The Topological Non-connectivity Threshold

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Recent Publications

- F. Borgonovi, G.L. Celardo, M. Maianti and E. Pedersoli Broken Ergodicity in Classically Chaotic Spin Systems Journ. of Stat. Phys. **116**, 235 (2004)
- G.L. Celardo, J. Barré, F. Borgonovi and S. Ruffo The non-ergodicity threshold: time scale for magnetic reversal cond-mat/0410119
- F. Borgonovi, G.L. Celardo, A. Musesti, R. Trasarti-Battistoni and P.Vachal, The Topological Non-Connectivity Threshold in long-range spin systems cond-mat/0505209
- F. Borgonovi, G.L. Celardo and G.P. Berman Quantum signatures of the Classical Disconnection Border cond-mat/0506233

Physical Backgrounds: Key Words

- NANO : How to describe statistically nano-sized ensembles of few atoms? Is temperature well defined and unique for such system?
- LONG-RANGE : Long-range interacting systems give rise to a non-additive thermodynamics. Canonical/Microcanonical ensemble give different results. How small a short range interacting system must be in order to be considered a long-interacting one?
- CHAOS : Is chaos enough in order to produce a statistical behavior in small systems thus avoiding the annoying $N \to \infty$ limit ?

Outlines

ABSTRACT

We show, in a well known statistical model (an extension of an X-Y anisotropic Heisenberg model with a spin constant decreasing with the spin distance as $|i-j|^{-\alpha}$) that :

1) finite-sized effects when driven by dynamical chaos can give predictions different from those of the Statistical Mechanics.

2) a topological transition occurs at $\alpha = d$.

3) the threshold can be mimicked in the quantized version of the model.

The Classical Model

$$H = -\frac{1}{2} \sum_{<i,j>} \frac{1}{|i-j|^{\alpha}} (S_i^y S_j^y - \eta S_i^x S_j^x), \qquad (1)$$

The key-ingredients

- anisotropy : $\eta \neq -1$ $\rightarrow$ easy axis of magnetization (in order to produce disconnection)
- long-range $\alpha < d$ where d is the dimensionality of the embedding space (in order to have a significant ratio in the thermodynamic limit)

from Broken Ergodicity $\longrightarrow$ Topological Non-connectivity Threshold

Definitions:

$$\begin{aligned} E_{min} &= Min[\ H\ ] \\ E_{dis} &= Min[\ H \mid \sum_i S_i^y = 0\ ] \\ r &= \frac{|E_{dis} - E_{min}|}{|E_{min}|} \end{aligned} \qquad (2)$$

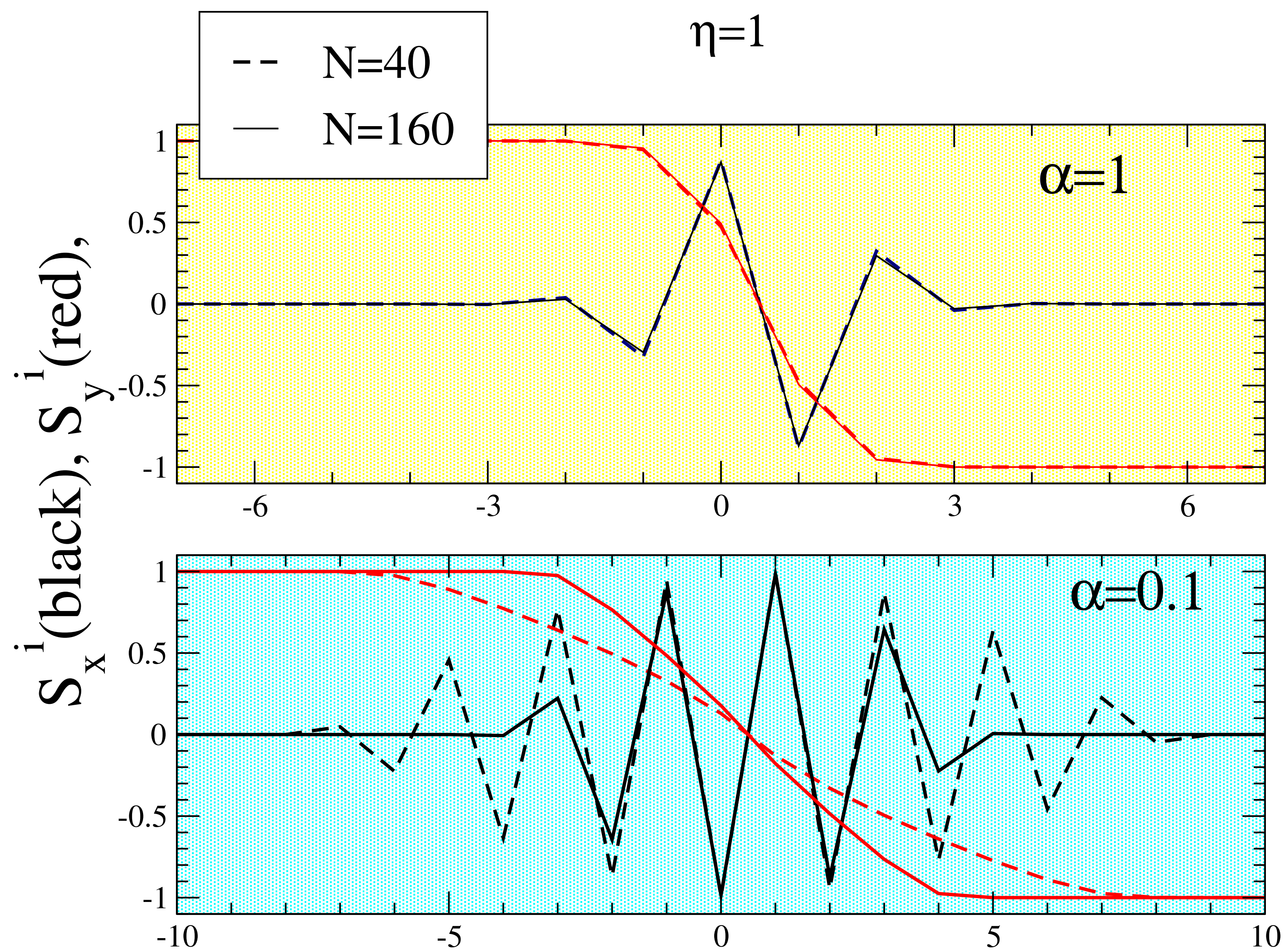
Results at finite number of particles

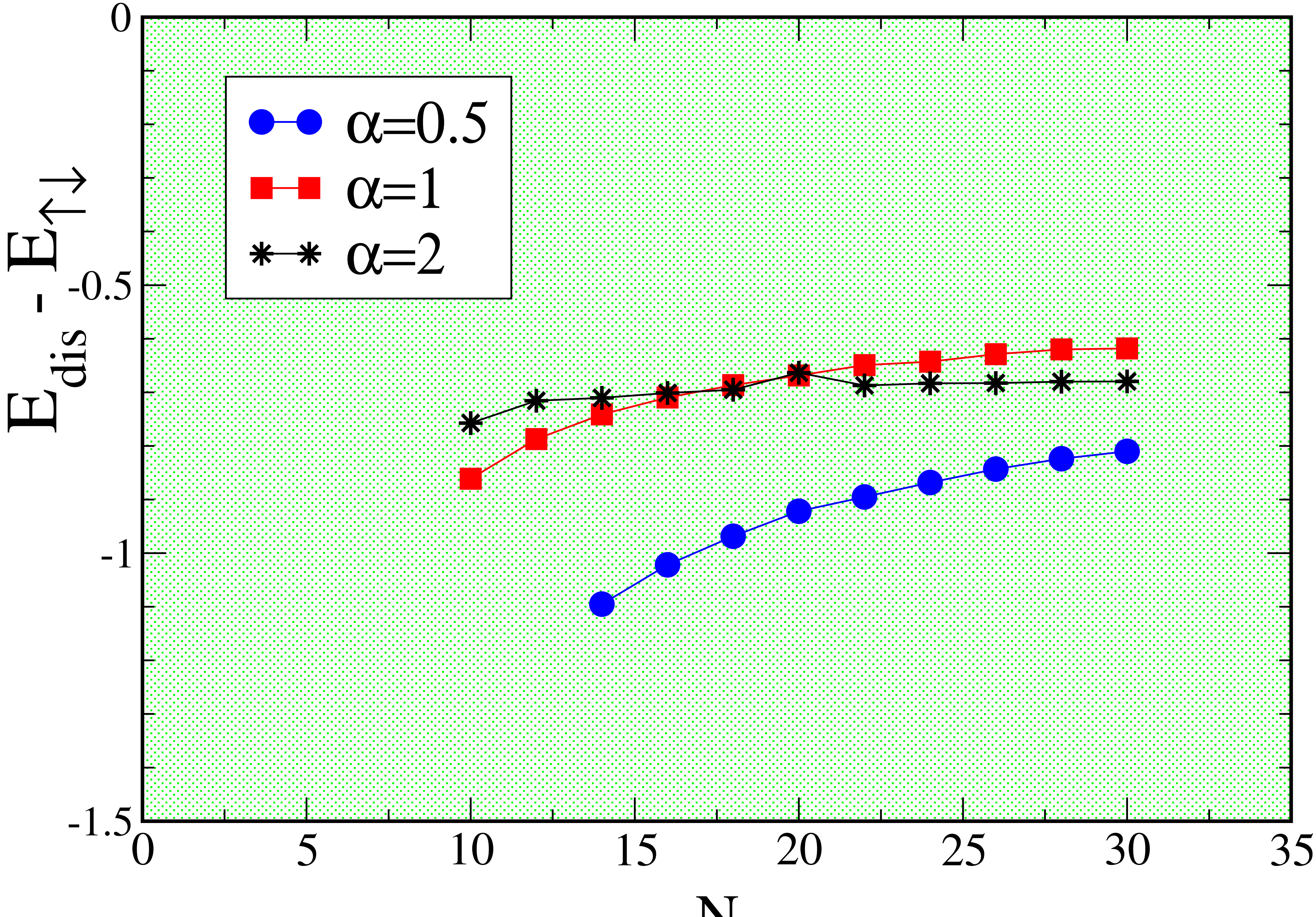
1) The phase space is disconnected in two regions $m_y = \sum_i S_i^y > 0$ and $m_y < 0$ for $E < E_{dis}$. Then, a trajectory with an initial sign of m_y cannot change it, since it cannot cross the $m_y = 0$ plane.

2) At the TNT spins configuration is half along the positive y-axis, half along the negative one, plus a domain wall whose size increases with the long range, but with a constant energy in the $N \to \infty$ limit. Also,

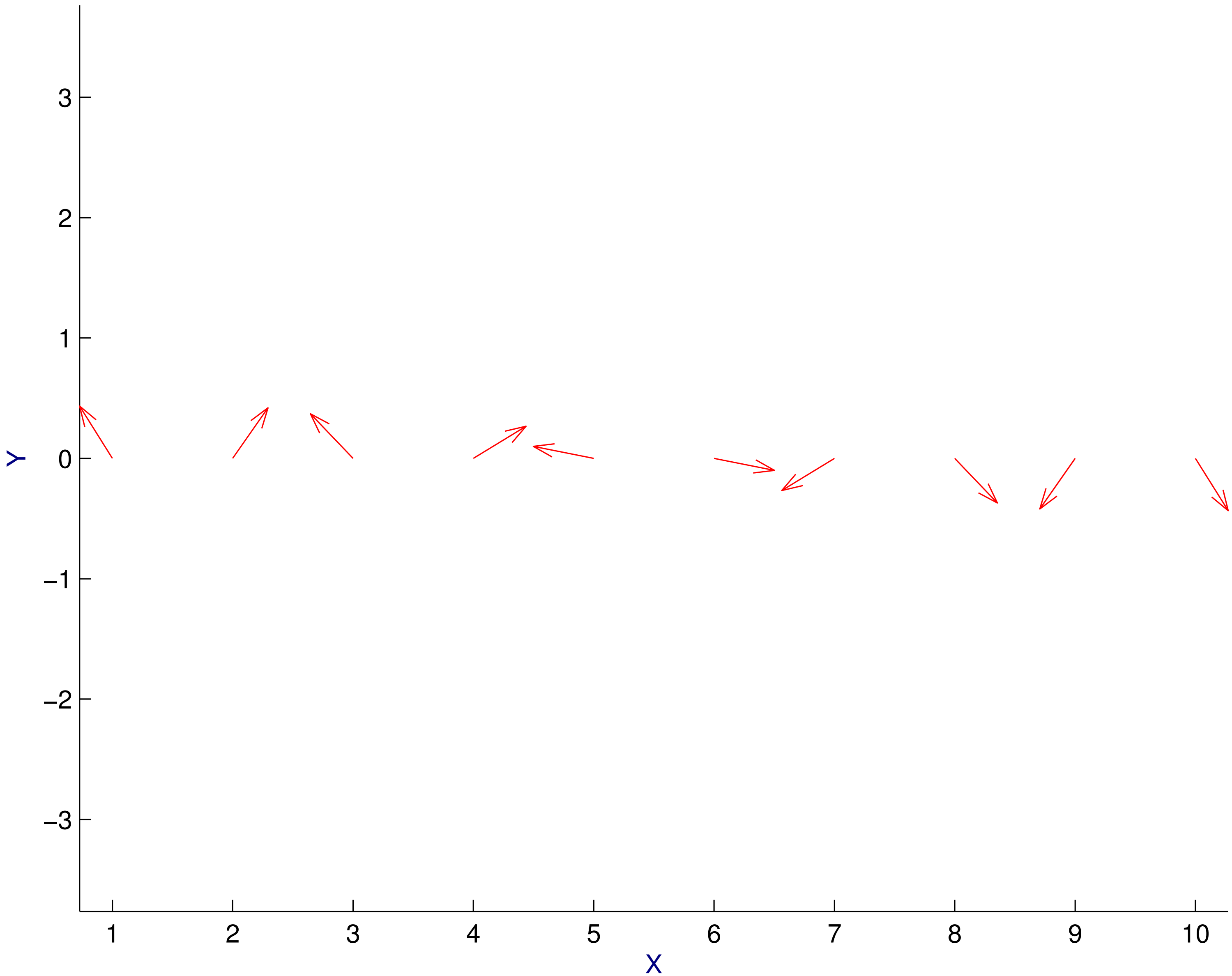
$$E_{dis} \simeq \begin{cases} N^2\eta/2 & \text{for} \quad \eta < 0 \\ 0 & \text{for} \quad \eta = 0 \\ -N\eta/2 & \text{for} \quad \eta > 0 \end{cases} \tag{3}$$

This is an example of broken ergodicity.

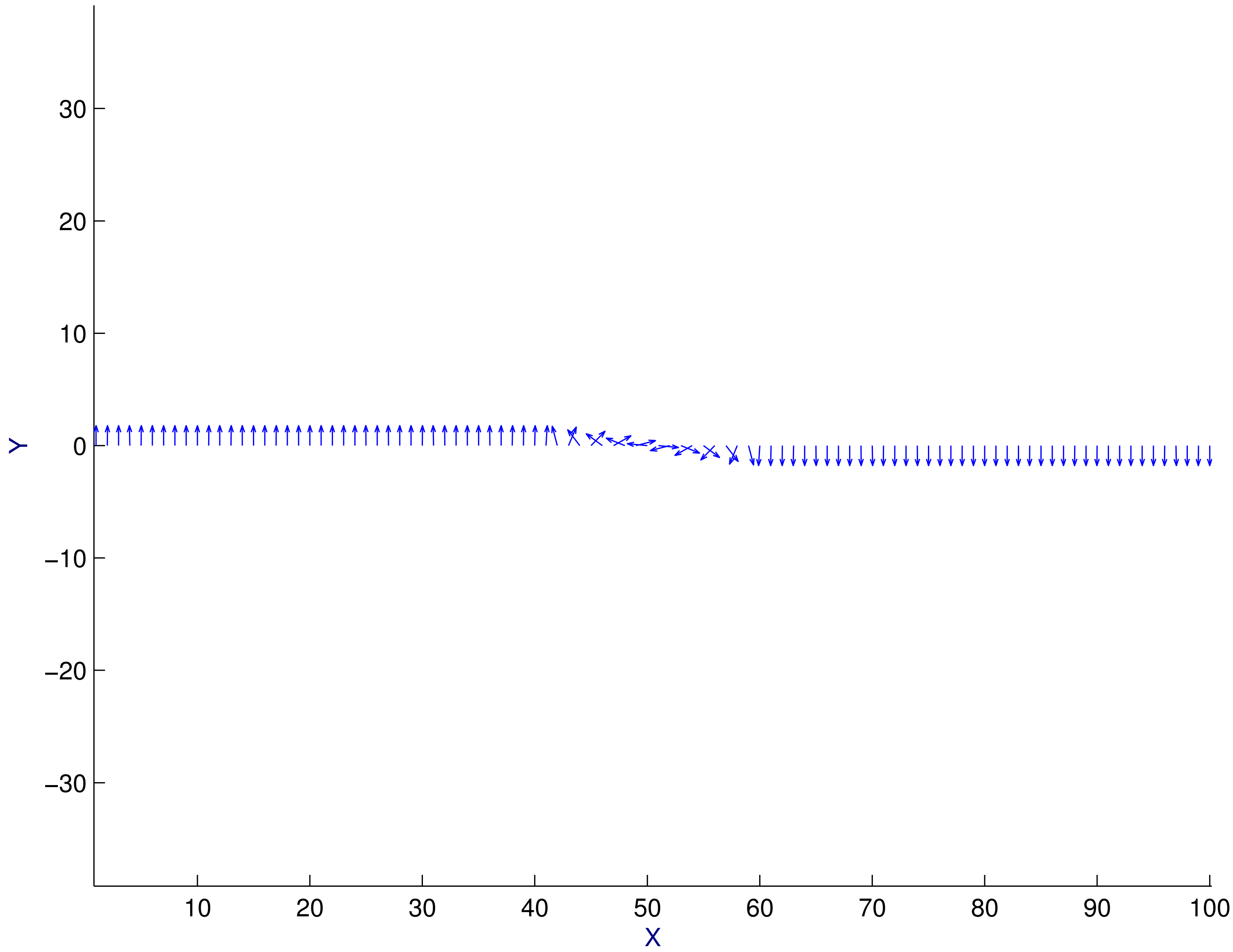

η=1
N=40
N=160
α=1
α=0.1
S_x^i(black), S_y^i(red),
1
0.5
0
-0.5
-1
-6
-3
0
3
6
-10
-5
5
10



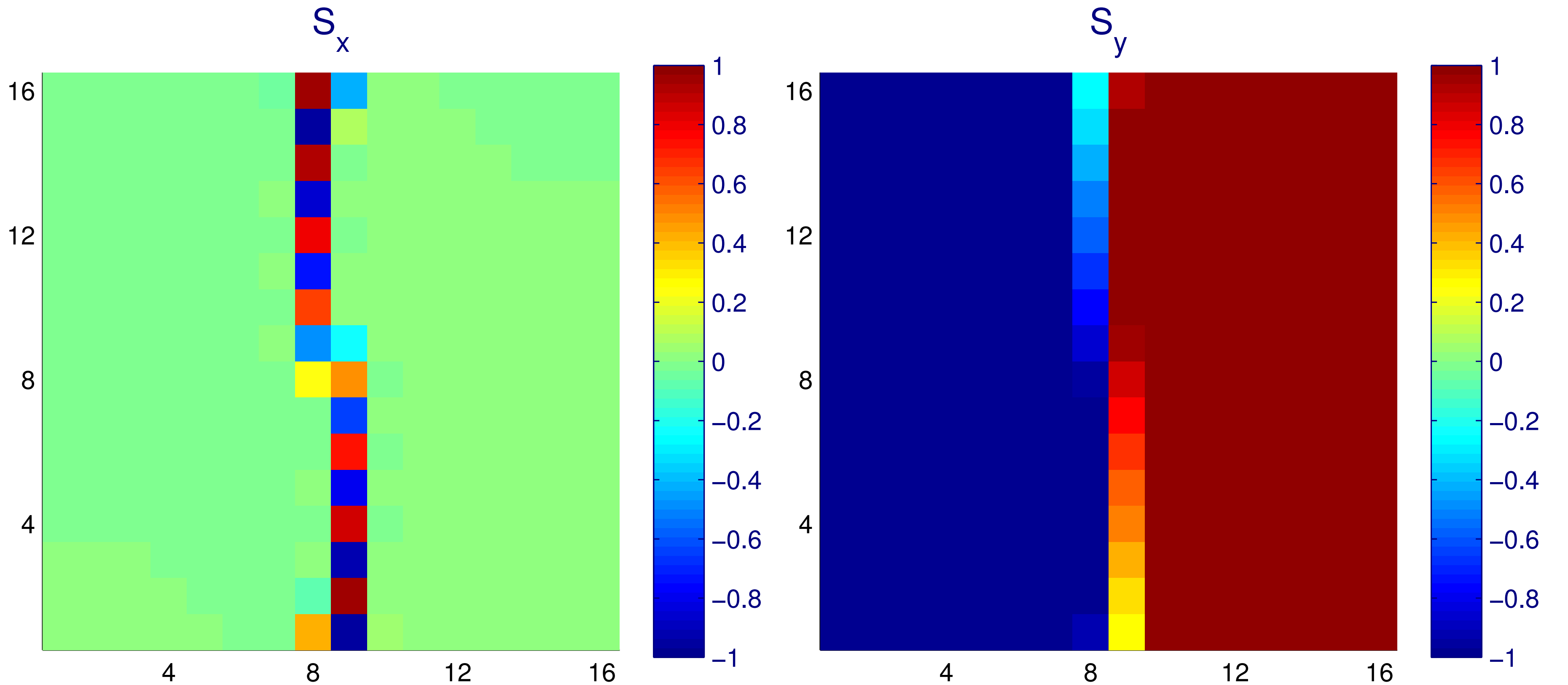
0
-0.5
-1
-1.5
0
5
10
15
20
25
30
35
N
E_dis - E_↑↓
α=0.5
α=1
α=2

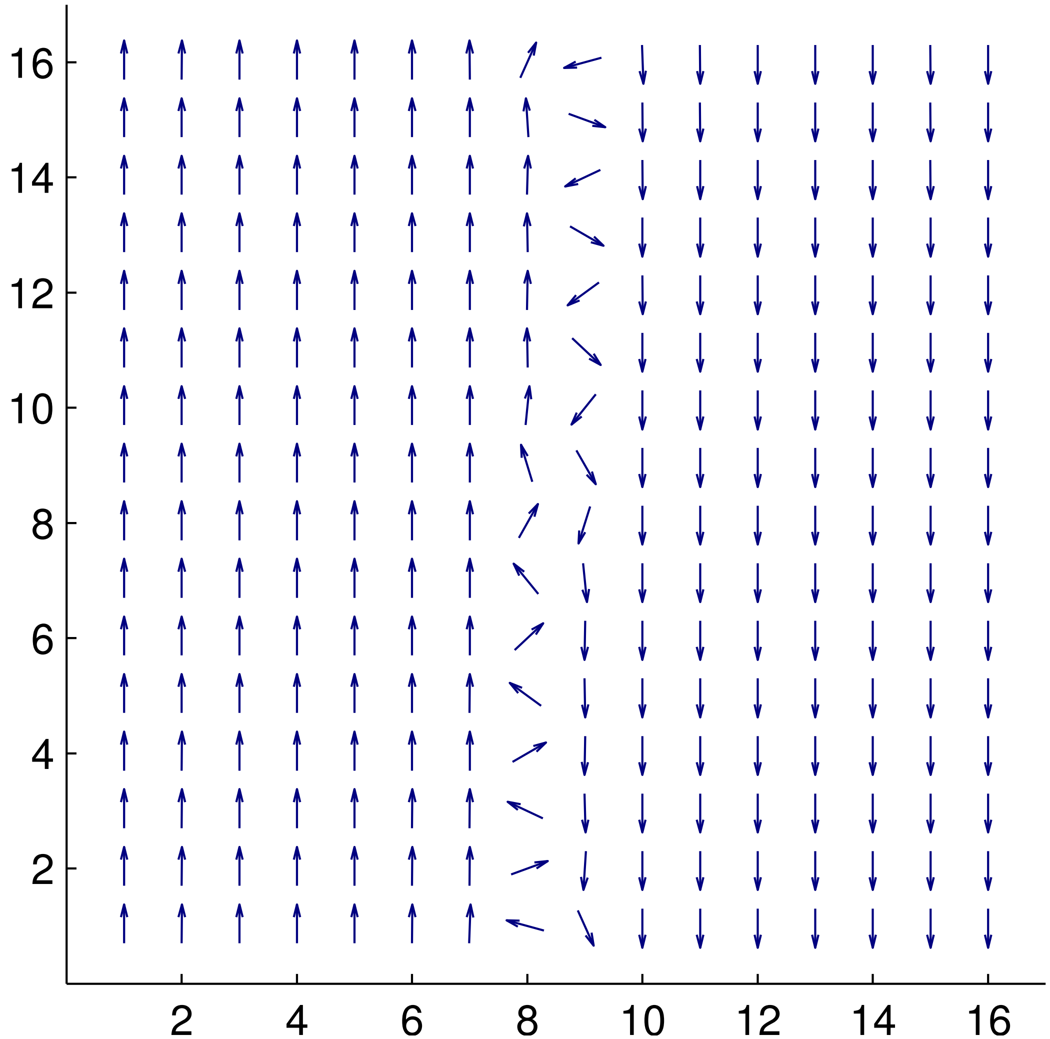


3
2
1
0
−1
−2
−3
Y
1
2
3
4
5
6
7
8
9
10
X



30
20
10
0
−10
−20
−30
Y
10
20
30
40
50
60
70
80
90
100
X


S_x
S_y
16
12
8
4
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1



16
14
12
10
8
6
4
2
2
4
6
8
10
12
14
16

Results in the thermodynamic limit $N \to \infty$

Even if E_{dis} exists, for any interaction range and anisotropy $\eta \neq 1$, a significant portion of the disconnected energy region survives at the thermodynamic limit, only in presence of long-range. Namely, for $N \to \infty$:

$$r = \frac{|E_{dis} - E_{min}|}{|E_{min}|} \to \begin{cases} 0 & \text{for} \quad \alpha \geq d \\ const. \neq 0 & \text{for} \quad \alpha < d \end{cases} \tag{4}$$

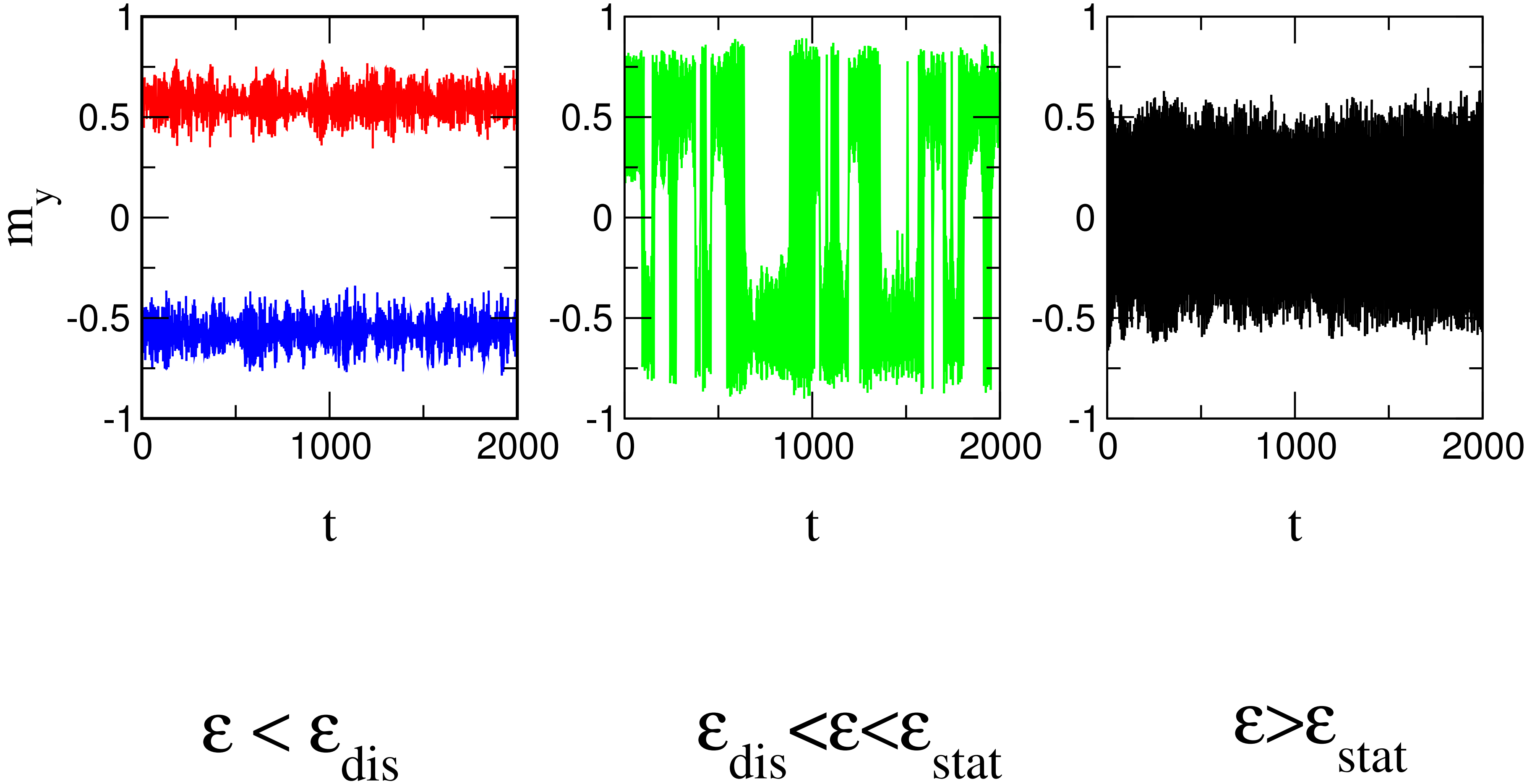
Dynamical consequences : Reversal time

Define the magnetization reversal time τ as the average lifetime in one region, say $m_y > 0$ before jumping to $m_y < 0$ (also called demagnetization time). Two major results:

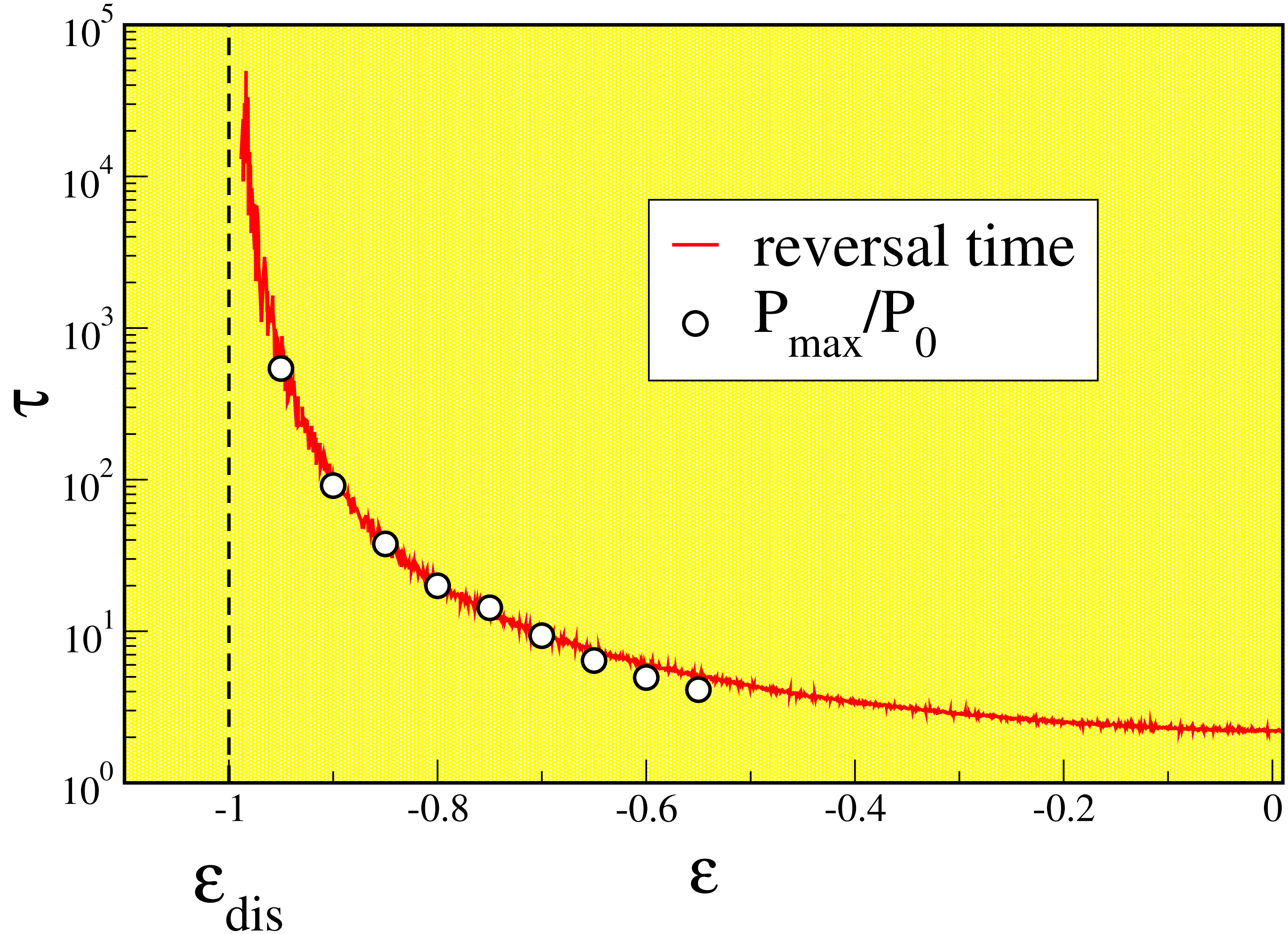
1. Reversal times τ occurs erratically, like those of a random telegraph noise, and are distributed according to a Poissonian law.

2. In analogy with phase transitions, demagnetization times diverge at the critical energy ϵ_{dis} as a power law :

$$\tau \sim \frac{1}{|\epsilon - \epsilon_{dis}|^{\alpha N}}, \qquad \alpha \sim 1 \tag{5}$$



m_y
1
0.5
0
-0.5
-1
0
1000
2000
t
t
t
$\varepsilon < \varepsilon_{dis}$
$\varepsilon_{dis} < \varepsilon < \varepsilon_{stat}$
$\varepsilon > \varepsilon_{stat}$



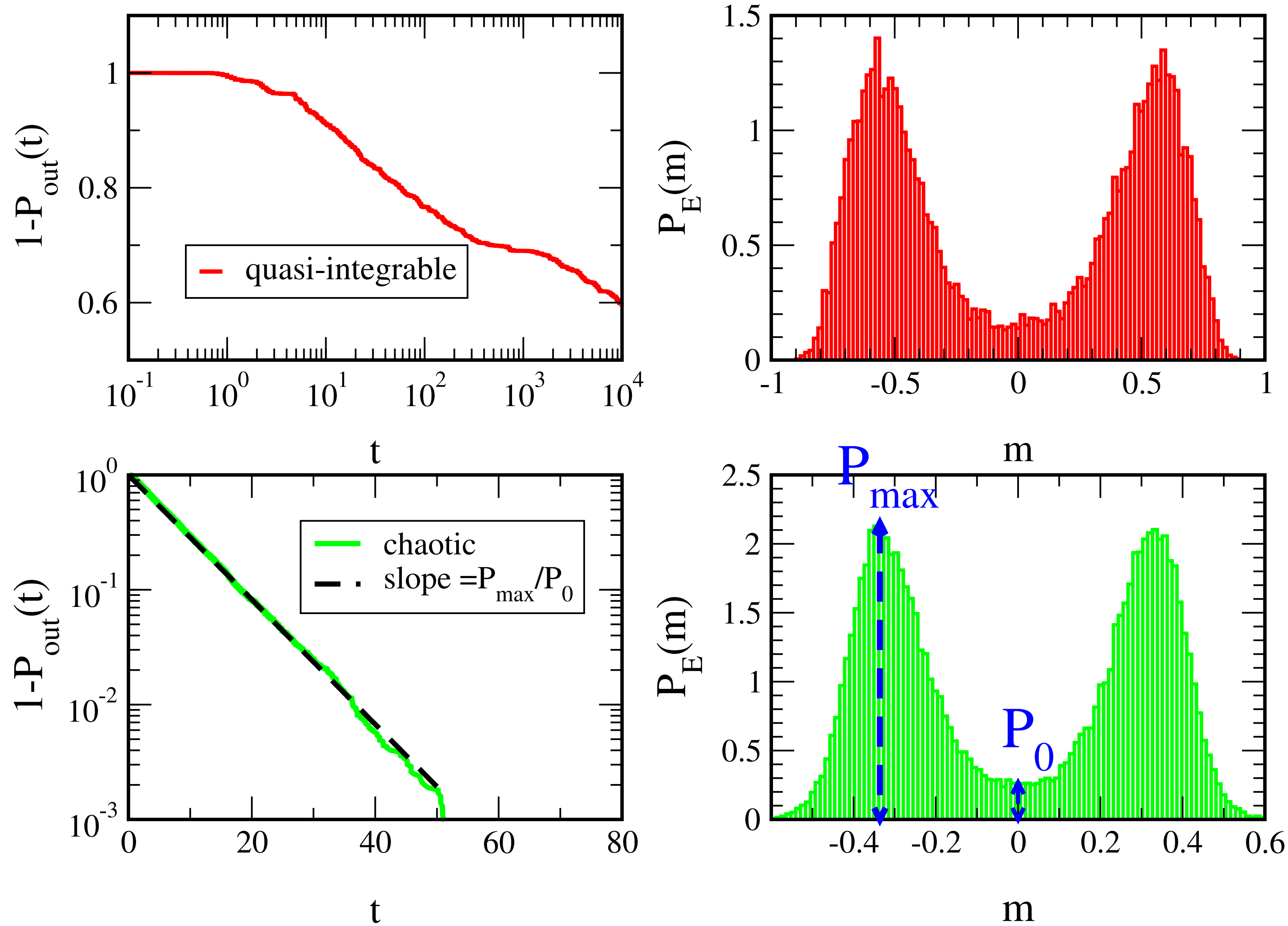
10^5
10^4
10^3
10^2
10^1
10^0
τ
reversal time
P_{max}/P_0
-1
-0.8
-0.6
-0.4
-0.2
0
ε_{dis}
ε

Relation with chaos

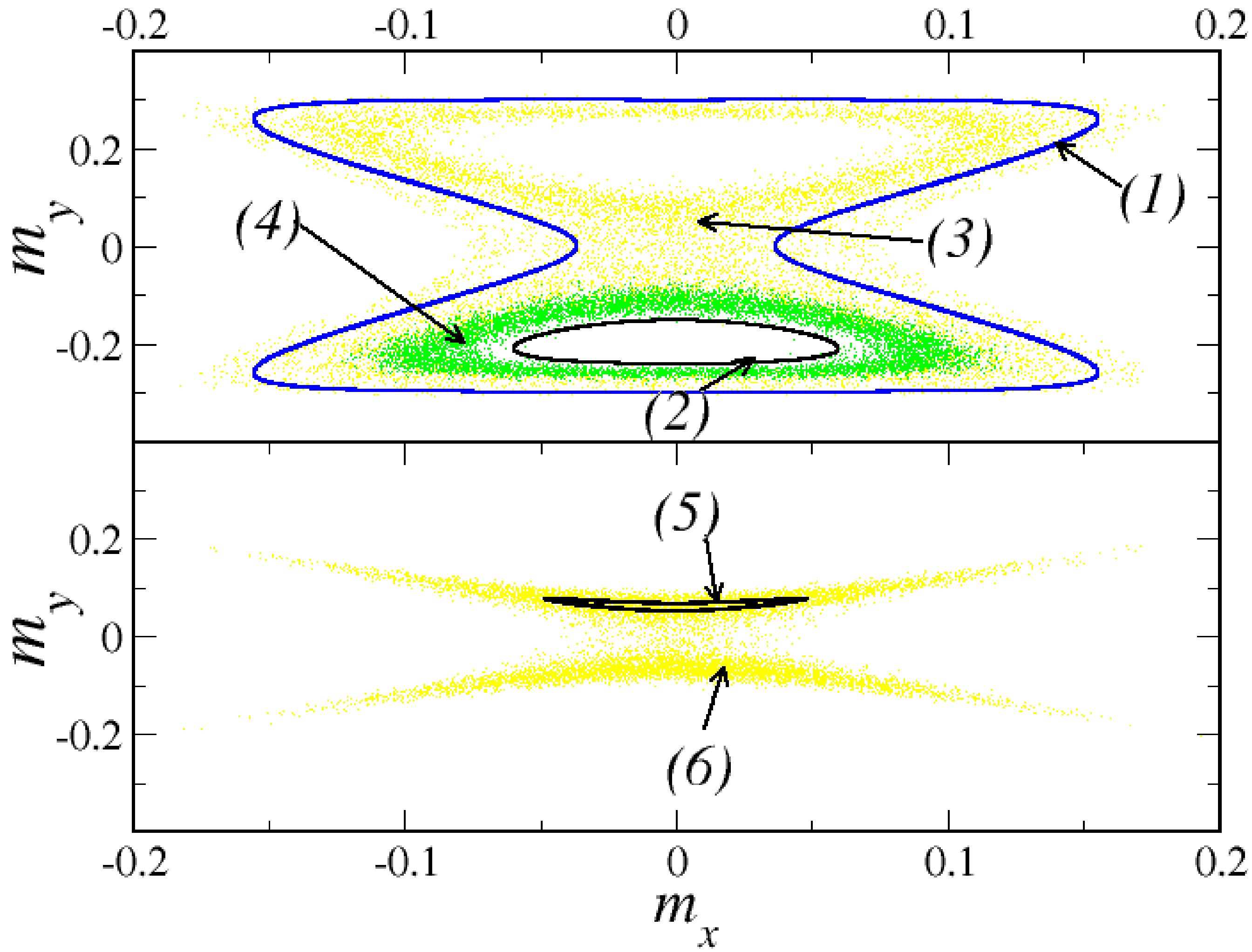
1. The system has a positive Lyapunov exponent for all parameters, even if it decreases approaching the minimal energy.

2. Despite chaoticity even above E_{dis} some trajectories do not cross the $m_y = 0$ plane up to our best simulation time $\rightarrow$ possible existence of invariant curves in the multidimensional space ?

Therefore we can distinguish between a chaotic and quasi-integrable regime, the latter characterized by a long law tail in the survival probability.



1-P_{out}(t)
t
quasi-integrable
P_E(m)
m
chaotic
slope =P_{max}/P_0
P_{max}
P_0



-0.2
-0.1
0
0.1
0.2
0.2
0
-0.2
(1)
(2)
(3)
(4)
(5)
(6)
m_y
m_y
m_x

Connection with Statistics

A simplified version of Hamiltonian, in terms of macroscopic variables, can be introduced for $\alpha = 0$ and $\eta = 1$.

$$H = BNm_z + \frac{1}{2}N^2\left(\eta m_x^2 - m_y^2\right)$$

and the entropy, counting the number of microscopic configurations, calculated, using the Large Deviation Theory. A second order phase transition, in the limit $N \to \infty$ occurs at $\epsilon = \epsilon_{stat}$. Specifically entropy has a two-peaked shape for $\epsilon < \epsilon_{stat}$ and is single peaked for $\epsilon > \epsilon_{stat}$.

Analytical Results (Mean Field) $\alpha = 0$, N large

1. ϵ_{stat} can be evaluated explicitly and it remains distinct from ϵ_{dis} even in the limit $N \to \infty$. (Is this a contradiction between dynamics and statistics?).

2. Reversal times can be evaluated assuming proportionality with transition probability [Landau]:

$$\tau \simeq \exp N\Delta s \simeq \frac{P_{max}}{P_0} \tag{6}$$

(when chaos is enough to destroy all invariant structures preventing the transitions between the two regions).

3. We predict close to the TNT

$$\tau \simeq \frac{1}{(\epsilon - \epsilon_{dis})^N} \tag{7}$$

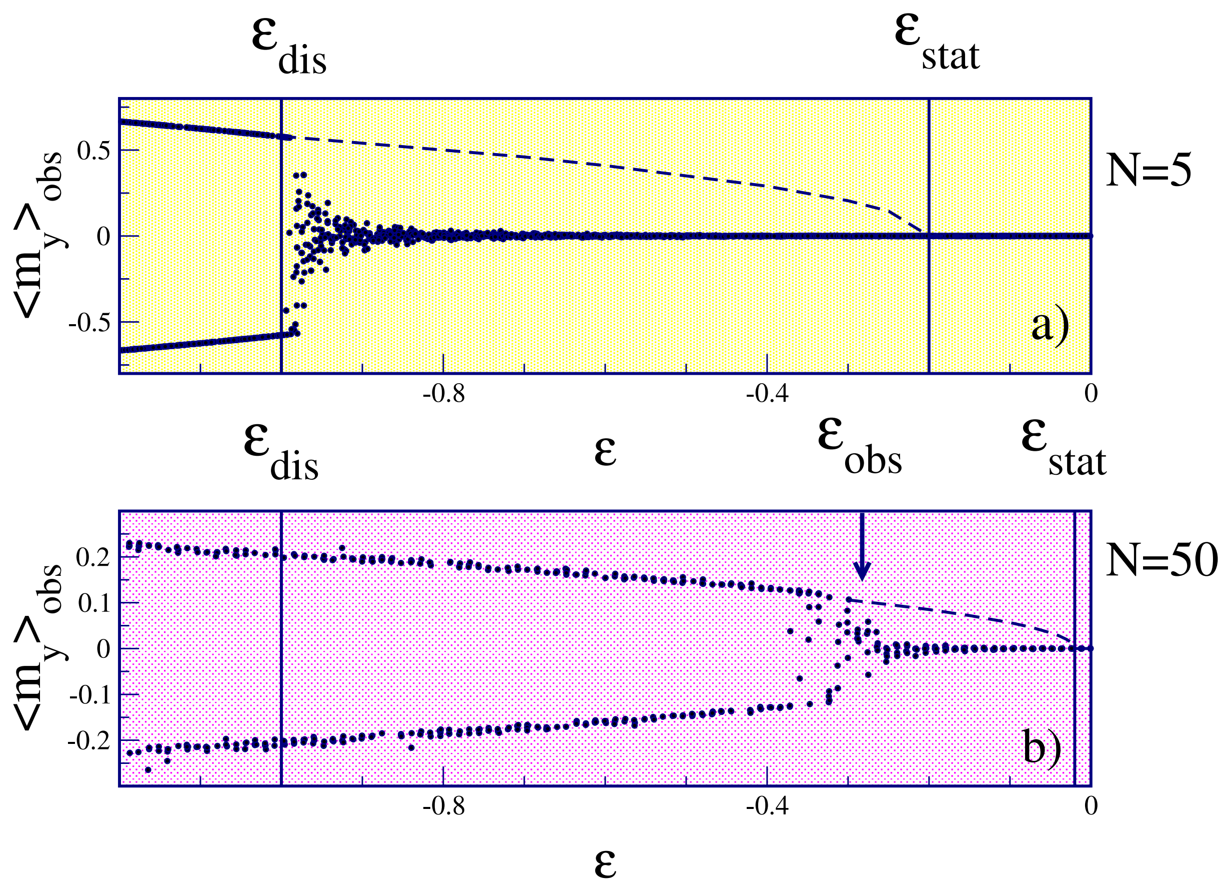
to be compared with the factor $-0.85N$ obtained numerically.

Question, at what energy is there a transition?

Define

$$\langle m_y \rangle_{obs} = \frac{1}{\tau_{obs}} \int_0^{\tau_{obs}} dt\; m_y(t). \tag{8}$$

Then the transition occurs at ϵ_{obs}.



ε_{dis}
ε_{stat}
N=5
$<m_y>_{obs}$
0.5
0
-0.5
a)
-0.8
-0.4
0
ε
ε_{dis}
ε_{obs}
ε_{stat}
N=50
0.2
0.1
0
-0.1
-0.2
b)
-0.8
-0.4
0
ε

Non-commutativity

We observe that, at any fixed N, in absence of invariant structures,

$$\lim_{\tau_{obs}\to\infty} \epsilon_{obs} = \epsilon_{dis} \quad (9)$$

while, for any fixed τ_{obs}

$$\lim_{N\to\infty} \epsilon_{obs} = \epsilon_{stat} \quad (10)$$

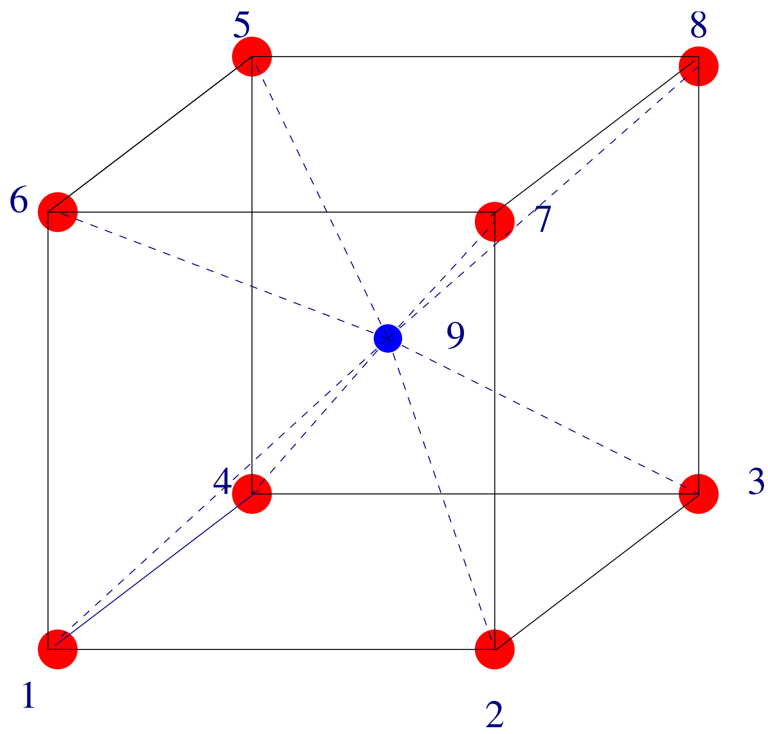
(the well known non-commutativity of the limits $N \to \infty$ and $t \to \infty$.)

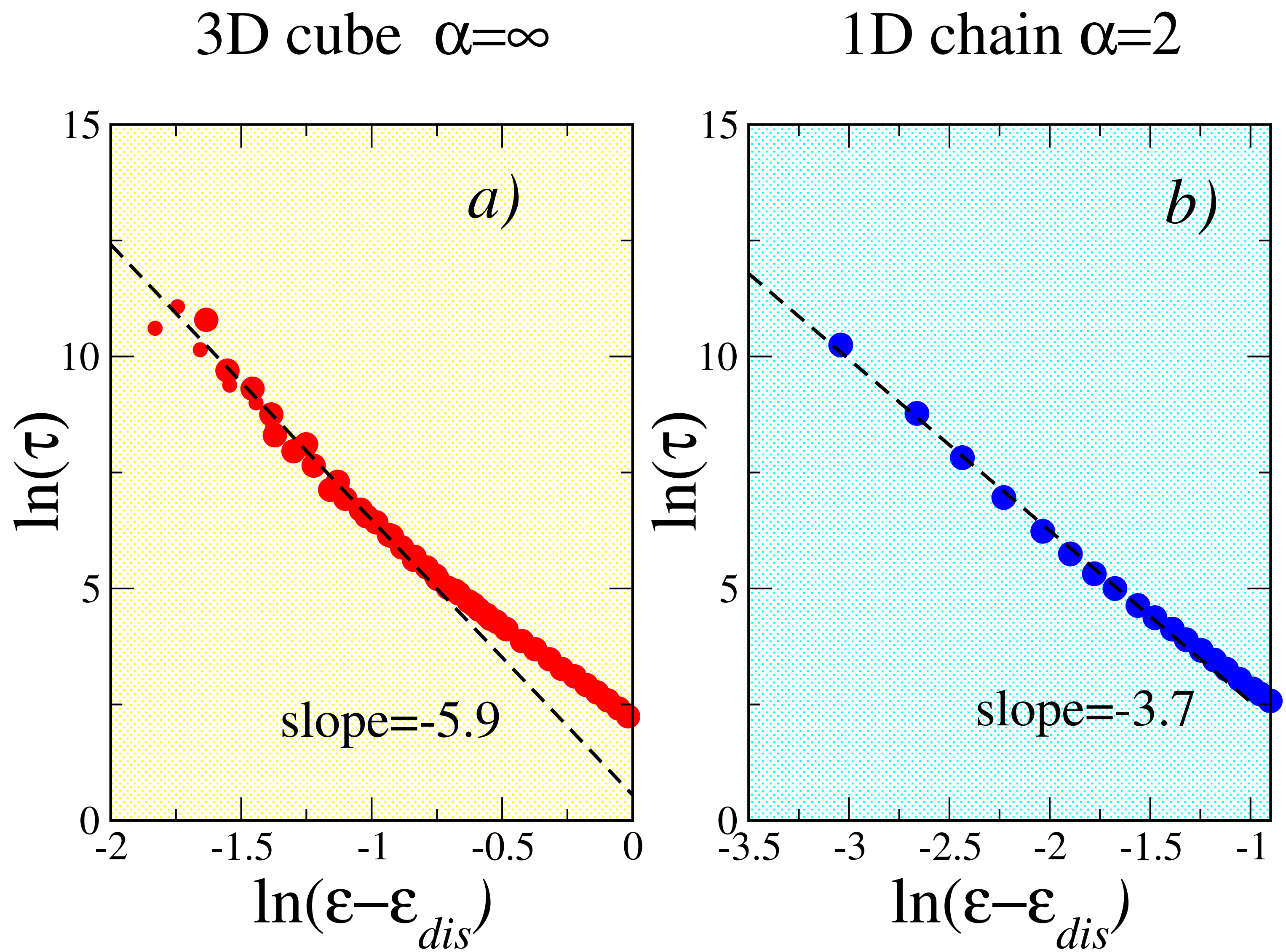
Extension to short-range and $d = 2, 3$.

1) Is there a transition in small short range systems?

2) Is there a transition in small 3D systems?

YES, THERE IS.





3D cube α=∞
1D chain α=2
a)
b)
slope=-5.9
slope=-3.7
ln(τ)
ln(ε−ε_dis)
15
10
5
0
-2
-1.5
-1
-0.5
0
-3.5
-3
-2.5
-2
-1.5
-1

Quantum Effects

We restrict our considerations to the case where all spins are interacting with all the others ($\alpha = 0$), and strongest anisotropy ($\eta = 1$). We also quantize the model according to Bose Statistics.

Open Questions:

1) Is there a TNT in the quantum model?

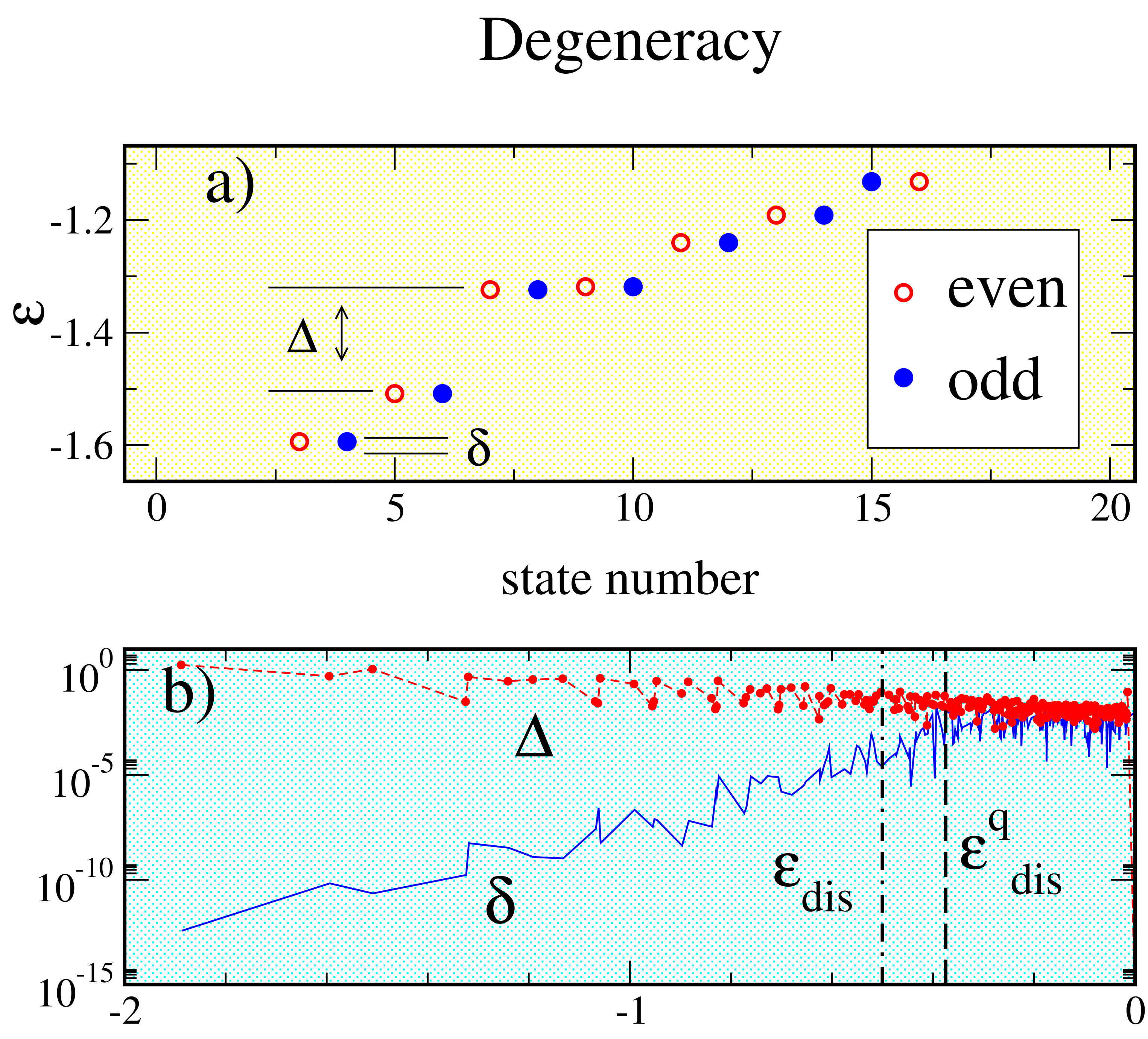
2) How to describe and compare dynamical times?

Quantization

Hamiltonian:

$$\hat{H} = \frac{\eta}{2} \sum_{i=1}^{N} \sum_{j \neq i} \hat{S}_i^x \hat{S}_j^x - \frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i} \hat{S}_i^y \hat{S}_j^y, \tag{11}$$

Classical limit is obtained with an appropriate rescaling of the Planck constant, $\hbar \to \hbar/|S_i| = 1/\sqrt{l(l+1)}$. With this choice, in the classical limit, $l \to \infty$ ($\hbar \to 0$), the spin modulus remains equal to 1.



Degeneracy
a)
-1.2
-1.4
-1.6
0
5
10
15
20
ε
Δ
δ
even
odd
state number
b)
10^0
10^-5
10^-10
10^-15
-2
-1
0
Δ
δ
ε_dis
ε^q_dis

Parity

An important property of the Hamiltonian (11) is its invariance under a π rotation about the z-axis : the Hamiltonian commutes with the operator $\exp(i\pi \sum \hat{S}_i^z)$, and its eigenstates can be labeled as odd (-) or even (+) according to whether they change or do not change sign under such rotation. Also:

$$\langle E_+ | \sum \hat{S}_i^y | E_- \rangle = 0$$

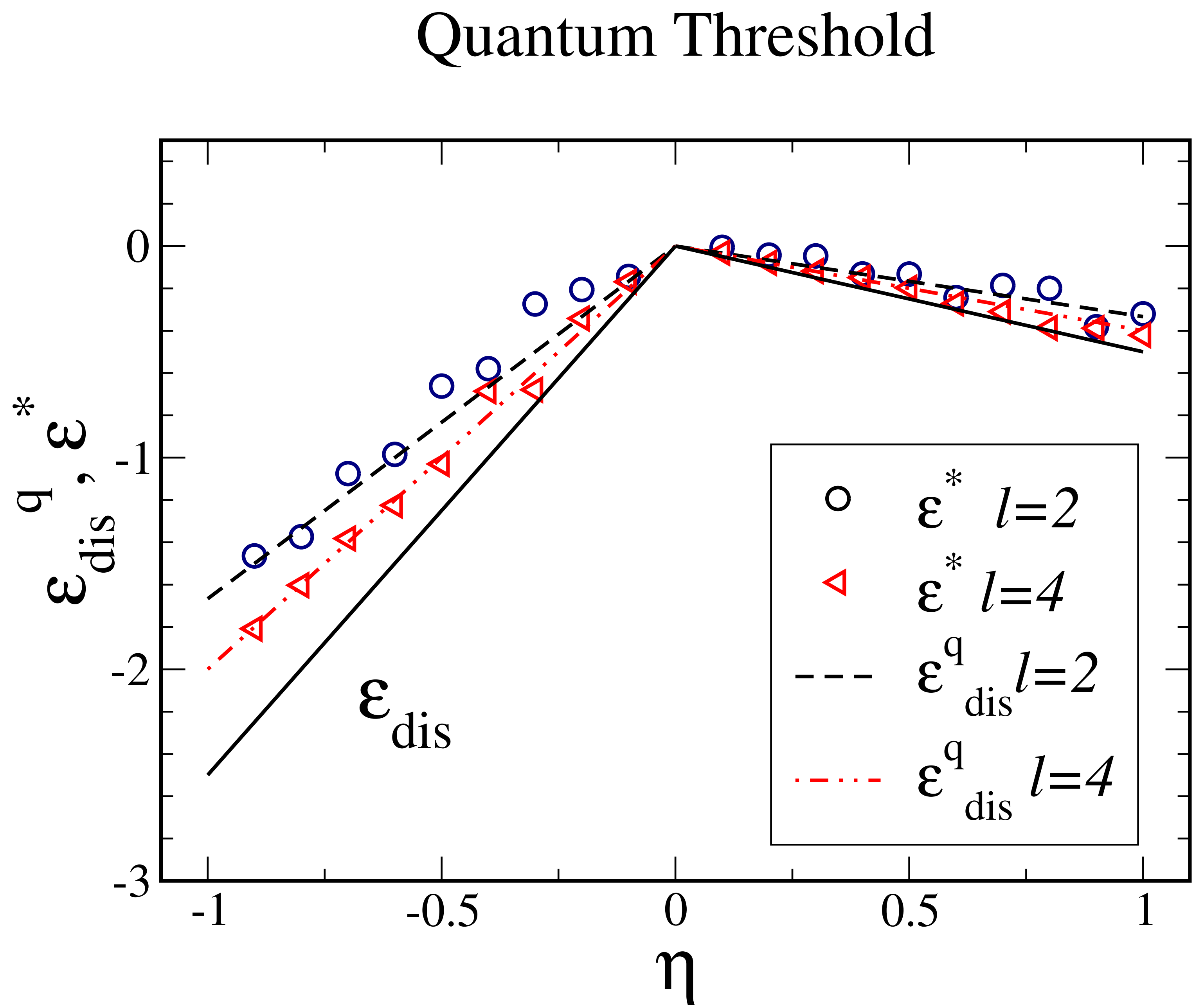
Quantum threshold

We may give two definitions:

1) considering the energy ϵ^* such that $\delta(\epsilon^*) \simeq \Delta(\epsilon^*)$

2) in the classical case, ϵ_{dis} has been obtained computing the minimum of $-(\eta/2)\sum(S_i^x)^2$ when $\eta > 0$, and of $(\eta/2)M_x^2 - (\eta/2)\sum(S_i^x)^2$ when $\eta < 0$. Thus, the lowest eigenvalue of the same operators could give an approximate quantum border.

$$\begin{aligned} \epsilon_{dis}^q &\sim -\frac{\eta}{2}(\hbar l)^2 \text{ for } \eta > 0 \\ \epsilon_{dis}^q &\sim \frac{\eta}{2}(N-1)(\hbar l)^2 \text{ for } \eta < 0. \end{aligned} \tag{12}$$



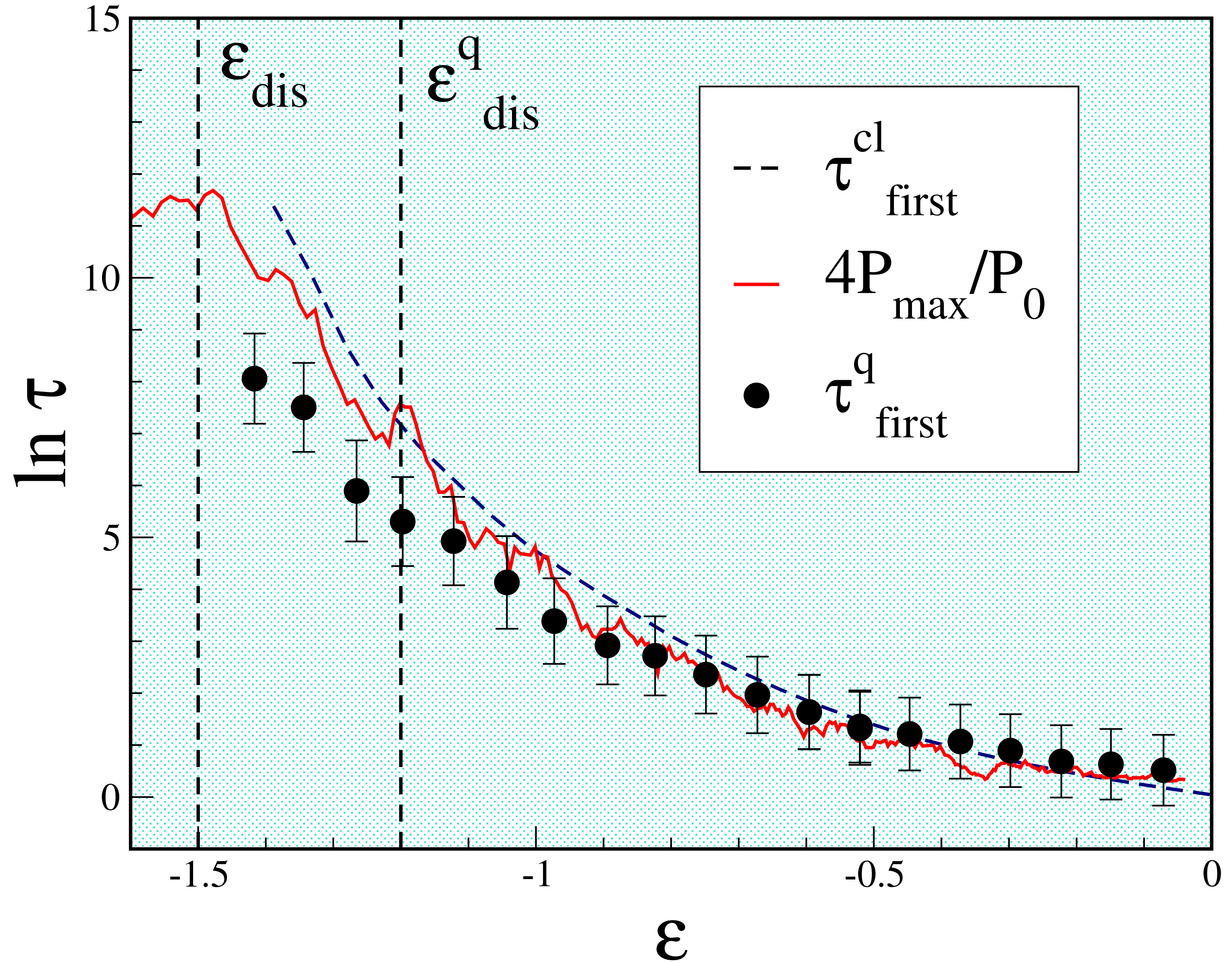
Quantum Threshold
0
-1
-2
-3
-1
-0.5
0
0.5
1
η
ε^q_dis, ε*
ε_dis
ε* l=2
ε* l=4
ε^q_dis l=2
ε^q_dis l=4

Quantum Dynamics

Since in the classical case the reversal times have been determined at a fixed energy (microcanical approach), we adopt here the same procedure and compute the reversal time of the quantum average magnetization starting from an ensemble of initial states, $|\psi\rangle$, obtained choosing randomly energy eigenstates in a narrow energy interval: $|\psi\rangle = \sum_E^{E+\Delta E} C_E|E\rangle$. The coefficients C_E have been randomly chosen in modulus and phase and such that $\sum_E^{E+\Delta E} |C_E|^2 = 1$. Since $\hat{M}_y$, connects only eigenstates with different parity, we have:

$$\langle M_y(t)\rangle = 2\mathcal{R}e\{\sum_{E_+,E_-=E}^{E+\Delta E} C^*_{E_+} C_{E_-} e^{-it(E_- - E_+)/\hbar}\langle E_+|\hat{M}_y|E_-\rangle\}, \quad (13)$$

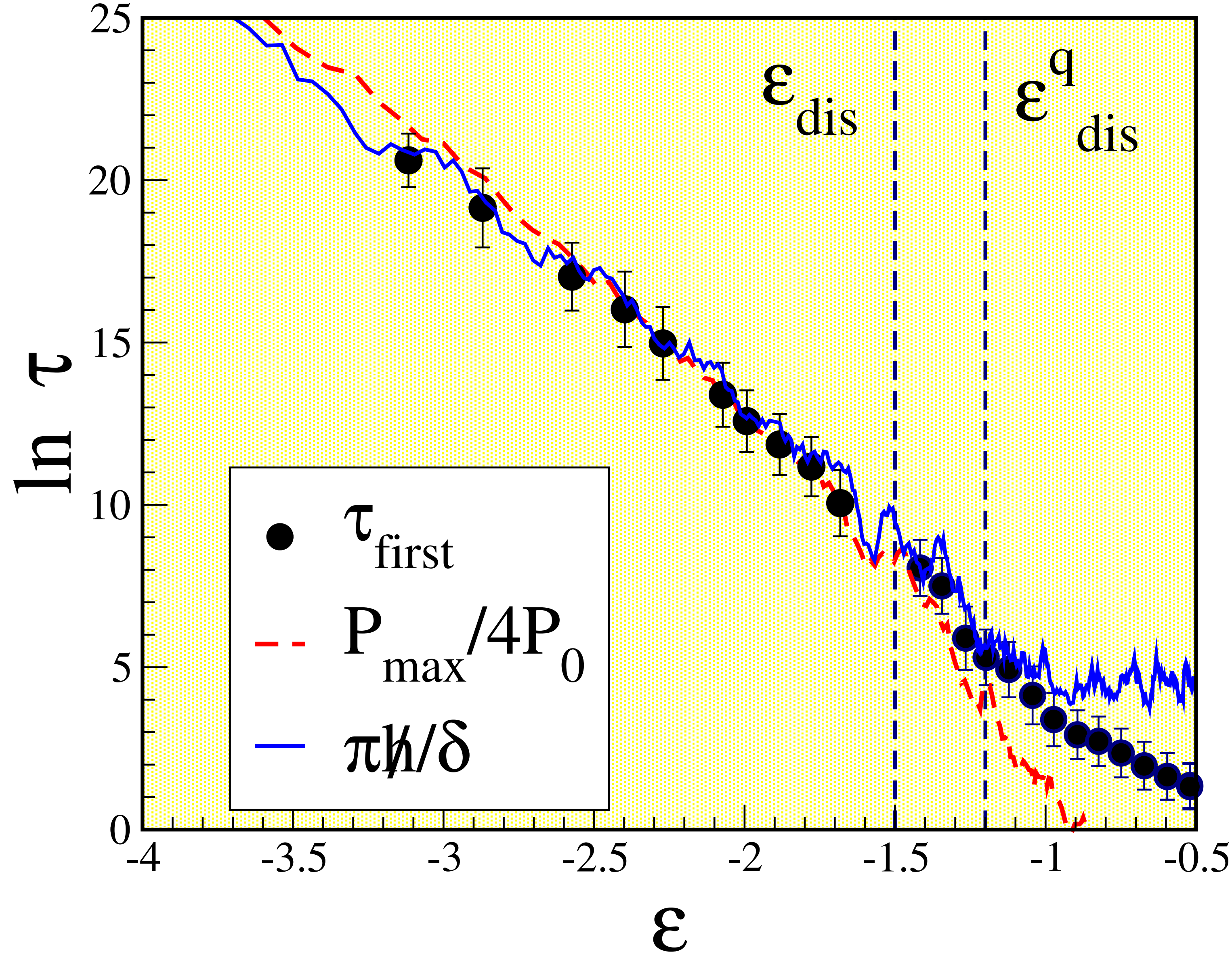
Above TNT : Semiclassical regime



Quantum regime : Macroscopic Tunnelling

In the low energy region of the spectrum, due to the intrinsic quasi-degeneracy the dynamics can be entirely characterized by the energy difference $|E_+ - E_-| = \delta$. The dynamics is thus oscillatory with a period given by $2\pi\hbar/\delta$. Indeed under this condition, the magnetization oscillates coherently between states with opposite sign, a phenomenon known as Macroscopic Quantum Coherence. This period represents the time for the first passage to zero of $\langle M_y(t) \rangle$. One thus can assume : $\tau \sim \pi\hbar/(2\delta)$. It is surprising that P_{max}/P_0 is proportional to the tunneling rates and to the reversal times, even in the region classically forbidden (below ϵ_{dis}) (the only mechanism allowing the jumping of the barrier is through Macroscopic Quantum Tunneling.)

Quantum Tunnelling



Open problems

- Experimental detection of TNT (nanomagnets)
- Introducing decoherence in the model (spin bath models)