Kharagpur Lecture 10
Lyapunov Instability , Spectra , Fractals
[continued and concluded]

0. Quotes from Alghero, Sardinia, 15 - 17 July 1991
1. Galton Board Evolution and Finite-Precision Stationary States
2. Galton Board Isomorphisms and Fluctuations
3. Baker Maps at and away from Equilibrium
4. Baker Map and the Fluctuation Theorem
5. Dimensionality Loss in 2D Maps and Particulate Flows
6. 0532 Model Spectra at and away from Equilibrium
7. The ϕ^4 Model Spectra and Dimensionality Loss
8. Summary

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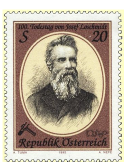
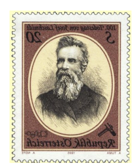
December 2016



0. Quotes from a NATO conference at Alghero, Sardinia, 15 - 17 July 1991



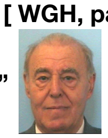
Resolving Loschmidt's (1821 - 1895) paradoxical question [slightly paraphrased] :
"How can time-reversible equations of motion have irreversible solutions ?" Note that

"The nonequilibrium simulations all show that a phase-space collapse to a fractal strange attractor occurs with a collapse rate given by the summed spectrum of Lyapunov exponents ." [WGH, page 61]

Round Table Discussion on Irreversibility and Lyapunov Spectra :

"Now, in the steady state it should be obvious that the [phase] volume, if it is changing, can only get smaller ." [WGH, page 334] "One of the characteristics of the attractors is that Gibbs' entropy always diverges in the nonequilibrium case, always minus infinity." [WGH, page 336]

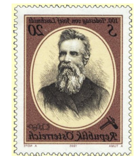
E. G. D. Cohen : "I do not think so ." [also page 336]
Joel Lebowitz : "Boundary conditions [are] only effective at the boundary"



Today :

"If most of the space is contracting the volume eventually vanishes !"

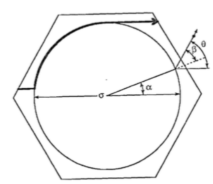
0. Quotes from a NATO conference at Alghero, Sardinia, 15 - 17 July 1991



"I know that most men , including those at ease with problems of the greatest complexity , can seldom accept even the simplest and most obvious truth if it be such as would oblige them to admit the falsity of conclusions which they have delighted in explaining to Colleagues , which they have proudly taught to others , and which they have woven , thread by thread , into the fabric of their lives ."

— Leo Tolstoy

1. Evolution of the Galton Board Fractal *



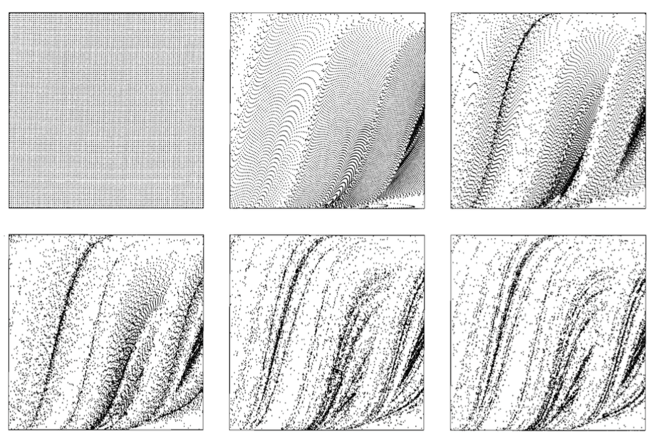
Cross section of the phase-space distribution after 0, 1, 2, 3, 5, 10 collisions with field = 3 . In The Beginning a uniform grid of 10,000 points was the set of initial conditions . Here the field Is perpendicular to a row of scatterers .

$$\Delta x = (p^2/mE)\ln(\sin\theta_0/\sin\theta),$$

$$\Delta y = (p^2/mE)(\theta_0 - \theta),$$

$$t = (p/E)\ln[\tan(\theta_0/2)/\tan(\theta/2)],$$

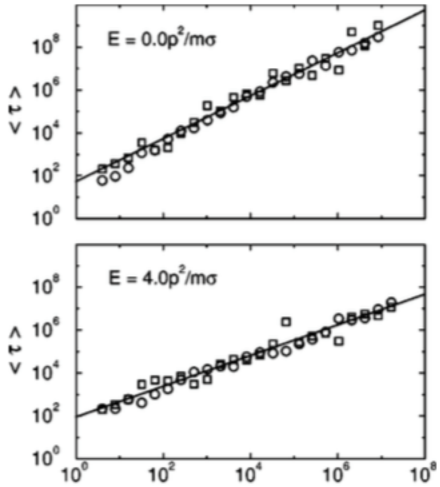
{ -1 < sin(β) < +1 as a function of 0 < cos(α) < π }



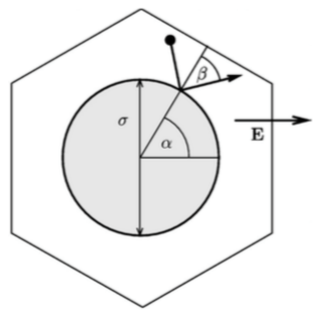
Exactly the same (Δx, Δy) equations apply for a *Hamiltonian* particle in an *exponential* field with $\mathcal{H} = \mathcal{K} - E\lambda e^{(x/\lambda)}$. This observation has a remarkable consequence : the moving particle arrives at infinity at a finite time !

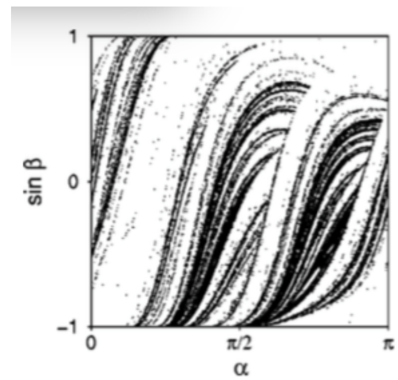
*** Hoover, Moran, Hoover, Evans, Physics Letters A 133, 114 - 120 (1988) .**

1. Finite-Precision Galton Board → Periodic Orbits ! *



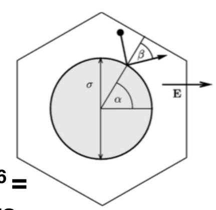
The field is parallel to a row of scatterers at 4/5 the close-packed density . The Box-Counting, Information, and Correlation dimensions are 2.00, 1.54, and 1.43 .

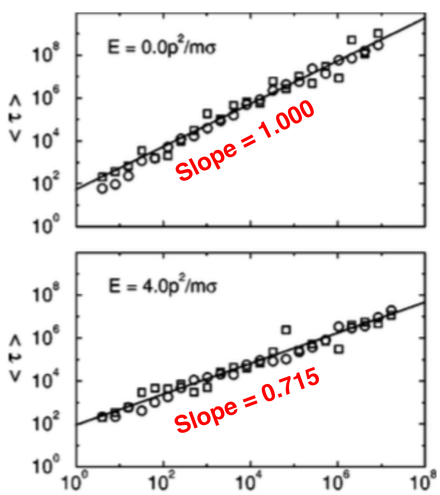




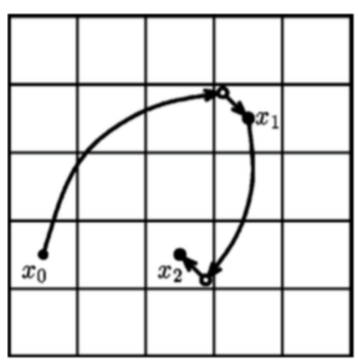
* Dellago and Hoover, Physical Review E 62, 6275-6281 (2000) .

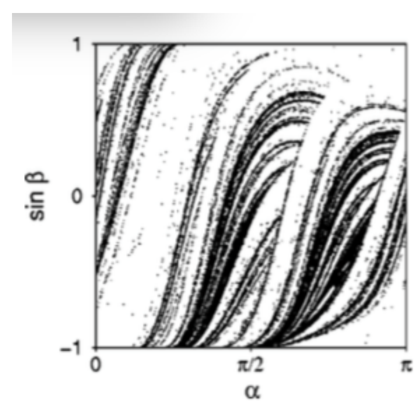
1. Finite-Precision Galton Board *





We carried out simulations with from 2^2 to 2^{46} = $8{,}388{,}608^2$ cells, mapping to the n^2 cell centers .





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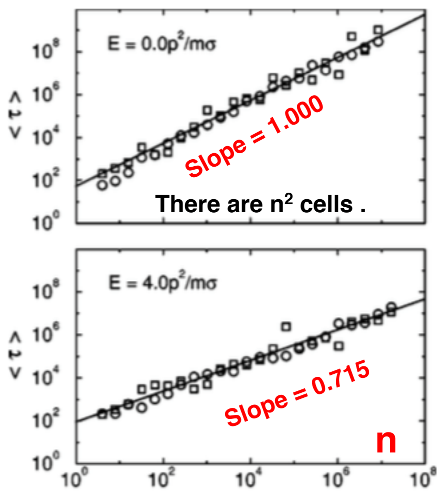
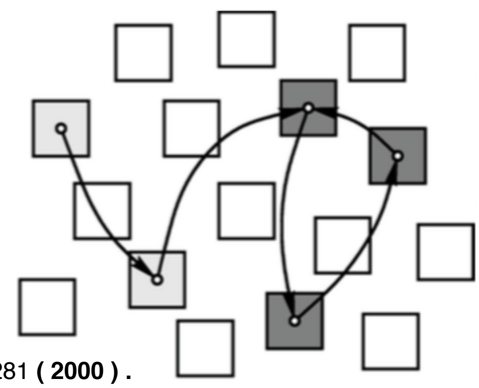
1. Finite-Precision Galton Board with n^2 Cells *



Now there is a deterministic mapping with a transient part (circles) and a period (squares) which agree with a stochastic model predicting slopes of one half the Correlation dimension, 2.000/2 and 1.430/2.0 for 0 and 4 . Notice that the circles and squares lie on the same lines .



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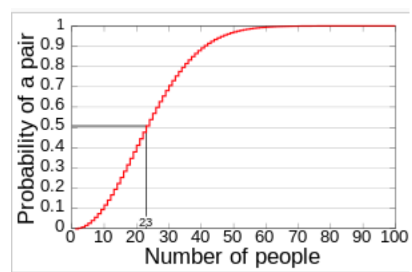
1. Finite-Precision Galton Board with n^2 Cells



The Birthday Problem shows that a group of 23 people is likely to have a pair with the same Birthday . If we have $N = n^2$ cells in phase space the number of pairs → N^2 . If we imagine a sequence of M cells with each of them different to all the predecessors the joint probability is

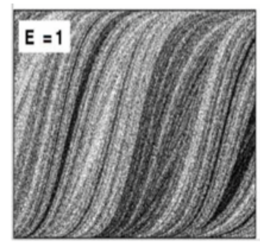
$$(1)(1 - 1/M)(1 - 2/M) \ldots \approx \exp[- M^2/2] \ .$$

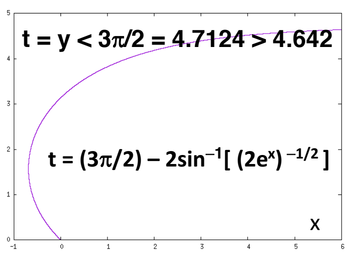
The probability that a new cell will be different from *all* the previous cells should be of order $N^{1/2}$ and in fact turns out to be $\tau = (\pi N/2)^{1/2}$ for large N .

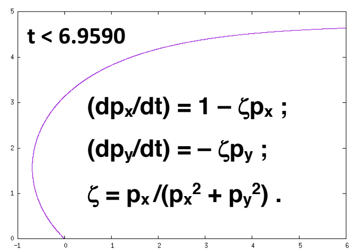
At equilibrium the fraction of states actually visited is $\Omega^{[-½]}$. The *number* diverges while the *fraction* goes to zero . Both the transient and the period vary as $\Omega^{[-½]}$. Nonequilibrium steady states, with a correlation dimension less than that of the space have a "basin of attraction" which is most of the space and relatively small transients and periods . Out of 2^{26} states the Galton Board attractor was made up Of 1836 points in all . Out of 10^{32} states we would expect to see only $10^{22.9}$ for E = 4 .

2. An Interesting Isomorphism for the Galton Board *

Consider a particle at the origin with momentum (-1,+1) with a gravitational field e^x : $(dx/dt) = p_x$; $(dy/dt) = p_y$; $(dp_x/dt) = e^x$; $(dp_y/dt) = 0$ with $\{ x,y,p_x,p_y \} = \{ 0,0,-1,+1 \}$ Evidently the motion in the y direction is uniform with $y = t$ and $p_y = 1$. The motion in the x direction involves solving $(d/dt)^2 x = e^x$. To solve it write the energy equation for the motion in the x direction only : $(dx/dt) = [2e^x - 1]^{1/2}$ with the solution from Pierce's Tables # 412 shown in the left panel below . Though the exponential field solution reaches infinity at time 4.7124 the constrained kinetic energy generates the same trajectory in an infinite time. Only a time of 6.9590 is shown in the right panel .





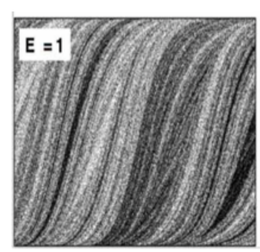


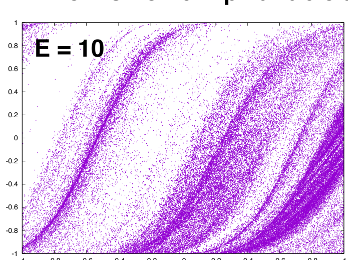
This same isomorphism holds for *any* field strength . It is another case in which *scaling the time* relates two different-seeming problems . The exponential field has a fractal spatial distribution but ⊕ is perfectly conserved !

* W G Hoover, B Moran, C G Hoover, and W J Evans, Physics Letters A 133, 114 - 120 (1988) .

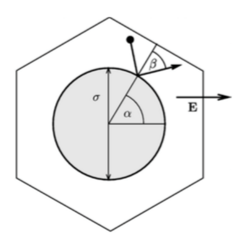
2. Interesting Model Variations for Transport*

Another way to generate nonequilibrium steady states is to extract heat by using a *constant* viscosity . Although this type of dynamics does not seem to be "reversible" it does fit our definition. Evidently changing the *sign* of the viscosity and running the trajectory backward would generate a mirror-image repellor while satisfying the same motion equations . Thus the constant-viscosity model shares many of its properties with the isokinetic Galton Board. The constant-viscosity phase space is more complicated, with four phase-space dimensions, with the momentum p variable at collisions characterized by α and β .





← Here is a projection of the viscous phase-space distribution onto the [α,sin(β)] plane . Here there is a wide range of kinetic energies so that the fractal structure is smeared a bit by the projection operation .



* W G Hoover, "Multifractals from Hamiltonian Many-Body Molecular Dynamics", Physics Letters A 235, 357 - 362 (1997) .

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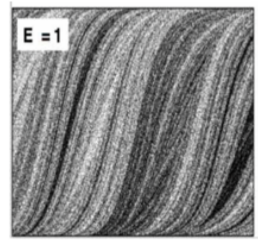
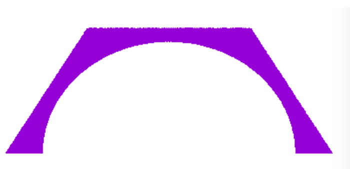
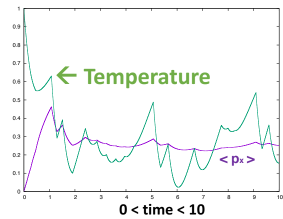




```
x = yy(1)
y = yy(2)
px = yy(3)
py = yy(4)
zeta = 0.001d00
yyp(1) = px
yyp(2) = py
yyp(3) = field - zeta*px
yyp(4) = - zeta*py
```



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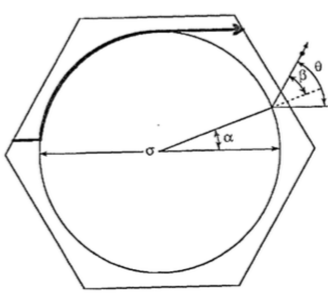
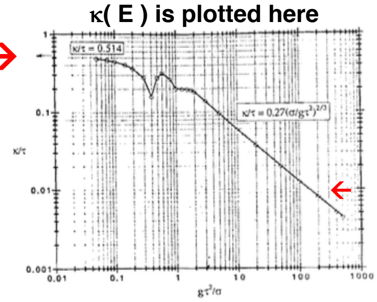
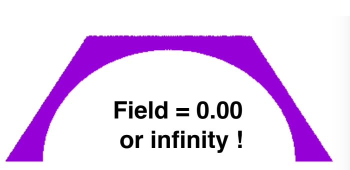


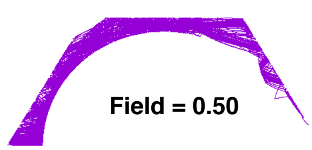
←Creep→

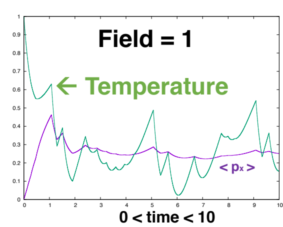
κ(E) is plotted here



← Green-Kubo







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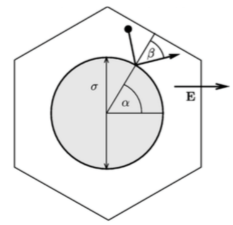
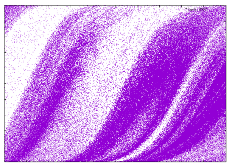
2. Interesting Model Variations for Transport

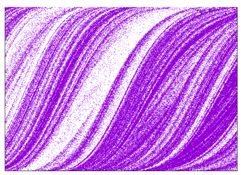


Because the 0532 and $\zeta\xi$ models provide ergodicity for the oscillator it is interesting to see how they do for the Galton Board. This increases the dimensionality by either one or two but we can still project the solutions onto the (α,sinβ) plane. Here is an 0532 sample for a field of 3 and T = 1 .



0532 Model with E = 3

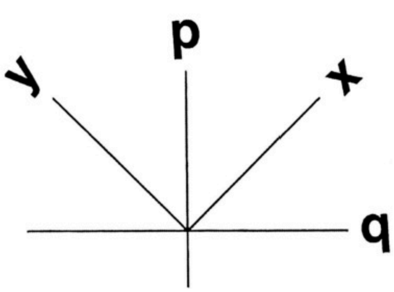
In two dimensions the generalization of the 0532 Model includes (dp/dt) = Force $-\zeta p[\ 0.05 + 0.032p^2\ ]$ where p^2 includes x and y . Likewise $(d\zeta/dt) = 0.05(\ p^2 - 2\ ) + 0.32(\ p^4 - 4p^2\ )$ with circularly symmetric $< p^2,p^4 > = (\ 2,8\ )$ rather than the one-dimensional (1,3) .



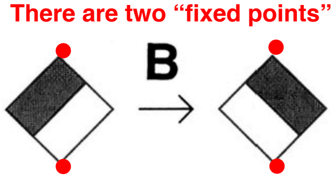
ZX Model with E = 3

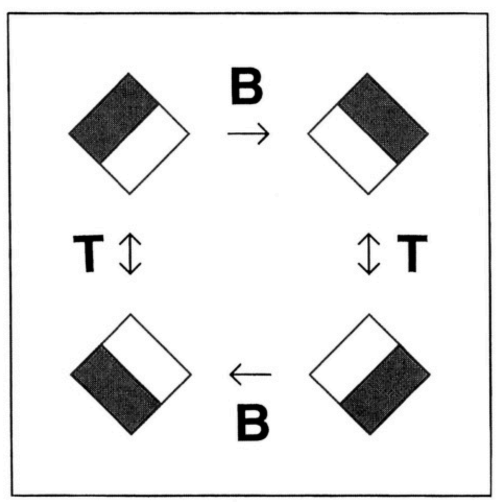
In two dimensions the generalization of the ZX Model includes (dp/dt) = Force $- \zeta p - \xi pp^2$ where p^2 includes x and y . Likewise $(d\zeta/dt) = (\ p^2 - 2\ )$ and $(d\zeta/dt) = (\ p^4 - 4p^2\ )$ with the circularly symmetric $< p^2,p^4 > = (\ 2,8\ )$, not the one-dimensional (1,3) .

3. An up-to-date Time Reversible Baker Map
[Chaos and Reversibility in Two Dimensions]

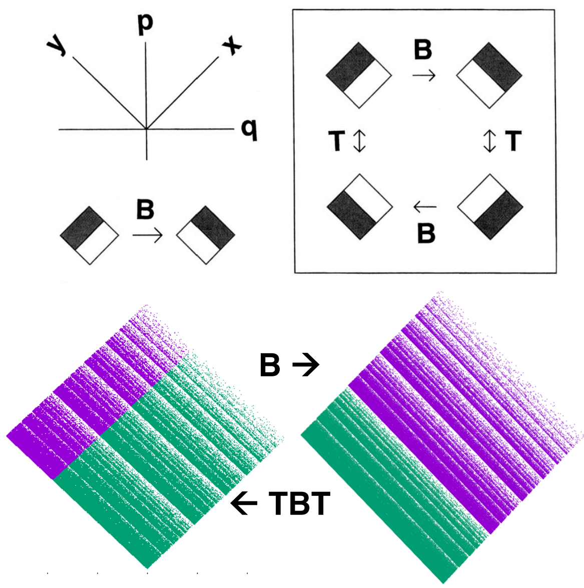


There are two "fixed points"





An Updated Version of the Baker Map



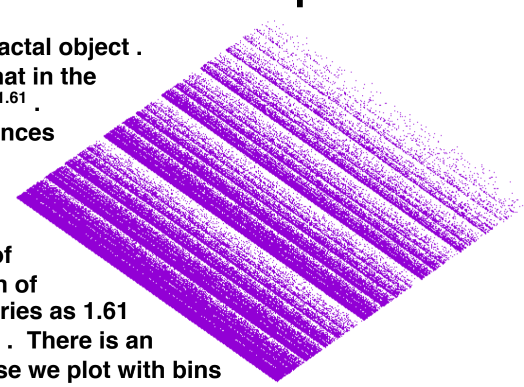
Equilibrium Chaos and Ergodicity
λ_1 = ln 2 = 0.69315 with no change in the comoving phase volume .

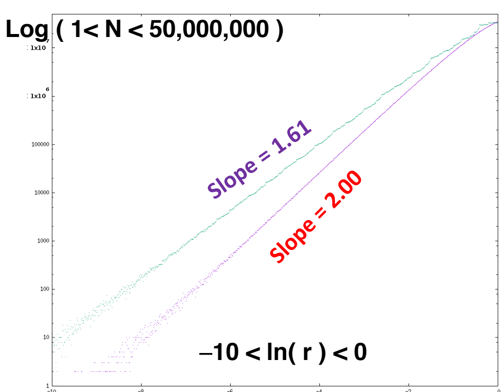
There is no qualitative difference between the Equilibrium and Nonequilibrium measures of chaos .

Nonequilibrium Chaos and Ergodicity
λ_1 = (1/3) ln 3 + (2/3) ln (3/2) = 0.63651 with volume changes of (1/2) (2/3) of the time and 2 (1/3) of the time . But of course the compression wins and a “strange attractor” is the result .

3. Equilibrium and Nonequilibrium Baker Maps

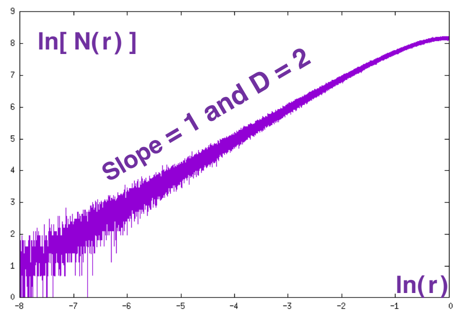
This dissipative time-reversible map → a nice ergodic fractal object . It has a correlation dimension of about 1.61 , meaning that in the vicinity of a point the number of other points varies as $r^{1.61}$. To see this we generate 100,000 points and bin the distances according to the value of ln(r) , using a bin width 0.01 .

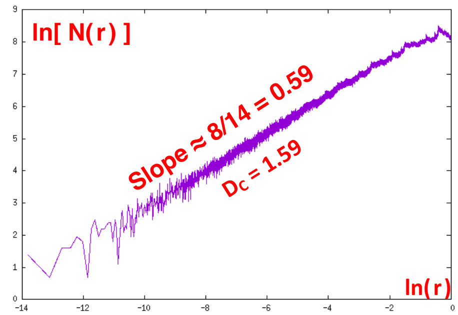




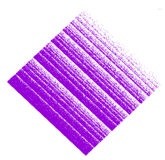
The number of points in a bin of width dln r varies as 1.61 or 2.00 power . There is an extra r because we plot with bins using dln(r) = dr/r . The correlation dimension is 2.00 at equilibrium and 1.61 for this nonequilibrium Baker Map . Because this map is designed to be time-reversible we can generate the repellor by changing the sign of the vertical coordinate p .

3. Correlation Dimension for Equilibrium and Nonequilibrium Baker Maps



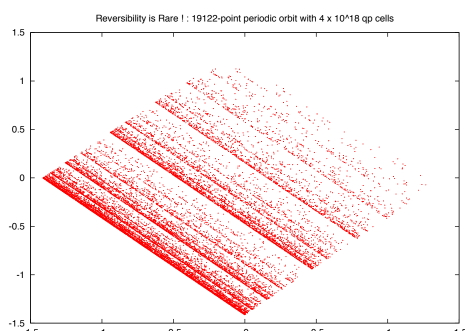


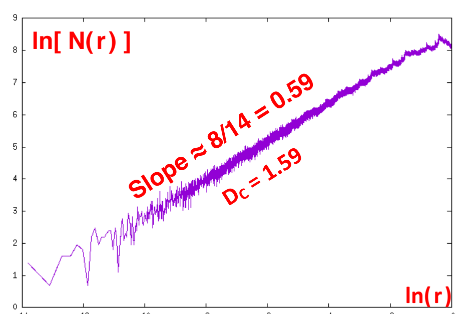
**Here is a comparison of the number of pairs of points in bins of fixed size dr at r .
From the Birthday Problem we expect the periodic orbit length to vary as $r^{1.59/2}$.
Grids of 200^2, 400^2, . . . 1000^2 gave irregular results with 249 the longest orbit .**

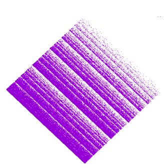


Even in this small two-dimensional problem , with a time-reversible mapping , the measure of trajectories which violate the Second Law [here corresponding to expansion rather than compression] is very small . We demonstrate this by spanning (qp) space with 4 x 10^{18} cells .

3. Correlation Dimension for Equilibrium and Nonequilibrium Baker Maps

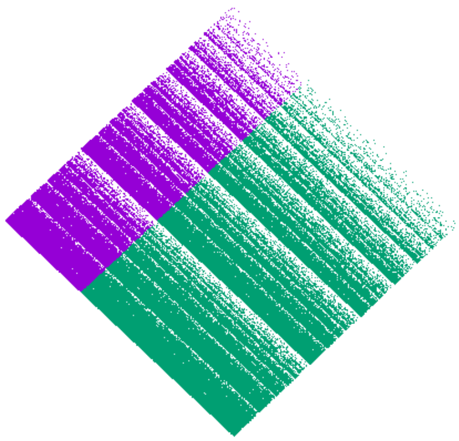




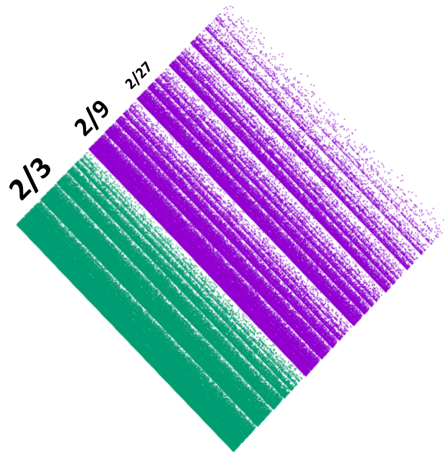


Even in this small two-dimensional problem , with a time-reversible mapping , the measure of trajectories which violate the Second Law [here corresponding to expansion rather than compression] is very small . We demonstrate this by spanning (q,p) space with 4 x 10^{18} cells . Starting with (q,p) = (0.6,0.8) we find a periodic orbit with 19,122 points . To make this reproducible let us look briefly at the details of the mapping .

3. The *Reversed* Nonequilibrium Baker Map



← TBT

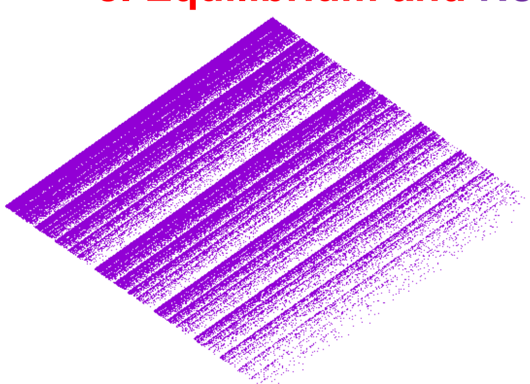


BEFORE

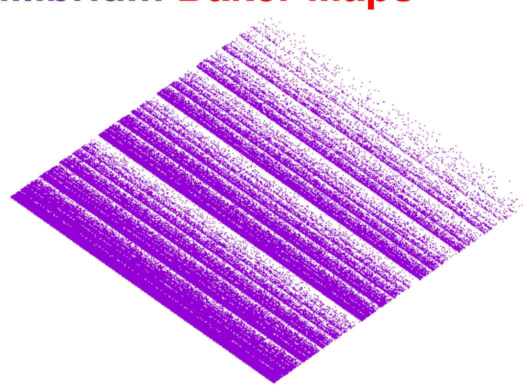
AFTER

ANY TRANSFORMATION THAT IS ERGODIC HAS *SOME* COMPRESSION AND EXPANSION .
MOST OF THE MAP CORRESPONDS TO COMPRESSION GIVING A STRANGE ATTRACTOR .

3. Equilibrium and Nonequilibrium Baker Maps



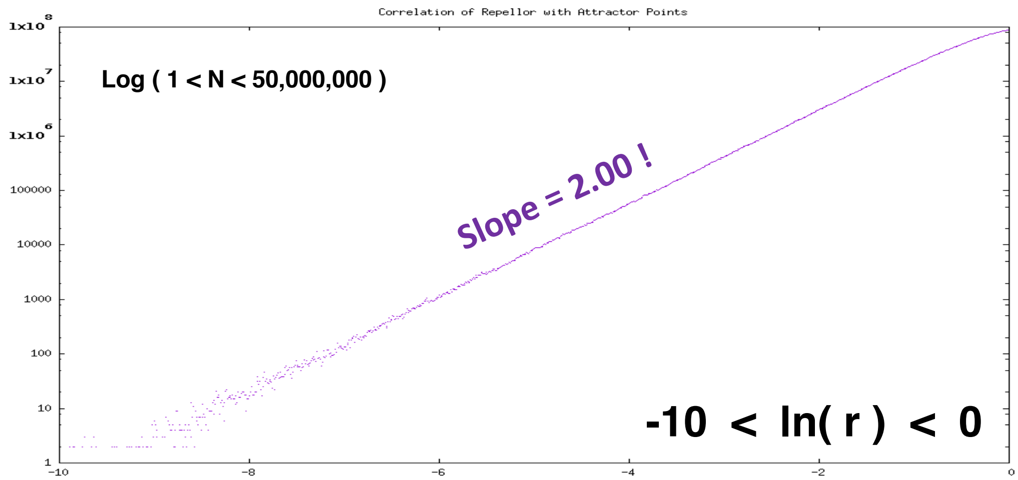
Repellor



Attractor

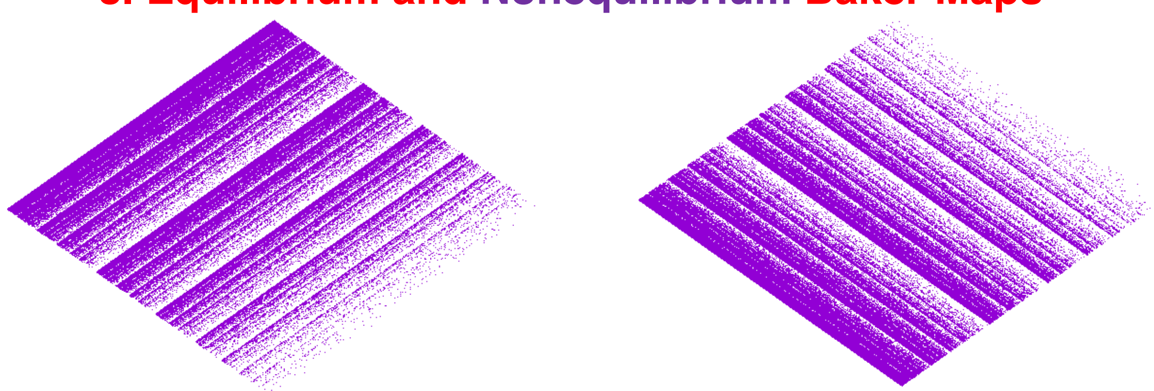
What do you suppose is the distribution of Attractor points near Repellor points ?

3. Equilibrium and Nonequilibrium Baker Maps



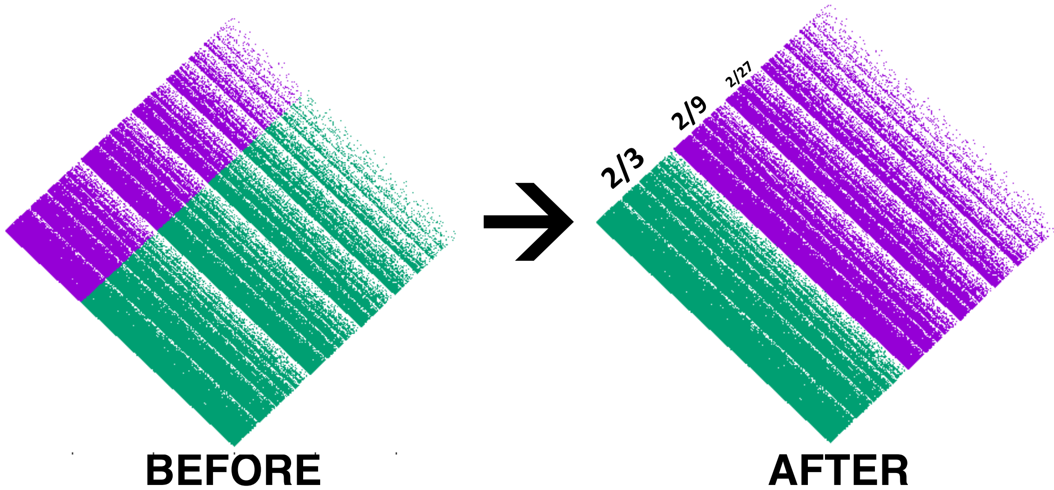
What do you suppose is the distribution of Attractor points near Repellor points ?

3. Equilibrium and Nonequilibrium Baker Maps



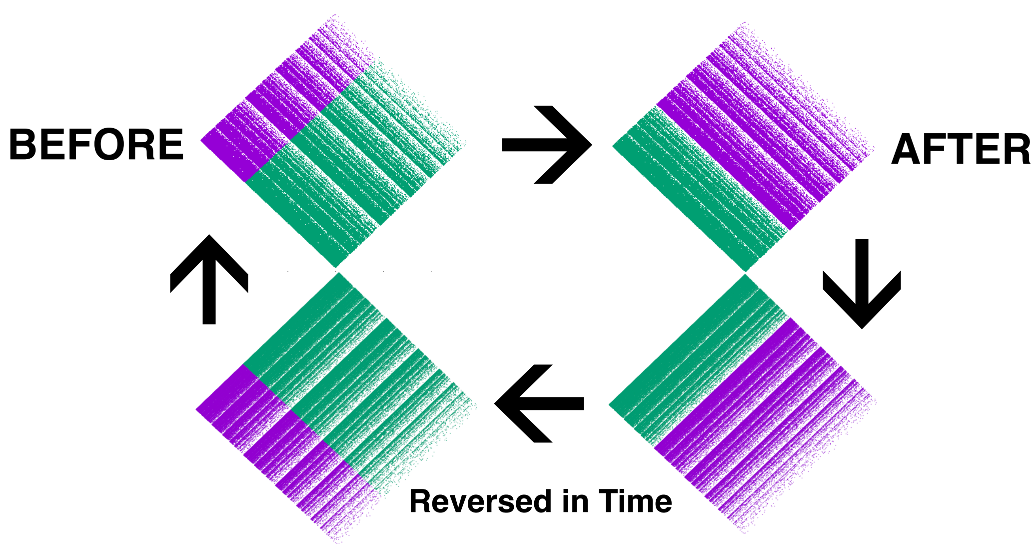
What do you suppose is the distribution of Attractor points near Repellor points ?
The distribution turns out to vary as r^2 ! There is ***no*** correlation between them !

3. The Nonequilibrium Baker Map



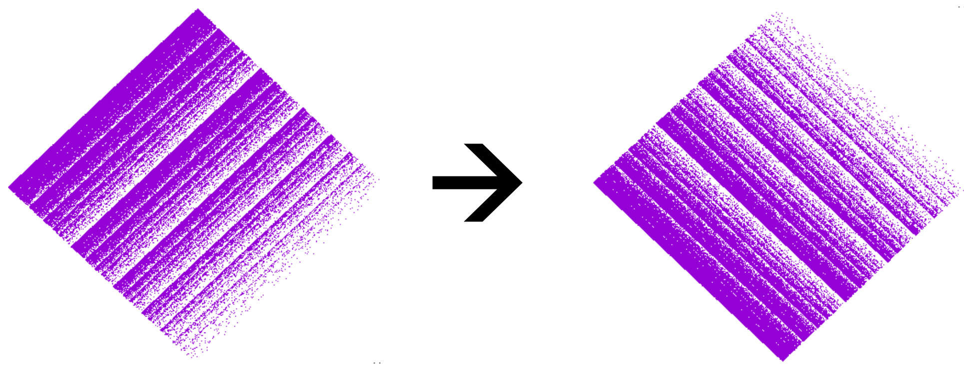
ANY TRANSFORMATION THAT IS ERGODIC HAS *SOME* COMPRESSION AND EXPANSION .
2/3 OF THE MAP CORRESPONDS TO COMPRESSION GIVING A STRANGE ATTRACTOR .

3. *Time Reversibility* of the Nonequilibrium Baker Map



ANY TRANSFORMATION THAT IS ERGODIC HAS *SOME* COMPRESSION AND EXPANSION .
MOST OF THE MAP CORRESPONDS TO COMPRESSION GIVING A STRANGE ATTRACTOR .

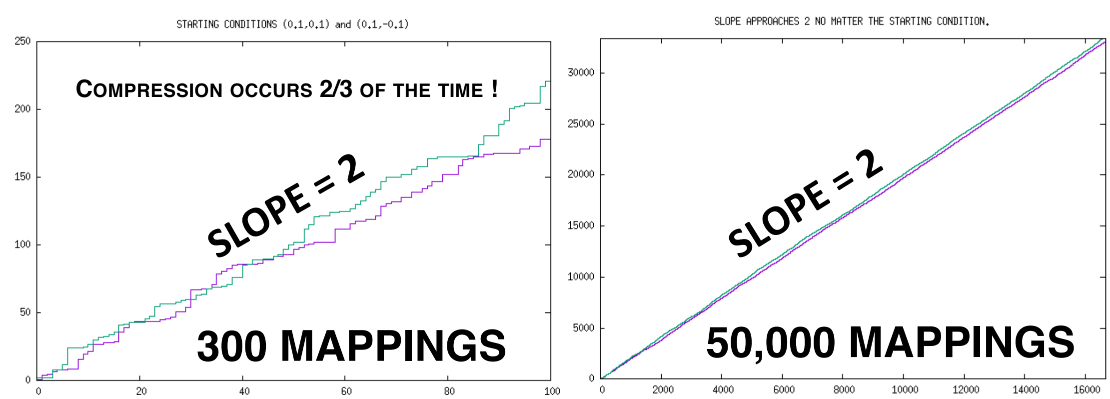
3. *Irreversibility* of the Nonequilibrium Baker Map



Repellor **Attractor**

ANY TRANSFORMATION THAT IS ERGODIC HAS *SOME* COMPRESSION AND EXPANSION .
MOST OF THIS MAP CORRESPONDS TO COMPRESSION GIVING A STRANGE ATTRACTOR .
THEREFORE THE STRANGE ATTRACTOR IS INEVITABLE AND THE REPELLOR IMPOSSIBLE !

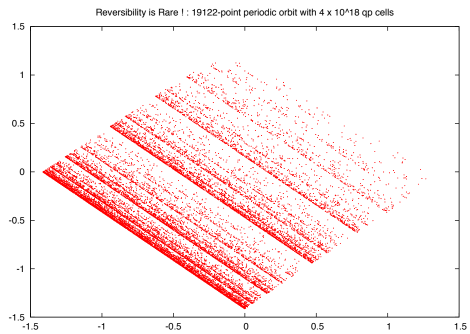
3. The Nonequilibrium Baker Map Compressions *versus* Expansions



The Second Law is Overwhelmingly Obeyed !

3. Correlation Dimension for Equilibrium and Nonequilibrium Baker Maps

n = 2 000 000 000 is the square root of Ω .




```
x = (+q + p)/dsqrt(2.0d00)
y = (-q + p)/dsqrt(2.0d00)
ixp = (x+1)*(n/2) + 1
iyp = (y+1)*(n/2) + 1
x = (ixp - 0.5d00*(n + 1))*(2.0d00/n)
y = (iyp - 0.5d00*(n + 1))*(2.0d00/n)

q = (x - y)/dsqrt(2.0d00)
p = (x + y)/dsqrt(2.0d00)
if(q.lt.p-dsqrt(2.0d00/9.0d00)) then
qp = 11*q/6.0d00 - 7*p/6.0d00 + dsqrt(49.0d00/18.0d00)
pp = 11*p/6.0d00 - 7*q/6.0d00 - dsqrt(25.0d00/18.0d00)
endif

if(q.gt.p-dsqrt(2.0d00/9.0d00)) then
qp = 11*q/12.0d00 - 7*p/12.0d00 - dsqrt(49.0d00/72.0d00)
pp = 11*p/12.0d00 - 7*q/12.0d00 - dsqrt( 1.0d00/72.0d00)
endif

x = (+qp + pp)/dsqrt(2.0d00)
y = (-qp + pp)/dsqrt(2.0d00)
```

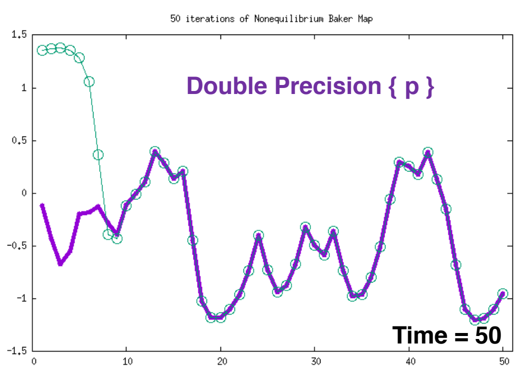
← **Here is the conversion to a grid**

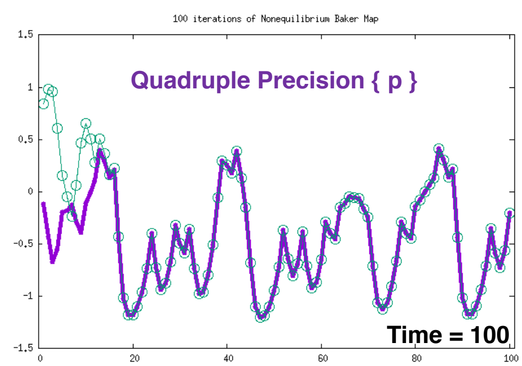
This solution is time-reversible . Using a reversed initial condition (0.6,-0.8) rather than (0.6,+0.8) finds itself on exactly the same periodic orbit of 19 122 points . But this is *not* what is meant by reversibility .

3. Summary from the Standpoint of the Baker Map

Compare the reversibility of the mapping using double and quadruple precision arithmetic .

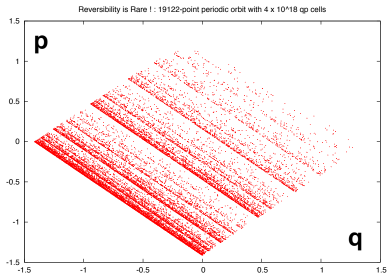
17 decimal digits in double precision and 38 decimal digits in quadruple precision

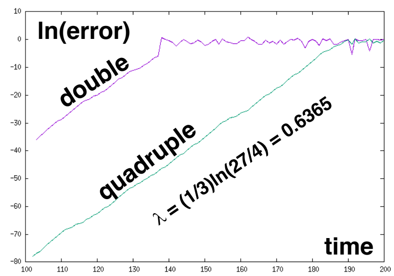




50 Double Precision and 100 Double Precision Iterations in Both Time Directions from (0,0)

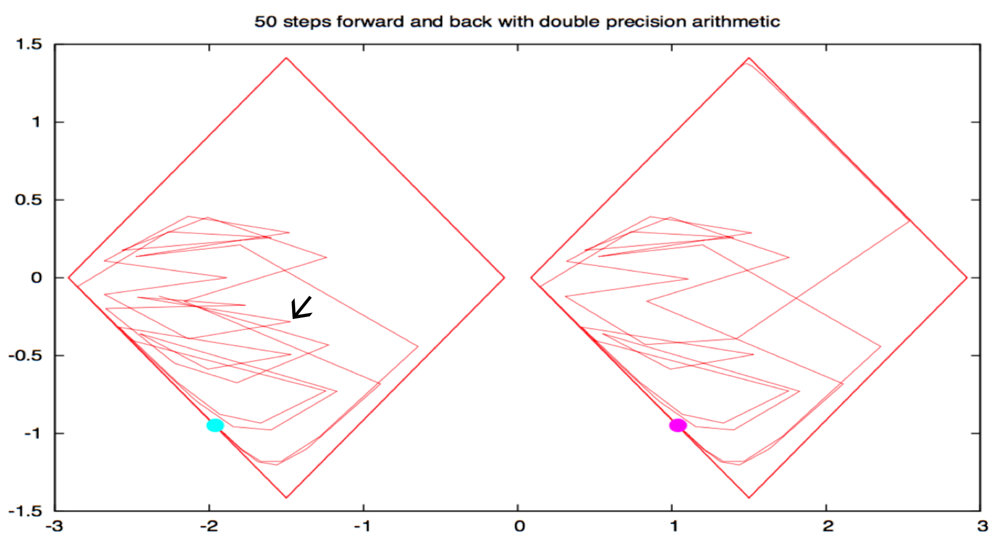
3. Correlation Dimension for Equilibrium and Nonequilibrium Baker Maps



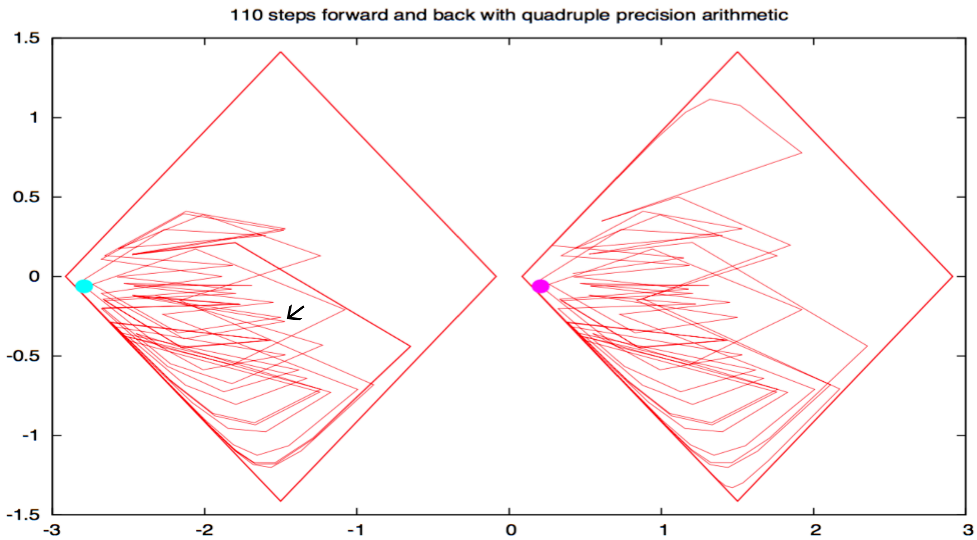


Running the map forward for 100 steps, reversing the momentum and running backward gives a separation between the forward and backward points which grows exponentially until the difference is "random" in size . About 40 iterations for double precision and 80 for quadruple precision are enough to eliminate correlation between the forward and backward trajectories . The *averaged* Lyapunov exponent over the entire map gives ln(3) one third of the time and ln(3/2) two thirds of the time but this small sequence gives a somewhat larger rate of divergence . No matter where one starts new information is generated by the stretching algorithm , soon overwhelming any remaining knowledge of the past . The existence of the periodic solutions is a consequence of the finite phase-space available computationally . The strange attractor is gradually approached by making the mesh finer and finer while the fraction of the mesh that is covered goes rapidly to zero as $\Omega^{D/2}/\Omega$.

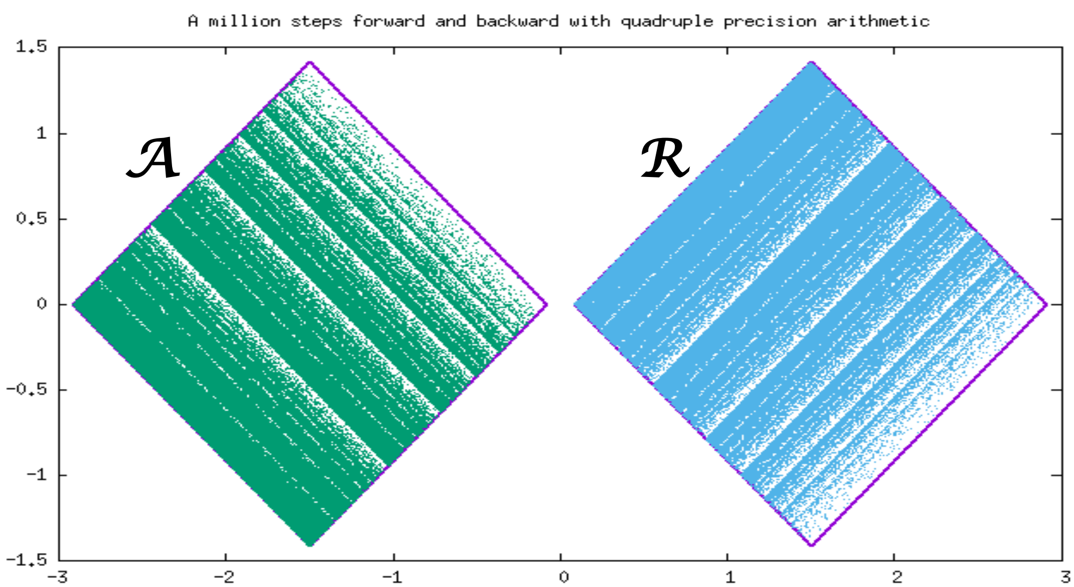
3. Summary from the Baker Map Using Double Precision and 50 Steps



3. Summary from the Baker Map Using Quadruple Precision and 110 Steps



3. Summary from the Standpoint of the Baker Map



3. Summary from the Standpoint of the Baker Map

The Baker Map is chaotic and ergodic , both at equilibrium and away .

The Lyapunov exponent is of order unity in both these cases .

The inverse of the Baker Map , TBT , can reverse for about 100 steps .

The forward map B converges to the Attractor with $D_C = 1.59$.

Once roundoff error is amplified by λ_1 the reversed map is a Repellor .

There is no fractal correlation between Attractor and Repellor points .

The areas of both the Attractor and Repellor are zero. They are *unlikely* .

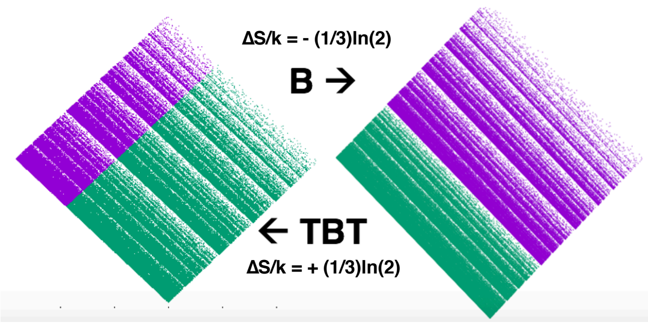
The number of states in the stationary state is of order $\Omega^{D_C/2}$.

4. The Fluctuation Theorem as seen with the Baker Map

In their seminal 1993 paper "Probability of Second Law Violations in Shearing Steady States" , [Physical Review Letters 71, 2401-2404 (1993)] Denis Evans, Eddie Cohen, and Gary Morriss formulated the relative measures of forward to backward motion in terms of entropy production :

$$\mu_{forward} / \mu_{backward} = e^{\Delta S/k}$$

Here the entropy follows Gibbs' statistical mechanics and corresponds to the logarithm of the phase-space volume, $S = k \ln \Omega$. We illustrate their idea using our time-reversible but dissipative Baker Map :

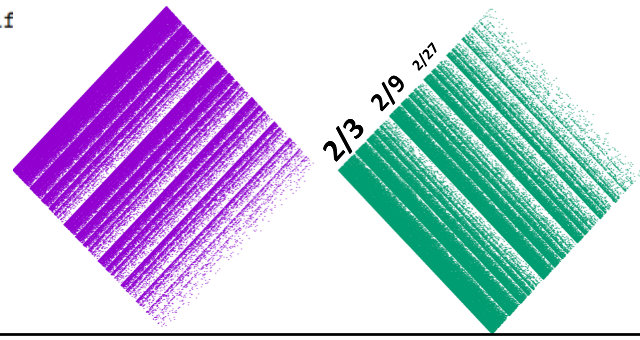


What about Einstein ?

4. The Fluctuation Theorem as seen with the Baker Map

```
if(q.lt.p-dsqrt(2.0d00/9.0d00)) then !  EXPANDING !
qp = 11*q/6.0d00 - 7*p/6.0d00 + dsqrt(49.0d00/18.0d00)
pp = 11*p/6.0d00 - 7*q/6.0d00 - dsqrt(25.0d00/18.0d00)
endif
if(q.gt.p-dsqrt(2.0d00/9.0d00)) then !  CONTRACTING !
qp = 11*q/12.0d00 - 7*p/12.0d00 - dsqrt(49.0d00/72.0d00)
pp = 11*p/12.0d00 - 7*q/12.0d00 - dsqrt( 1.0d00/72.0d00)
endif
```

Repellor →



← Attractor

4. The Fluctuation Theorem as seen with the Baker Map

This time-reversible dissipative Baker Map contracts 2/3 of the time and expands 1/3 , behaving just like an RL random walk . To show this consider 27 000 000 iterations of the Baker Map confirming the sequences' frequencies to an accuracy of 3 or 4 figures :

R = 18M , L = 9M ;
RR = 12M , RL = LR = 6M , LL = 3M ;
RRR = 8M , RRL = RLR = LRR = 4M , RLL = LRL = LLR = 2M , LLL = 1M

The Evans + Cohen + Morriss Fluctuation Theorem * relates the relative probabilities of forward and backward trajectory segments to the entropy production for those segments :

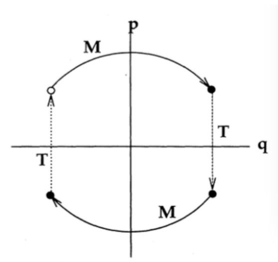
$$\mu_{forward}/\mu_{backward} = e^{\Delta S/k} = \Delta\Omega$$

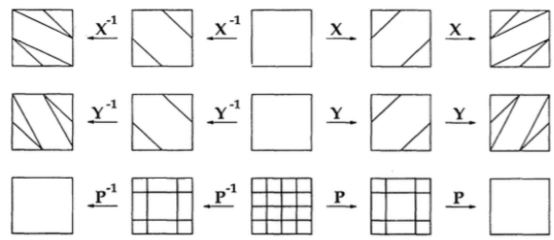
R/L = 2 corresponds to the twofold changes in area
RR/LL = 4 corresponds to the fourfold changes in area
RRR/LLL = 8 corresponds to the eightfold changes in area

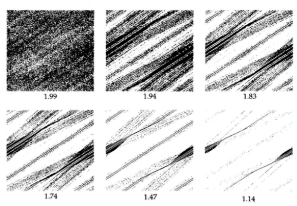
The Fluctuation Theorem describes the change in Gibbs' entropy due to a time-reversible dissipative process . There is a voluminous literature on this subject !

*** "Probability of Second Law Violations in Shearing Steady States" ,**
[D J Evans + E G D Cohen + G Morriss , Physical Review Letters 71, 2401-2404 **(1993)]**
There is much related work on "Crooks' Fluctuation Theorem" and "Jarzynski's Equality"

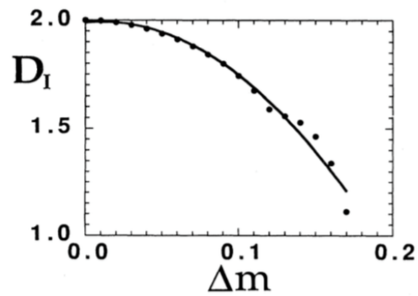
5. Dimensionality Loss in Time-Reversible Maps*





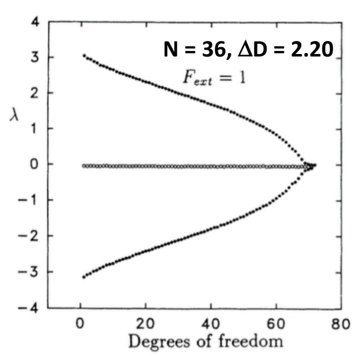


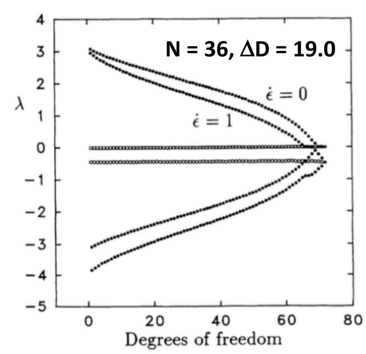
XYPYX with six values of Δm :
0.01, 0.05, 1/12, 0.10, 0.15, 0.17
[m = 0.25 is "equilibrium" $\Delta m = 0$]



* W. G. Hoover, O. Kum, and H. A. Posch, Physical Review E 53, 2123 – 2129 (1996) . TRCSAC .

5. Dimensionality Loss in Color Conductivity and Steady Shear Simulations*
Nonequilibrium Steady States Occupy a Vanishing Phase-Space Volume !





A wide variety of systems shows phase-space dimensionality losses from the Lyapunov spectrum .
The N = 100 dimensionality losses are 8.38 and 53.1 for the same field and the same strain rate .
In order to see whether or not the loss persists in the large-system limit the dependence on the number of thermostated particles was studied and found to suggest that the loss is real , and was minimized when all of the particles were thermostated , as in the results above . $\phi(r) = 100(1 - r^2)^4$.

* W. G. Hoover and H. A. Posch, Physical Review E 49 , 1913 - 1920 (1994) .

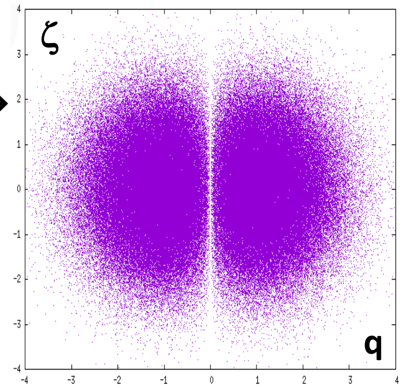
6. 0532 Model Spectra at and away from Equilibrium

These are ergodic equations for an oscillator with T = 1 :

$$(dq /dt) = p \; ; \; (dp /dt) = - q - \zeta [0.05p + 0.32(p^3/T)] \; ;$$

$$(d\zeta /dt) = 0.05[(p^2/T) - 1] + 0.32[(p^4/T^2) - 3(p^2/T)] \; .$$

The Poincaré Section has no holes .
Section with p = 0 has a "nullcline" →



0532 Model is time-reversible as well as deterministic : Change the signs of dt, p, and ζ . (dq/dt) changes sign ; (dp/dt) is unchanged as is also ($d\zeta$ /dt) . This also applies away from equilibrium where $T \equiv 1 + \varepsilon \tanh(q)$. The equilibrium distribution is Gaussian in q , p , and ζ .

6. 0532 Model Spectra at Equilibrium

These are ergodic* equations for an oscillator with T = 1 :

$$(dq /dt) = p \; ; \; (dp /dt) = - q - \zeta [0.05p + 0.32(p^3/T)] \; ;$$

$$(d\zeta /dt) = 0.05[(p^2/T) - 1] + 0.32[(p^4/T^2) - 3(p^2/T)] \; .$$

$$f(q,p,\zeta) = (2\pi)^{-3/2} \exp[- (q^2/2) - (p^2/2) - (\zeta^2/2)]$$

* Ergodic, time- reversible, and chaotic

[0] All (q,p,ζ) can be reached by the time-reversible dynamics .

[1] At equilibrium the distribution is Gaussian in q , p , and ζ .

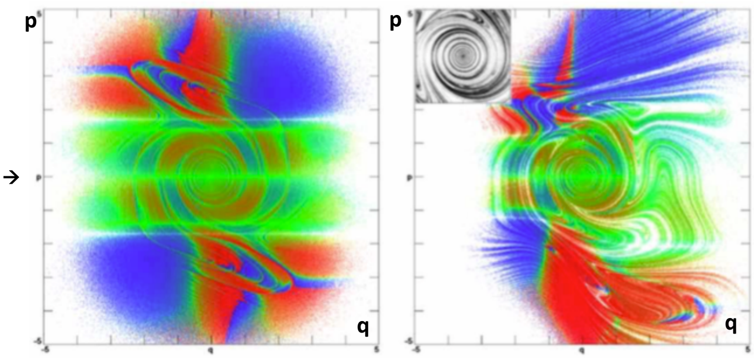
[2] The Lyapunov exponent $\lambda_1 = \langle \lambda_1(t) \rangle$ is independent of ($qp\zeta$)$_0$.

[3] The Poincaré Section has no holes .

6. 0532 Model z = 0 Sections At and Away from Equilibrium

$$(d\ln\oplus/dt) = \lambda_1(t) + \lambda_2(t) + \lambda_3(t) = -\zeta\,[\,0.05 + 0.96p^2\,]$$

Inversion symmetry →



$\varepsilon = 0.00$
$\{ 0.144, 0, -0.144 \}$
Ergodic Gaussian Distribution

$\varepsilon = 0.50$
$\{ 0.113_5, 0, -0.145_4 \}$
Multifractal Strange Attractor

Notice that changing the sign of p does not just change the sign of $\lambda_1(t)$!

6. 0532 Model Thermodynamics Away from Equilibrium

1. Consider the change of Gibbs entropy of the System due to heat loss :

$$(dS/dt) = +\zeta\,[\,0.05(p^2/T) + 0.32(p^4/T^2)\,]$$

2. Consider the change of Phase Volume of the System due to heat loss :

$$(d\ln\oplus/dt) = -\zeta\,[\,0.05 + 0.96(p^2/T)\,]$$

3. Notice that a time average relates the expressions 1 and 2 :

$$\langle \zeta(d\zeta/dt) \rangle = 0 = \langle \zeta \{ 0.05[(p^2/T) - 1] + 0.32[(p^4/T^2) - 3(p^2/T)] \} \rangle$$

so that $\langle \zeta\,[\,0.05(p^2/T) + 0.32(p^4/T^2)\,] \rangle = \langle \zeta\,[\,0.05 + 0.96(p^2/T)\,] \rangle$

$$\langle (dS/dt) \rangle_{\text{HEAT}} = \langle (d\ln\oplus/dt) \rangle_{\text{DYNAMICS}}$$

Standard Thermodynamics applies to the 0532 Model so long as the results are independent of initial conditions !

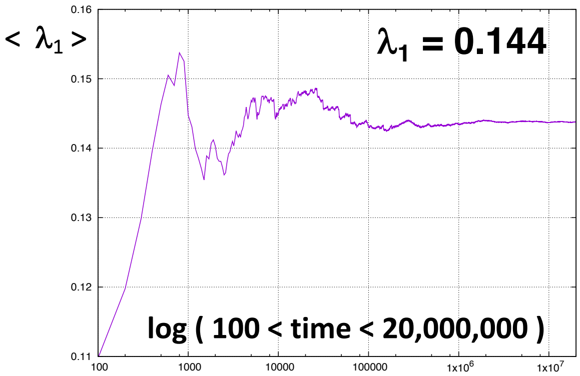
6. 0532 Model Spectrum away from Equilibrium

$(dq/dt) = p \; ; \; (dp/dt) = -q - \zeta [0.05p + 0.32(p^3/T)] \; ;$

$(d\zeta/dt) = 0.05[(p^2/T) - 1] + 0.32[(p^4/T^2) - 3(p^2/T)]$ with

$\langle (d\ln \oplus /dt) \rangle = -\zeta [0.05 + 0.96(p^2/T)] = \lambda_1 + \lambda_2 + \lambda_3 < 0$.

Because λ_2 *must vanish* $\lambda_1 + \lambda_3 < 0$.

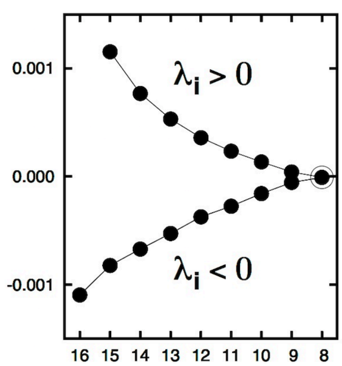


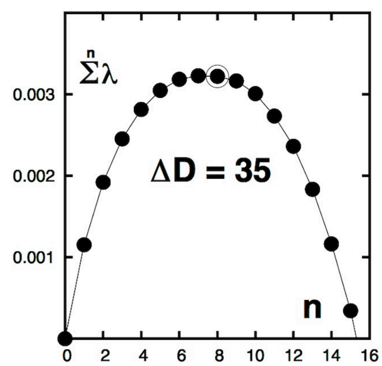
Because the motion is ***ergodic*** linear-response theory can be applied to the model . One way to obtain nonequilibrium simulations is to set the temperature equal to $T(q) = 1 + \varepsilon \tanh(q)$. This turns out to generate a hot-to-cold heat current which can be related to fluctuations through Green and Kubo's theory . We expect a strange attractor or a limit cycle to result .

7. ϕ^4 Model for Chaos and Heat Conduction with Substantial Fractal Dimensionality Loss*

$$\mathcal{H} = K + \Phi_{\text{tethers}} + \Phi_{\text{pairs}} = \sum_i^N [\, (p_i^2/2) + (q_i^4/4) \,] + \sum_{i<j}^{\text{pairs}} (q_i - q_j)^2/2$$

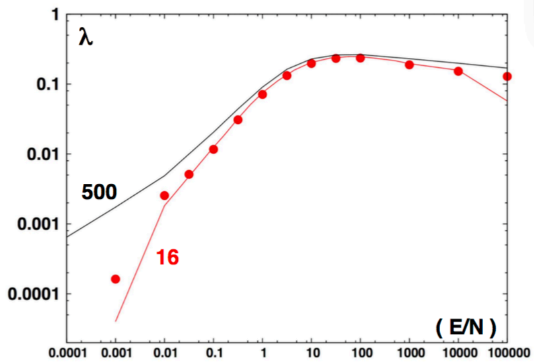
There are 24 particles in the chain, 24 coordinates, 24 momenta, and two friction coefficients, one cold and one hot, so that the phase space has 50 dimensions in all . Temperatures are 0.003 and 0.027 .

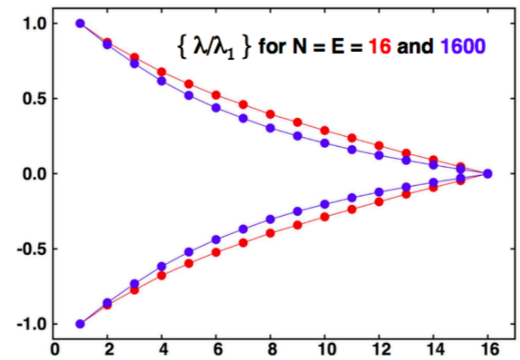




* Hoover and Aoki, Order and Chaos in the One-Dimensional ϕ^4 Model : N-Dependence and the Second Law of Thermodynamics = arXiv 1605.07721 submitted to PRE (2016) .

7. ϕ^4 Model for Chaos and Heat Conduction *





The Model is chaotic over a wide range of energies despite its Hamiltonian character . The spectrum of Lyapunov exponents has a relatively simple structure . Its chaotic nature makes it possible to obey Fourier's law of heat conduction, $Q_x = -\kappa(\, dT/dx\,)$ over a wide range of energy and dimensionality .

* W G Hoover and K Aoki, "Order and Chaos in the One-Dimensional ϕ^4 Model" = arXiv 1605.07721 .

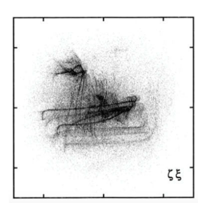
7. ϕ^4 Model for Chaos and Heat Conduction *

The ϕ^4 Model was the first that I know of that produced overwhelming evidence of the pervasive fractal structures in nonequilibrium steady states. Other models, where Newtonian particles were driven by a few boundary particles at the corners, or on the edges, typically showed fractal dimensions only a bit less than the full dimensionality of the phase space .

Kaplan and Yorke suggested that the fractal dimension be determined by interpolating between the last positive sum of exponents and the first negative sum . Although this idea works well for some attractors there are others for which it definitely fails . For a doubly-thermostated oscillator with two friction coefficients and a temperature which varies as $0 < T(q) = 1 + \tanh(q) < 2$ the Kaplan-Yorke interpolation gives $D_{KY} = 2.80$ while the precise bin-counting measurement gave an information dimension $D_I = 2.56$.

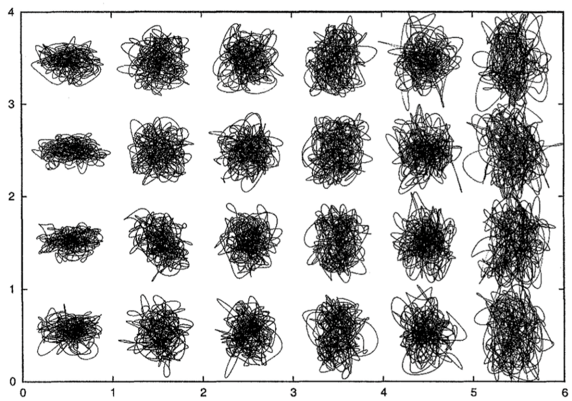
$(dq/dt) = p$; $(dp/dt) = -q - \zeta p - \xi p^3$; NOTE THAT (p^3/T) IS BETTER !

$(d\zeta/dt) = p^2 - T$; $(d\xi/dt) = p^4 - 3p^2T$



This projection of the fractal into the (ζξ) plane is taken from Hoover, Hoover, Posch, and Codelli, Communications in Nonlinear Science and Numerical Simulation (2005) .

7. ϕ^4 Model for Chaos and Heat Conduction *



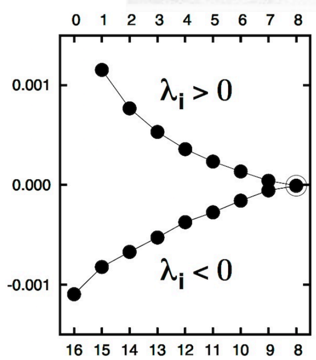
The leftmost four particles are "cold" While the rightmost four are "hot" , using two Nosé-Hoover thermostat variables. The remaining 16 particles are Newtonian . All nearest-neighbor pairs interact with Hooke's-Law springs and every particle is tethered to its own lattice site with a quartic potential .

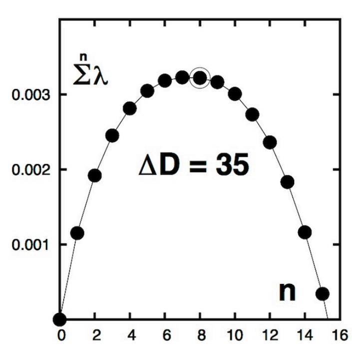
The one-dimensional version of this Model gave the first deterministic and time-reversible simulations in which a majority of the phase-space dimensions were missing in the nonequilibrium strange attractor .

* Hoover, Aoki, Hoover, de Groot, [Physica D 187, 253 (2004)] includes a comparison of 7 thermostats .

7. ϕ^4 Model for Chaos and Heat Conduction *

The one-dimensional version of the ϕ^4 Model provided the first simulations in which most of the phase-space dimensions were missing in the nonequilibrium strange attractor .





We consider a 24-particle chain with two Nosé-Hoover particles at the ends (with temperatures of 0.003 and 0.027) with D = 50 .

The (48 + 2) dimensional phase space contains a 15-dimensional strange attractor corresponding to the loss of 35 dimensions ! ROTATION of the δ vectors *must* be the cause of this great loss .

* Simulation and Control of Chaotic Nonequilibrium Systems (2015) , page 205 .

8. Summary

In 1987 it became obvious that time-reversible deterministic steady-state simulations of mass, momentum, and energy flows *always* obey the Second Law of Thermodynamics, forming a phase-space strange attractor and a mirror-image repellor. The fractal repellor is unobservable in that it occupies zero phase-space volume and has also an *unstable* Lyapunov spectrum with a positive sum : $\Sigma\lambda = -\#\zeta = -d\ln f/dt = d\ln\oplus/dt = d(S/k)/dt$.

1. The Galton Board exhibits both adiabatic and isokinetic Time-Reversible Fractals .
2. Finite-Precision stationary states are related to the D_C and to $\sqrt{\Omega}$ at equilibrium .
3. Reversible Baker Maps provide a 2D version of ergocity, chaos, and the Second Law .
4. 0532 Model Spectra at and away from Equilibrium provide ergodic 2D sections .
5. At and away from Equilibrium ϕ^4 Model spectra provide vivid dimensionality losses .
6. These models suggest many promising research areas .

In retrospect it is "obvious" that a constant-viscosity homogeneous simulation of mass , momentum , or energy flows would lead to about the same dimensionality loss without any ambiguity . One merely needs to accept the presence of a heat sink in the equations of motion, $\{ (dp/dt) = F - \zeta p \}$. Remember that Hamiltonian systems permit no heat flow .

8. Summary Continued . . .

[1] It is a useful exercise to show that the two-dimensional generalizations of the 0532 and $\zeta\xi$ models are consistent with Gibbs' canonical distribution by using Liouville's continuity equation in the many-dimensional phase space. This is "straightforward but tedious" .

[2] A somewhat paradoxical feature of mechanics is that observing a section of trajectory does not reveal whether or not the comoving volume is changing . On the other hand, by extending the trajectory, so as to fill the accessible part of the phase space , we can generate the "natural measure" or distribution and figure out whether the flow is "conservative", in the sense of keeping the comoving volume constant, or "dissipative" , in the sense of allowing the comoving volume to change , sometimes generating a strange attractor .

[3] Evidently the motion equations cannot be determined from the trajectory . We just saw that the exponential field and the constant field with an isokinetic constraint provide isomorphic trajectories . The one-dimensional trajectory and the many-dimensional flow are not the same , although evidently either can be determined by studying the other .

[4] It is amusing that the local Lyapunov exponents for flows vary in a fractal manner !

8. Summary Continued . . .

[4 , continued] It is amusing that the local Lyapunov exponents for flows vary in a fractal manner ! The two examples below are Taken from our study of the ergodic MKT harmonic oscillator , explored with Dennis Isbister and published in January of 2001 .

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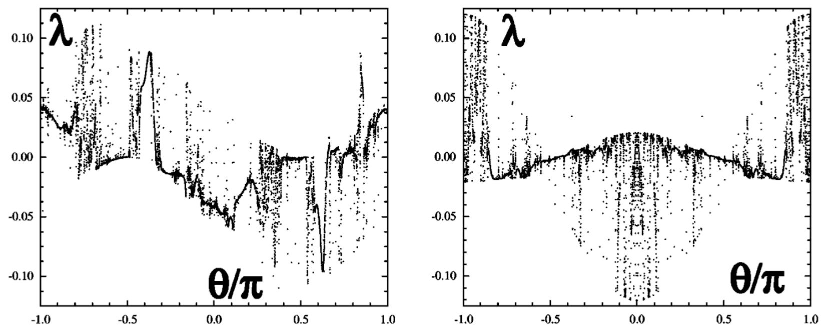

FIG. 2. Variation of the local (instantaneous) Lyapunov exponents $\lambda_1(\theta)$ along two circles in phase space. At the left both q and ζ are $0.1\cos\theta$ while p and ξ are $0.1\sin\theta$. At the right q and $-p$ are $-0.1\sin\theta$ while ζ and $-\xi$ are $-0.1\cos\theta$. In both cases the phase-space location parameter θ varies from $-\pi$ to $+\pi$. Each of the 10^4 points represents a reversed trajectory of 10^6 time steps with $dt=0.001$.