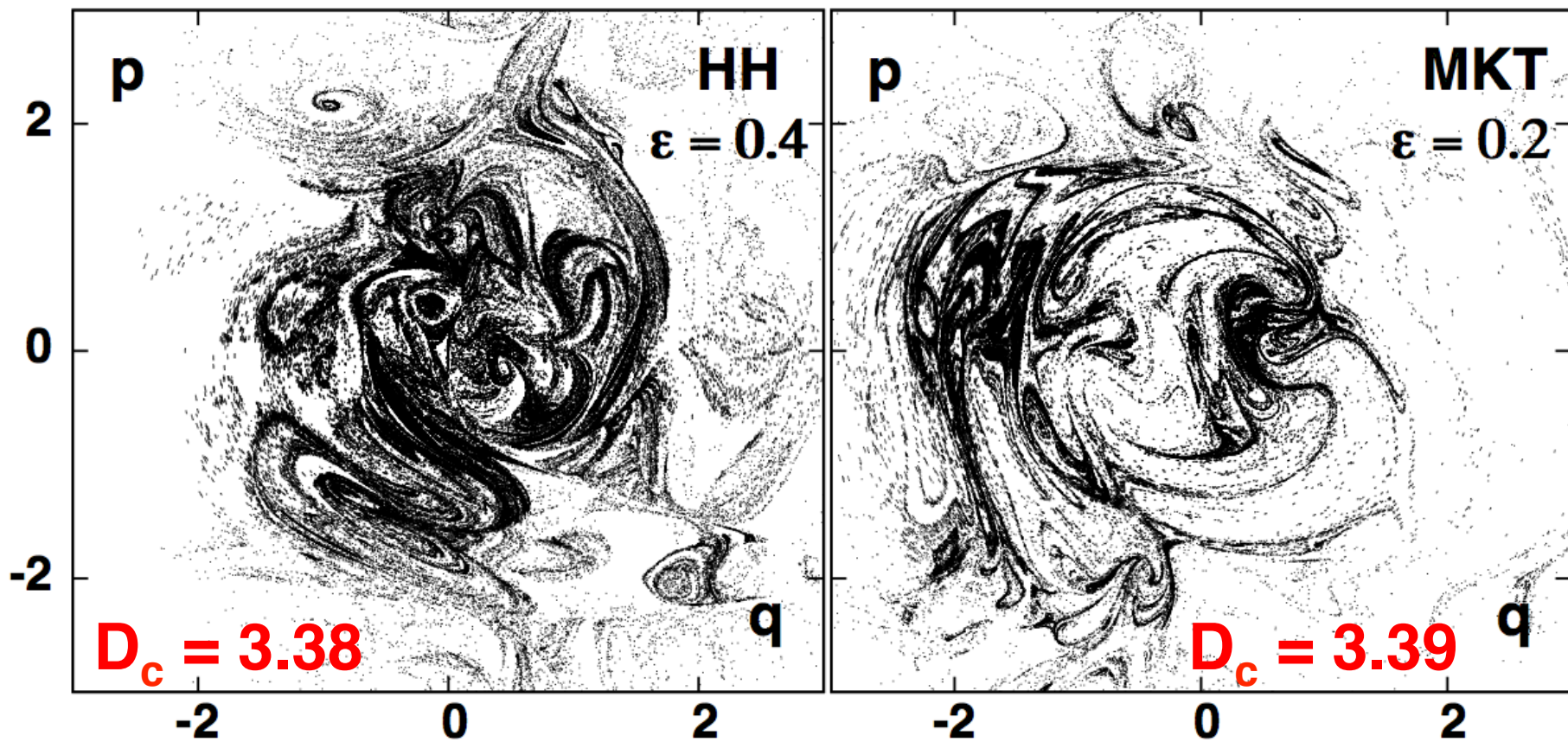
$$\dot{\xi} = \zeta^2 - T$$

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

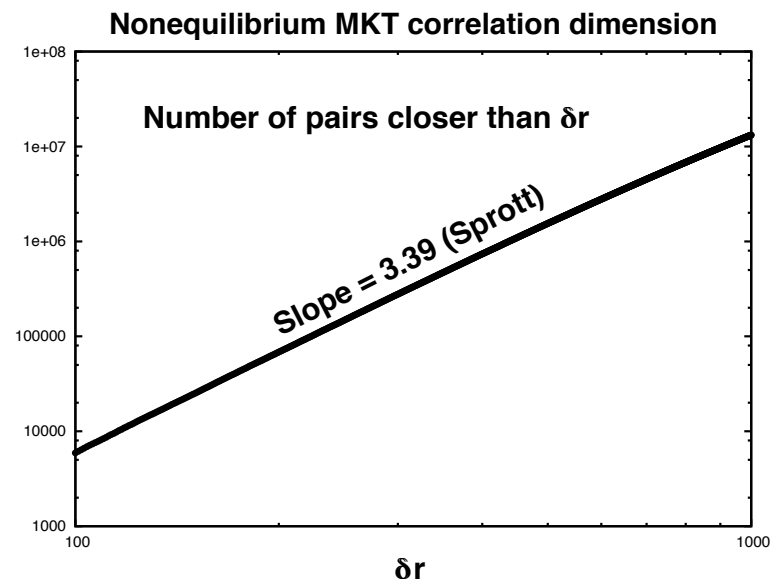
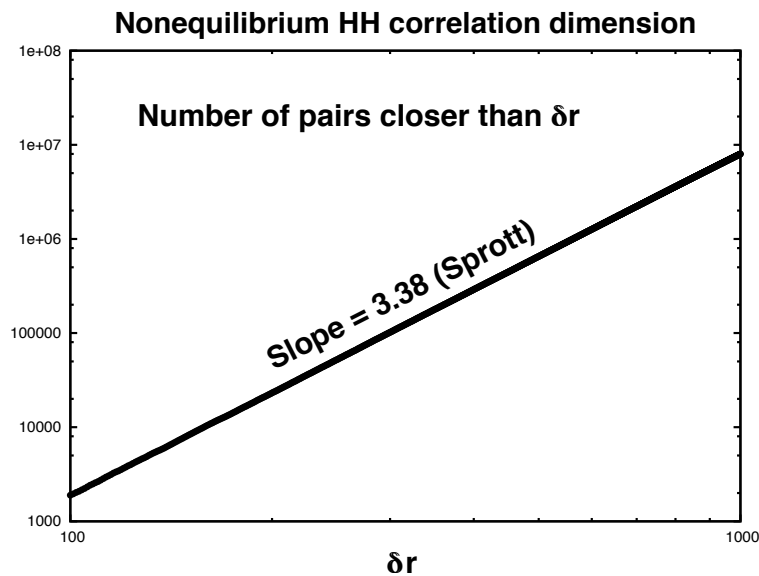
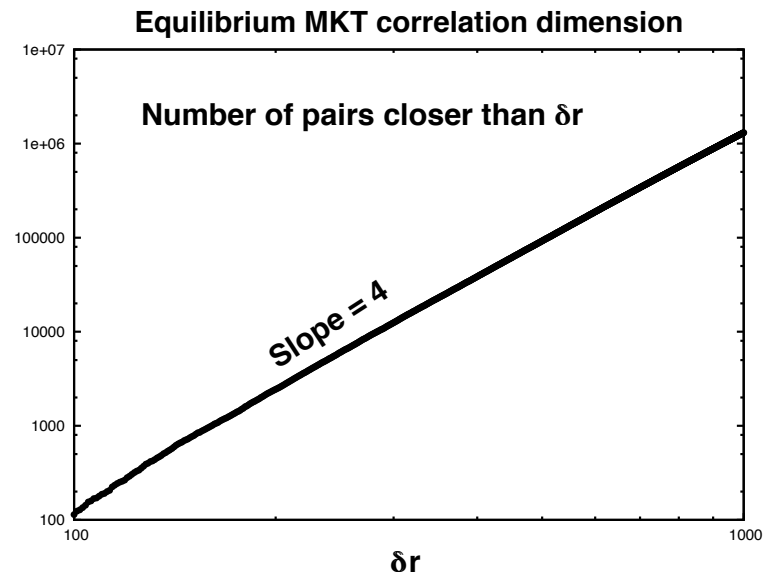
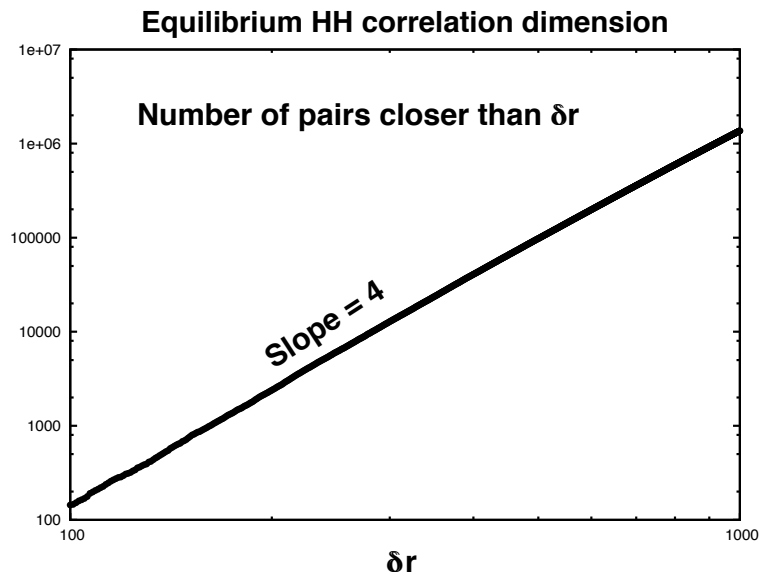
Steady state with a temperature gradient .



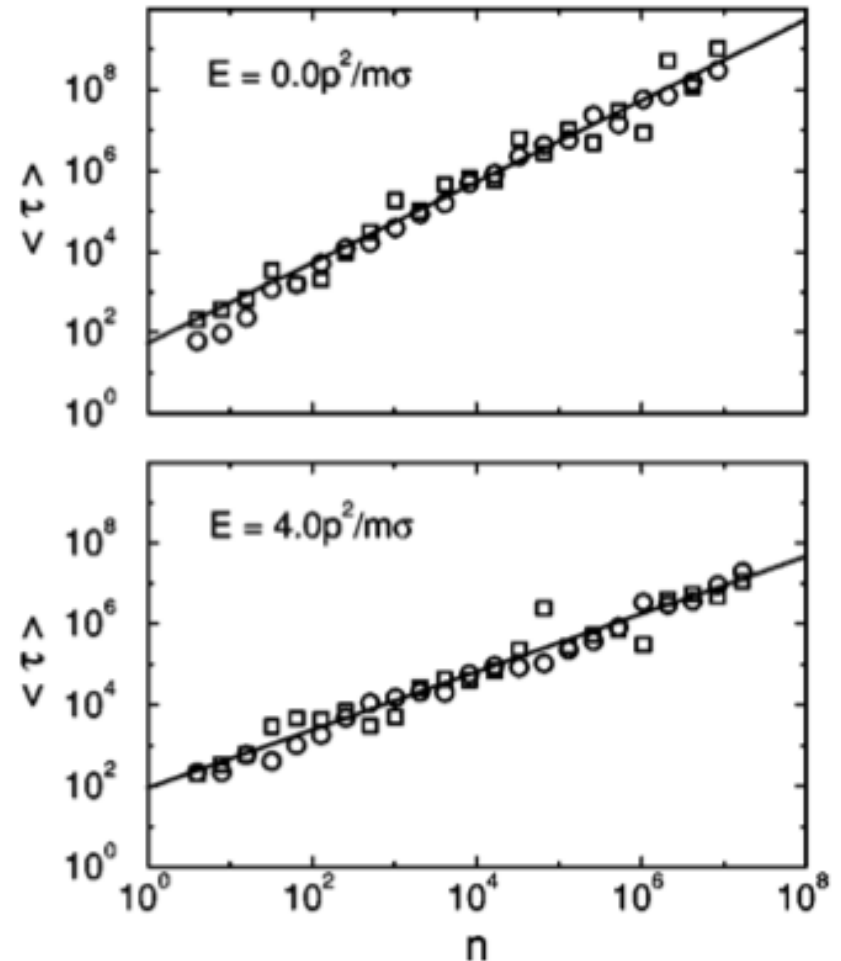
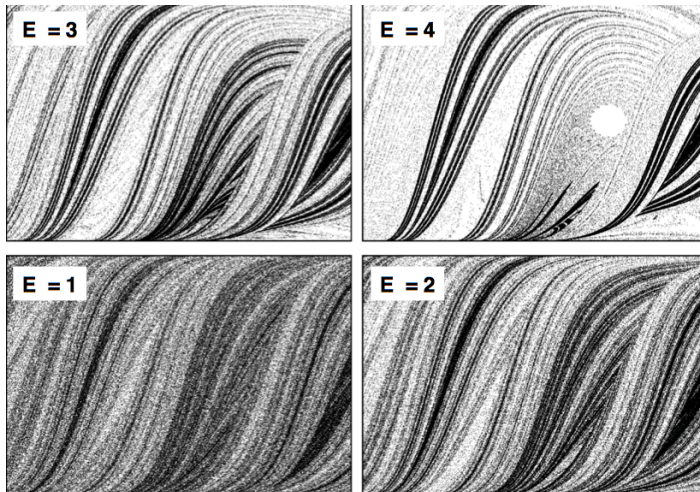
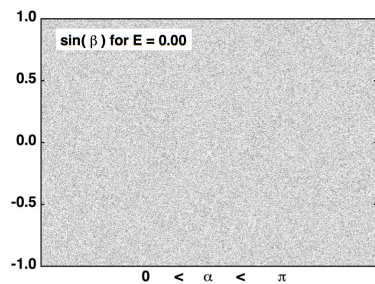
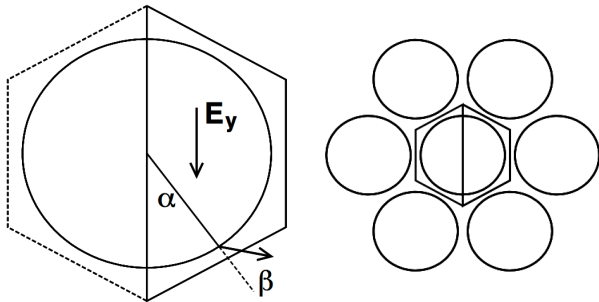
HH and MKT (qp00) for the four-dimensional oscillator with a temperature gradient



Correlation dimension for equilibrium and nonequilibrium oscillators



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



$$D_c / 2 = (1.0 \text{ and } 0.715)$$

Accessible states, periodic orbits and the Birthday Problem

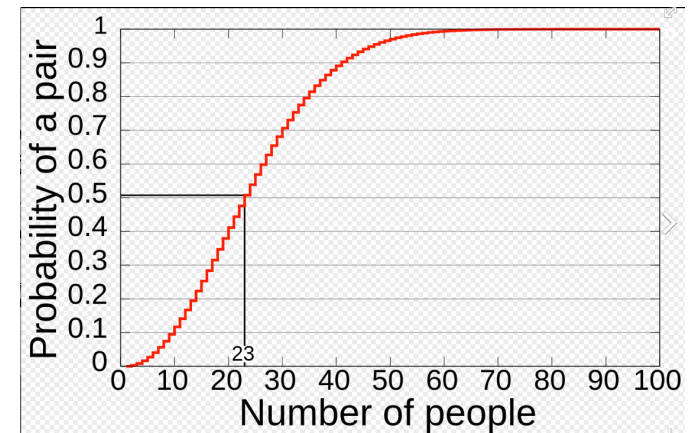
In a set of n randomly selected people, what is the probability that a pair will not have the same birthday?

$$\begin{aligned}
 p(n) &= 1 \times \left(1 - \frac{1}{365}\right) \left(1 - \frac{2}{365}\right) \dots \left(1 - \frac{n-1}{365}\right) \\
 &= \frac{365 \times 364 \times \dots \times (365 - n + 1)}{365^n} = \frac{365!}{365^n (365 - n)!}
 \end{aligned}$$

$$\begin{aligned}
 &= \frac{365!}{365^n (365 - n)!} = \frac{365!}{365^n} \frac{1}{(365 - n)!} \\
 &= \frac{365!}{365^n} \frac{1}{(365 - n)!}
 \end{aligned}$$

$$\Omega_{\text{orbit}} = \sqrt{(\pi / 2) \Omega_{\text{total}}}$$

$$\Omega_{\text{orbit}} \cong \Omega_{\text{periodic}} + \Omega_{\text{transient}}$$



Gibbs' entropy *versus*

Finite-Precision entropies for periodic orbits

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

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

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

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

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

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

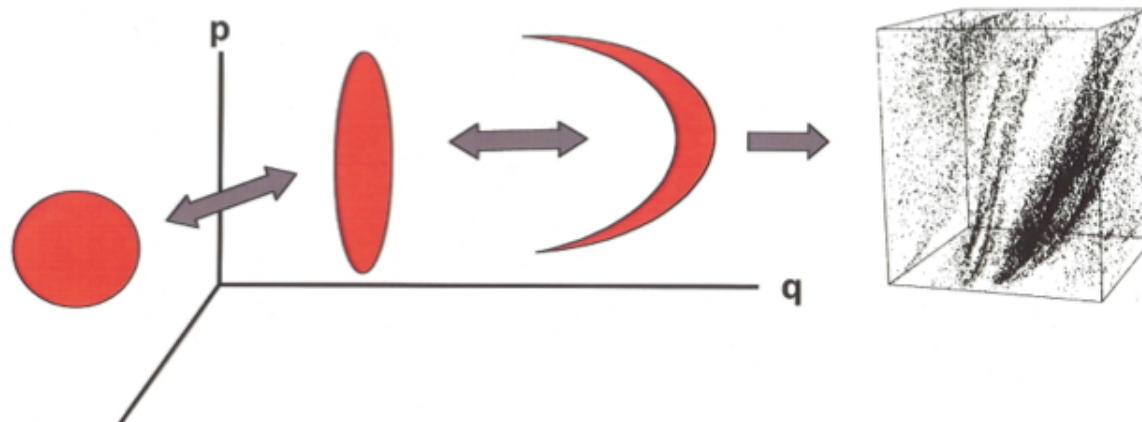
But in fact entropy does not even exist for fractals !!

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 !

Generic Nonequilibrium Phase Space Flow



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:

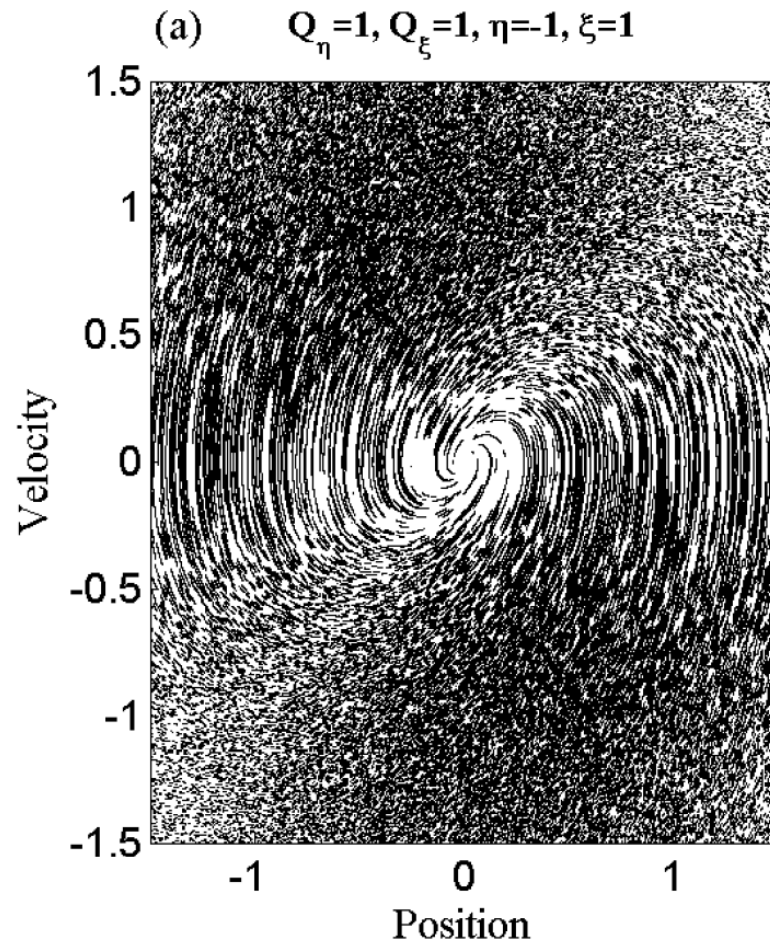
Details of the challenge problem are in an arxiv publication [arXiv:1408.0256](https://arxiv.org/abs/1408.0256). Submit solutions to www.arxiv.com before 1 January 2015 or to Computational Methods in Science and Technology . For further details see www.williamhoover.info

Shuichi Nosé
(1951 – 2005)

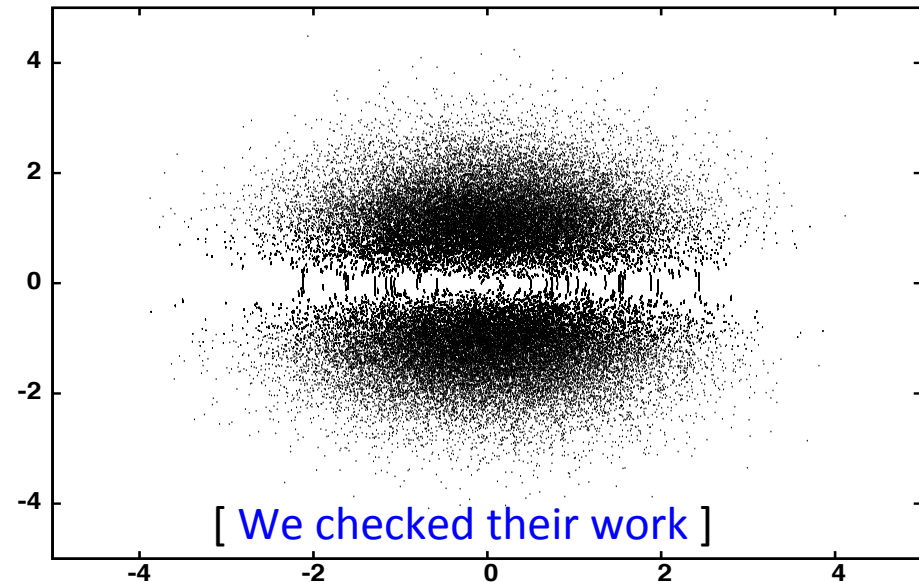


Ian Snook
(1945 – 2013)

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”.