Chapter 5

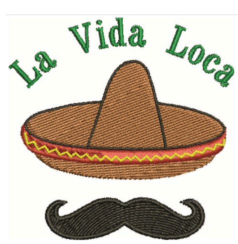
Kharagpur Lectures

1. Ergodicity and Its Importance in Small Systems
2. Gibbs' Ensembles and Linear-Response Theory
3. Ergodicity of Hard-Disk and Soft-Disk Cell Models
4. Nosé-Hoover Oscillator and the Chaotic Sea
5. Complicated Tori discovered by Wang and Yang
6. Ergodicity of Oscillator Models : 1984 - 2016
7. Singly-Thermostated Ergodicity : Logistic Thermostat

William G. Hoover
Ruby Valley Nevada
December 2016

Kharagpur Lectures

1. Ergodicity and Its Importance in Small Systems



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1. Ergodicity and Its Importance in Small Systems

Gibbs' microcanonical (constant energy) and canonical (constant temperature) ensembles include all phase-space states , an ellipse or a Gaussian distribution for the harmonic oscillator . This is an important consideration for small systems , where fluctuations are large . Nosé's idea was to extend the (q,p,s,ζ*) phase space in order to make all of the states accessible with Gibbs' distribution :

$$f(q,p) \propto e^{[- (1/2)(q^2 + p^2)]}$$

This attempt failed . The simpler Nosé-Hoover approach, with just (q,p, ζ) and

$$f(q,p,\zeta) \propto e^{[- (1/2)(q^2 + p^2 + \zeta^2)]}$$

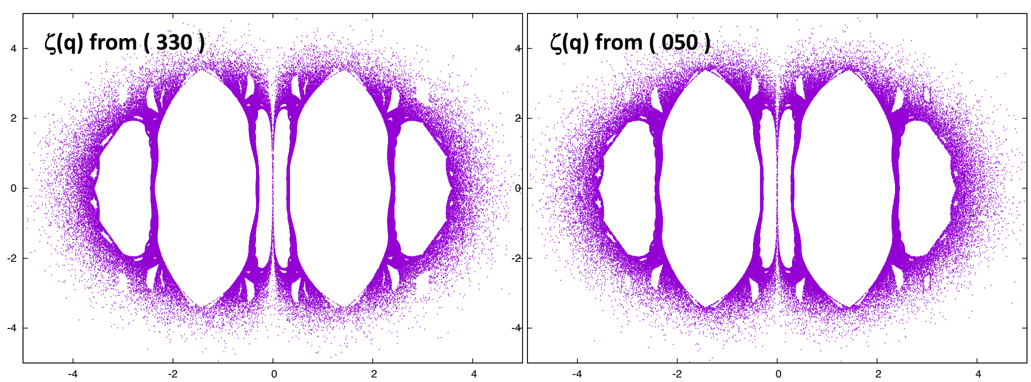
is equally far from ergodic . This can be seen by looking at a chaotic Poincaré section , choosing (q,ζ) points to plot whenever p changes sign . Two chaotic initial conditions are (3,3,0) and (0,5,0) . Let us look at the Poincaré sections .

*** Remember that ζ is the "conjugate momentum" associated with the time-scaling s .**

Ergodicity and Its Importance in Small Systems

Nosé-Hoover Poincaré Sections with initial (qpζ) = (330) and (050)

{ (dq/dt) = p ; (dp/dt) = – q – ζp ; (dζ/dt) = p² – 1 }



About 250 000 points appear in each of these (q 0 ζ) sections from trajectories of 1 000 000 000 steps of 0.001 each .

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2. Gibbs' Ensembles and Linear-Response Theory

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Perturbation Theory Based on Gibbs' Canonical Distribution

Gibbs' distribution, like the Maxwell-Boltzmann velocity distribution, provides a basis for perturbation theory , the "Green-Kubo" linear-response theory, based on adding a perturbation to the Hamiltonian. When the distribution is *linearized* so that

$$e^{[-(\mathcal{H}+d\mathcal{H})/kT]} \rightarrow e^{[-(\mathcal{H}/kT)]}[1-(d\mathcal{H}/kT)+\ldots]$$

It becomes possible to find the linear response, typically in the form of a time correlation function which is to be evaluated in the equilibrium Gibbs' ensemble .

By choosing appropriate perturbations (a constant field can drive diffusion and a constant strain rate , with x velocity proportional to y , can drive viscosity) the transport coefficients can all be written in terms of equilibrium correlation functions .

This convenient perturbation theory is not so easily interpreted if the equilibrium distribution is not actually realized by the system dynamics . Ergodicity is vital .

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3. Ergodicity of Hard-Disk and Soft-Disk Cell Models

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3. Ergodicity of Hard-Disk and Soft-Disk Cell Models

Nándor Simányi has written a 58-page paper , arXiv:math/0008241 , entitled "Proof of the Boltzmann-Sinai ergodic hypothesis for typical hard disk systems" . This 2003 work goes back to 1970 and is noteworthy for its complexity . There is no reason to doubt that this ergodicity is due to the effect of scattering from a convex surface , as was demonstrated in Carol's second lecture .

Back in 1996 Harald Posch , Franz Vesely , and I speculated that a two-dimensional soft-disk system was likewise ergodic in our work on the "Canonical Dynamics of the Nosé Oscillator" , Physical Review A 33 , 4253-4265 **. Unlike the "event-dominated" hard-disk problem the soft-disk problem , with $\phi(r) = 3(1 - r)^4$ and an energy of unity is a good example . How do we best test such models' ergodicity ?**

3. Ergodicity of Hard-Disk and Soft-Disk Cell Models

How do we best test such models' ergodicity ?

An effective approach is to choose random initial conditions , all with the same microcanonical energy or from the same canonical distribution and to look for differences in their long time behavior (moments, Lyapunov exponent , . . .) .

With a soft-disk cell model problem it is apparent that regular solutions can be obtained for specially symmetric initial conditions such as a velocity nearly parallel to the cell axes . So long as these conditions have a finite measure (not just a single orbit , but a measurable collection of orbits) there is no possibility of ergodicity and the phase-space dynamics will be a messy collection of chaotic and regular regions .

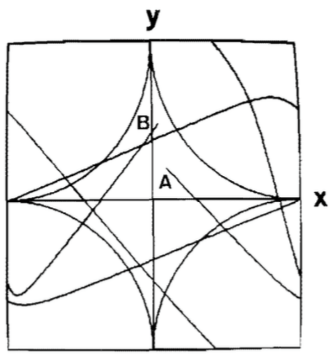
3. Ergodicity of Hard-Disk and Soft-Disk Cell Models

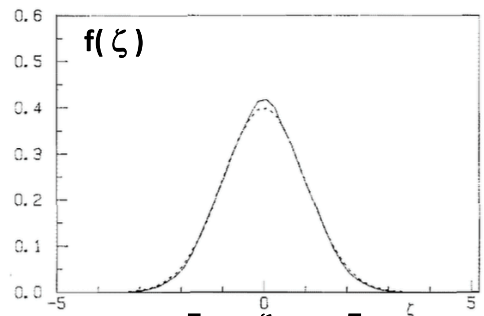
Simányi's result is interesting in view of this mixed nature of the soft-disk phase space (part chaotic and part regular) . Is it the case that gradually making the potential steeper (approaching the hard-disk limit) will eventually lead to ergodicity ? Another approach to the same problem is to examine the stability of the glancing-collision solutions .

A similar "focusing" of orbits was observed by Vineyard in his radiation damage studies . Motion parallel to rows of atoms is evidently stable to small transverse perturbations .

It is noteworthy that simulations provide conclusions much more rapidly than do theoretical analyses .

A Soft-Disk Cell Model as of 1986 *





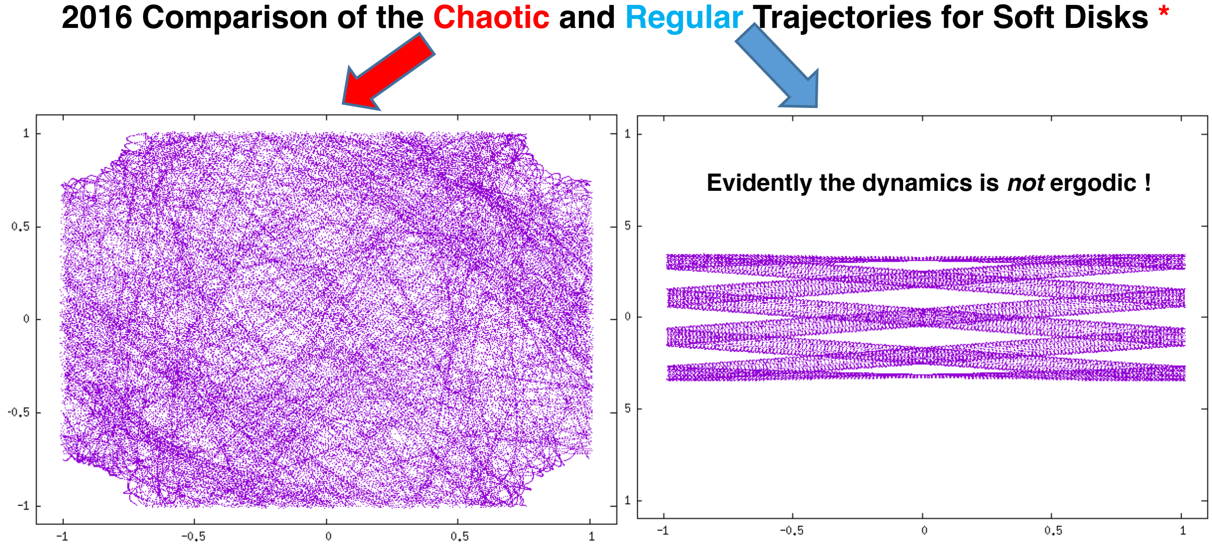
$-5 < \zeta < +5$

$\phi(r) = 3(1 - r)^4$ with $(x, y, p_x, p_y, \zeta) = (0.1, 0.2, +1, -1, 0)$. Is it ergodic ?

Probability density for ζ compared to the Gaussian distribution (dashes) .

* **Posch, Hoover, Vesely, Physical Review A 33,** 4253-4265 **(1986) .** Compare to 2016 →

2016 Comparison of the Chaotic and Regular Trajectories for Soft Disks *



$\lambda_1 = 0.788$ **$\lambda_1 = 0.000$**

* The energy is conserved to six figures in both these 2 000 000 timestep simulations .

George Vineyard's Radiation-Damage Studies *

Structure of static defects as well as highly energetic "Knock-On" Collisions in Metals
Physical Review 120, 1229 - 1253 (1960)

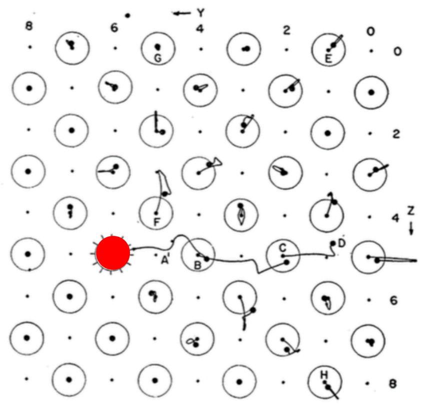
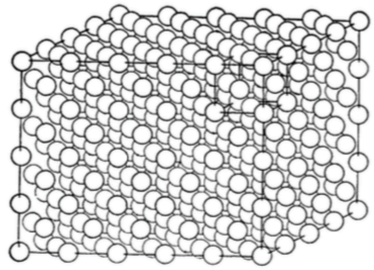
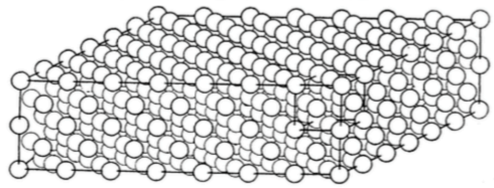


FIG. 6. Atomic orbits produced by shot in (100) plane at 40 ev.



* $\dot{v}_i(t) \cong [v_i(t+\Delta t/2) - v_i(t-\Delta t/2)]/\Delta t,$

$\dot{x}_i(t+\Delta t/2) \cong [x_i(t+\Delta t) - x_i(t)]/\Delta t.$ *



* Using the "Verlet" algorithm before Verlet !

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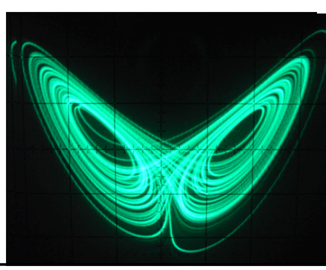
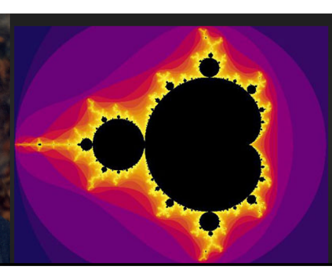
4. Nosé-Hoover Oscillator and the Chaotic Sea

{ (dq/dt) = p ; (dp/dt) = – q – ζp ; (dζ/dt) = p^2 – 1 }

Why is it that *three* dimensions are required for Chaos ? What about "maps" rather than "flows" ?



4. Nosé-Hoover Oscillator and its Chaotic Sea

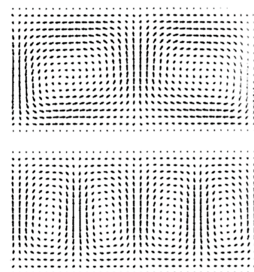
Structures of a few of the simpler tori , courtesy of Wang and Yang *, who chose to examine $\alpha = 10$:

$$\{ (dq/dt) = p \; ; \; (dp/dt) = -q - \zeta p \; ; \; (d\zeta/dt) = \alpha(p^2 - 1) \}$$

The constant parameter α is related to frequency^2 :

$$\alpha = \nu^2 = 1/\tau^2$$

The existence of multiple solutions for hydrodynamic problems like Rayleigh-Bénard convective flows → shows that molecular dynamics can have multiple chaotic seas . No such degeneracy has yet been seen in physically interesting small-system situations .



* L Wang and X-S Yang , arXiv 1501.03375 (2015) .

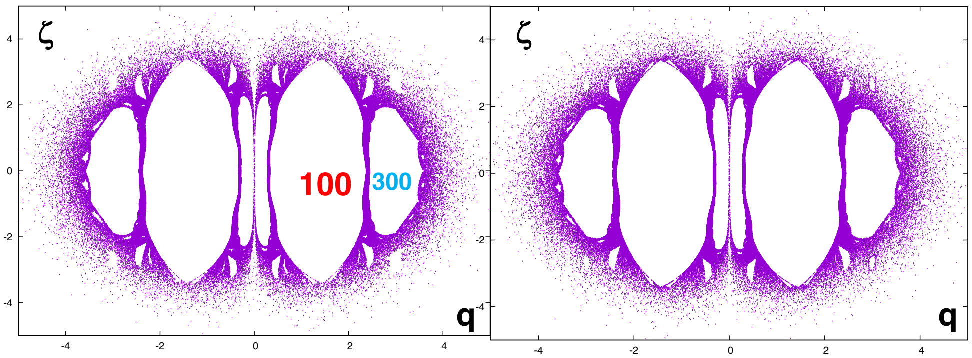
Four Ways to Test for Ergodicity

1. Compare average values of E , P , < p^2 > , < q^4 >
2. Determine whether or not regular solutions are present
3. See whether or not λ_1 depends upon the initial conditions
4. Look at Poincaré sections for holes

Toroidal initial condition	Chaotic initial condition
`x(1)  =  0.0d00`	`x(1)  =  0.1d00`
`y(1)  =  0.0d00`	`y(1)  =  0.2d00`
`px(1) = +dsqrt(1.98d00)`	`px(1) = +1.0d00`
`py(1) = +dsqrt(0.02d00)`	`py(1) = -1.0d00`

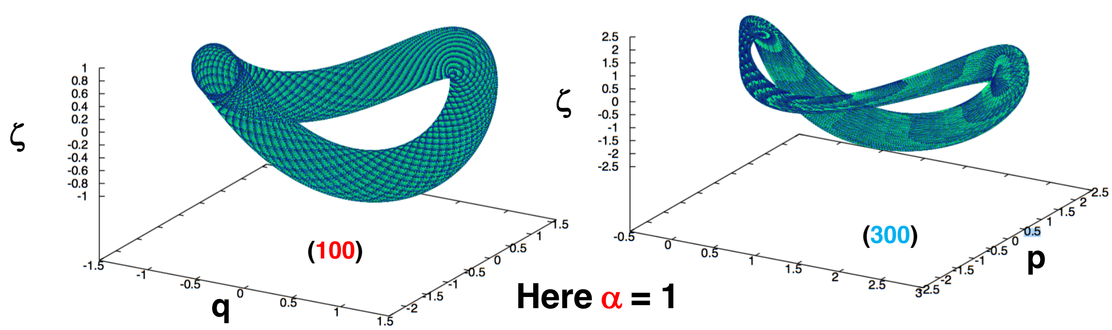
Two million steps with RK4 dt = 0.01d00 . Analyze last half .

251 426 (330) points and 252 348 (050) Nosé-Hoover Poincaré section points*
Both simulations used 1 000 000 000 timesteps with dt = 0.001 using RK4 .
The *holes* in these sections suggest two interesting things to do :
[1] magnifying the sea to see its structure more clearly and the
[2] starting with the (100) and (300) tori to see their complexity .



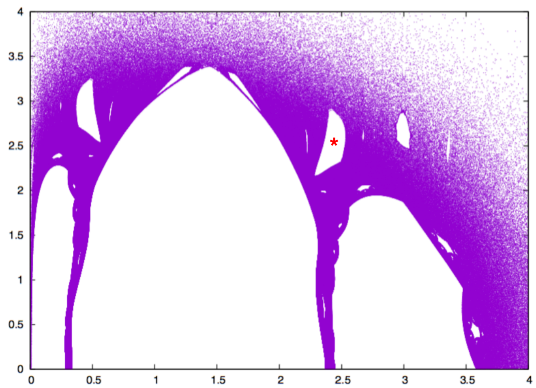
*These are points along the trajectory where p vanishes , detecting a negative pold*pnew .
(330) and (050) are the initial values of (qpζ) used to obtain these (q0ζ) section data .

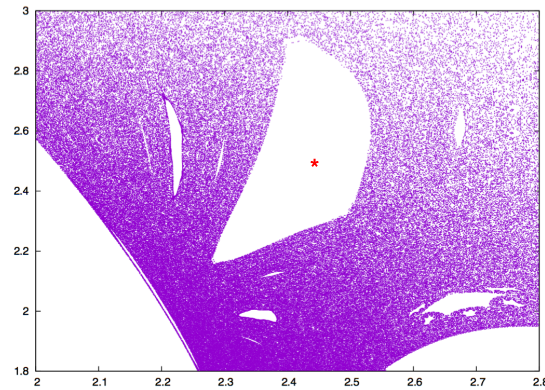
Here we plot every 1000th point out of 1 000 000 000 starting with (100) and (300) = (qpζ) . Both simulations produce nonchaotic tori . Both used dt = 0.001 with RK4 .



Notice the different scales, with the 300 torus occupying mostly positive values of the coordinate q . The 100 torus is symmetric about the origin . Very recently Lei Wang and Xiao-Song Yang "The invariant tori of knot type and the interlinked invariant tori in the Nosé-Hoover system" (arXiv 1501.03375) have identified six Nosé-Hoover tori and have found that they are interlinked (wrapped around one another) . This new finding underlines the complexity present in a simple model .

Magnified view of the chaotic sea with the RK4 dt = 0.0001 for additional clarity

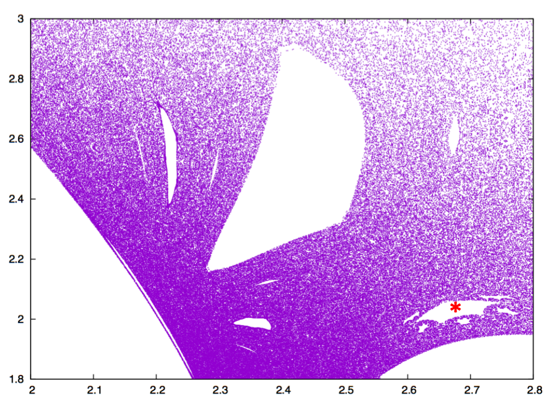


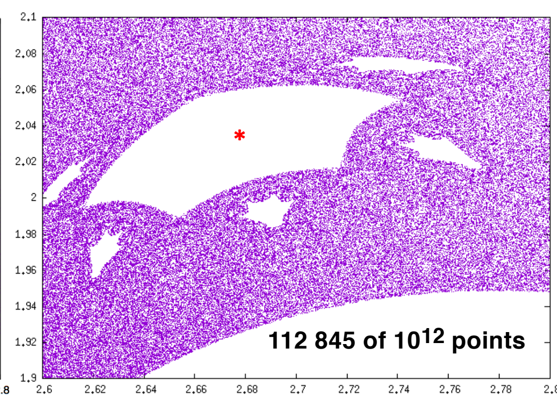


The 2 522 740 (lql, 0, lζl) section points reveal tiny holes *
Notice that the chaotic sea displays fourfold symmetry .

The ultrasimplified 'Logistic Map' , y = α y (1 – y) , has similar features .

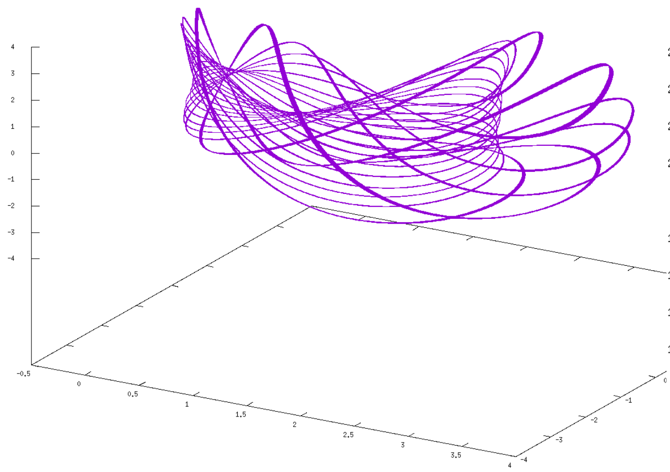
Magnified view of the chaotic sea with the RK4 dt = 0.0001 for additional clarity

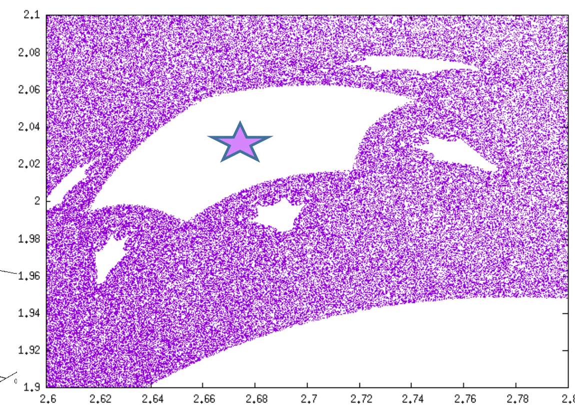




The 2 522 740 (lql, 0, lζl) section points reveal tiny holes . The extreme closeup to the right reveals that the holes themselves contain small islands . This "structure on all scales" is characteristic of Hamiltonian Chaos , which is inherited from the Nosé-Hoover-Dettmann equations .

Here is the torus which fits into the large pentagonal hole * .
The initial N-H conditions are (q, p, ζ) = (2.68, 0.00, 2.03)





112 845 of 10^{12} points

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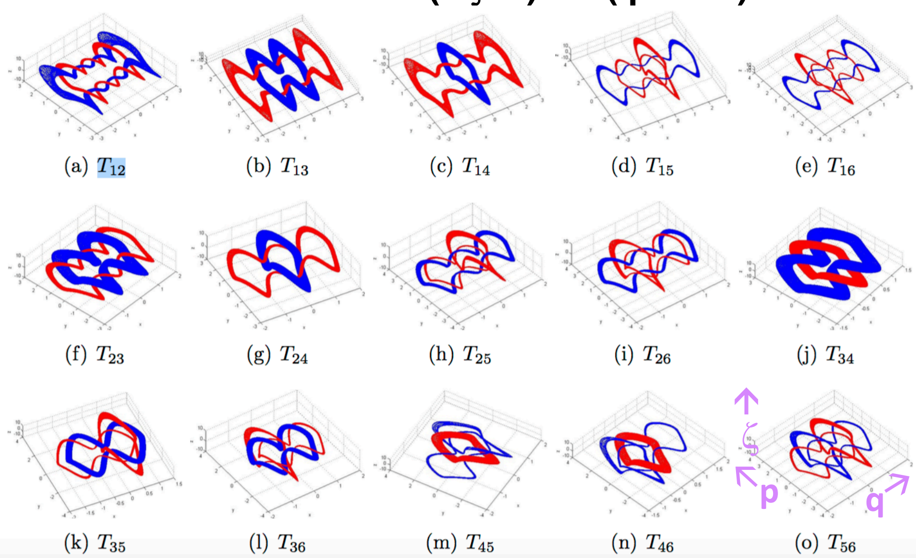
5. More complicated Tori were discovered by Wang and Yang *
In 2015 by solving the Nosé-Hoover equations with $\alpha = 10$.

$$(dq/dt) = p \; ; \; (dp/dt) = -q - \zeta p \; ;$$
$$(d\zeta/dt) = 10(p^2 - 1)$$

* Lei Wang, Xiao-Song Yang, "The invariant tori of knot type and the interlinked invariant tori in the Nosé-Hoover system" arXiv 1501.03375

Illustrations of the 6 x 5/2 = 15 interlinked tori pairs from the Wang-Yang arXiv paper

Here $\alpha = 10$ where $(d\zeta/dt) = \alpha(p^2 - 1)$.



(a) T_{12} (b) T_{13} (c) T_{14} (d) T_{15} (e) T_{16}

(f) T_{23} (g) T_{24} (h) T_{25} (i) T_{26} (j) T_{34}

(k) T_{35} (l) T_{36} (m) T_{45} (n) T_{46} (o) T_{56}

Kharagpur Lectures

6. Ergodicity of Oscillator Models : 1984 - 2016

6. Ergodicity of Oscillator Models : 1984 - 2016
Nosé and Nosé-Hoover Oscillators
Martyna-Klein-Tuckerman Oscillator
Kusnezov-Bulgac-Bauer papers
Sergi-Ferrario (qp) Oscillator
Sergi-Ezra-Patra-Bhattacharya Oscillator
Weak (qp) and (p^2, p^4) Oscillator Control
(Including solutions of Nosé's problem)
'Logistic Thermostat' and the Mexican Hat

Nosé and Nosé-Hoover oscillators : 1984 - 1986

Question : Nosé's Hamiltonian model added s and ζ to the harmonic oscillator, giving more complexity , 6% chaotic and 94% toroidal . How do we know ?

Answer : Choose 1 000 000 initial conditions from the solution of Liouville's flow equation f α exp[-$\mathcal{H}$(q,p,s,ζ)/kT] . About 60 000 of these have nonzero Lyapunov exponents .

To do this use Giancarlo Benettin's Lyapunov Algorithm : Propagate two nearby trajectories, rescaling their separation after each timestep . Compute < λ(t) > = < -ln(factor)/dt > and determine whether or not it is significantly different to zero . The two trajectories have weights from exp[-$\mathcal{H}$(q,p,s,ζ)/kT] .

Giancarlo Benettin’s Lyapunov Algorithm (1980)

The simplest programming propagates two nearly identical (`q,p,z`) vectors for a time of 20 000 using dt = 0.01 . The distance between them ,

```
r = dsqrt( (q1-q2)**2 + (p1-p2)**2 + (z1-z2)**2 )
```

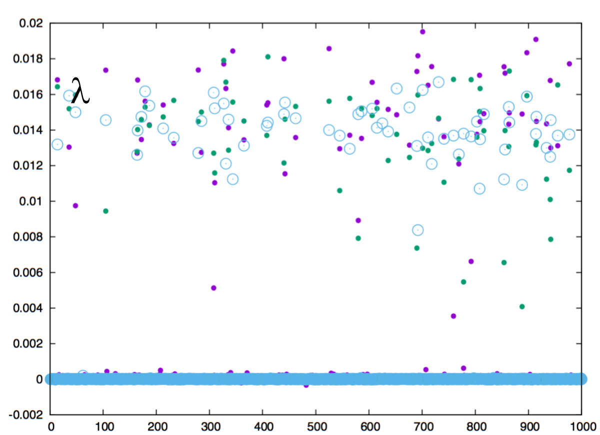
is then returned to `0.000001d00` by “scaling” :

```
q2 = q1 + factor*(q2 – q1)
p2 = p1 + factor*(p2 – p1)
z2 = z1 + factor*(z2 – z1)
```

where `factor = (0.000001d00/r) .`

The Lyapunov exponent is the mean value of `-ln(factor)/dt` using data from the last of half each run, with runtimes 20K , 80K , and 160K . The λ expression follows from exponential dependence : r α exp[+λt] .

Giancarlo Benettin’s Lyapunov Algorithm



← 1000 Initial Conditions →

Nosé-Hoover Chaos is 6%

20K → 62 / 1000 chaotic

80K → 63 / 1000 chaotic

320K → 64 / 1000 chaotic

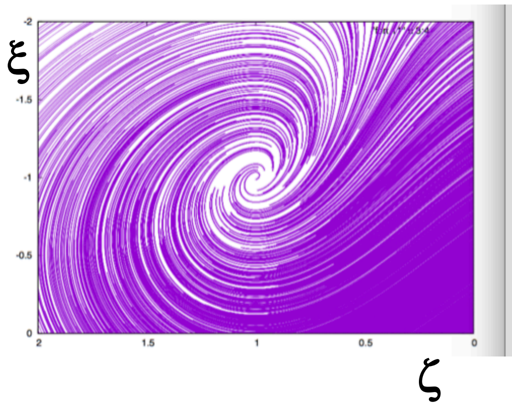
λ is between 0.013 and 0.014 . We tabulate the fraction greater than 0.002 .

Ergodicity of the Martyna-Klein-Tuckerman Chain Thermostat (1992)

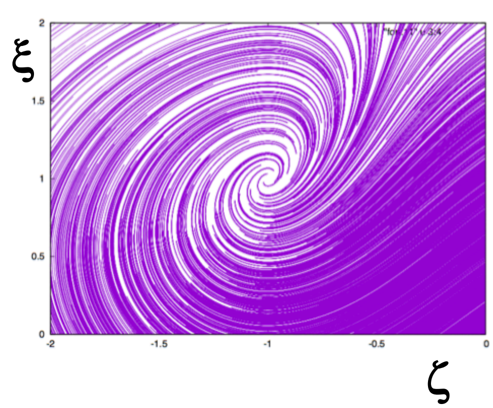
{ (dq/dt) = p ; (dp/dt) = – q – ζp ; (dζ/dt) = p^2 – 1 – ξζ ; (dξ/dt) = $ζ^2$ – 1 }

There are two fixed points at (q, p, ζ, ξ) = (0, 0, +1, – 1) and (0, 0, – 1, +1)

Shown below are the (ζ, ξ) for $q^2 + p^2 < 0.01$



Exponentially unstable in ζ and ξ



Exponentially unstable in q and p

Ergodicity of the Martyna-Klein-Tuckerman Chain Thermostat

The (qpζξ) fixed points are of two types ,
stable in qp unstable in ζξ *vs* unstable in qp stable in ζξ .

qp = 0,0 → { (dζ/dt) = – 1 – ζξ ; (dξ/dt) = $ζ^2$ – 1 } ← ISO
ζξ = +1,–1 → { (dq/dt) = p ; (dp/dt) = – q – p }
ζξ = –1,+1 → { (dq/dt) = p ; (dp/dt) = – q + p }
Both fixed points are unstable in one 2x2 plane .

The ζξ plane equations are isomorphic to a falling mass :
{ (dv/dt) = – 1 – ζv ; (dζ/dt) = v^2 – 1 } ← ISO

Ergodicity of the Martyna-Klein-Tuckerman Chain Thermostat

Let us look at typical ζξ orbits in the (q,p) = (0,0) plane from the falling-particle standpoint :

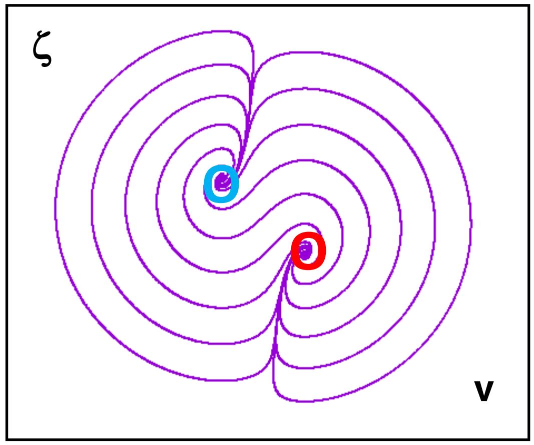
$$(dv/dt) = -1 - \zeta v$$

$$(d\zeta/dt) = v^2 - 1$$

The stability is easy to establish By linearization, for example :

$v = -1 + dv \; ; \; \zeta = +1 + d\zeta$

$v = +1 + dv \; ; \; \zeta = -1 + d\zeta$



Flow is from Red to Blue .

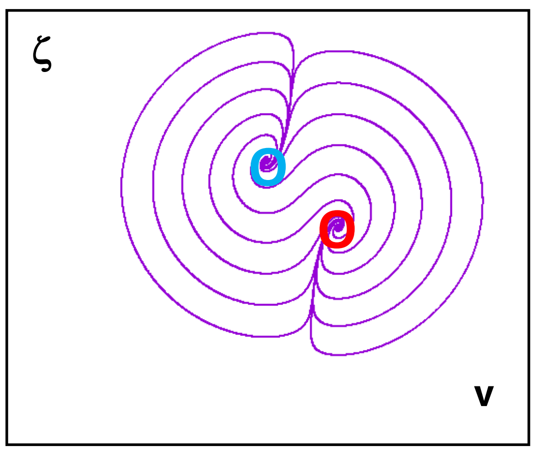
This is a good homework or examination problem . For details see TRCSAC .

Ergodicity of the Martyna-Klein-Tuckerman Chain Thermostat

Linear Stability Analysis* involves truncating Taylor's series for differential equations after the linear terms . We will give the detailed analysis for this thermostated "Falling Particle" problem on the succeeding slide . The idea is to analyze the dynamics in the vicinity of a "fixed point" in order to see whether or not the point Is "stable". For ergodicity we need instability .

$v = -1 + dv \; ; \; z = +1 + dz$

$v = +1 + dv \; ; \; z = -1 + dz$



* Such problems are good homework or examination problems .
For details see *Time Reversibility, Computer Simulation, and Chaos*.

Ergodicity of the Martyna-Klein-Tuckerman Chain Thermostat*

$(d^2x/dt^2) = + / - (dx/dt) - 2x$ are the unstable / stable cases .

To begin, expand the equations $\{ \dot{v} = -1 - \zeta v \ ; \ \dot{\zeta} = v^2 - 1 \ \}$ around $(v, \zeta) = (-1, +1)$:

$$\dot{\delta}_v \approx -\zeta \delta_v - v \delta\zeta \approx -\delta_v + \delta_\zeta \ ; \ \dot{\delta}_\zeta \approx 2v\delta_v \approx -2\delta_v \ .$$

Differentiation and substitution gives second-order differential equations for δ_v and δ_ζ :

$$\ddot{\delta}_v = -\dot{\delta}_v - 2\delta_v \ ; \ \ddot{\delta}_\zeta = -2\dot{\delta}_v = 2\delta_v - 2\delta_\zeta = -\dot{\delta}_\zeta - 2\delta_\zeta \ .$$

Both variables obey the same damped-oscillator motion equations at the stable fixed point. In the reversed motion we expect instability. To analyze this we expand around $(+1, -1)$:

$$\dot{\delta}_v = \delta_v - \delta_\zeta \ ; \ \dot{\delta}_\zeta = 2\delta_v \ .$$

Just as before we differentiate in order to get second-order motion equations :

$$\ddot{\delta}_v = \dot{\delta}_v - 2\delta_v \ ; \ \ddot{\delta}_\zeta = 2\dot{\delta}_v = 2\delta_v - 2\delta_\zeta = \dot{\delta}_\zeta - 2\delta_\zeta \ .$$

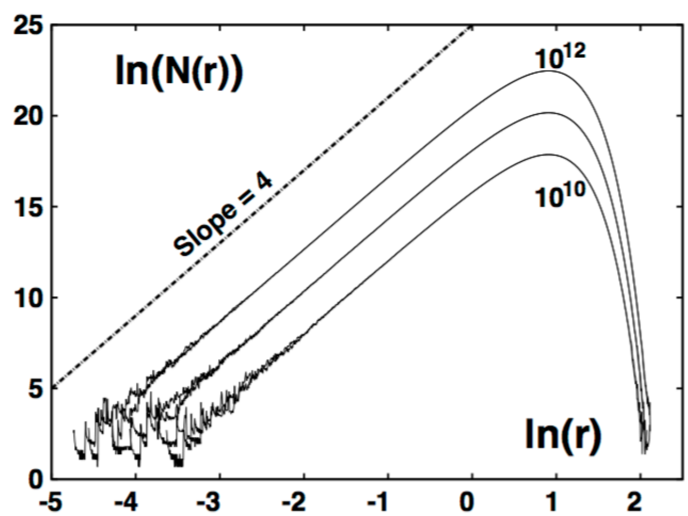
This fixed point is unstable. It is interesting that in the neighborhood of both fixed points, stable and unstable, the perturbed equations have *exactly the same form* for both variables.

*** This is a good homework or examination problem . For details see TRCSAC .**

Ergodicity of the Martyna-Klein-Tuckerman Chain Thermostat *

The apparent "holes" in the vicinity of the fixed points are misleading !

Determining the ergodicity of this problem was the 2014 Snook Prize Problem .

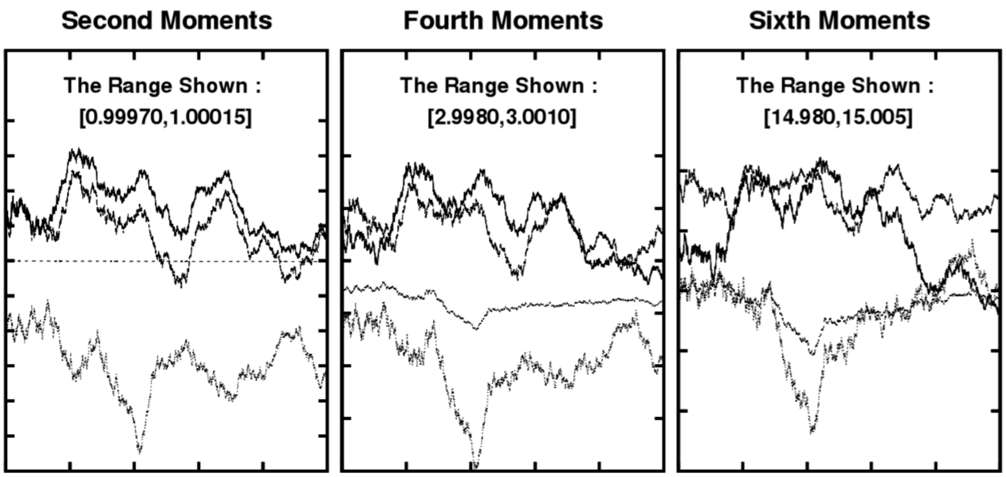


Simulations with from 10^{10} to 10^{12} timesteps show the dimension of the probability density near the fixed points is uniform .

*** CMST 21 (2015)**

Ergodicity of the Martyna-Klein-Tuckerman Chain Thermostat

Checking the moments (for all four variables) is another good test .



Time range shown is 100 000 000 to 200 000 000

Ergodicity of the Martyna-Klein-Tuckerman Chain Thermostat

The fixed points are all unstable .
The measures around the fixed points are uniformly space-filling .
The moments agree with Gibbs' canonical distribution .
The Lyapunov exponent is positive and universal .

This evidence is convincing . The MKT Chain Thermostat is ergodic .
We did not consider investigating *double* cross sections . These are now feasible on laptop machines . Let's look at an example * :

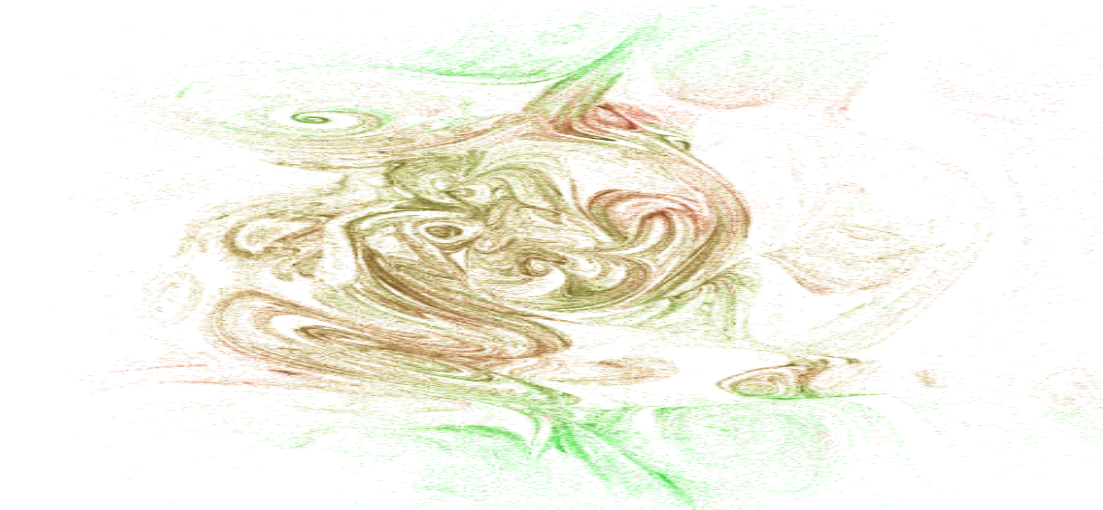
$$(dq/dt) = p \;;\; (dp/dt) = -q - \zeta p - \xi p^3 \;;$$

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

$$\text{where } T = 1 + 0.4\tanh(q)$$

* ***Simulation and Control of Chaotic Nonequilibrium Systems (2015)***
[Frontispiece illustration with $\zeta = \xi = 0$ courtesy of Clint Sprott]

Simulation and Control of Chaotic Nonequilibrium Systems
[Frontispiece illustration of p(q) courtesy of Clint Sprott]



The Information Dimension of this Nonequilibrium Hoover-Holian Attractor is 3.687 .

Kusnezov-Bulgac-Bauer papers

D. Kusnezov, A. Bulgac, and W. Bauer, "Canonical Ensembles from Chaos" , Annals of Physics (NY) 204 and 214 , (1990 and 1992) .

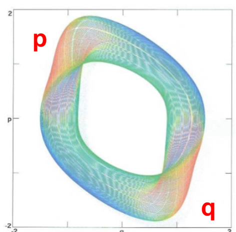
These two comprehensive papers treat many examples , including the Mexican Hat potential , which has a double well , and the diffusion of a Brownian particle , which requires three thermostat variables rather than two . At the time the papers were written it was unknown that simple problems like the oscillator could be thermostated ergodically with a single additional control variable , a nonlinear hyperbolic tangent .

Their papers emphasize that the motion equations can made consistent with Gibbs' canonical distribution by applying the continuity equation in The three- , four- , or five-dimensional "extended" phase space .

In 2001 Sergi and Ferrario (Physical Review E 64, 056125) introduced a set of four-dimensional motion equations which coupled the coordinate and momentum of an harmonic oscillator in an unusual way :

{ $(dq/dt) = p(1 + \zeta)$; $(dp/dt) = -q - \zeta p$; $(d\zeta/dt) = p^2 - 1 - qp$; $(ds/dt) = \zeta$ }

They included several parameters all of which we have set equal to 1 . Because the variable "s" plays no role in the solution we can ignore it . Sergi and Ferrario thought their equations ergodic , perhaps because they considered all four dimensions in their numerical work . But starting with $(qp\zeta) = (111)$ gives a nice torus ! The projection here shows p(q) .



Though not ergodic , this model suggested the useful idea of combining controls of momenta with controls of coordinates (or, better yet , forces) which led to further work , which was ultimately successful .

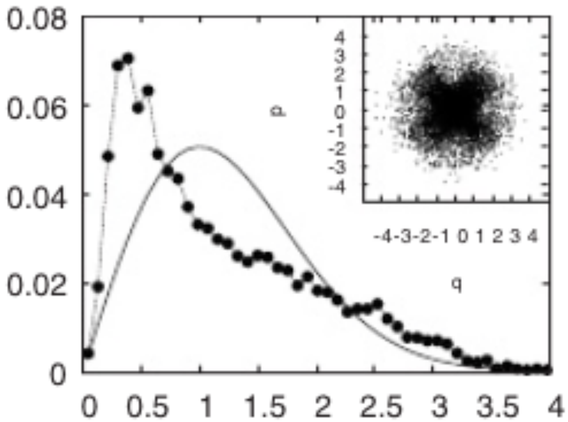
The Sergi-Ezra-Patra-Bhattacharya Oscillator was an attempt (2010 and 2014) to thermostat the momentum and the coordinate (or force) in a symmetric way :

{ $(dq/dt) = p - \xi q$; $(dp/dt) = -q - \zeta p$; $(d\zeta/dt) = p^2 - 1$; $(d\xi/dt) = q^2 - 1$ }

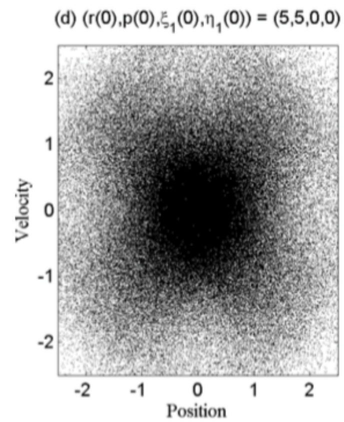
Oddly enough the (qp) distribution turns out *not* to be circularly symmetric so that this approach is not ergodic . It appears that simple modifications , using cubic forces , are enough to attain ergodicity for the oscillator . Patra and Bhattacharya have studied a large family of control variables and we have carried out many collaborations with them and with Clint Sprott at Madison Wisconsin .

The Sergi-Ezra = Patra-Bhattacharya Oscillator

{ $(dq/dt) = p - \xi q$; $(dp/dt) = -q - \zeta p$; $(d\zeta/dt) = p^2 - 1$; $(d\xi/dt) = q^2 - 1$ }



Sergi-Ezra



Patra-Bhattacharya

Weak (qp) and (p^2, p^4) Oscillator Control
(Including solutions of Nosé's problem)

Probably influenced by the earlier work various combinations of ourselves with Patra and Bhattacharya and Sprott developed weak controls of oscillator moments . It is easy to find combinations that are consistent with the phase-space continuity equation and some of them are ergodic . I will skip the (qp) controls and focus on joint control of $\langle p^2 \rangle$ and $\langle p^4 \rangle$, omitting $\langle p^6 \rangle$ as the equations tend to be stiff . It is convenient to use a Monte Carlo approach , starting with

{ $(dq/dt) = p$; $(dp/dt) = -q - \zeta(\alpha p + \beta p^3)$; $(d\zeta/dt) = \alpha(p^2 - 1) + \beta(p^4 - 3p^2)$ }

The parameters α and β can be varied between reasonable limits such as [0,1] and one can watch a movie of the Poincaré sections with 100 or so frames , choosing good looking examples for more investigation . In this way I found that $\alpha = 0.05$ and $\beta = 0.32$ "0532 Model" is ergodic .

7. Singly-Thermostated Ergodicity

From J Willard Gibbs' 1902 text , *Elementary Principles in Statistical Mechanics* , page 183 :

"If a system of a great number of degrees of freedom is microcanonically distributed in phase, any very small part of it may be regarded as canonically distributed."

From Gibbs' time until relatively recently it was thought that a large system "Thermodynamic Limit" had to be taken in order to model the "Microstates" found in Gibbs' canonical or microcanonical ensemble . Now it is known that few-body singly- or doubly-thermostated systems can exhibit these ergodic properties so that the thermodynamic limit is thoroughly obsolete .

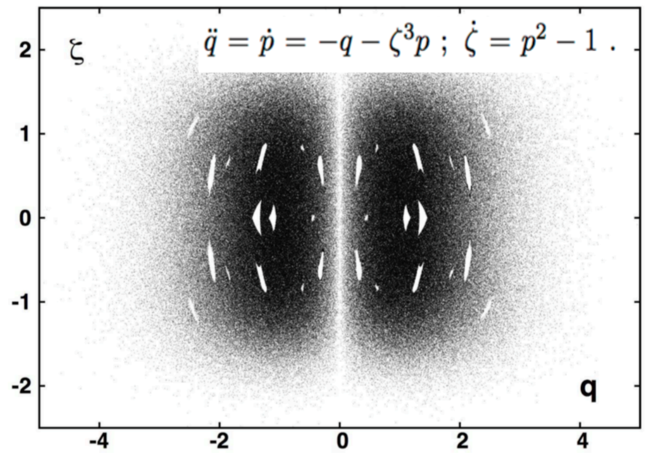
7. Singly-Thermostated Ergodicity → Logistic Thermostat *

With an ergodic oscillator it is natural to try to extend the weak control idea to a pendulum and to the Mexican Hat problem . All is well with the pendulum but even the quartic potential seems difficult to treat ! I tried *thousands* of combinations of parameters ($\alpha\beta\gamma$) without success on the quartic potential . With the cooperation of the Poznan Institute of Bioorganic Chemistry of the Polish Academy of Sciences Carol and I offered the 2016 Ian Snook Prize of $1000 for the most interesting contribution toward single-thermostat control of more complicated nonlinear problems like the quartic potential or the Mexican Hat .

Just last month Tapias , Bravetti , and Sanders * took up this challenge and formulated a new "Logistic Thermostat", which solves the problem.

* Tapias , Bravetti , and Sanders "Ergodicity of One-Dimensional Systems … " = arXiv 1611.05090
The "logistic equation" $dx/dt = \alpha x (1 - x)$ resembles the 'logistic map' $x = \alpha x (1 - x)$.

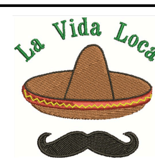
7. Singly-Thermostated Ergodicity : 2016 Snook Prize



IAN SNOOK (1945 – 2013) Tasmania and Melbourne OZ

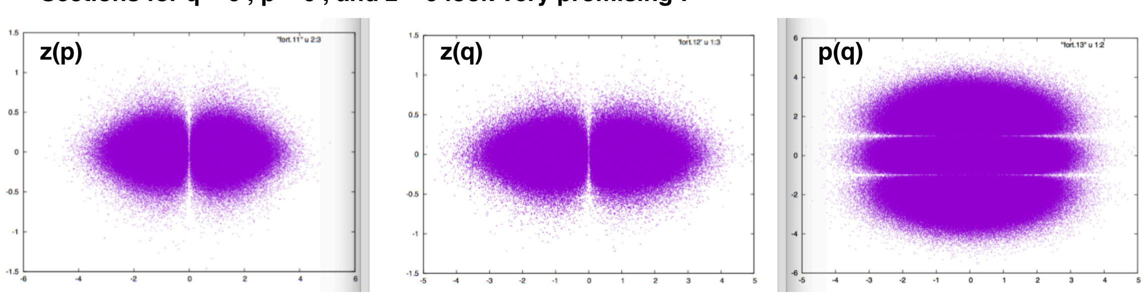
Cubic forces provide mechanisms enhancing ergodicity , as stressed by Bulgac and Kusnezov In their informative papers in the 1990 and 1992 Annals of Physics .

The Logistic Thermostat *



Logistic functions and distributions are applied in statistics, physics, hydrology, and chess . A special case is $e^x/(1 + e^x)^2 = (1/4)\mathrm{sech}^2(x/2)$, and a slight modification evidently provides an Ergodic Distribution for the harmonic oscillator, the quartic oscillator and the Mexican Hat !

In the case of the harmonic oscillator Tapias + Bravetti + Sanders solve three equations : { (dq/dt) = p ; (dp/dt) = – q – αp ; (dz/dt) = p^2 – 1 } where $\alpha = 10e^{10z}/(1 + e^{10z})^2$. The Poincaré Sections for q = 0 , p = 0 , and z = 0 look very promising :

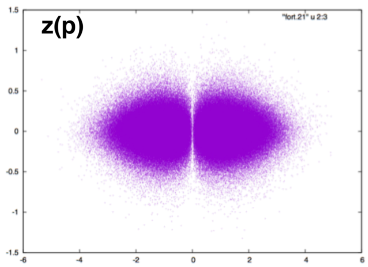


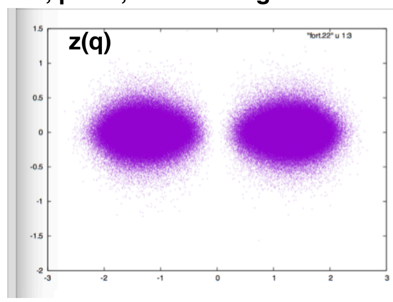
*** Tapias, Bravetti, and Sanders "Ergodicity of One-Dimensional Systems … " = arXiv 1611.05090**

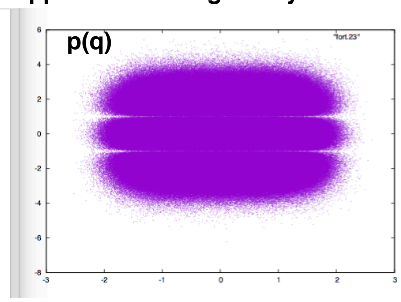
The Logistic Thermostat for the Quartic Potential *

Although the moment-based thermostats are apparently insufficient for the quartic and Mexican Hat potentials , the Logistic Thermostat can be used to solve those problems .

In the case of the quartic oscillator Tapias + Bravetti + Sanders solve three equations :
{ $dq/dt) = p$; $(dp/dt) = -q^3 - \alpha p$; $(dz/dt) = p^2 - 1$ } where just as before $\alpha = 10e^{10z}/(1 + e^{10z})^2$.
The Poincaré Sections for q = 0 , p = 0 , and z = 0 again have the appearance of ergodicity :







A simpler way to think about this thermostat is that the probability $e^{-H/kT}/\cosh(z)$ is consistent with a nonlinear friction coefficient $\tanh(z)$. This control is stiffer than the linear or cubic or quintic versions that were unable to thermostat the quartic and Mexican Hat potentials . It seems to work !

*** Tapias, Bravetti, and Sanders "Ergodicity of One-Dimensional Systems … " = arXiv 1611.05090**

The Logistic Thermostat for several potentials *

The use of an even logistic function , a solution of $d\ln f/dx = 1 - f(x)$ provides flexible models for saturated growth . The logistic map $x_+ \alpha\, x_o(1 - x_o)$ is a discrete form of the same idea . It can be written in terms of hyperbolic functions [as we formulated temperature in the case of the thermostated oscillator , with $T = 1 + \tanh(q)$] , or in terms of exponentials , as with $T = 1 + (e^{+q} - e^{-q})/(e^{+q} + e^{-q}) = 2/(1 + e^{-2q})$. Wikipedia has applications for flows and maps .

The Harmonic Oscillator

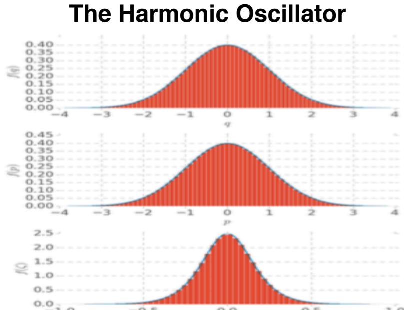


FIG. 4. Histograms compared with exact marginal distributions (solid line) for the harmonic potential.

The Mexican Hat

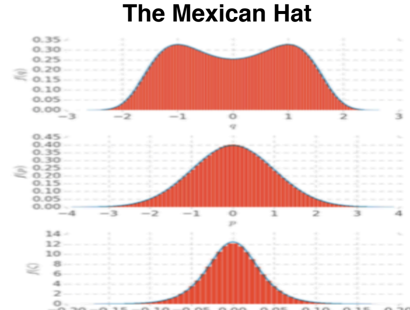


FIG. 6. Histograms compared with exact marginal distributions (solid line) for the Mexican hat potential.

Tapias, Bravetti, and Sanders "Ergodicity of One-Dimensional Systems … " = arXiv 1611.05090

Please think about suggestions for the 2017 Ian Snook Prize !

A Useful Exercise : Relating Sound Velocity to the Bulk Modulus

Calculation of the Sound Velocity c from the Adiabatic Bulk Modulus B

Define displacement $u(x,t)$ in a rightward traveling sound wave with wave vector k , frequency ω , and sound velocity $c = (\omega/k)$ as follows :

$$u = \sin(kx - \omega t) \ ; \ k \equiv (2\pi/\lambda) \ ; \ \omega \equiv 2\pi\nu \ .$$

Substitution of this traveling wave into the equation of motion relates the sound velocity to the (adiabatic) bulk modulus B :

$$\rho\ddot{u} = -\nabla P = B\nabla^2 u \longrightarrow -\rho\omega^2 u = -Bk^2 u \longrightarrow c = (\omega/k) = \sqrt{(B/\rho)} \ .$$