Chaos and thermalization of confined Hard rods

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(A work in progress)

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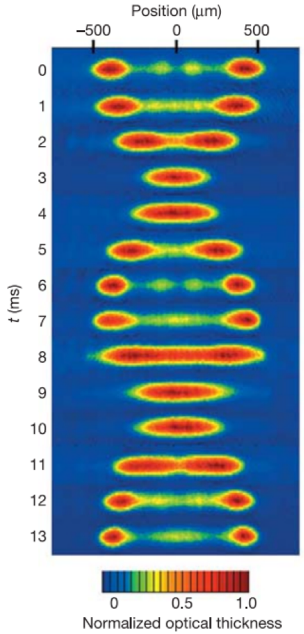
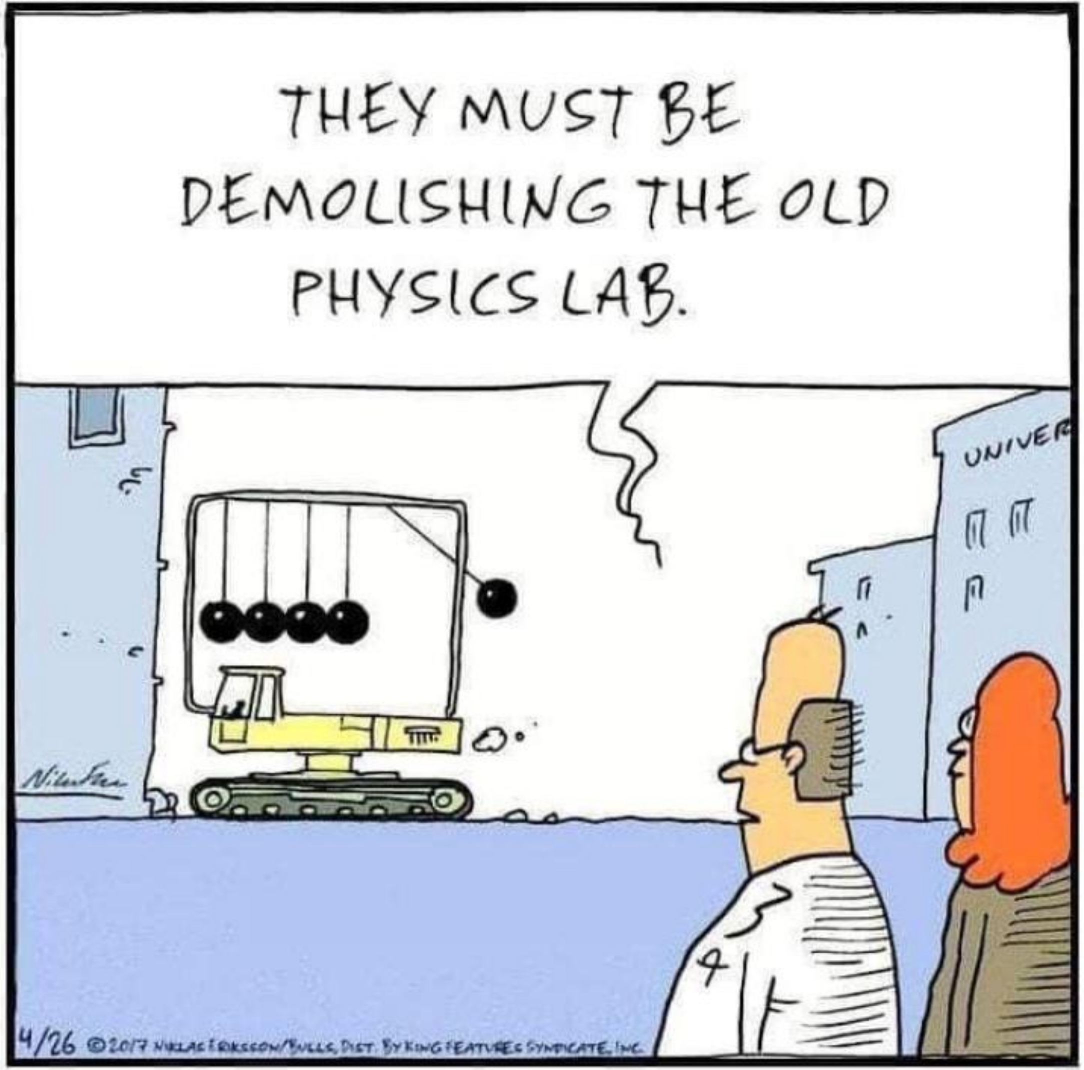
- Integrable systems have infinitely many conserved quantities.
- Realistic systems are not integrable.

Question: What is the effect of Integrability breaking?

The effect of integrability breaking on Chaos, Ergodicity, Thermalization and Transport properties have been studied.

- Chaos and Ergodicity: KAM theory [A. N. Kolmogorov (1954), (1979 for English)]
- Thermalization:
  1) Fermi-Pasta-Ulam-Tsingou equipartition problem [Fermi, E, Pasta P., Ulam S., Tsingou M., document LA-1940 (1955)].
  2) Quantum: Newton's Cradle [Kinoshita T, Wenger T Weiss D S, Nat. Letts. (2006)].
  3) Classical: Hard rods in Harmonic trap [Cao X, Bulchandani B V, Moore J E, PRL (2019)].





Credit: Internet

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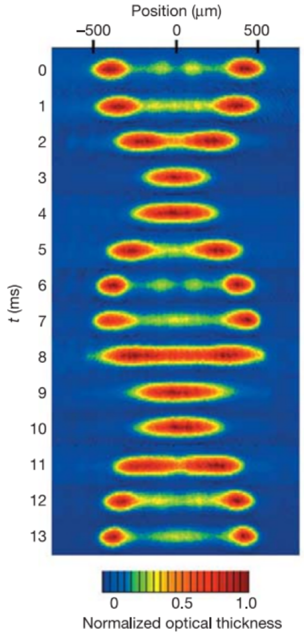


Hard Rods

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + \sum_{i=1}^{N} U(x_i) + \sum_{i=1}^{N-1} \Theta(x_{i+1} - x_i)$$

$$\Theta(r) = \begin{cases} \infty & \text{for } r \le a, \\ 0 & \text{for } r > a \end{cases}$$

(Particles collide elastically)

Here $U(x) = k\frac{x^\delta}{\delta}$ is the confining trap and we consider

(1) $\delta = 2$ for harmonic trap,

(2) $\delta = 4$ for quartic trap.

Q. Chaos and Thermalization of isolated Integrable systems when confined to external trap.

Sub Q.

1) Free energy and density at equilibrium.
2) Are these systems chaotic, ergodic?
3) Do they thermalize to the Gibbs state?

Free Energy and average density at Equilibrium

Difficult to solve the partition function exactly in the presence of external trap.

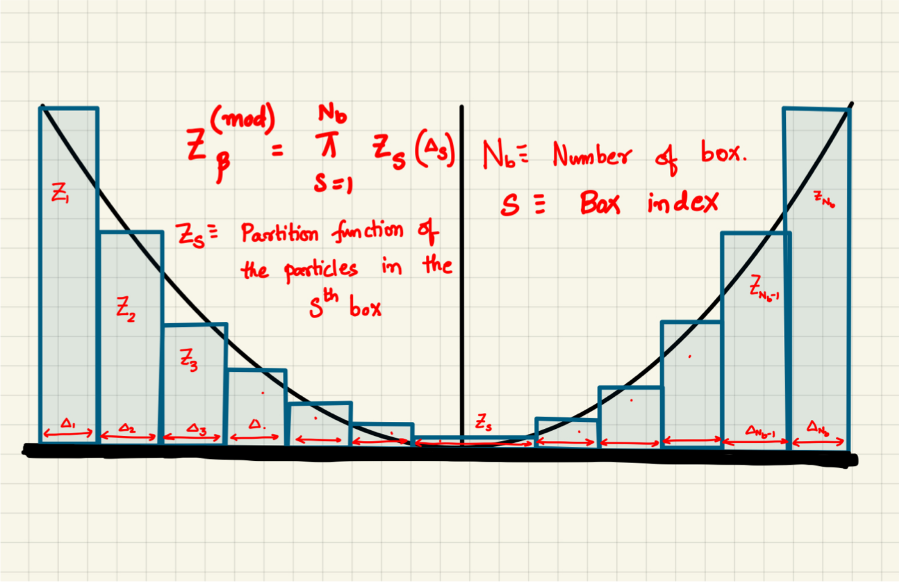
Assumption:

1) Trap breaks all the conservation laws except the Energy conservation. (Will be verified post hoc when we study thermalization.)

An approximate scheme:

Assumption:

2) The partition function can be written as a product of partition function of smaller subsystems.
3) Each subsystem experiences a constant potential $(V(x_s+\Delta) - V(x_s) < K_B T)$



Average thermal density is obtained by minimising the Free energy with the normalization constraint.

$$F_R[\rho(x),T] = \int_{-\infty}^{\infty} dx\,\rho(x)\left(U(x) - T\log\left(\frac{1-a\,\rho(x)}{\rho(x)}\right)\right)$$

Minimizing **free energy** with density along with normalization constraint gives

$$\mu^* = \frac{x^\delta}{\delta} - T\left[\log\left(\frac{1-a\,\rho^*(x,T)}{\rho^*(x,T)}\right) - \frac{1}{1-a\,\rho^*(x,T)}\right].$$

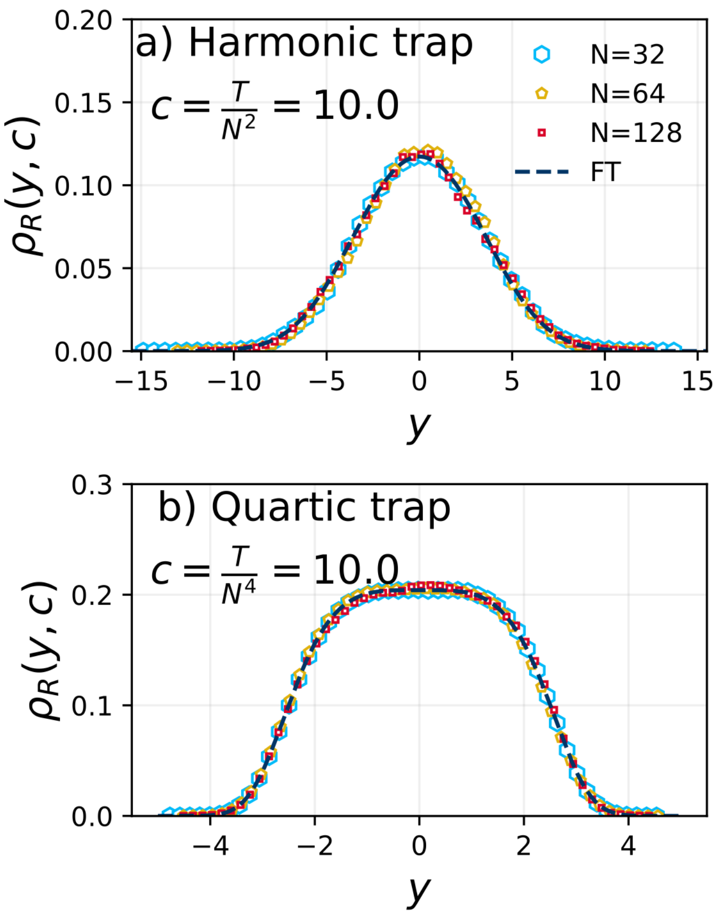
[Percus JK. J. Stat. Phys. (1976) 197615(6):505-11]

We find that in the rescaled variables the density takes a scaling form given by

$$\rho^*(x,T) = N^{1-\alpha}\rho_R(y,c) \text{ and } \mu^* = N^\lambda \mu_R$$

where $y = \frac{x}{N^\alpha}$ and **rescaled temperature** $c = \frac{T}{N^\gamma}$ with $\alpha = 1$ and $\gamma = \lambda = \delta$.

$$\mu_R = \frac{y^\delta}{\delta} - c\left[\log\left(\frac{1-a\,\rho_R(y\,,c)}{\rho_R(y\,,c)}\right) - \frac{1}{1-a\,\rho_R(y\,,c)}\right].$$



[arXiv:2209.13769. 2022 **JK**, Bagchi D, Dhar A, Kulkarni M, Kundu A (accepted in PRE)]

Dynamics of hard rods

$$E = \sum_{i=1}^{N} \left(\frac{\dot{x}_i^2}{2} + k \frac{x_i^\delta}{\delta} \right)$$

It is convenient to work in rescaled units
$\boldsymbol{x_i} \mapsto \boldsymbol{a}\, \boldsymbol{x_i}$ and $\boldsymbol{t} \mapsto \boldsymbol{\tau}\, \boldsymbol{t}$
where rod length is a and $\tau = \left(k a^{\delta-2}\right)^{-\frac{1}{2}}$.

$$E = k a^\delta \sum_{i=1}^{N} \left(\frac{\dot{x}_i^2}{2} + \frac{x_i^\delta}{\delta} \right)$$

The **ground state energy** $E \sim N^{\delta+1}\, k\, a^\delta$. The only relevant parameters then are the rescaled energy $\mathrm{e} = \frac{E}{N^{\delta+1} k\, a^\delta}$ and the number of particles N.

Turns out for harmonic confinement **energy of the centre of mass**

$$E_{CM} = \frac{1}{2}\left(\left(\sum_{i=1}^{N} x_i \right)^2 + \left(\sum_{i=1}^{N} p_i \right)^2 \right),$$

is also **conserved**. However it is not conserved for quartic confinement.

We use molecular dynamics simulations (event driven for harmonic confinement) to study the chaos, ergodicity and thermalization properties.

Integrability, chaos and Ergodicity

The maximum Lyapunov exponent

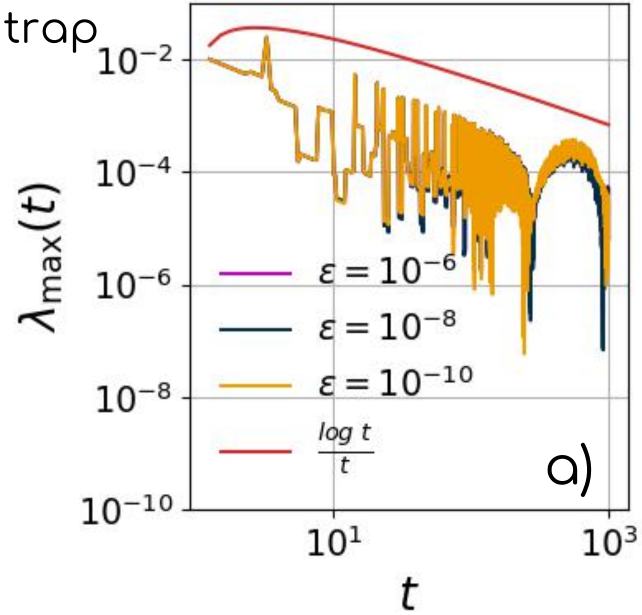
$$\lambda_{max}(t) = \lim_{\epsilon \to 0} \frac{1}{t} log \left| \frac{d_t}{\epsilon} \right|,$$

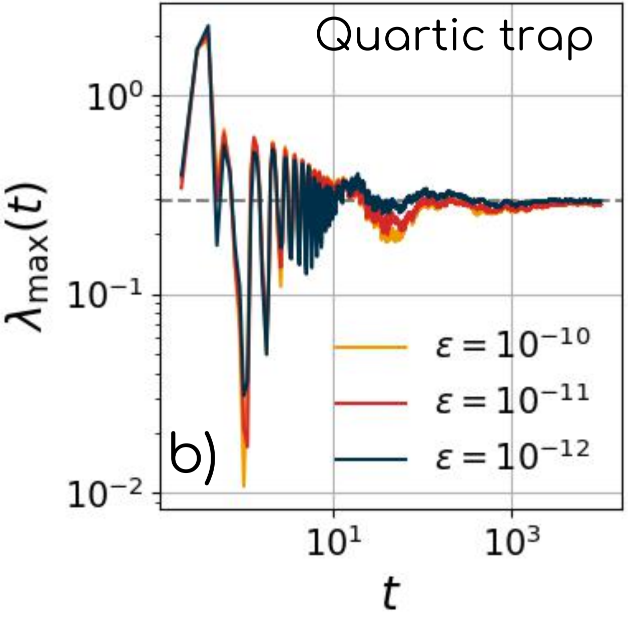
quantifies whether a system is chaotic ($\lambda_{max}(t \to \infty) > 0$) or not.

Benettin G, Galgani L, Strelcyn JM. Phys. Rev. A. 1976.

$N = 3$

Harmonic trap

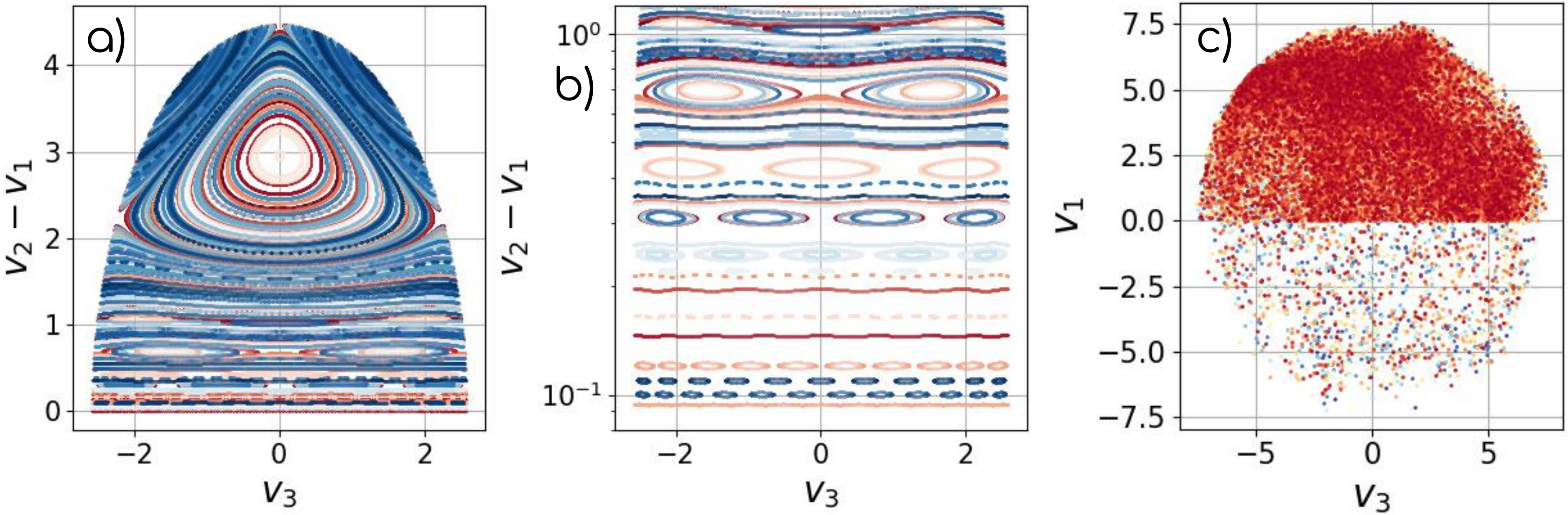




Poincare sections

Harmonic trap

Quartic trap



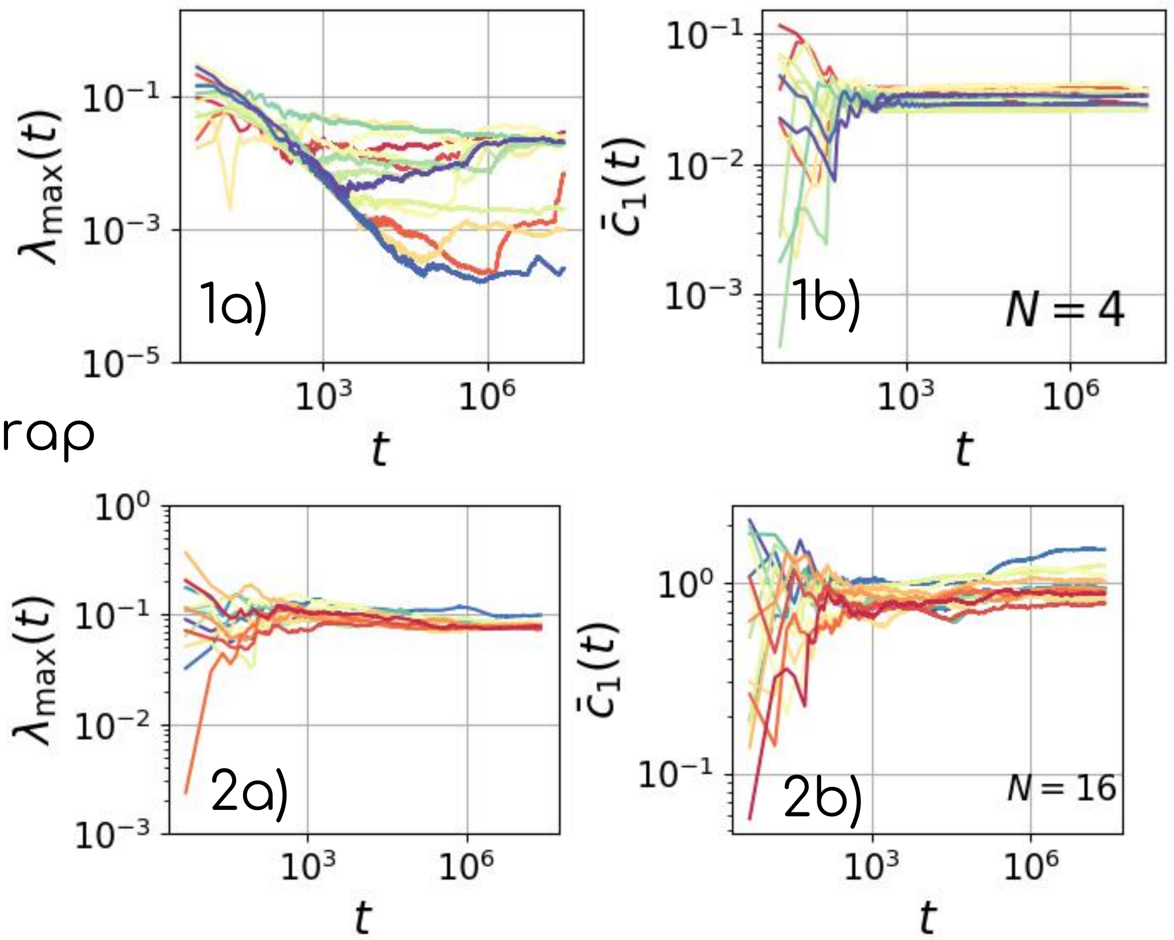
Regular orbits: Integrable dynamics

[Cao X., Bulchandani B. V., Moore J. E., PRL (2019)].

Dusty: Chaotic dynamics

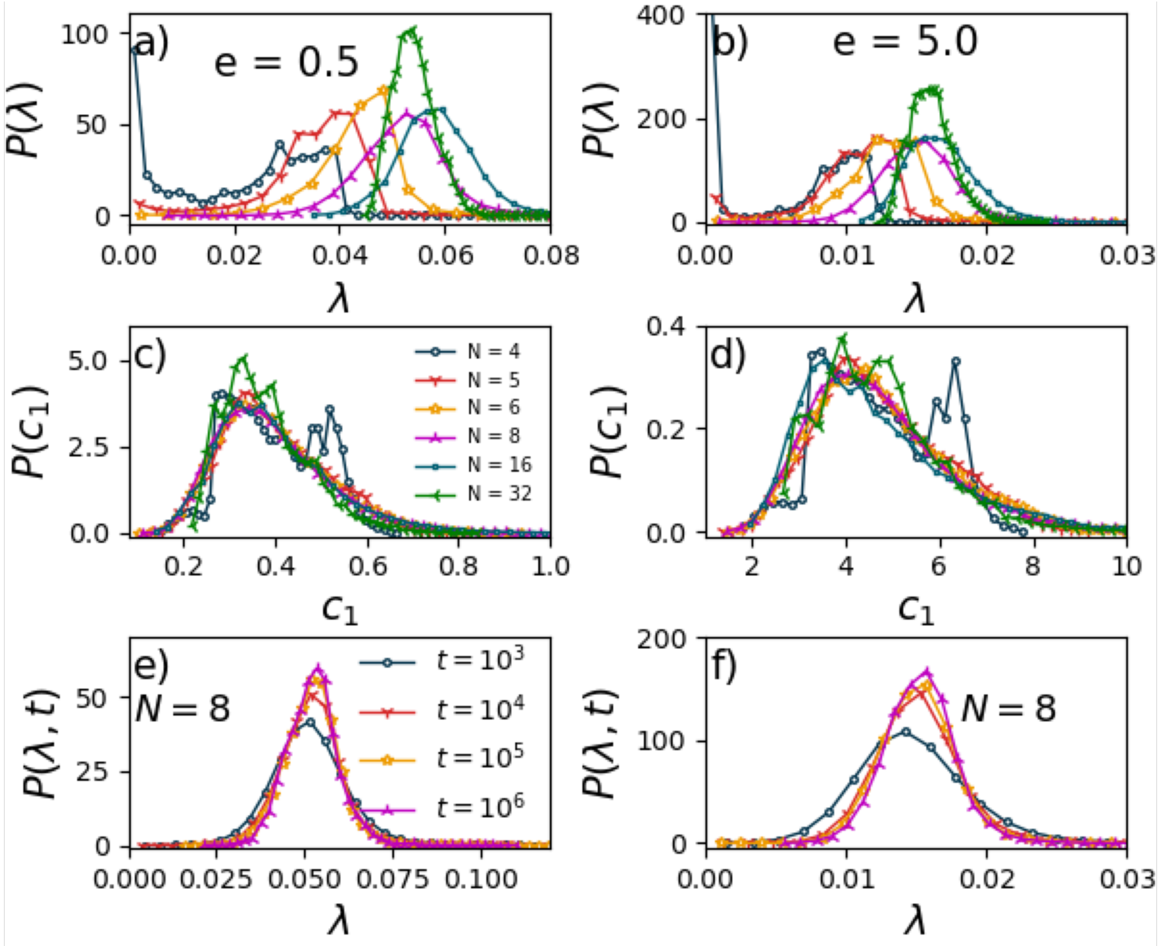
$N \geq 4$

Harmonic trap



Distribution of the Lyapunov exponent and temperature: Harmonic trap

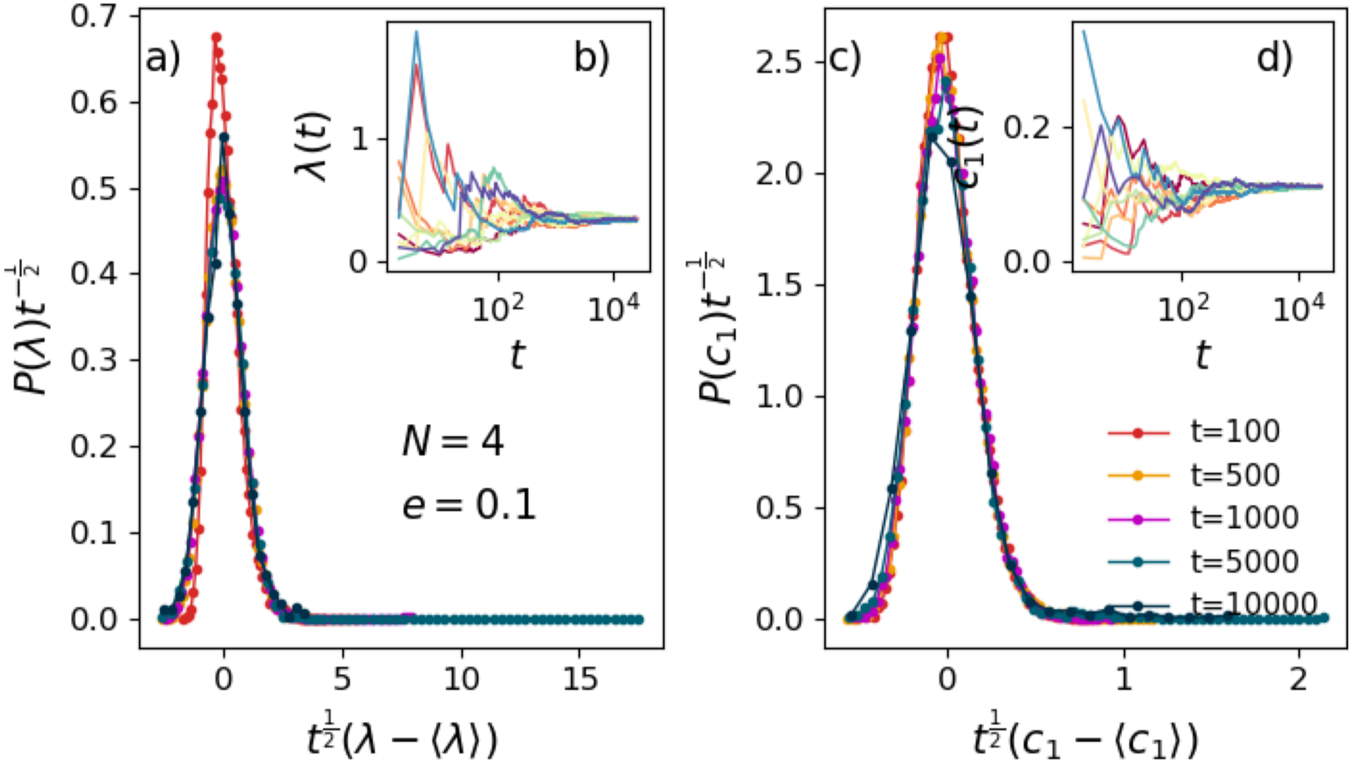
$\mathrm{N} \geq 4$



Harmonic trap:
Chaotic but
non-ergodic

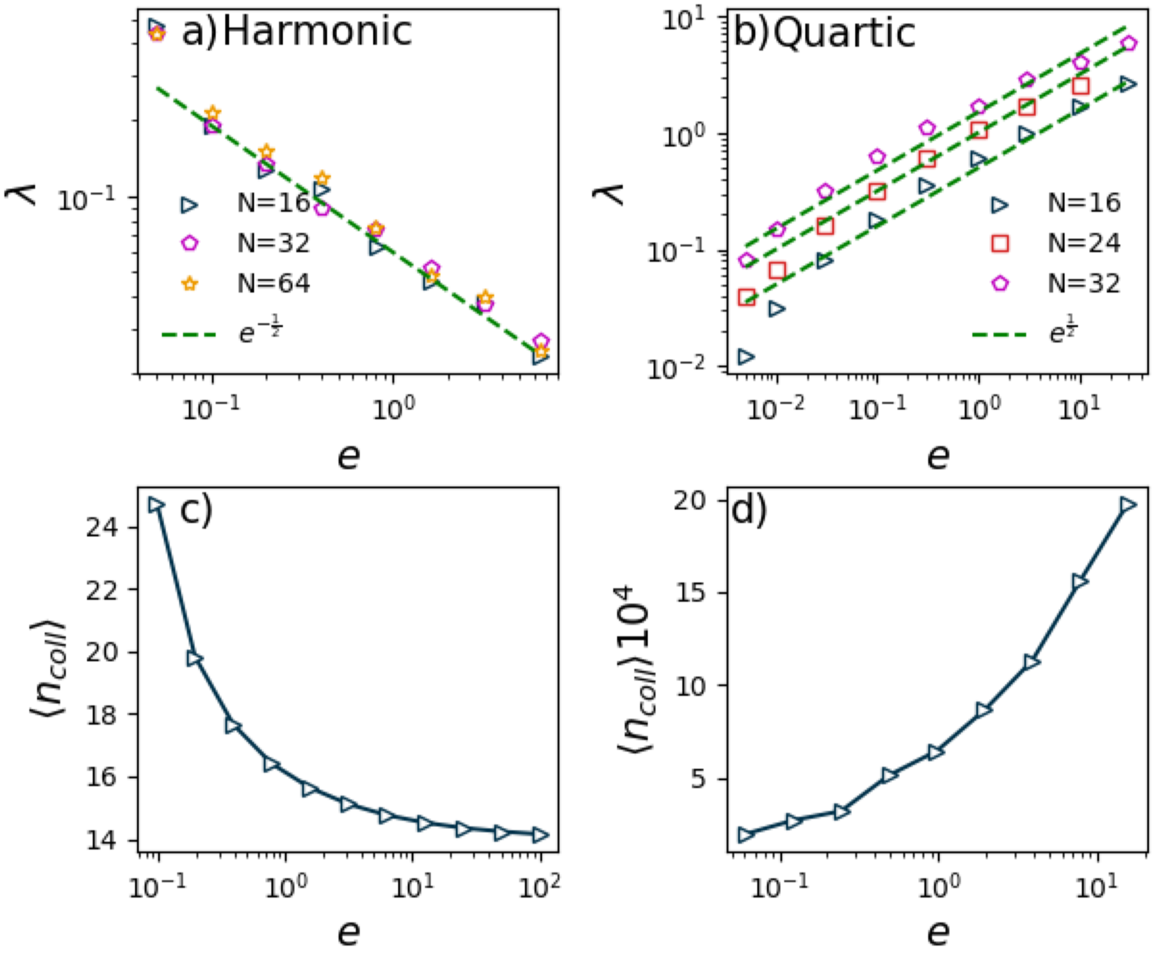

Γ ≡ (E, Ecm)
Γ1 = (E, Ecm, Q1)
Γ2 = (E, Ecm, Q2)
Γ3 = (E, Ecm, Q3)
Γ4 = (E, Ecm, Q4)

Distribution of the Lyapunov exponent and temperature: Quartic trap



Energy dependence of Lyapunov exponent

[Dong Z, Moessner R, Haque M. J Stat Mech. (2018) 063106.]

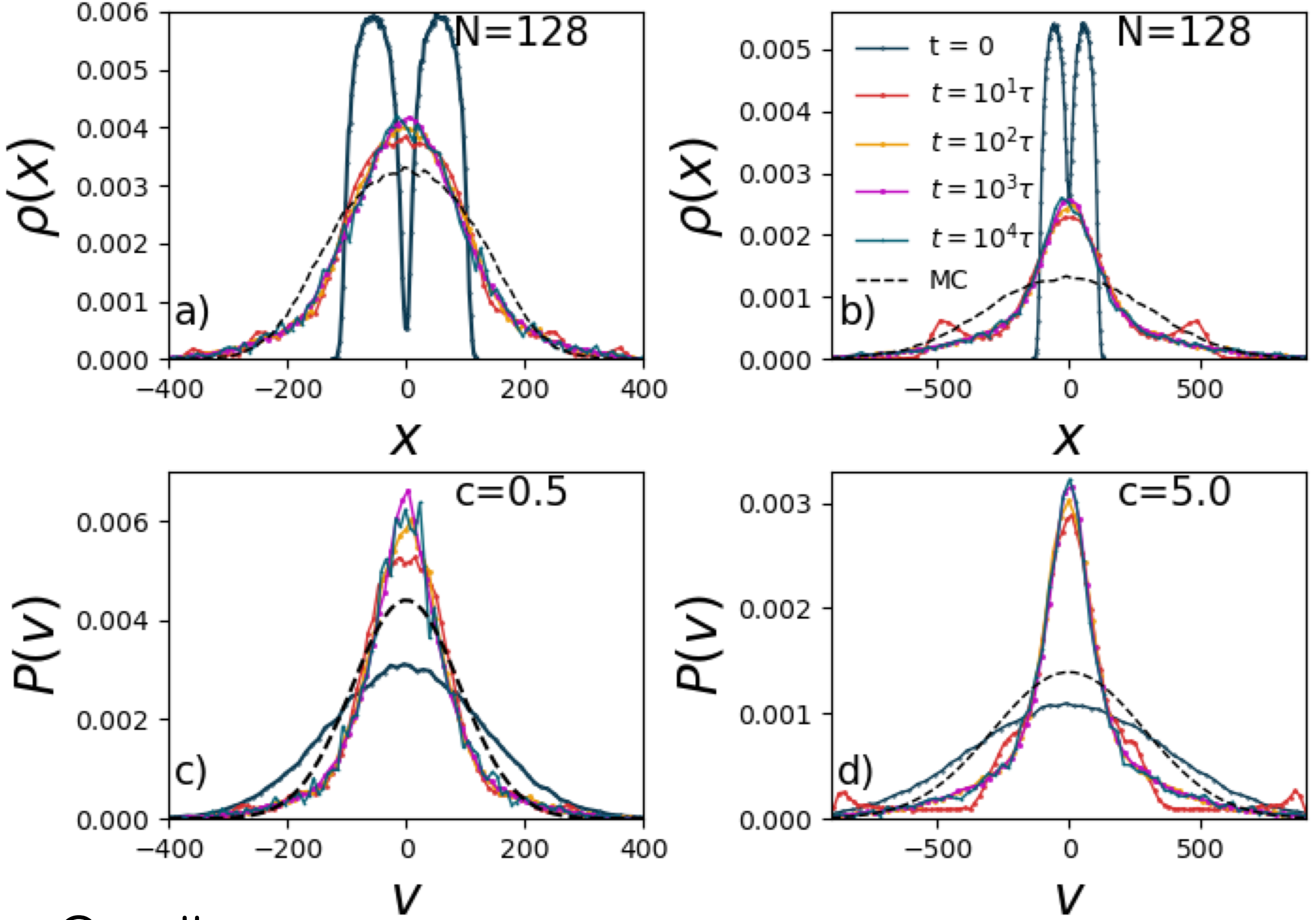


[Kurchan J. J. Stat phys (2018) 171(6):965-79].

Average number of collisions decrease with increasing rescaled energy (e): Less Chaotic

Average number of collisions increase with increasing rescaled energy (e): More Chaotic

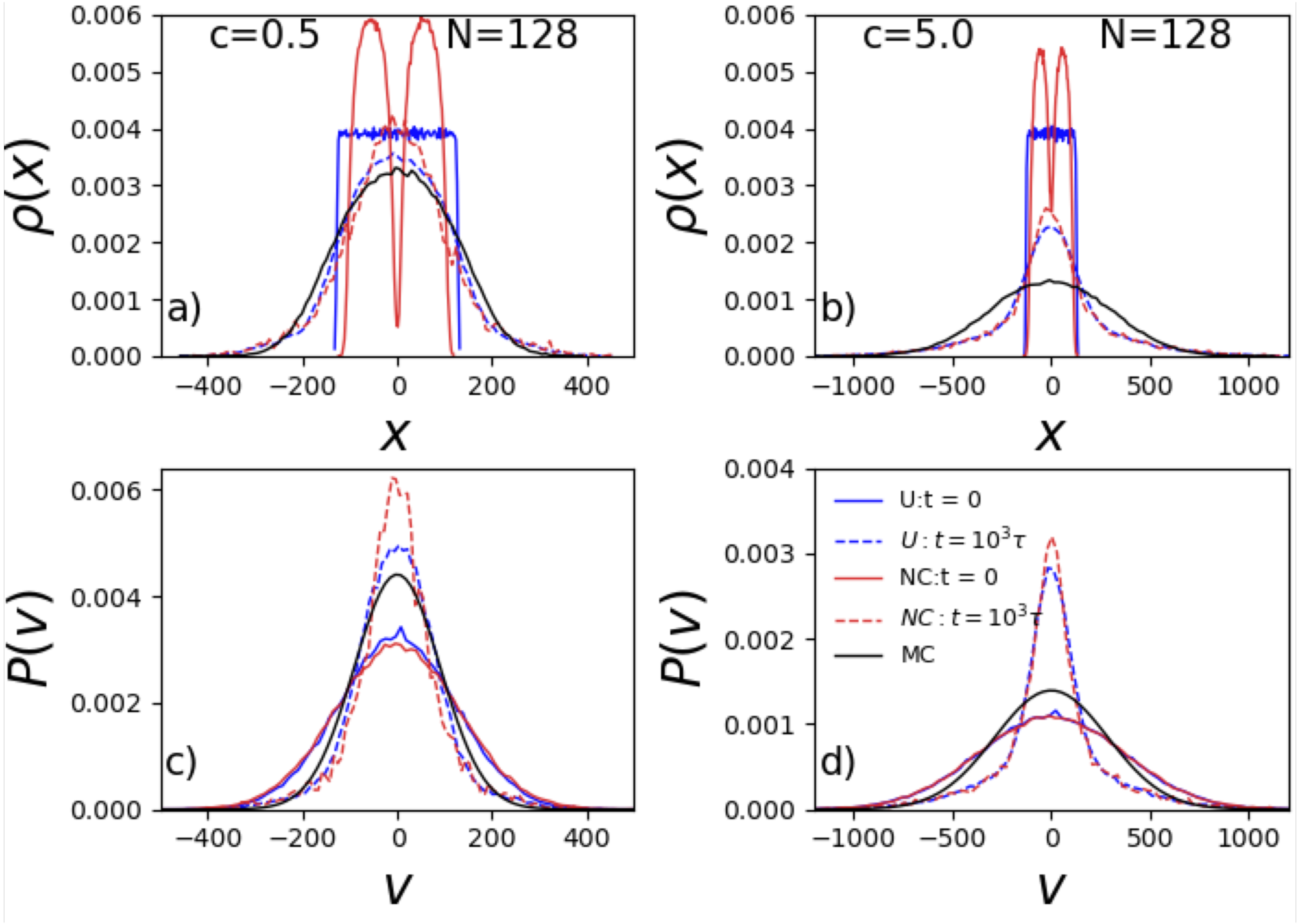
Macroscopic variables



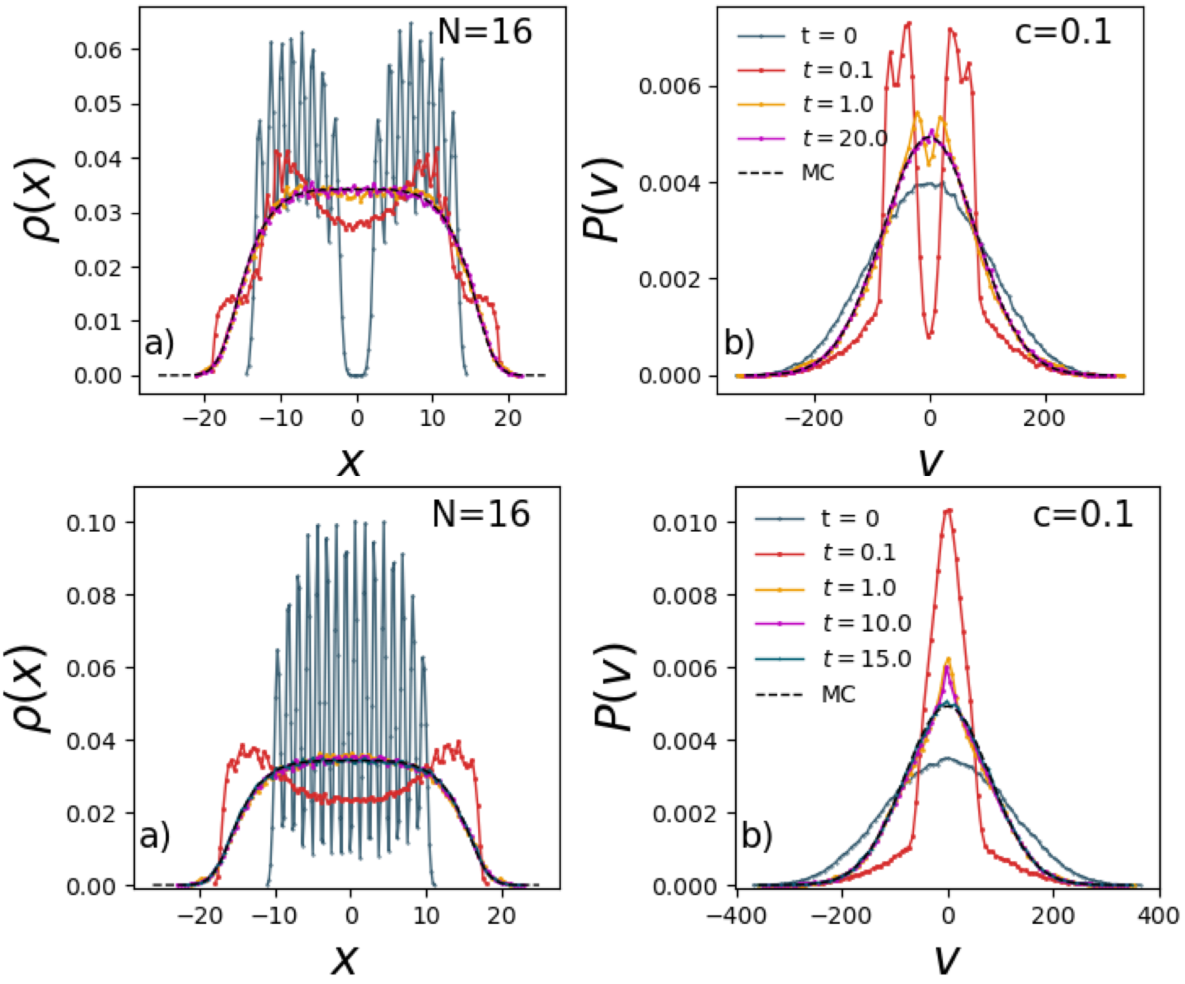
Newtons Cradle

Harmonic:
Not Gibbs
equilibrium

Initial condition dependence



Quartic: Gibbs equilibrium



Newtons Cradle

Uniform

Conclusions

- Equilibrium description
- Rescaled energy e and rescaled temperature c are the is the only relevant parameter.

Harmonic confinement and Quartic confinement have very different behaviour.

- $N = 3$, particle systems with harmonic confinement is integrable (we still don't know the third conserved quatity) however quartic trap is chaotic.

- $N \geq 4$, particle systems in harmonic confinement is chaotic but non-ergodic. For the quartic confinement we find the distribution of lyapunov exponent is sharply peaked.

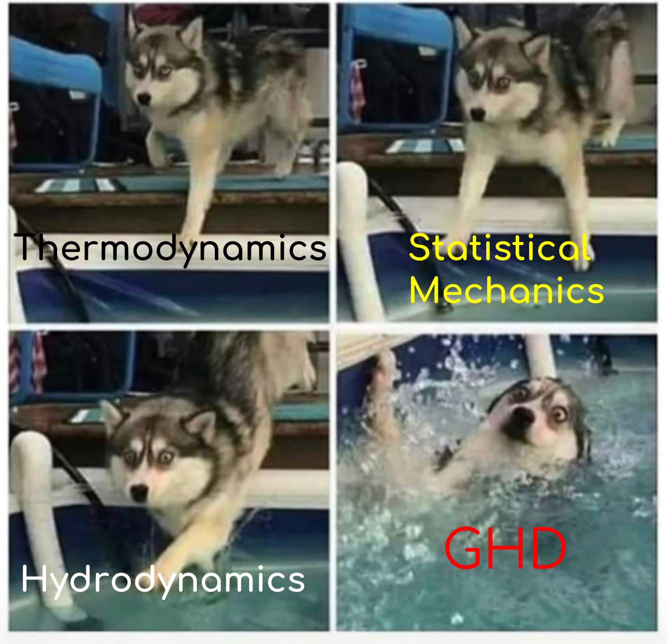
- The long time density profile is different from Gibbs expectation and initial condition dependent, for harmonic confinement. Quartically confined system thermalizes to the Gibbs state.

Properties	$N = 3$		$N \geq 4$	
	Harmonic	Quartic	Harmonic	Quartic
Chaotic	No	Yes	Yes (No)	Yes
Ergodic	No	Yes	No (→ Yes)	Yes
Steady state	(Not Gibbs)	(Gibbs equilibrium)	Not Gibbs	Gibbs equilibrium

Generalized Hydrodynamics with trapping potential

Q. Would modified GHD for harmonic confinement explain the different non-Gibbs states we observe?

Q. What are its results for quartic trap?
SubQ. Hydrodynamic description with 3 conservation laws



Thank you