NEXT 2003

News and Expectations in Thermostatistics

21-28 Settembre 2003 - Villasimius (CA)

Anomalous and Glassy behavior in Hamiltonian Dynamics

A. Pluchino

in collaboration with A. Rapisarda and V. Latora

Dipartimento di Fisica e Astronomia and INFN sezione di Catania
Università di Catania - **Italy**

CACTUS
Chaos And Complexity Theoretical University Study
Group
Catania

E-mail: *alessandro.pluchino@ct.infn.it* - ***Group web page:*** *www.ct.infn.it/~cactus*

Outline of the talk

- Introduction: Thermodynamics and Dynamics of the HMF model
- Negative specific heat & Metastable Quasi-Stationary States
- Slow dynamics, Anomalous diffusion & Velocity PDF

Main focus on some particular DYNAMICAL ANOMALIES :

- Role of initial conditions on the QSS dynamics
- Correlations, Dynamical frustration, Power Law Relaxation & Aging

…and on their INTERPRETATION :

- Links with generalized (non extensive) q-statistics scenario
- Weak ergodicity breaking and Spin-glass phase interpretation of the QSS regime

The HMF Model

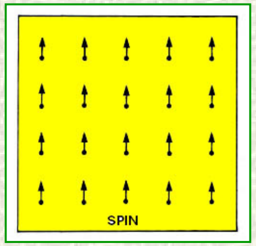
The

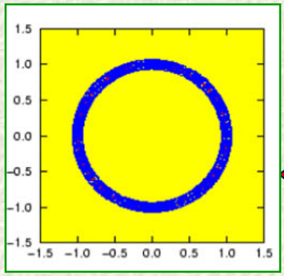
HAMILTONIAN MEAN FIELD (HMF) MODEL

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + \frac{1}{2N} \sum_{i,j=1}^{N} [1 - \cos(\vartheta_i - \vartheta_j)]$$

Antoni and Ruffo PRE 52 (1995) 2361

…is a simple XY model of fully-coupled classical spins (rotators),





or interacting particles moving on the unitary circle

Its behavior seems to be paradigmatic for a large class of non extensive systems, as for example nuclear and astrophysical systems, but also fragmenting nuclei and atomic clusters.

Thermodynamics

Taking as order parameter the modulus M of the total magnetization:

$$\vec{M} = \frac{1}{N}\sum_{i=1}^{N}\vec{m}_i$$

where the single spin is:

$$\vec{m}_i = (\cos\vartheta_i, \sin\vartheta_i)$$

the canonical solution of the model shows a second-order phase transition, passing from a CLUSTERED (ferromagnetic) phase to a HOMOGENEOUS (paramagnetic) one as a function of Energy Density U:

Caloric curve ⟹

$$U = \frac{E}{N} = \frac{\partial(\beta F)}{\partial \beta} = \frac{1}{2\beta} + \frac{1}{2}\left(1 - M^2\right)$$

Antoni and Ruffo, PRE 52 (1995) 2361

$F = free\,energy$

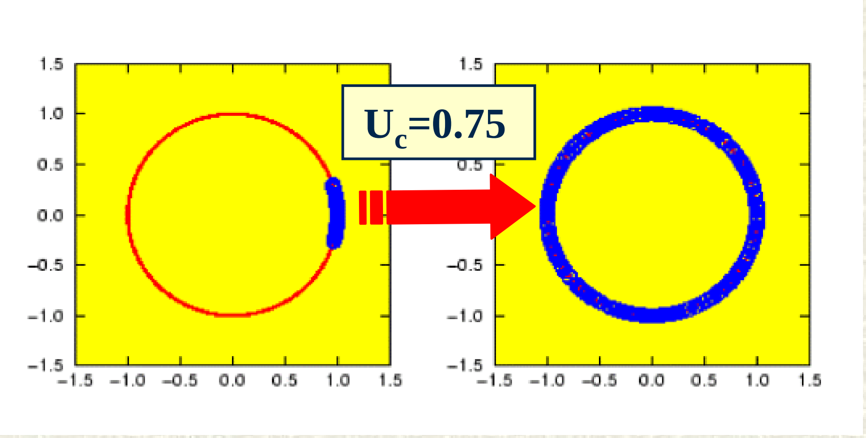
$\beta = \frac{1}{k_B T}$

$T = temperature$

M ~ 1

Low Energy Density

Clustered phase



M ~ 0

High Energy Density

Homogeneous phase

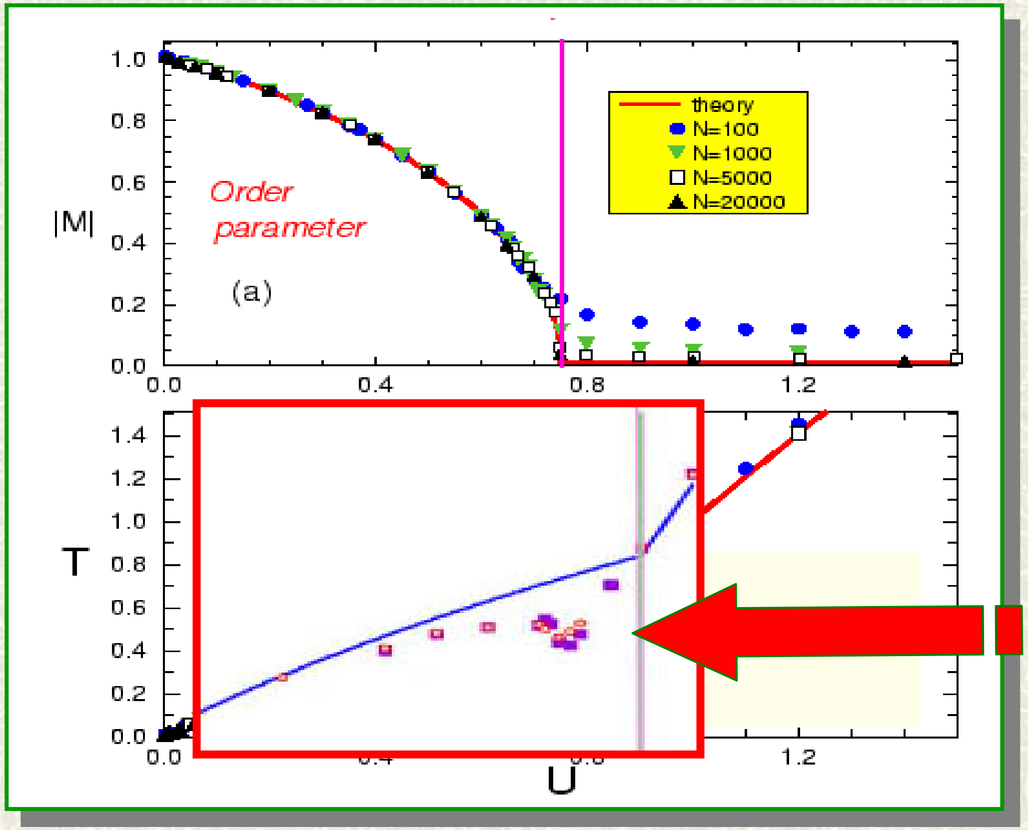
Dynamics and Equilibrium

Equations of motion

$$
\begin{cases}
\dfrac{\partial \theta_i}{\partial t} = p_i \\
\dfrac{\partial p_i}{\partial t} = -M_x \sin\theta_i + M_y \cos\theta_i
\end{cases}
$$

The equations are solved numerically by using a fourth order simplectic algorithms (Yoshida , Physica A **150** (1990) 262).

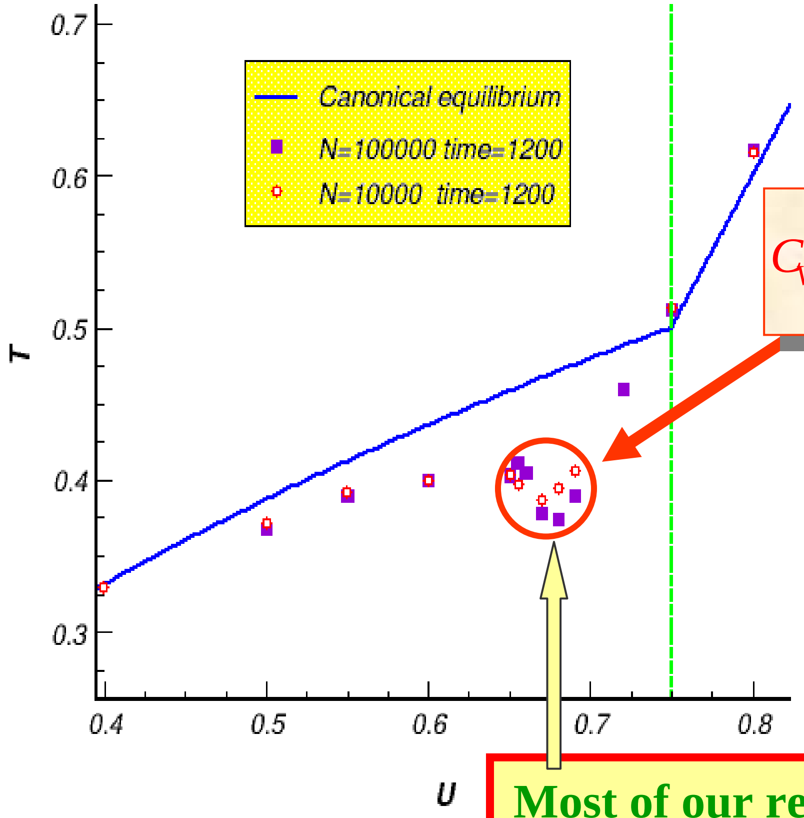
Good agreement between exact canonical solution and numerical microcanonical simulations at equilibrium for various sizes N of the system…



…but…

When the system is started with **initial conditions very far from equilibrium**, we observe many **dynamical anomalies.** In particular we focus on an energy range below the critical point (0.5 < U < 0.75).

Negative specific heat



$$C_V = \left(\frac{\partial U}{\partial T}\right)_V < 0$$

Most of our results will refer to the case U=0.69

In such a region the specific heat becomes negative.

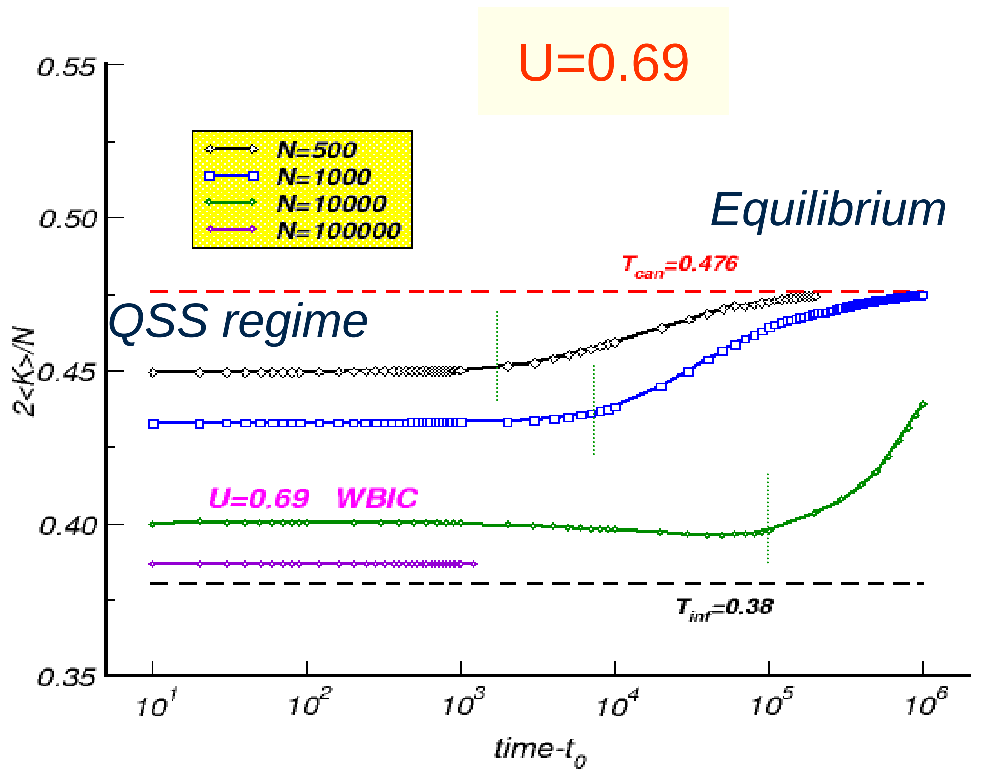
In fact the temperature decreases, by increasing the energy density.

This phenomenon has been observed in multifragmentation nuclear reactions and atomic clusters, but also in self-gravitating stellar objects, i.e. for non extensive systems.

See for example:

- Thirring, Zeit. Physik 235 (1970) 339
- Lynden-Bell, Physica A 263 (1999) 293
- D.H.E.Gross, *Microcanonical Thermodynamics: Phase transitions in Small systems*, World Scientific (2001).
- M. D'Agostino et al, Phys. Lett. B 473 (2000) 279
- Schmidt et al, Phys. Rev. Lett. 86 (2001) 1191

Metastable QSS



Starting far from equilibrium, the system remains trapped for a very long time in *METASTABLE QUASI STATIONARY STATES* (QSS) whose temperature, defined as:

$$T = \frac{2<K>}{N}$$

is smaller than the equilibrium one.

THE LARGER N, THE LONGER THE QSS LIFETIME.

Finally, for $N \rightarrow \infty$ the QSS temperature tends to $T_{QSS} = 0.38$ and the system never reaches the equilibrium regime!

Order in the limits

Our simulations clearly show that, in going towards the thermodynamic limit, it is very crucial the order of taking the size limit and the time limit…

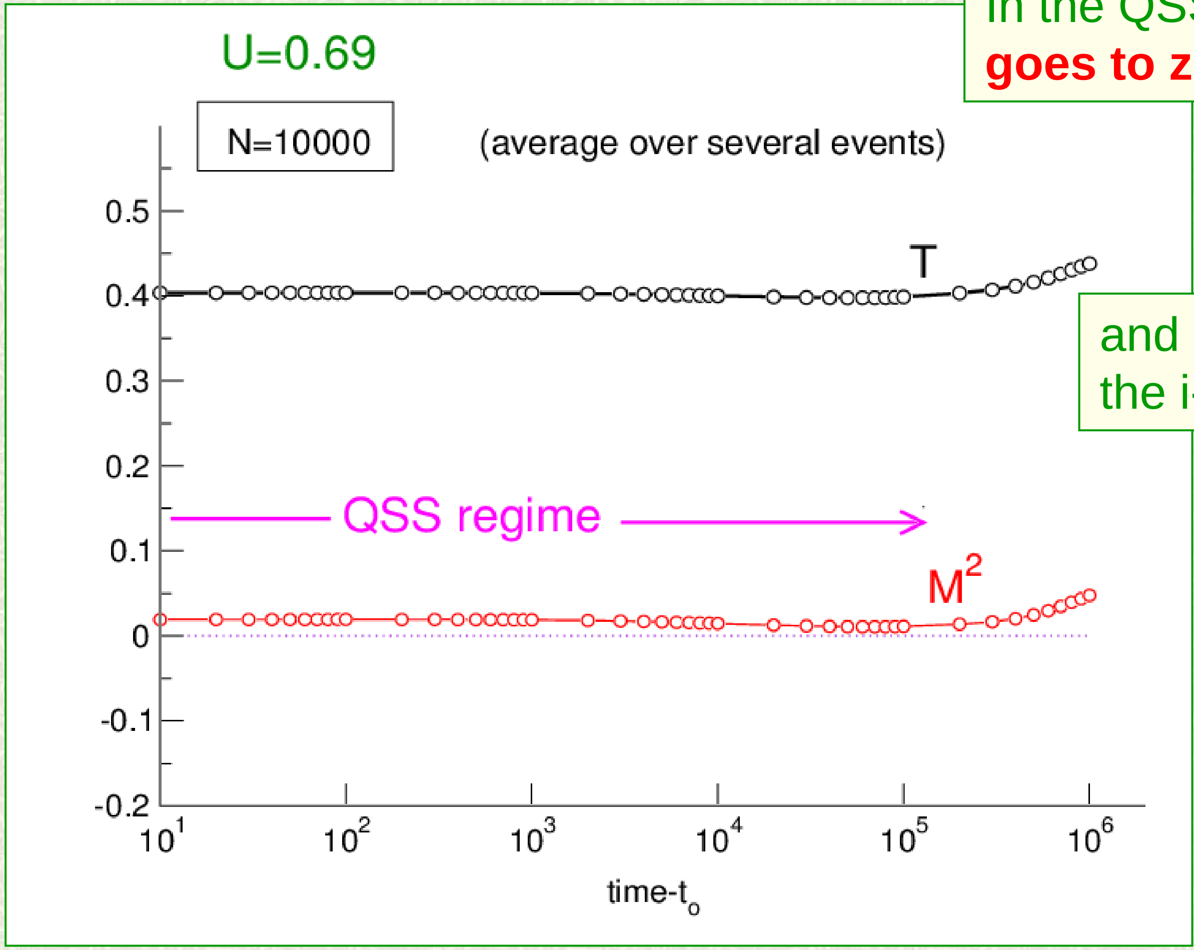
In general, the two limits do not commute:

$$N \to \infty \; t \to \infty \quad \neq \quad t \to \infty \; N \to \infty$$

Boltzmann-Gibbs equilibrium

QSS

Slow dynamics



In the QSS regime the **magnetization goes to zero** with the size N:

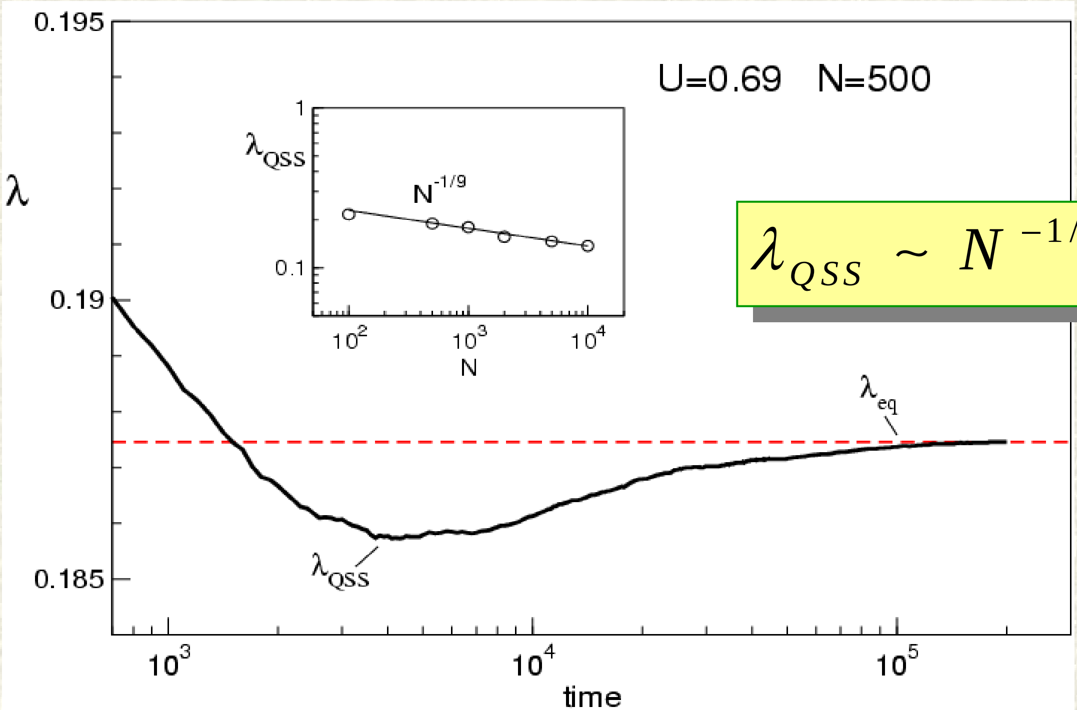
$$M_{QSS} \sim N^{-1/6}$$

and so does also **the force F_i** on the i-th spin, being:

$$F_i = -M_x \sin\theta_i + M_y \cos\theta_i$$

Thus the QSS dynamics is slower and slower by increasing N.
For $N \to \infty$ the system remains frozen in the QSS regime.

Vanishing Lyapunov exponents



$$\lambda_{QSS} \sim N^{-1/9}$$

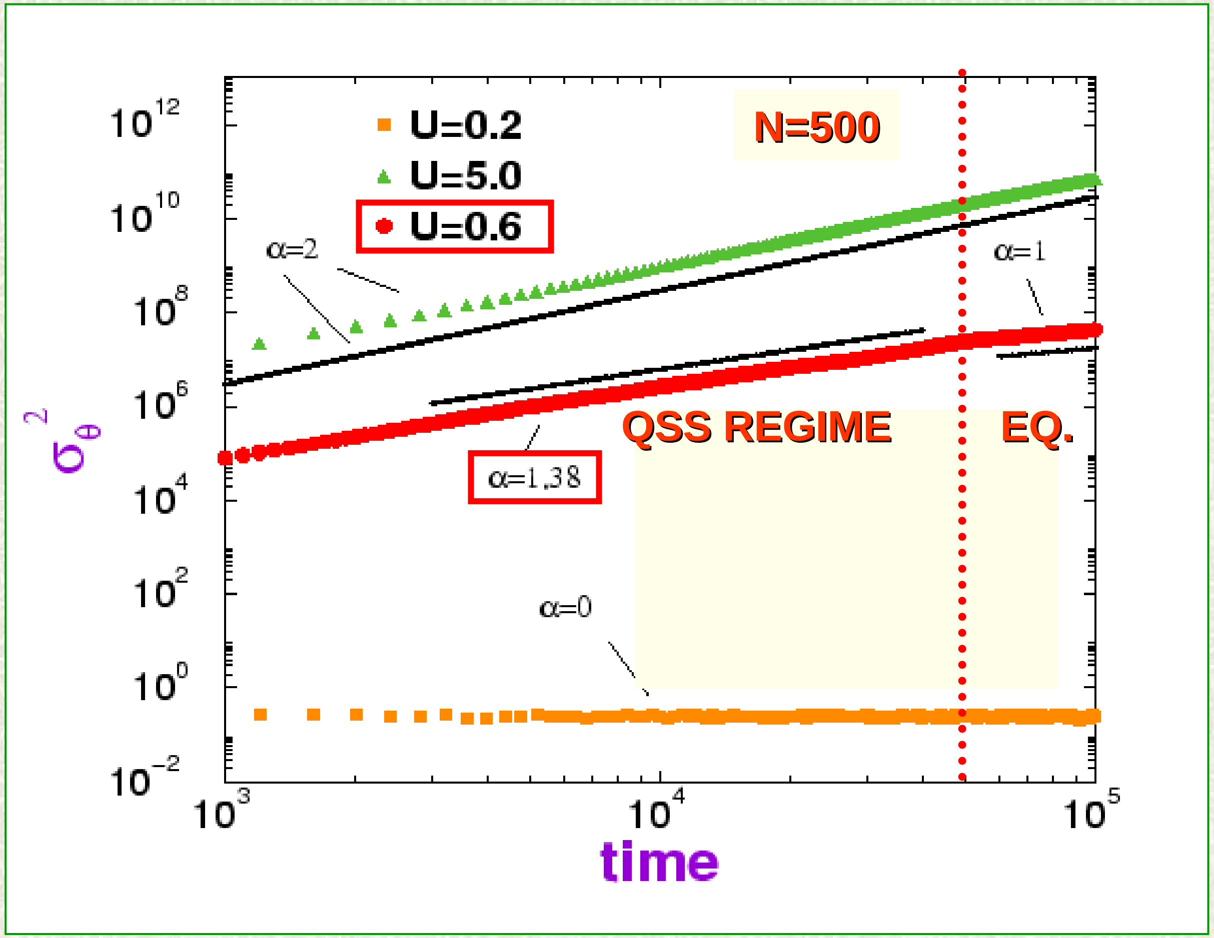
In the QSS regime the largest Lyapunov exponent tends to zero as the size of the system tends to infinity

This scaling can be obtained considering that…

$$\lambda \propto M^{2/3} \propto \left(N^{-1/3}\right)^{1/3} = N^{-1/9}$$

See Latora, Rapisarda, Tsallis Physica A 305 (2002) 129

Anomalous Diffusion



Latora, Rapisarda and Ruffo, PRL 83 (1999) 2104

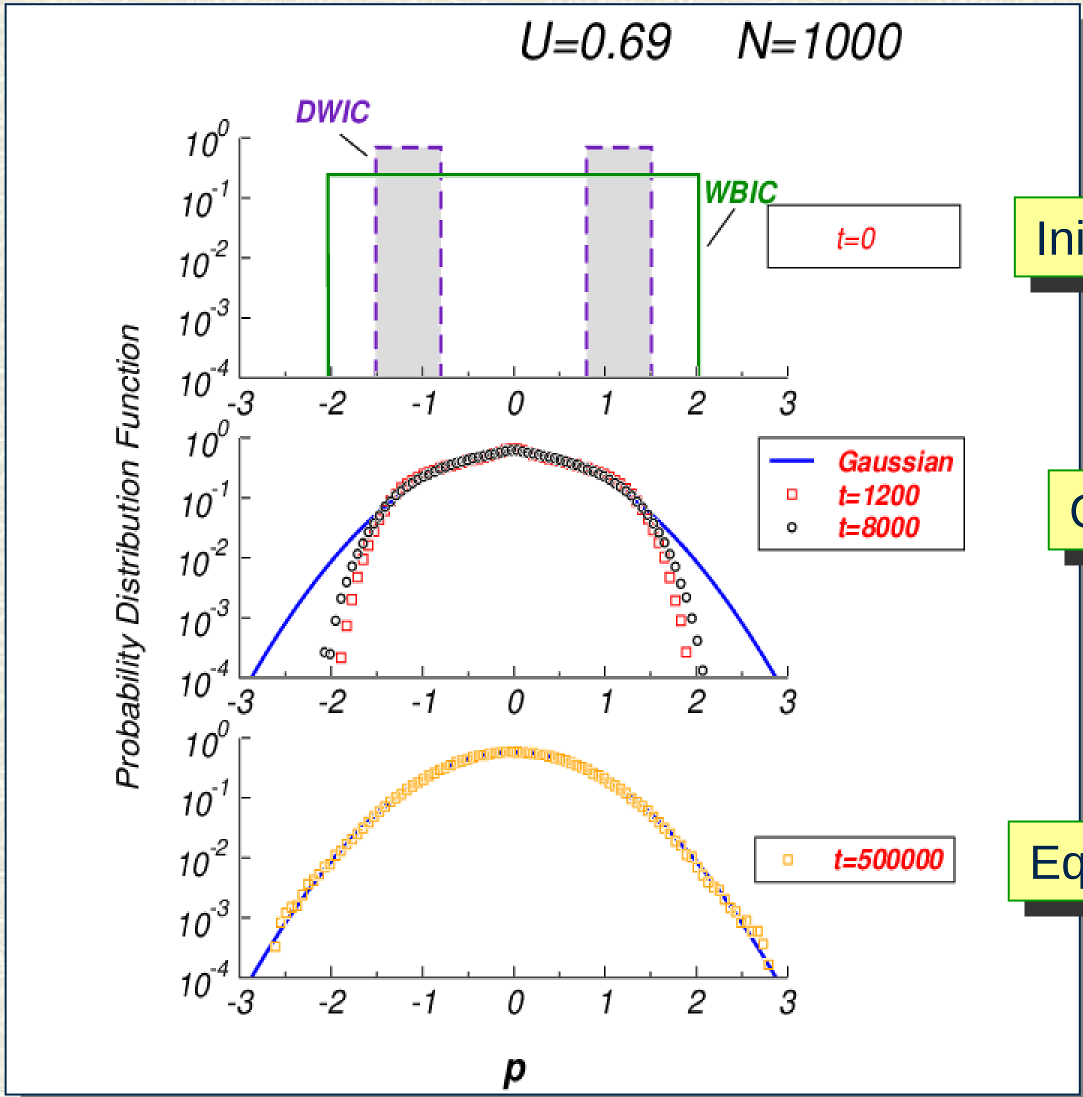
$$\sigma^2(t) \propto t^\alpha$$

$\alpha = 1$	Normal diffusion
$\alpha \neq 1$	Anomalous diffusion

In correspondence of the **QSS regime** we get **superdiffusion** with an exponent **α=1.38.**

The diffusion becomes **normal** when the system reaches the equilibrium

Non Gaussian Velocity PDFs



Initial conditions

QSS regime

Equilibrium regime

CACTUS Chaos And Complexity Theoretical University Study Group Catania

Outline of the talk

- Introduction: Thermodynamics and Dynamics of the HMF model
- Negative specific heat & Metastable Quasi-Stationary States
- Slow dynamics, Anomalous diffusion & Velocity PDF

Main focus on some particular **DYNAMICAL ANOMALIES** :

- Role of initial conditions on the QSS dynamics
- Correlations, Dynamical frustration, Power Law Relaxation & Aging

…and on their **INTERPRETATION** :

- Links with generalized (non extensive) q-statistics scenario
- Weak ergodicity breaking and Spin-glass phase interpretation of the QSS regime

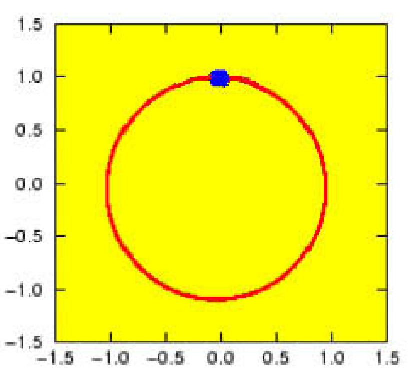
Role of initial conditions

We have recently studied the nature of the metastable QSS regime by starting from **two classes of initial conditions** with different magnetization values:

M1ic

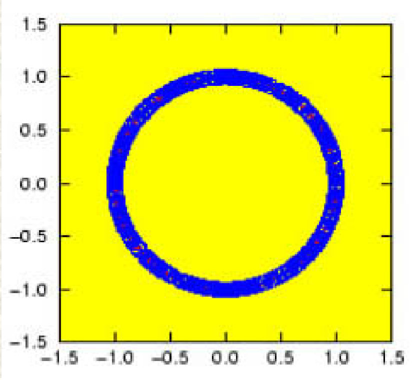
M(0)=1

The old one



all the angles = 0

M0ic



angles uniformly distributed

M(0)=0

The new one

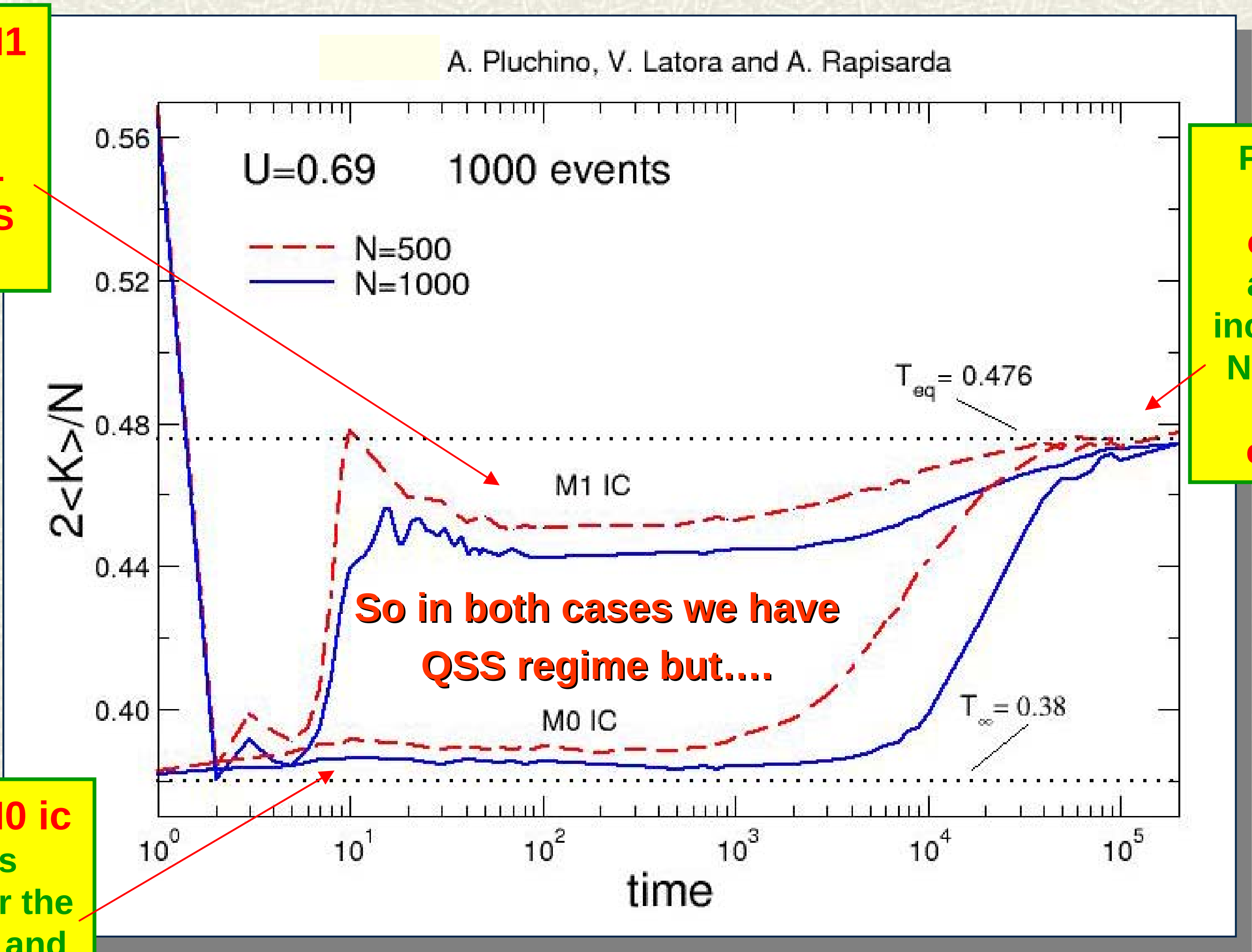
See Dauxois' talk…

(in both cases we consider the usual uniform distribution in velocity – water bag).

Pluchino, Latora and Rapisarda, Physica D (2003) in press [cond-mat/0303081]

QQS for M1 & M0 IC

Starting from **M1 ic** the system dynamically reaches the **N-dependent QSS** plateaux



So in both cases we have QSS regime but….

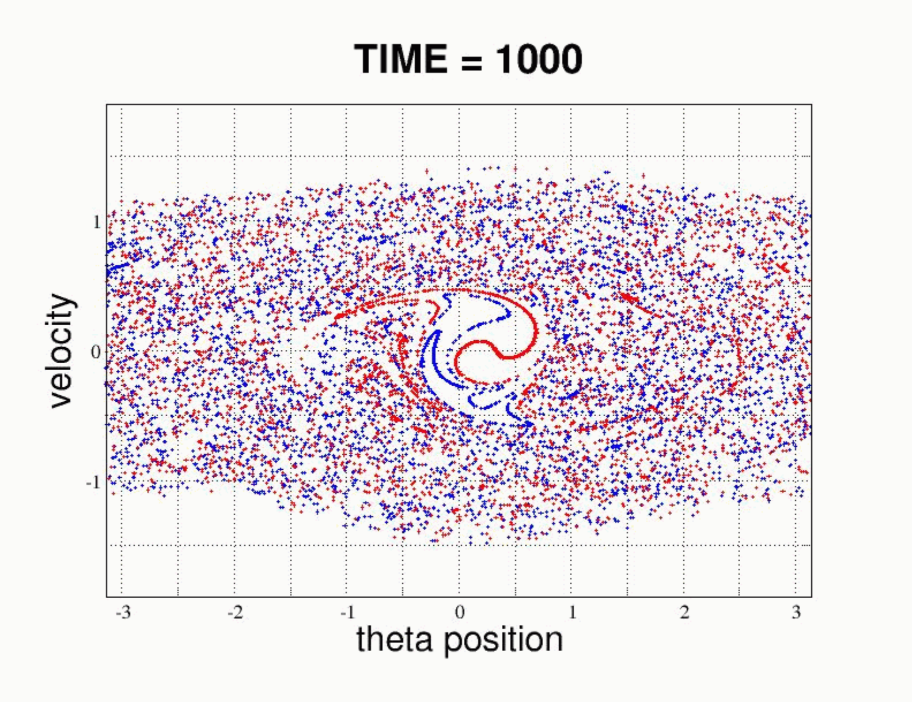
For **both the initial conditions**, after a time increasing with N, the system relaxes to **equilibrium**

Starting from **M0 ic** the system is directly put near the state with **M ~0** and **T~0.38**, and stays here for a while

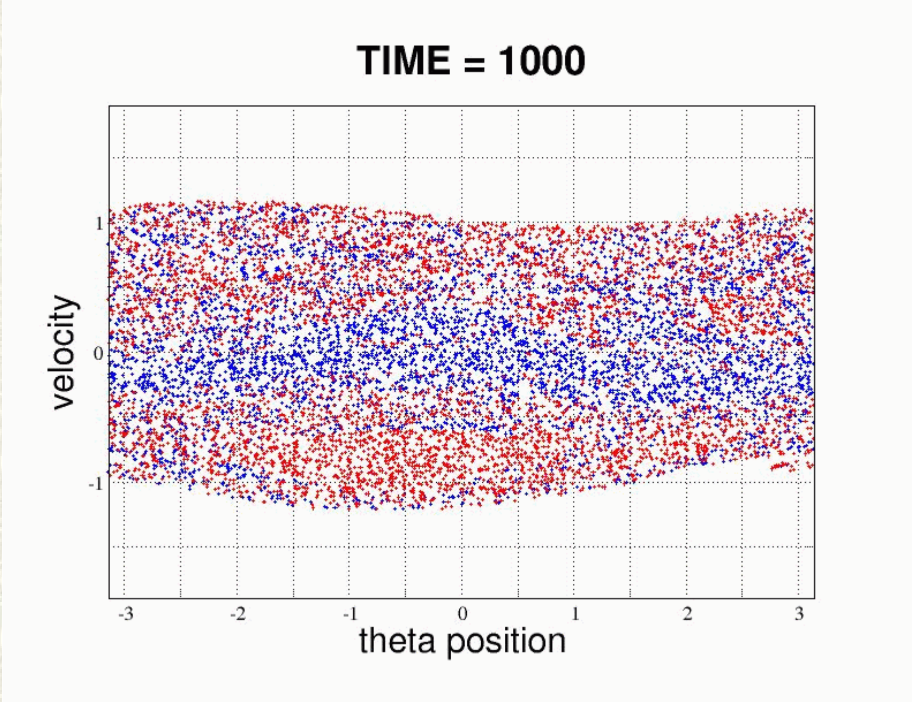
Correlations in phase-space

…structures in phase-space appears, in the QSS regime, only for M1 IC, *and not for M0 IC*

M1 ic



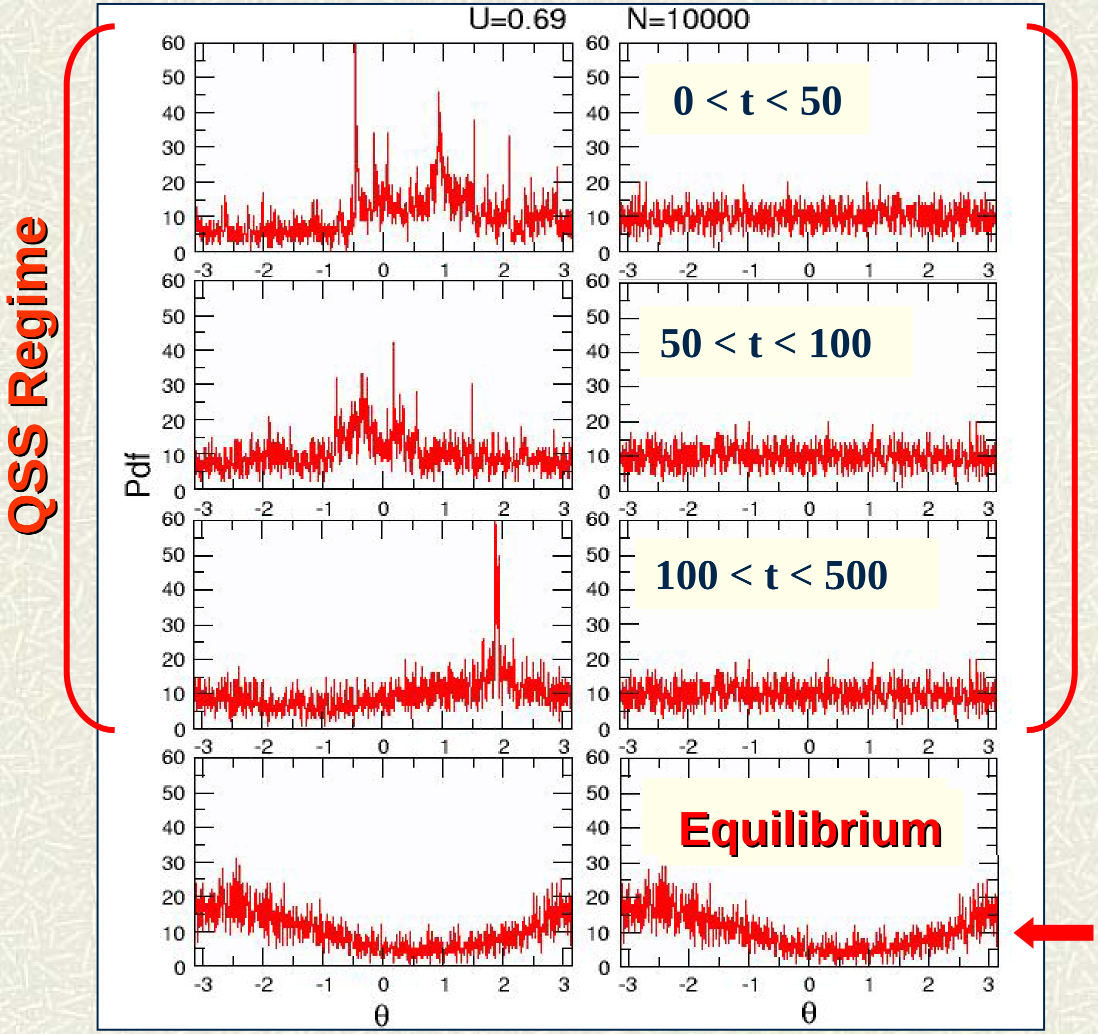
M0 ic



- **High velocity particles at t = 0**
- **Low velocity particles at t = 0**

Dynamical frustration

M1 IC   M0 IC

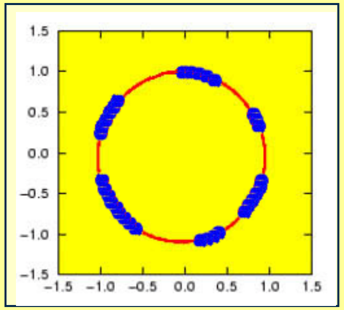


ANGLES PDFs

M=1 initial conditions:

- Competition between clusters of rotating particles in the QSS regime

- Each cluster tries to capture the maximum number of particles in order to reach the final equilibrium configuration:



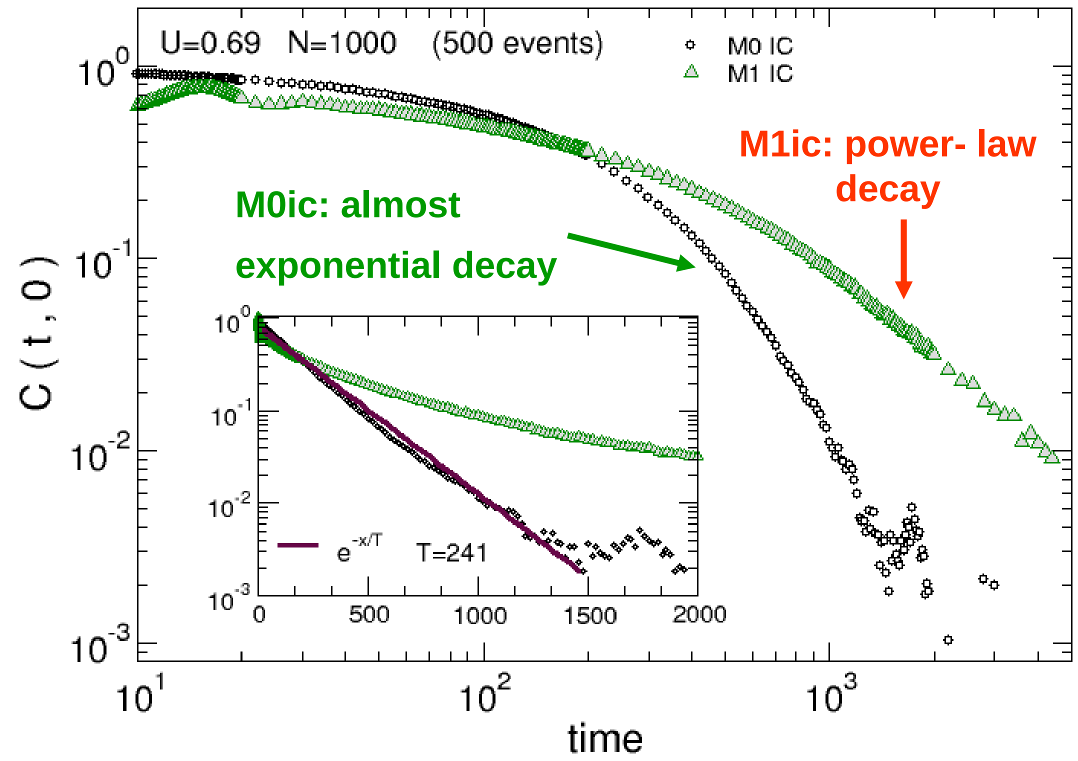
This competition leads to a ***DYNAMICAL FRUSTRATION*** in the QSS regime!

M=0 initial conditions:

No competition and no frustration are present

At equilibrium only one big rotating cluster is present for both the IC

Relaxation to equilibrium



Velocity auto-correlation functions:

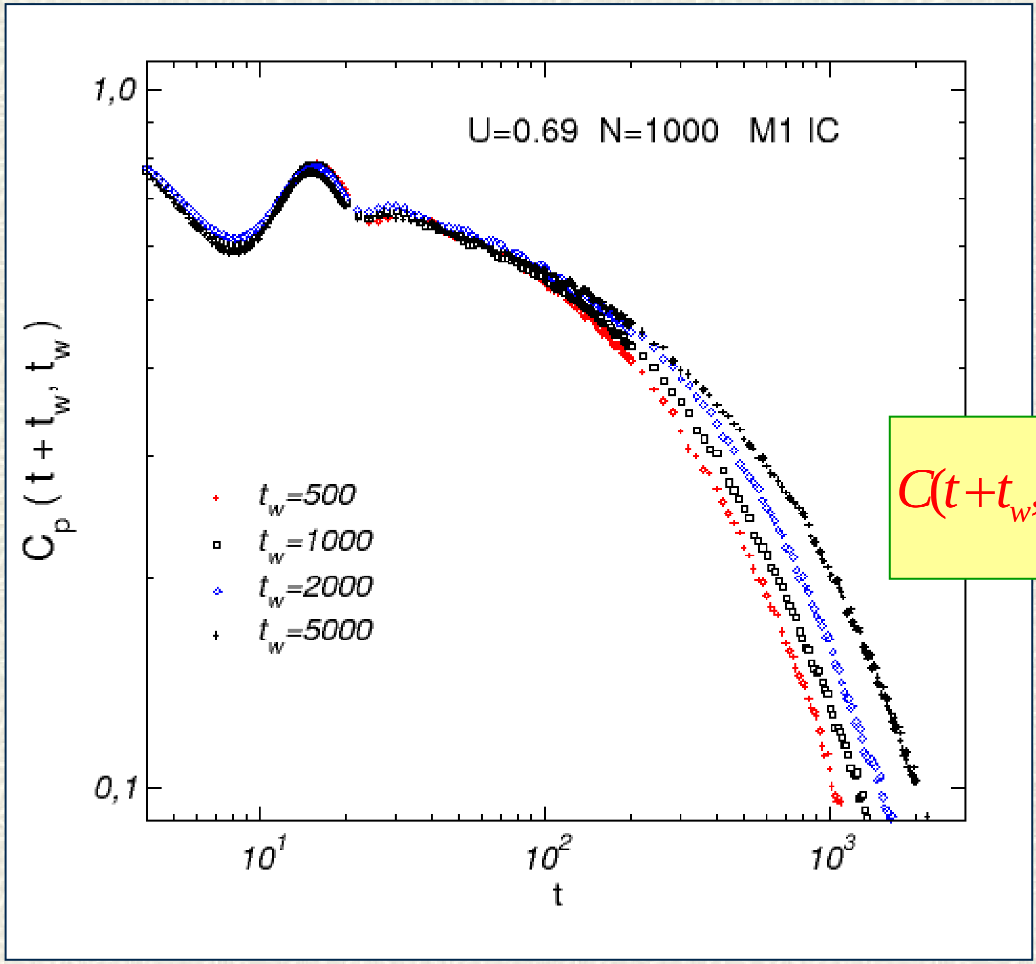
$$C(t,0) = \frac{<\mathbf{P}(t)\mathbf{P}(0)> - <\mathbf{P}(t)><\mathbf{P}(0)>}{\sigma(t)\sigma(0)}$$

where:

$$\mathbf{P}(t) = (p_1, p_2, \ldots p_N)$$

is the **velocity vector**, the brackets indicate an average over the events, and $\sigma(t)$ is the standard deviation at time t.

Memory effects & Aging



Pluchino, Latora and Rapisarda, Physica D (2003) in press [cond-mat/0303081]

See also: Montemurro, Tamarit and Anteneodo PRE 67 (2003) 031106

Only for M=1 initial conditions:

The system, in going towards equilibrium, shows **memory effects** and **aging**, i.e. the velocity auto-correlation functions decay depend on the waiting time t_w :

$$C(t+t_w,t_w) = \frac{<\mathbf{P}(t+t_w)\mathbf{P}(t_w)> - <\mathbf{P}(t+t_w)><\mathbf{P}(t_w)>}{\sigma(t+t_w)\sigma(t_w)}$$

So, **figuratively**, we can say that, in the QSS regime for finite N, the system **lives** for a while in a metastable condition, **ages** and finally **dies** relaxing to equilibrium…

(Thanks to prof. C.Tsallis for this suggestive metaphor!)

Outline of the talk

- Introduction: Thermodynamics and Dynamics of the HMF model
- Negative specific heat & Metastable Quasi-Stationary States
- Slow dynamics, Anomalous diffusion & Velocity PDF

Main focus on some particular DYNAMICAL ANOMALIES :

- Role of initial conditions on the QSS dynamics
- Correlations, Dynamical frustration, Power Law Relaxation & Aging

…and on their INTERPRETATION :

- Links with generalized (non extensive) q-statistics scenario
- Weak ergodicity breaking and Spin-glass phase interpretation of the QSS regime

Tsallis generalized formalism

In the last decade a lot of effort has been devoted to understand if **thermodynamics** can be **generalized** to nonequilibrium complex systems.

In particular one of these attempts is that one started by **Constantino Tsallis** with his seminal paper J. Stat. Phys. 52 (1988) 479

The **generalized Tsallis entropy** is:

$$S_q = \frac{1 - \sum_i p_i^q}{q - 1}$$

S_q **is non extensive**, i.e. for two independent systems A and B one gets:

$$S_q(A+B) = S_q(A) + S_q(B) + (1-q) S_q(A) S_q(B)$$

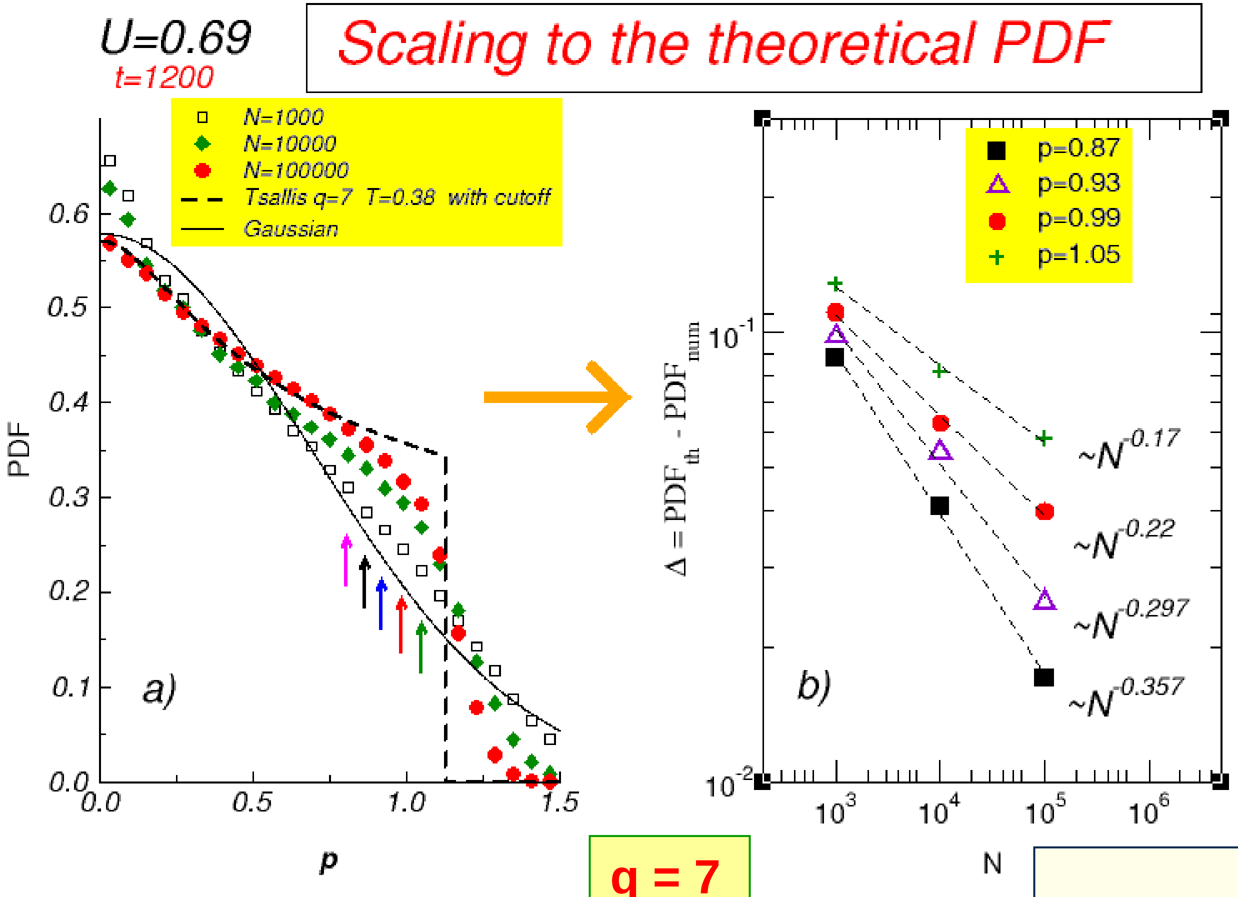
where S_q reduces to the Boltzmann entropy for $q = 1$

The **Boltzmann weight** is also generalized (q-exponential) and reads

[illegible]

In general the standard statistical mechanics formalism is **q-invariant**

Generalized velocity pdf

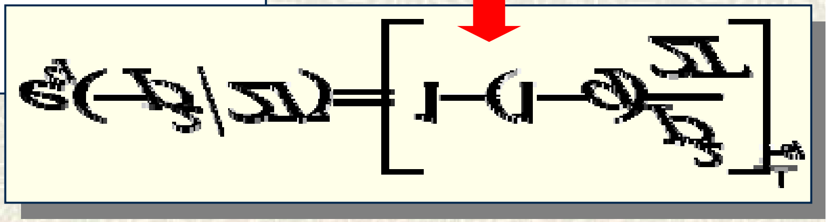


q = 7

The anomalous QSS regime is the effect of non extensivity or, in other words, of the long-range character of the interaction.

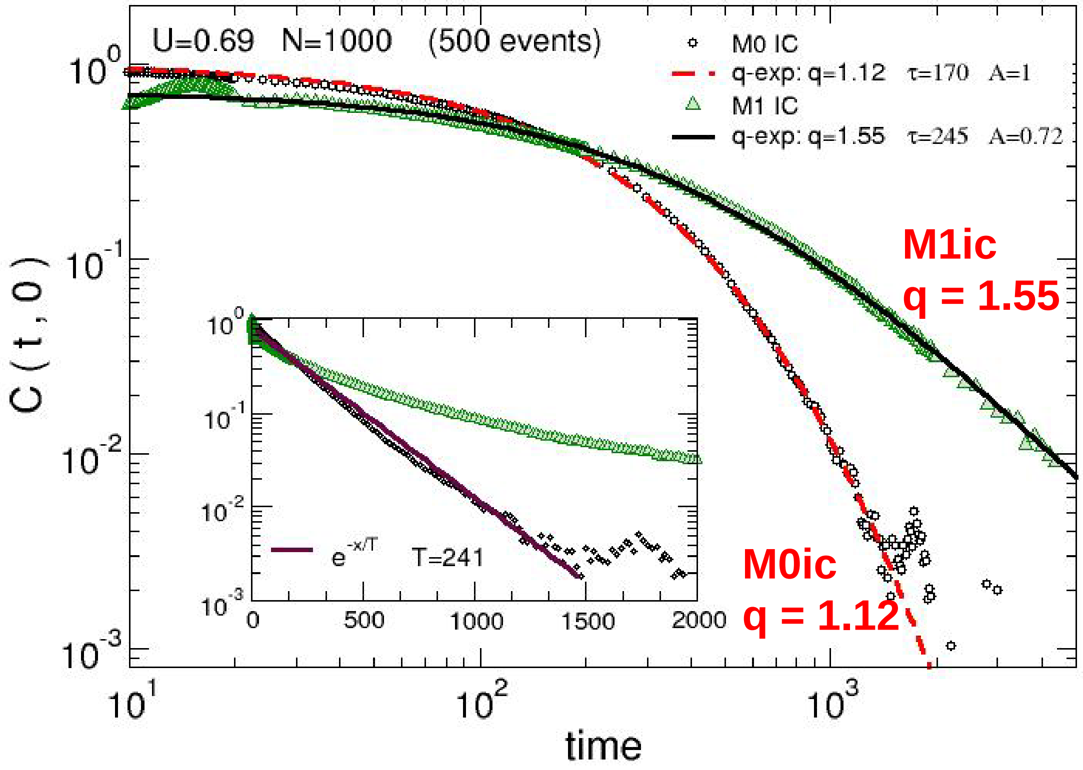
Thus, when long range correlations and fractal structures in phase space are present, the Tsallis' generalized thermodynamics formalism could provide a first interpretation of QSS.

In fact, for the M1ic, the non gaussian velocity pdfs show a q-exponential asymptotical behavior:



Latora, Rapisarda, Tsallis, Phys. Rev. E 64 (2001) 056134.

q-exponential decay of C(t,0)



M1ic q = 1.55

M0ic q = 1.12

[1] Tsallis and Buckman PRE 54 (1996) R2197

Also the decay of the velocity correlation function seems to be reproduced very well by means of the generalized q-exponential:

$$Ae_q(x) = A[1+(1-q)x]^{\frac{1}{1-q}}$$

with $x = -t/\tau$.

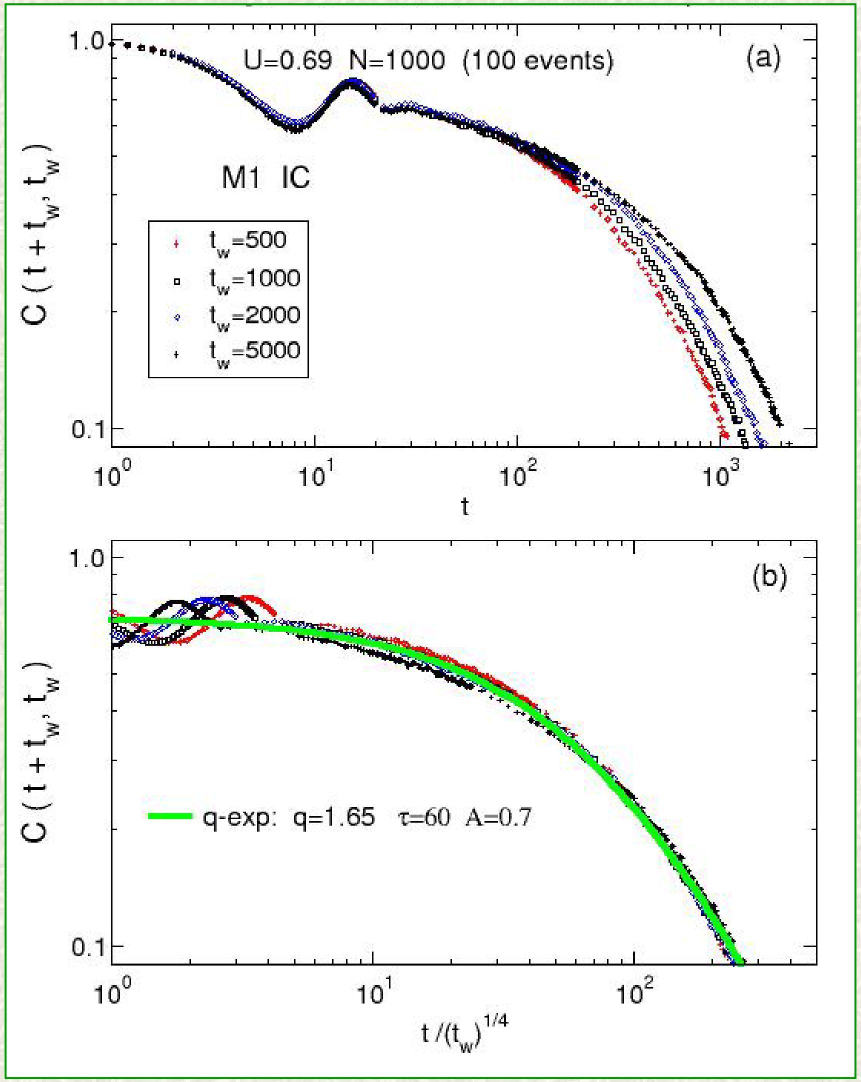
Within a generalized Fokker-Plank equation which generate Tsallis q-exponential pdfs [1], one can extract the following relation between the exponent α of the anomalous diffusion and q:

$$\alpha = \frac{2}{3-q}$$

In QSS regime, for M1ic, we had α=1.38-1.4 thus we expect q=1.55-1.6, which is confirmed by the fit.

On the other hand, for M0ic the decay is almost exponential and in fact the fit gives a value of q near to 1.

q-exponential decay for aging

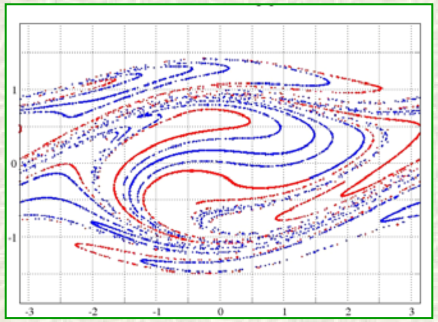


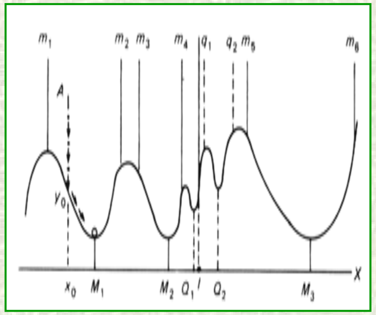
And also for the aging behavior, the power law decay of the M1ic correlation functions, after a proper rescaling, can be reproduced with a q-exponential function.

In this case we get **q = 1.65**.

QSS & Weak ergodicity breaking

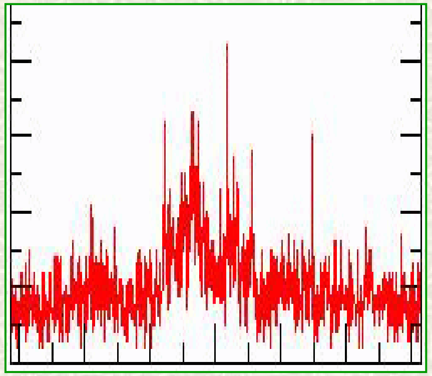
The onset of aging and slow relaxation dynamics in the QSS regime for M1 ic, and also the links with Tsallis' thermostatistics, are so evidently related with the complex (fractal) structure of the region of phase-space visited in time by the system.





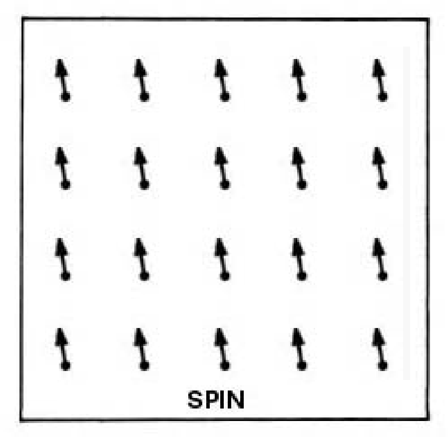
Such a scenario, in which the system doesn't explore all the *a-priori* available phase-space, strongly suggests a further link with the weak ergodicity breaking tipical of spin glass systems, where the complexity of the energy landscape is usually associated with quenched disorder and/or frustration.

In HMF model, despite the fact that neither disorder nor frustration are present *a-priori* in the interactions, the weak ergodicity breaking could be related to the complex dynamics generated by the vanishing Lyapunov exponent and by the dynamical frustration due to the competition between clusters in the QSS regime.

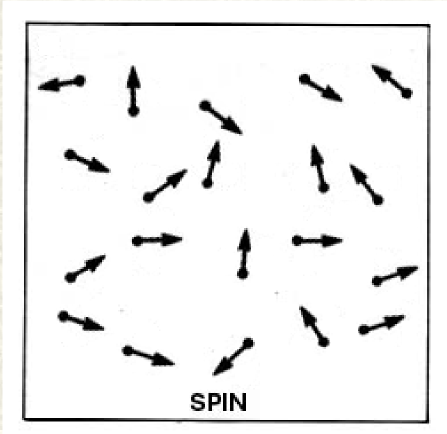


Spin Glass Phase

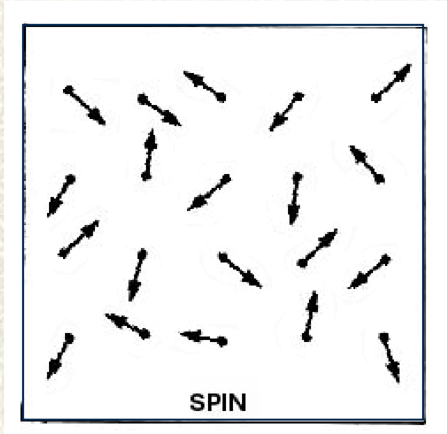
FERROMAGNETIC PHASE:



PARAMAGNETIC PHASE:



SPIN GLASS PHASE:



QUENCHED DISORDER & FRUSTRATION

$M \neq 0$ $M = 0$ $M = 0$

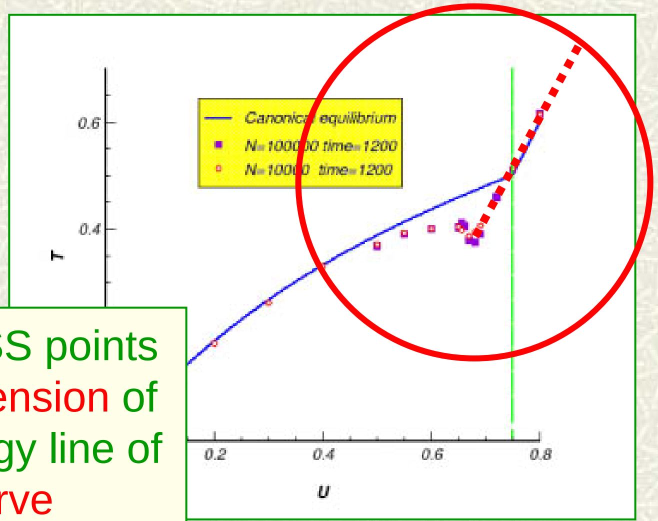
$$M = \frac{1}{N}\left|\sum_{i=1}^{N} \vec{s}_i\right|$$

How to discriminate between Paramagnetic and Spin Glass phase?

Polarization in HMF model

As previously seen, the QSS regime is characterized by a value of magnetization that vanishes with the size of the system (as in the paramagnetic regime):

$$M_{QSS} \sim N^{-1/6}$$



In fact the QSS points lie on the extension of the high energy line of the caloric curve

So, in order to better characterize the QSS regime of the HMF model (with M1 ic), we introduce a new quantity, the "*elementary polarization*":

$$< \vec{s}_i > = \frac{1}{\tau} \int_0^\tau \vec{s}_i(t)\, dt$$

i.e. the temporal average, over a time interval τ, of the successive positions of each elementary spin vector (rotator).

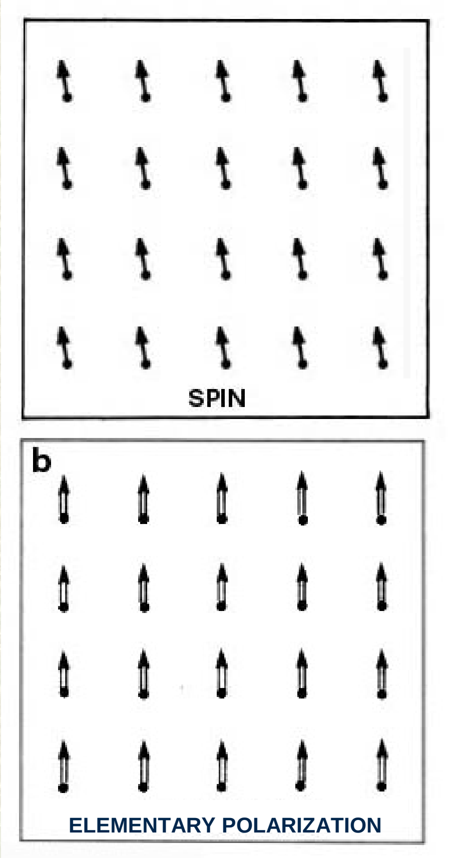
The modulus of the *elementary polarization* has to be furtherly averaged over the N spin configuration, to finally obtain the ***"polarization" p***:

$$p = \frac{1}{N} \sum_{i=1}^{N} \left| < \vec{s}_i > \right|$$

SG phase in the HMF model?

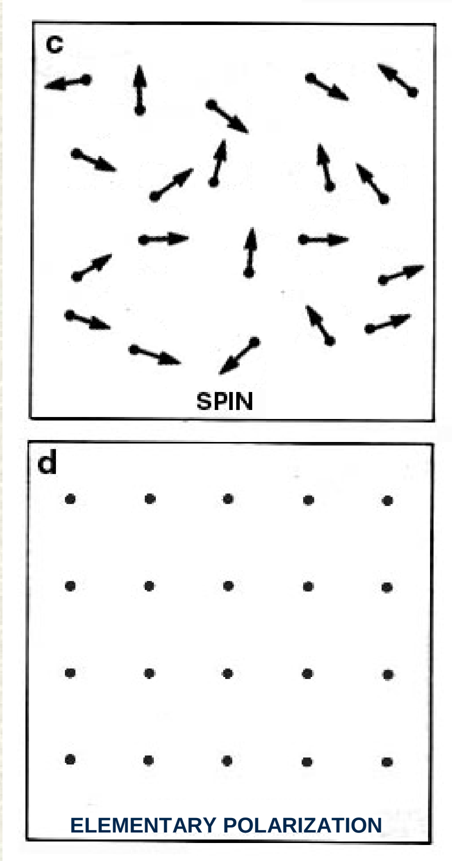
FERROMAGNETIC PHASE:

$M \neq 0 \qquad p \neq 0$



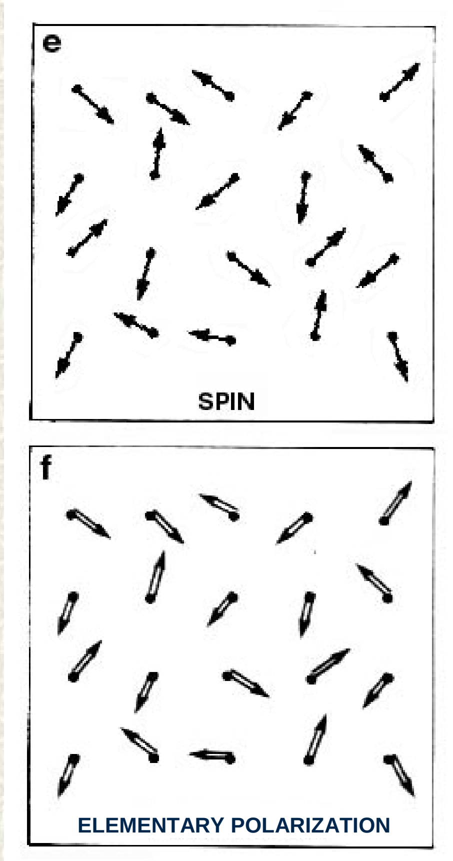
PARAMAGNETIC PHASE:

$M = 0 \qquad p = 0$



SPIN GLASS PHASE:

$M = 0 \qquad p \neq 0$



If we were in presence of a spin glass-like phase, the polarization p shouldn't vanish with M, so measuring the freezing of the rotators

$$p = \frac{1}{N}\sum_{i=1}^{N}\left|<\vec{s}_i>\right|$$

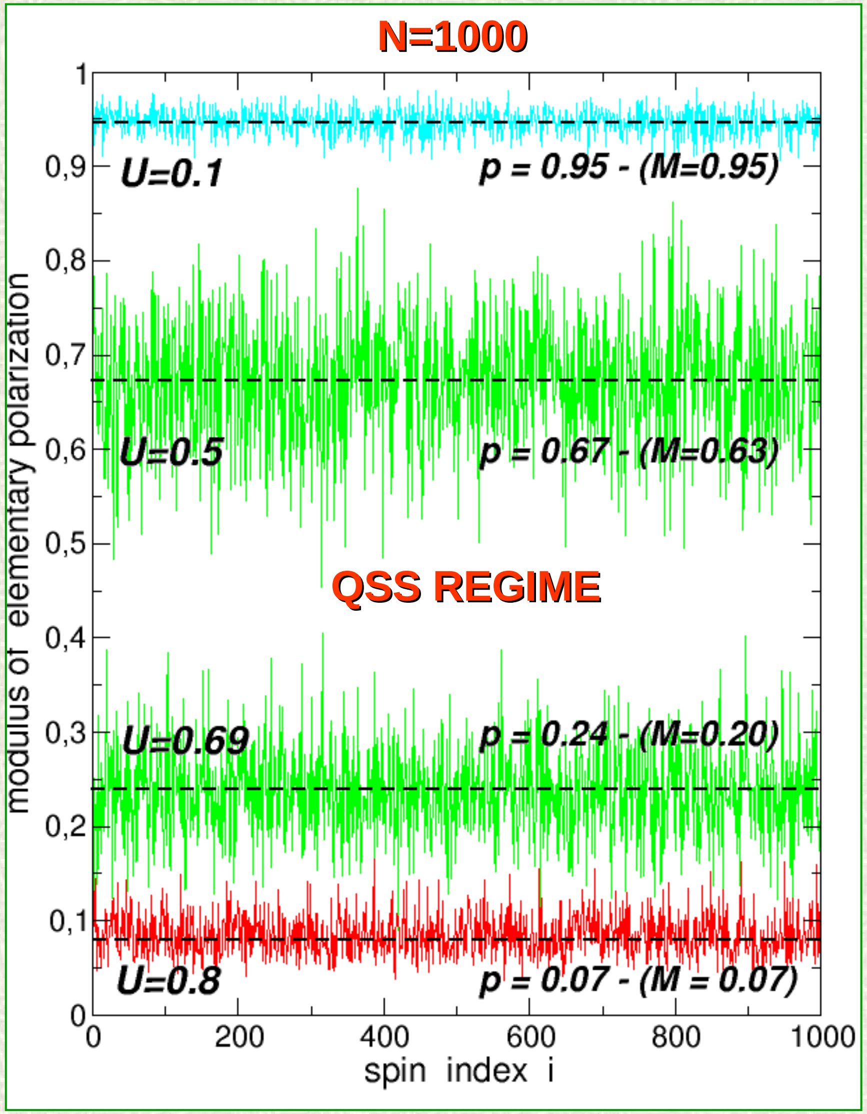
ELEMENTARY POLARIZATION: $<\vec{s}_i> = \frac{1}{\tau}\int_0^{\tau}\vec{s}_i(t)\,dt$

Polarization and QSS

Effectively, from our simulations with **M(0)=1** ic the ***polarization p*** results to be different from M only in the ***QSS regime***, where seems to stay also different from zero:

Phase		
FERRO	$p = M \neq 0$	
PARA	$p = M \approx 0$	
QSS regime	$p \neq 0$	$M \longrightarrow 0$

But… does *p* remain different from zero if the size of the system grows to infinity?



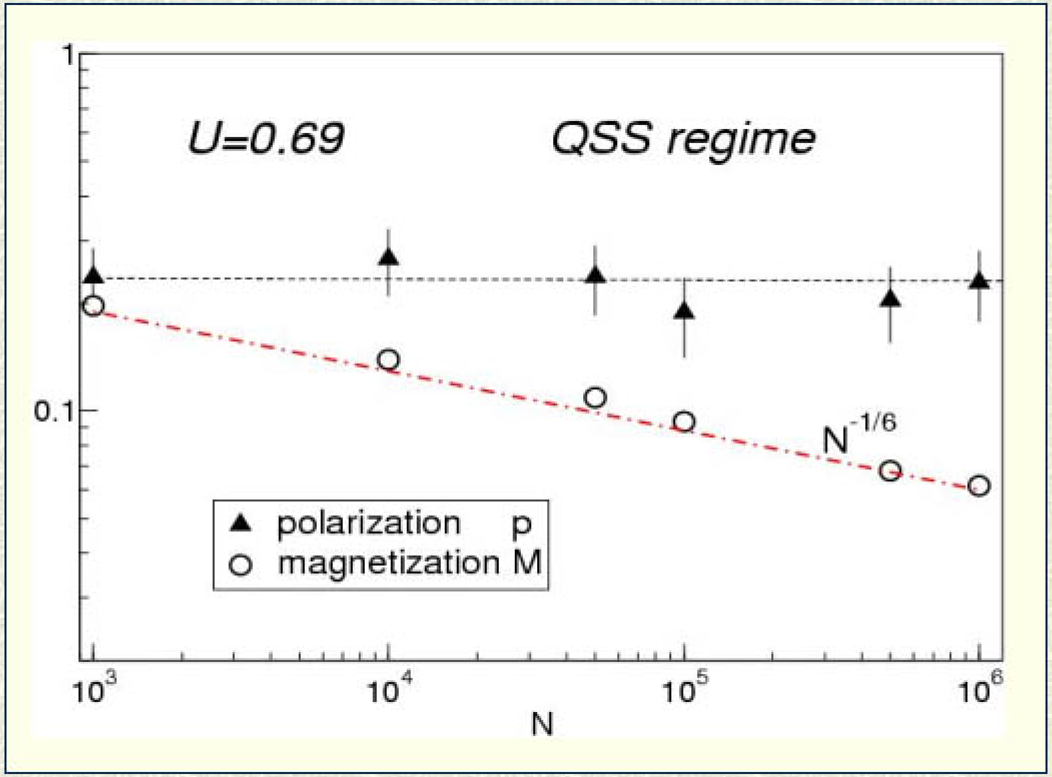
p and M vs N

We found that, increasing the size of the system…
…the polarization remains constant and different from zero:

$$p \sim 0.24$$

while the magnetization, as expected, vanishes with N:

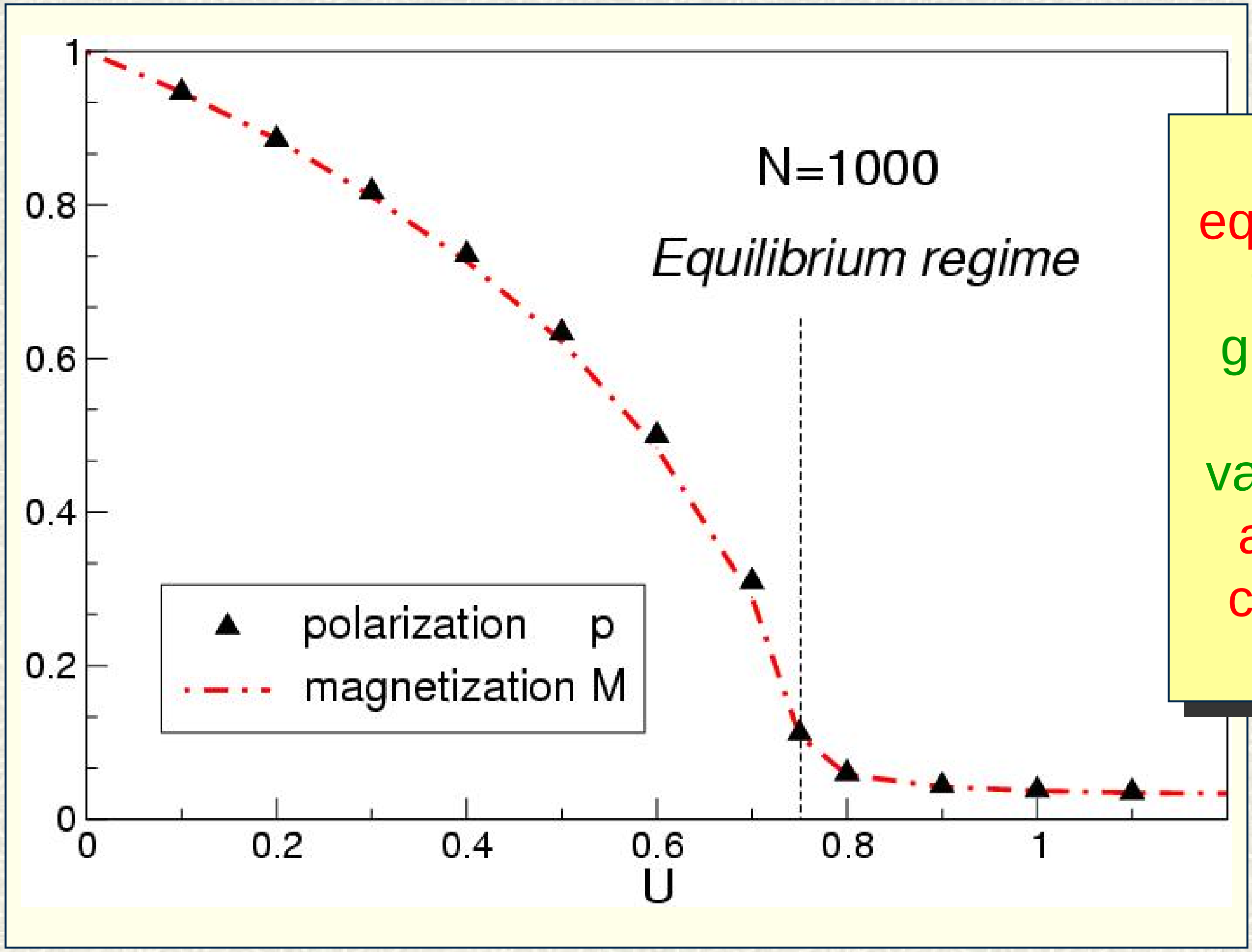
$$M \propto N^{-\frac{1}{6}}$$



Thus, we can confidently consider QSS regime as equivalent to a Spin Glass Phase of the HMF model, related to the dynamical frustration between clusters

Pluchino, Latora, Rapisarda, [cond-mat/0306374].

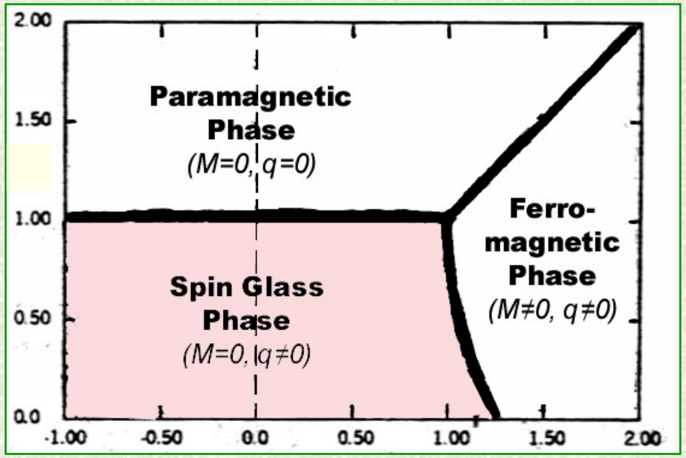
p and M at Equilibrium



As expected, at equilibrium, when any trace of QSS and glassy behavior has disappeared, the values of polarization and magnetization coincides for all the energies.

SK Model

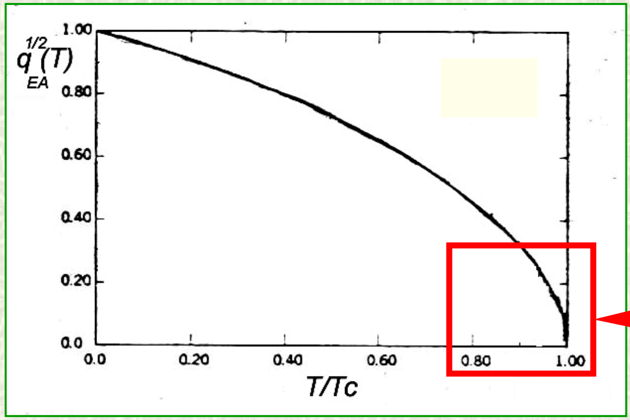
In conclusion, if we look at the Sherrington Kirpatrick (SK) model, the first solvable infinite range spin glass model, the analogous of polarization is the famous:



Edwards Anderson order parameter:

$$q_{EA} = << S_i >^2 >_d$$

<…> = thermal average ; $<\ldots>_d$ = average over the spatial disorder



The comparison between the QSS polarization (U=0.69) and the square root of q_{EA} in the SG phase of the SK model, gives us values in the same range (taking $T=T_{QSS}(N)$ and $T_C = T_{EQ}$).

Of course it would be interesting to understand how deep is the connection between glassy systems and non extensive hamiltonian ones.

And at the moment we are just working in this direction…


….ehm, maybe not EXACTLY at THIS moment…☺

Conclusions

- Summarizing, the Hmf model represents a paradigmatic model for non extensive i.e. long-range interacting systems, as for example self-gravitating objects, nuclear and atomic systems.

- Several dynamical metastable anomalies are present: QSS regime, negative specific heat, slow dynamics, anomalous diffusion, power-law relaxation, aging and weak mixing.

- This anomalous behavior is very sensible to the initial conditions. Even if QSS are present for both M1 and M0 i.c. we found structures in phase-space, dynamical frustration and correlations only for the M1 initial conditions.

- Links with Tsallis generalized q-statistics were found in the velocity pdf and in the velocity correlation functions for M1 ic.

- Interpretation of the QSS regime as a spin-glass phase was proposed, by the introduction of a new order parameter, the polarization, as a measure of the degree of freezing of the system.

Main References

- Antoni and Ruffo, Phys. Rev. E 52 (1995) 2361.
- Latora, Rapisarda, Ruffo, Phys. Rev. Lett. 80 (1998) 698.
- Latora, Rapisarda, Ruffo Physica D 131 (1999) 38.
- Latora, Rapisarda, Ruffo, Phys. Rev. Lett. 83 (1999) 2104.
- Latora, Rapisarda, Tsallis, Phys. Rev. E 64 (2001) 056134.
- Dauxois, Latora, Rapisarda, Ruffo,Torcini, Lectures Notes in Phys., Springer 602 (2002).
- Tsallis, Rapisarda, Latora, Baldovin, Lectures Notes in Phys., Springer 602 (2002).

For the role of initial conditions and the Spin Glass interpretation of QSS:

- Pluchino, Latora, Rapisarda, Physica D (2003) in press, [cond-mat/0303081].
- Pluchino, Latora, Rapisarda, [cond-mat/0306374].

For the generalized version of the HMF model see:

- Anteneodo and Tsallis, Phys. Rev. Lett. (1999)
- Campa, Giansanti and Moroni, J. Phys. A 36 (2003) 6897 and refs. therein.