The role of thermal fluctuations and dissipation in producing NTS

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Workshop on Non-Equilibrium Processes at Negative Temperature
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The role of nonlinearity (i.e. nonlinear excitations) in determining thermodynamic equilibrium and nonequilibrium properties of a Hamiltonian system.

The Fermi-Pasta-Ulam nonlinear chain and long-time relaxation time scales to equilibrium in the limit of small energies and long-wavelength initial excitations: KAM and the Strong Stochasticity Threshold. Lack of ergodicity has no practical effects on thermodynamics, while fluctuations in stationary nonequilibrium conditions yield anomalous heat-transport properties.

The FPU problem in the limit of short-wavelength initial excitations can be mapped onto the Discrete-Nonlinear-Schrodinger Equation (that conserves both the energy and the number of particles): it exhibits a dynamical phase where breaking of ergodicity yields spontaneous relaxation to nonequilibrium multi-breather states that are characterized by negative temperature.

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The DNLS Hamiltonian on a lattice made of M sites with p.b.c.

$$H = \sum_{j=1}^{M} [(p_j^2 + q_j^2)^2 + 2 (p_{j+1} p_j + q_{j+1} q_j)]$$

Two conserved quantities:

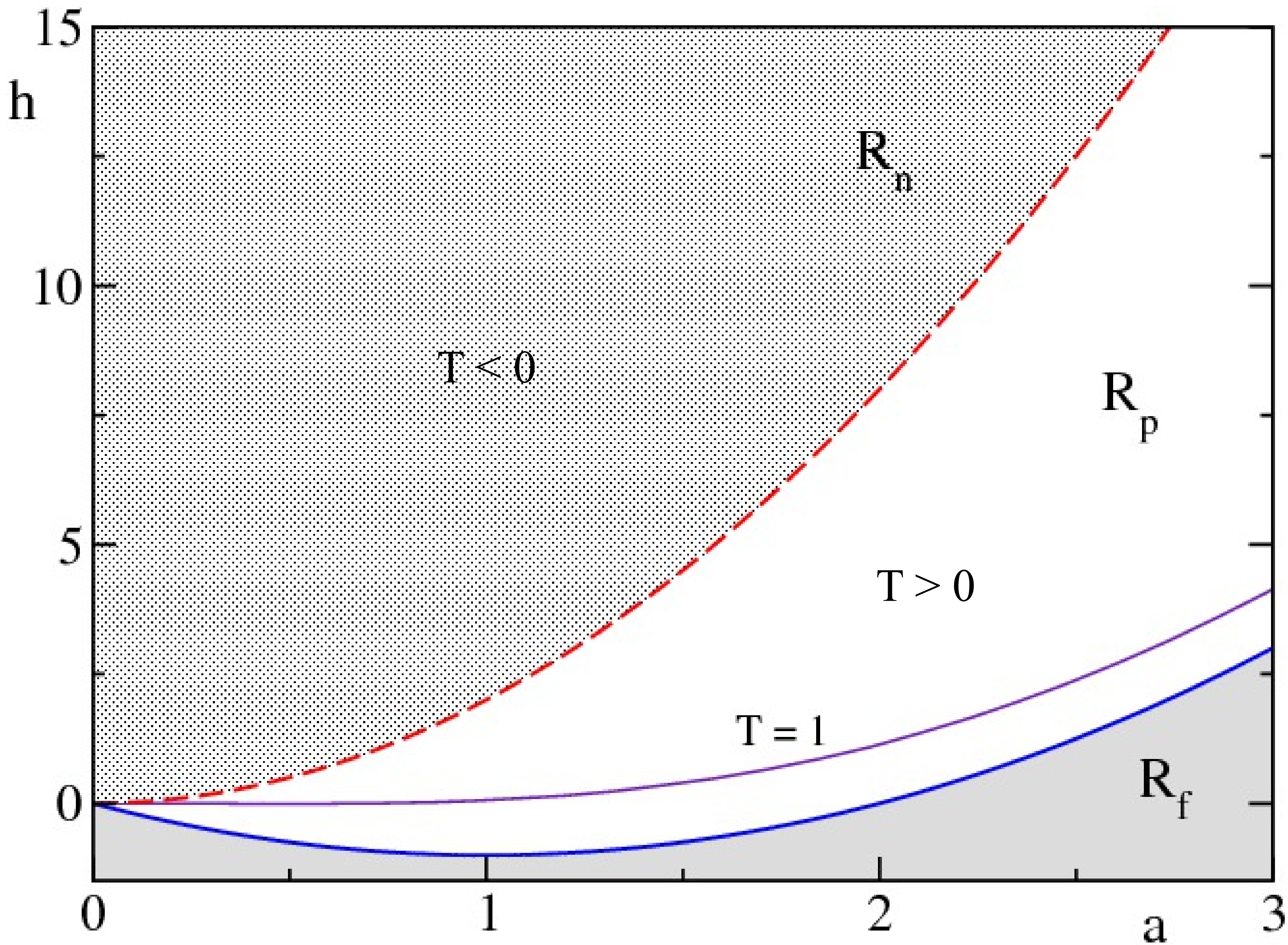
Energy = H

Mass = $\sum_{j=1}^{M} (p_j^2 + q_j^2)$

Model for BEC in optical lattices (Gross-Pitaevskij)
and for light propagation in coupled wave-guides

$$\mathrm{H} = \sum_{i=1}^{M} [U |z_i|^4 + \xi_i |z_i|^2] - \frac{T}{2} \sum_{i=1}^{M-1} (z_i^* z_{i+1} + c.c.) \qquad \text{with} \qquad \{ z_j^*, z_k \} = \frac{i}{\hbar} \delta_{j,k}$$

Energy density h vs. Mass density a



It was conjectured that R_p and R_n correspond to positive and negative temperatures, respecively: breathers were associated to the latter case.

K.O. Rasmussen et al., Phys. Rev. Lett. **84**, 3740 (2000)

It was shown later, by entropic arguments, that negative temperature equilibrium states cannot exist in R_n : the equilibrium state collapses onto a background at infinite temperature, while the excess energy is stored into a single breather state.

B. Rumpf, Phys. Rev. E 69, 016618 (2004); Europhys. Lett. 78, 26001 (2007)

What does it happen in R_n ?

Peculiar relaxation properties in models with two conseved quantities: e.g., nonlinear oscillators and Heisenberg spin chains.

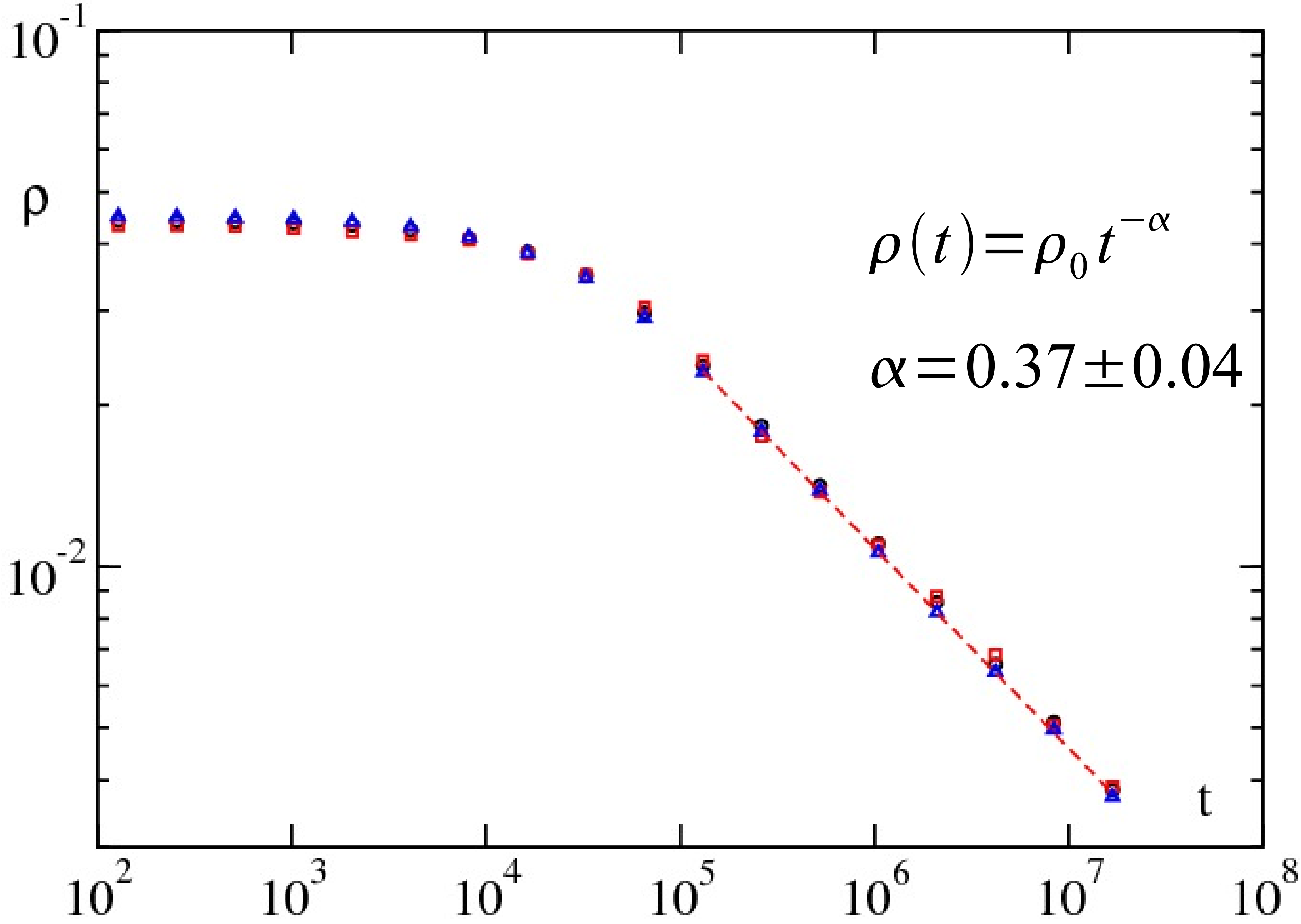
G.P. Tsironis ans S. Aubry, Phys. Rev. Lett. **77**, 5225 (1996)
B. Rumpf and A.C: Newell, Phys. Rev.Lett. **87**, 54102 (2001)

Microcanonical MC study of the weak coupling limit (null hopping) allows to separate entropic effects from dynamical slowing-down in the process of relaxation to thermodynamic equilibrium.

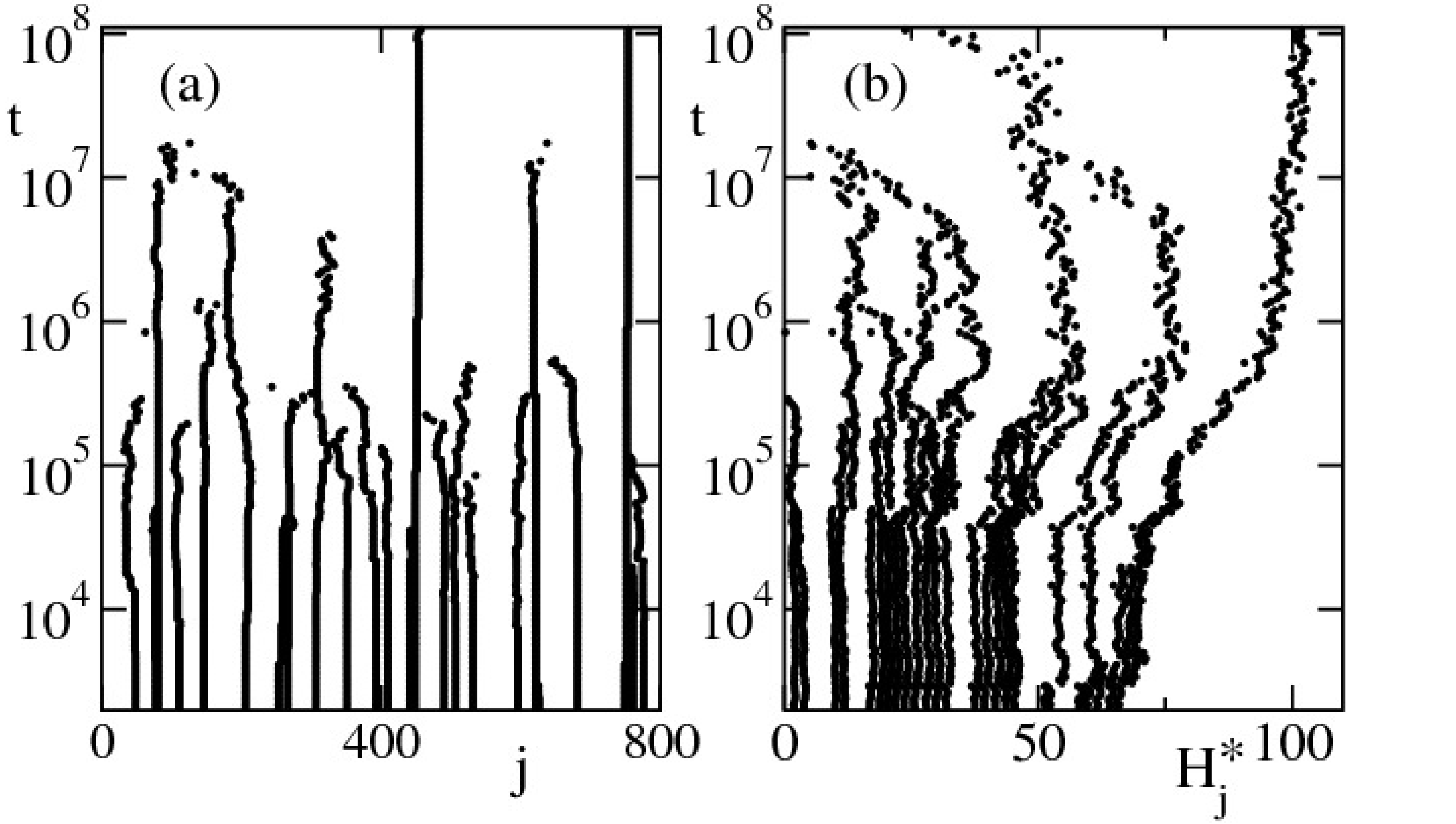
In R_p one observes fast relaxation to a positive temperature state without breathers.

Conversely, in R_n one observes a coarsening process yielding a single final breather: scaling exponent close to 1/3 (Cahn-Hilliard)

Density of sites ρ with amplitude $A_j > 10$ (breathers)

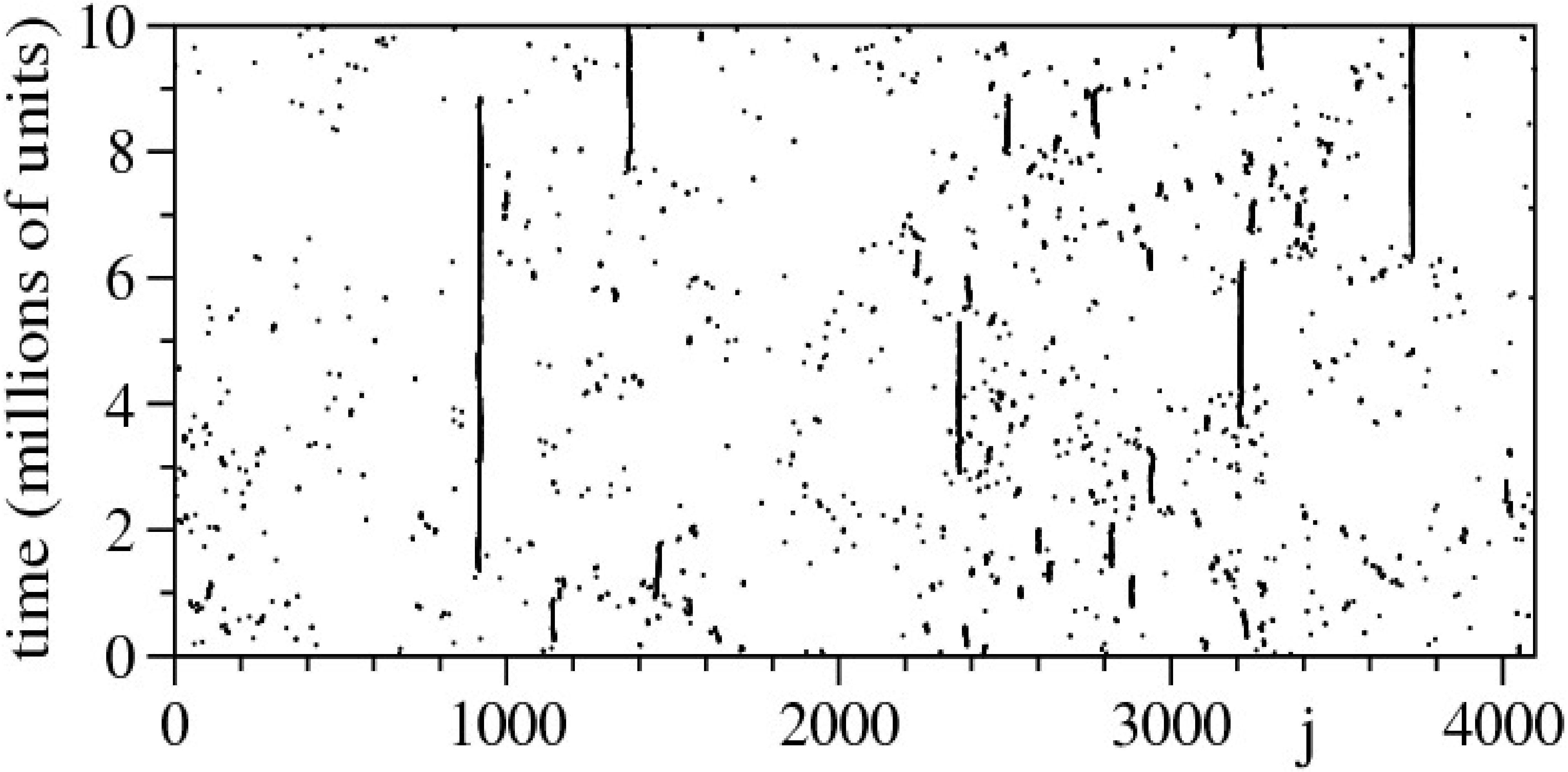


Coarsening Dynamics



The hamiltonian dynamics relaxation process becomes by far much slower than the MMC coarsening dynamics

Parameter values h = 2.4 and a = 1



Such metastable states are characterized by a finite density of breathers and by negative temperatures (microcanonical definition)

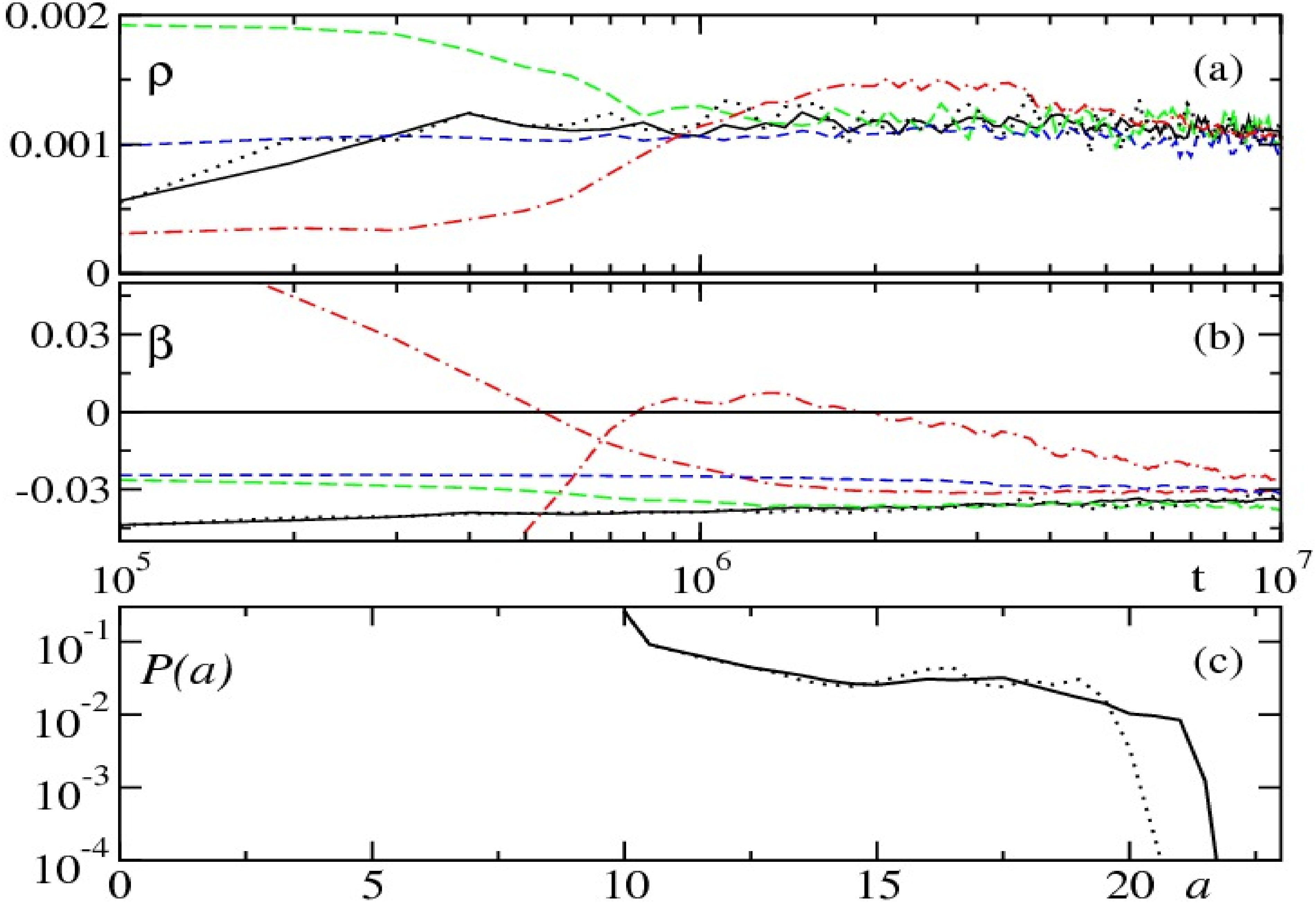
$$\beta = \frac{1}{T_\mu(E,C)} = \left\langle \frac{W|\vec{\xi}|}{\vec{\nabla} H \cdot \vec{\xi}} \vec{\nabla} \cdot \left(\frac{\vec{\xi}}{|\vec{\xi}| W} \right) \right\rangle_\mu$$

where

$$\vec{\xi} = \frac{\vec{\nabla} H}{|\vec{\nabla}| H} - \frac{(\vec{\nabla} H \cdot \vec{\nabla} A) \vec{\nabla} A}{|\vec{\nabla} H| |\vec{\nabla} A|^2}$$

$$W = \left\{ \sum_{j,k} \left(\frac{\partial H}{\partial x_j} \frac{\partial A}{\partial x_k} - \frac{\partial H}{\partial x_k} \frac{\partial A}{\partial x_k} \right) \right\}^{1/2}$$

Temperature measurements can be performed by collecting phases and amplitudes of the atomic condensate or of the light in waveguides.


0.002
ρ
(a)
0.001
0
0.03
β
(b)
0
-0.03
10^5
10^6
t
10^7
10^-1
P(a)
(c)
10^-2
10^-3
10^-4
0
5
10
15
20
a

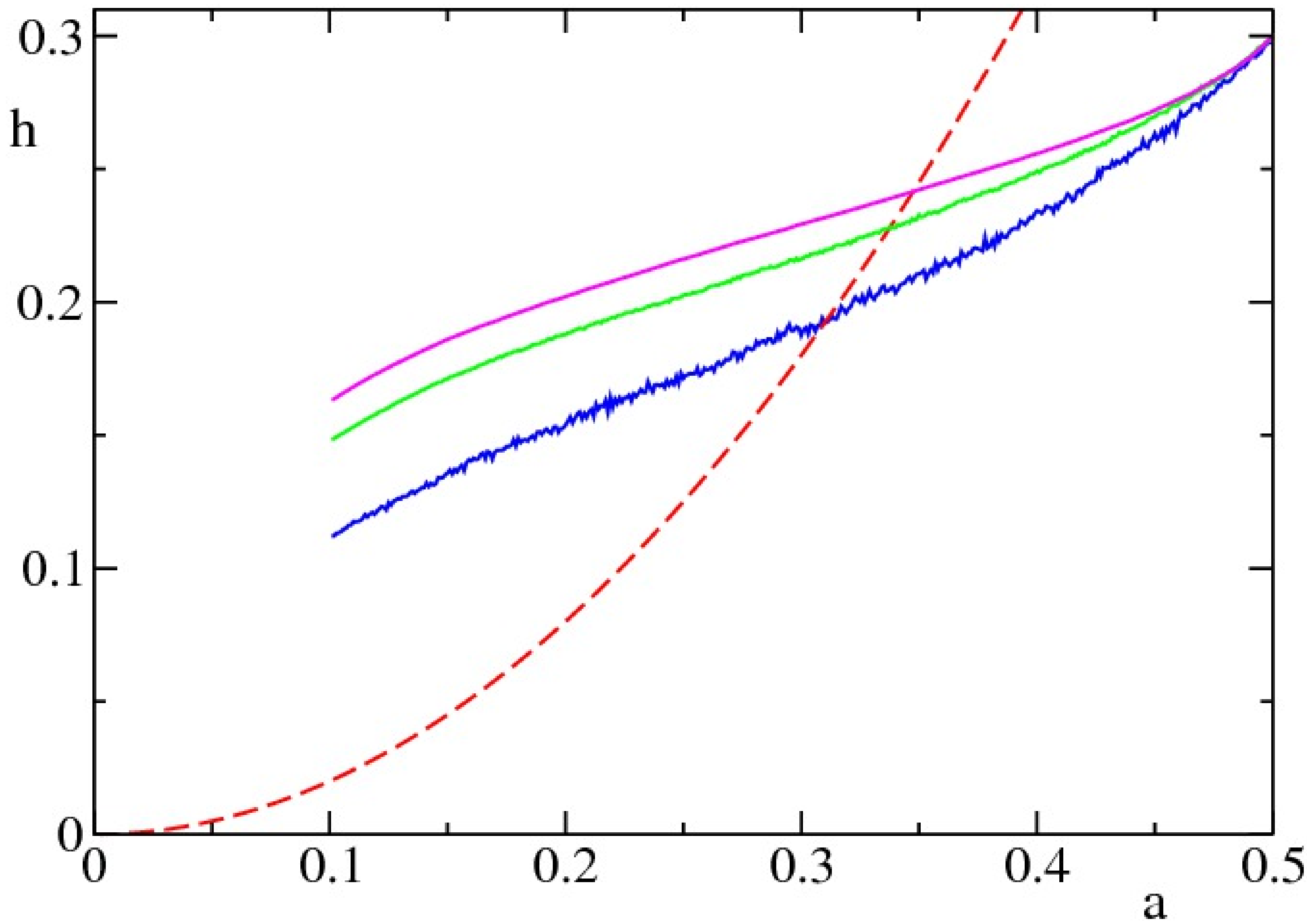
These metastable negative temperature states survive over 10^9 proper time units, without exhibiting any tendency of relaxation to thermodynamic equilibrium !

How can one produce such states?

- "Cooling" from a positive to a negative temperature state by free expansion in a partially empty lattice

- Mass (i.e. amplitude) dissipation from the boundaries

R. Livi, R. Franzosi, and G.-L. Oppo, Phys. Rev. Lett. **97**,060401 (2006)

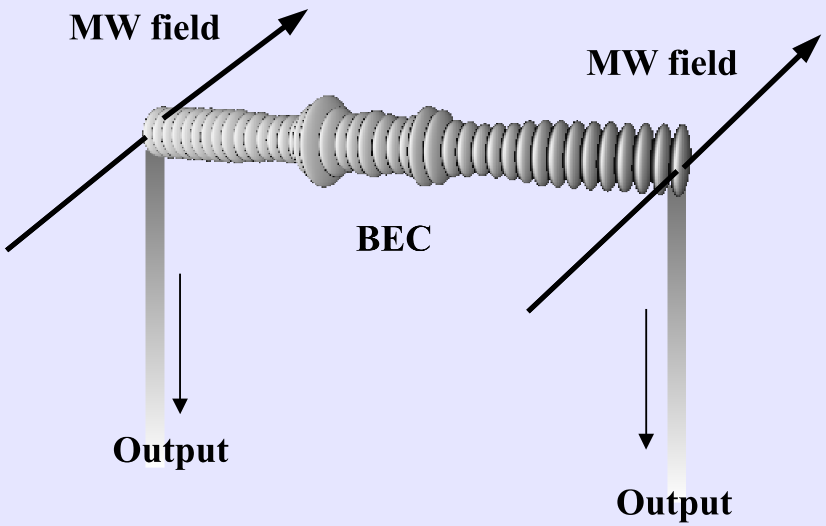

0.3
h
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
a

DNLSE with boundary dissipations

$$i\frac{d}{d\tau}z_j = \Lambda|z_j|^2 z_j - \frac{1}{2}\left(z_{j+1}+z_{j-1}\right) \boxed{- i\gamma z_j\left(\delta_{j,1}+\delta_{j,M}\right)}$$

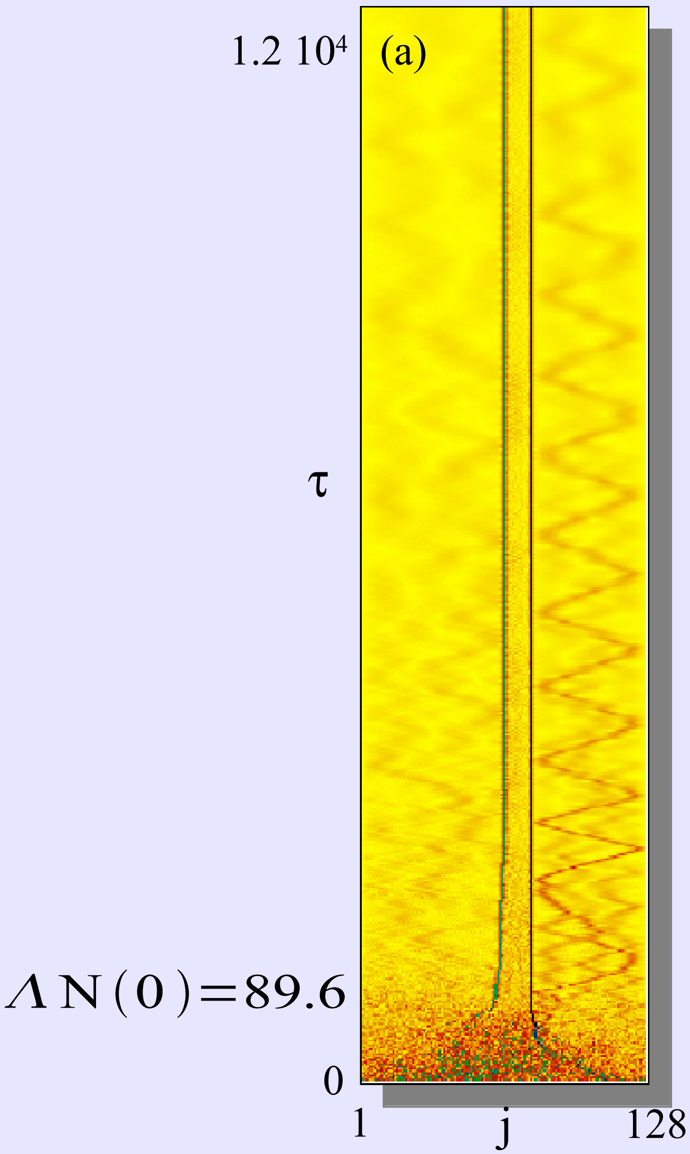
$$\tau = \frac{t\,T}{\hbar} \quad \Lambda = \frac{2U}{T}$$

- The output coupling depends on the
- microwave (Raman Laser) intensity
- High trap frequency essentially yields
- local exponential decay
- Under such conditions the
- ‘bound mode’ is basically empt



R. Livi, R. Franzosi, and G.-L. Oppo, **Phys. Rev. Lett.** 97, 060401 (2006)

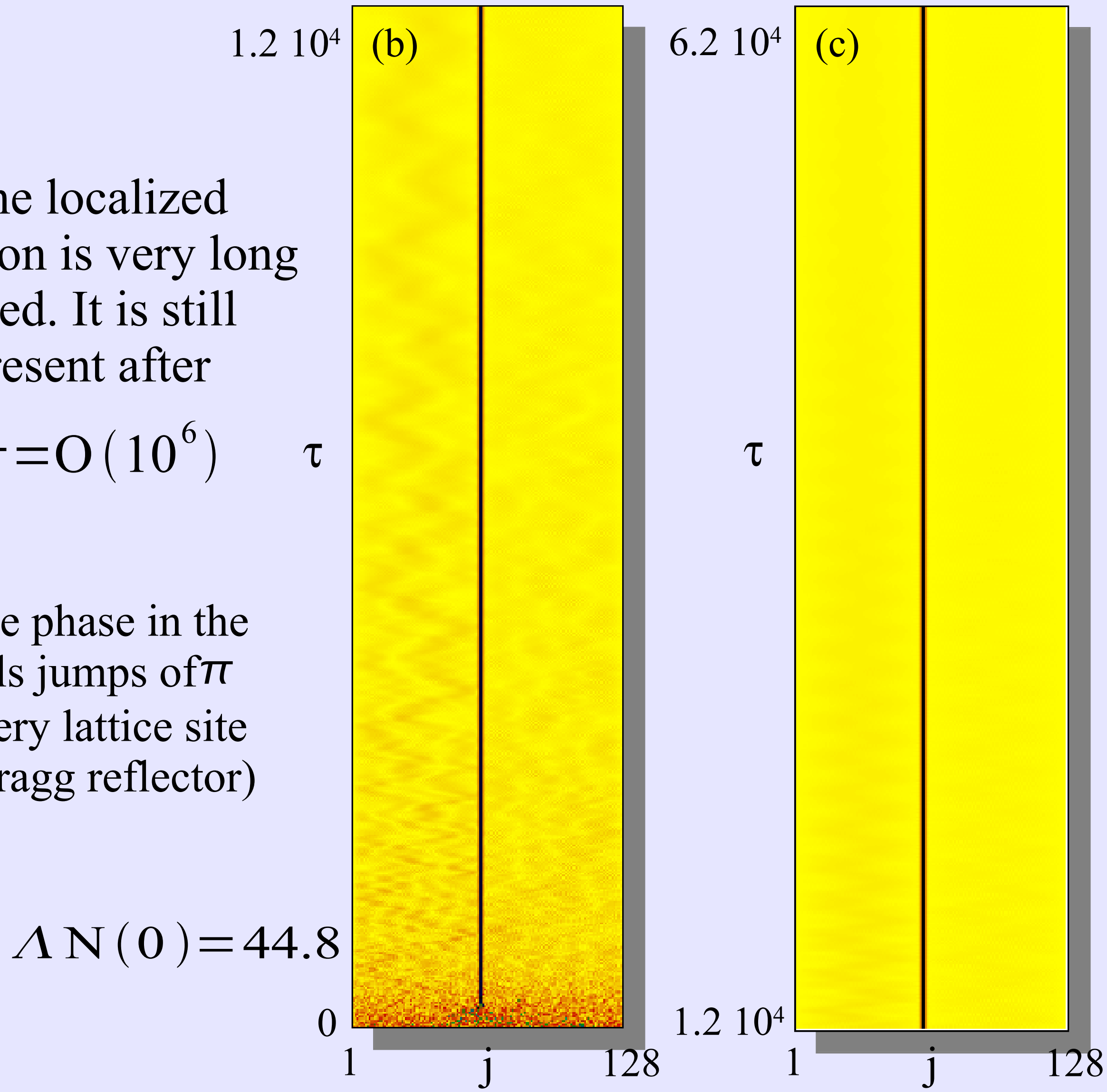
The effect of boundary dissipation



The localized solution is very long lived. It is still present after

$$\tau = O(10^6)$$

The phase in the tails jumps of π every lattice site (Bragg reflector)

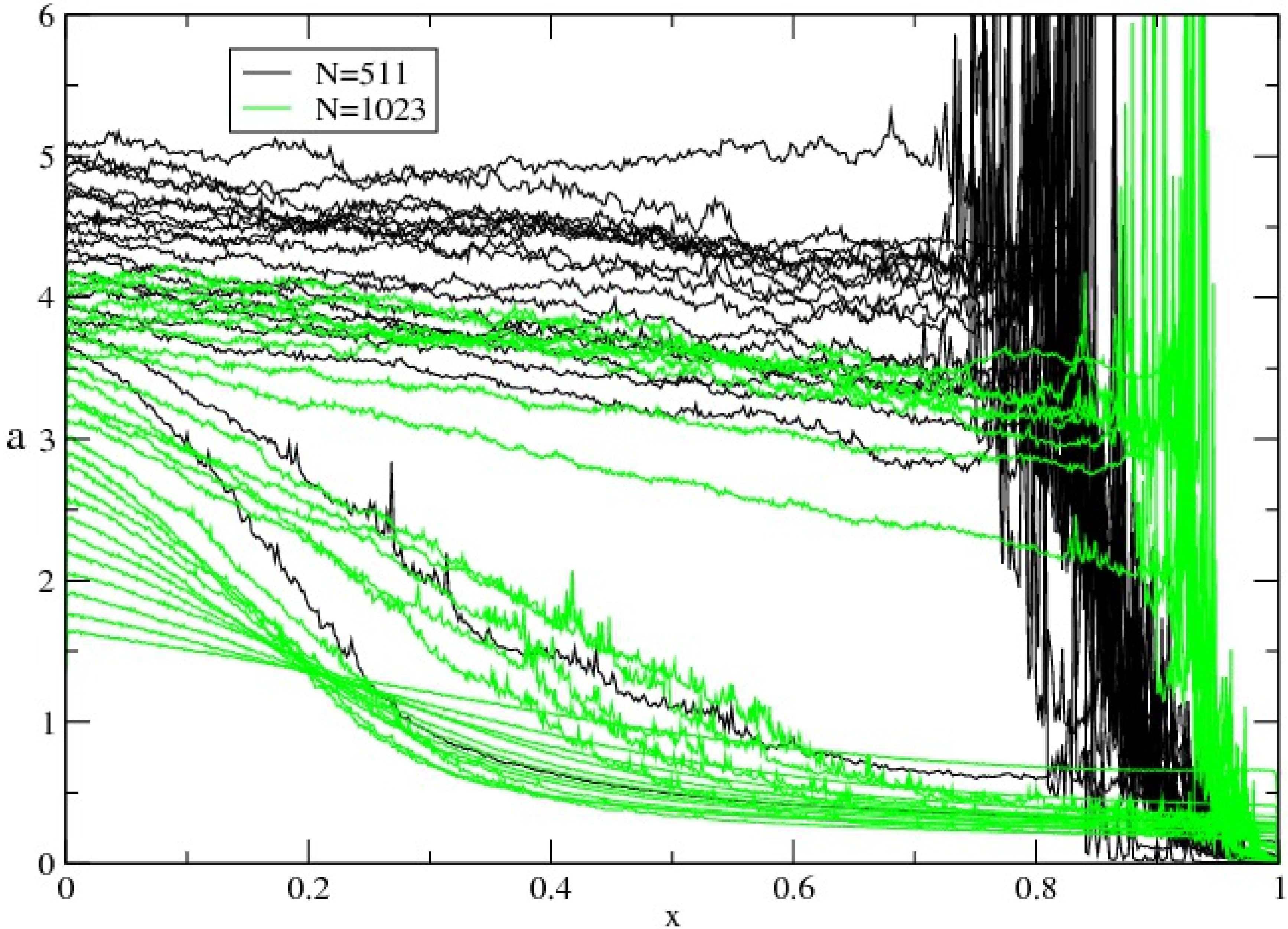


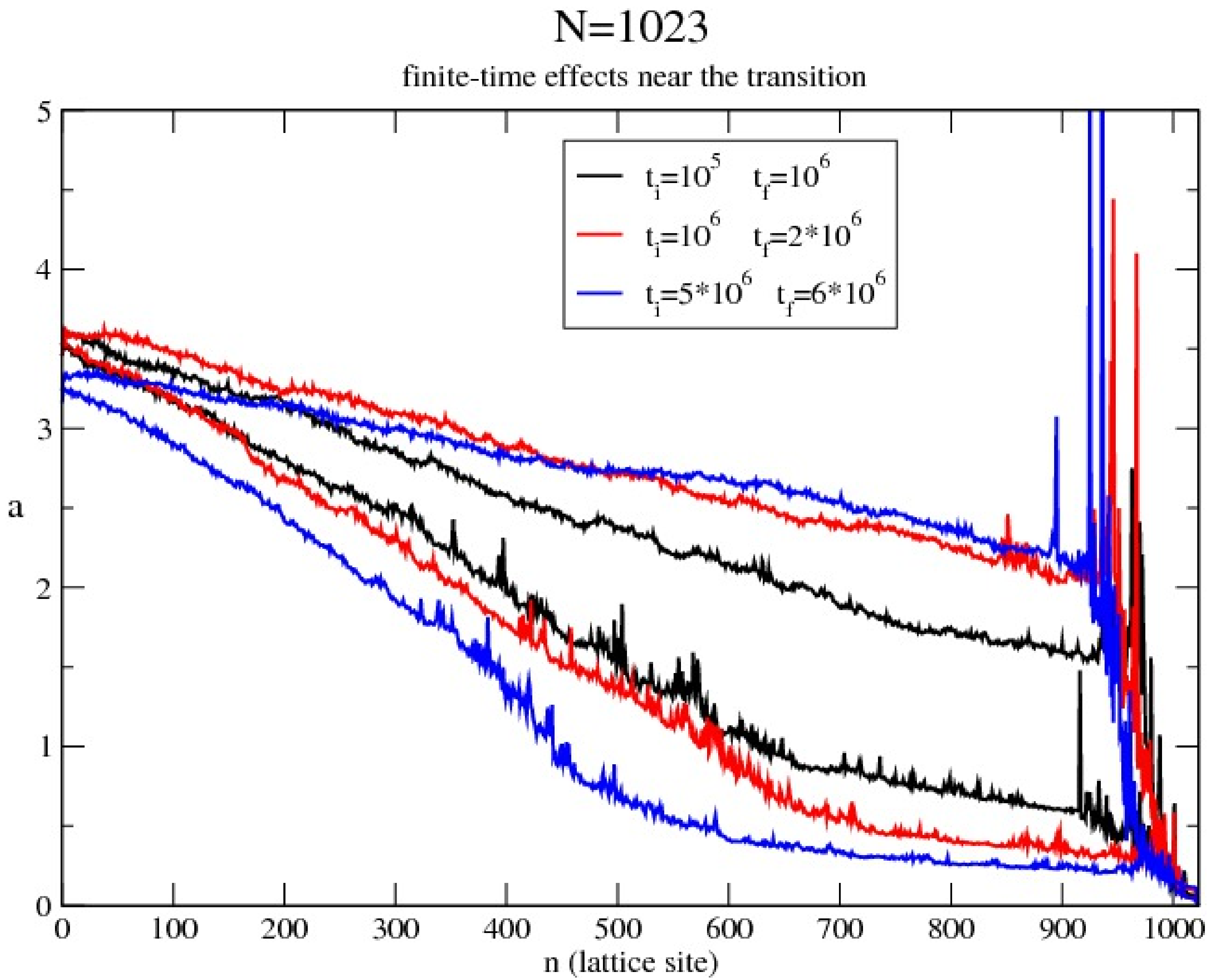
Conductor/insulator transition mediated by the spontaneous formation of breathers

SETUP:
A heat bath at positive temperature T+ acts at one boundary, while a pure dissipator acts at the other boundary.

When T+ is increased one observes a crossover from a standard temperature profile (compatible with Fourier law) to an almost flat temperature profile, segregated from the dissipator by the formation of a (fluctuating) breather state.

The crossover occurs at T+ = 10 (in our dimensionless units)


N=511
N=1023
a
x
0
1
2
3
4
5
6
0.2
0.4
0.6
0.8
1



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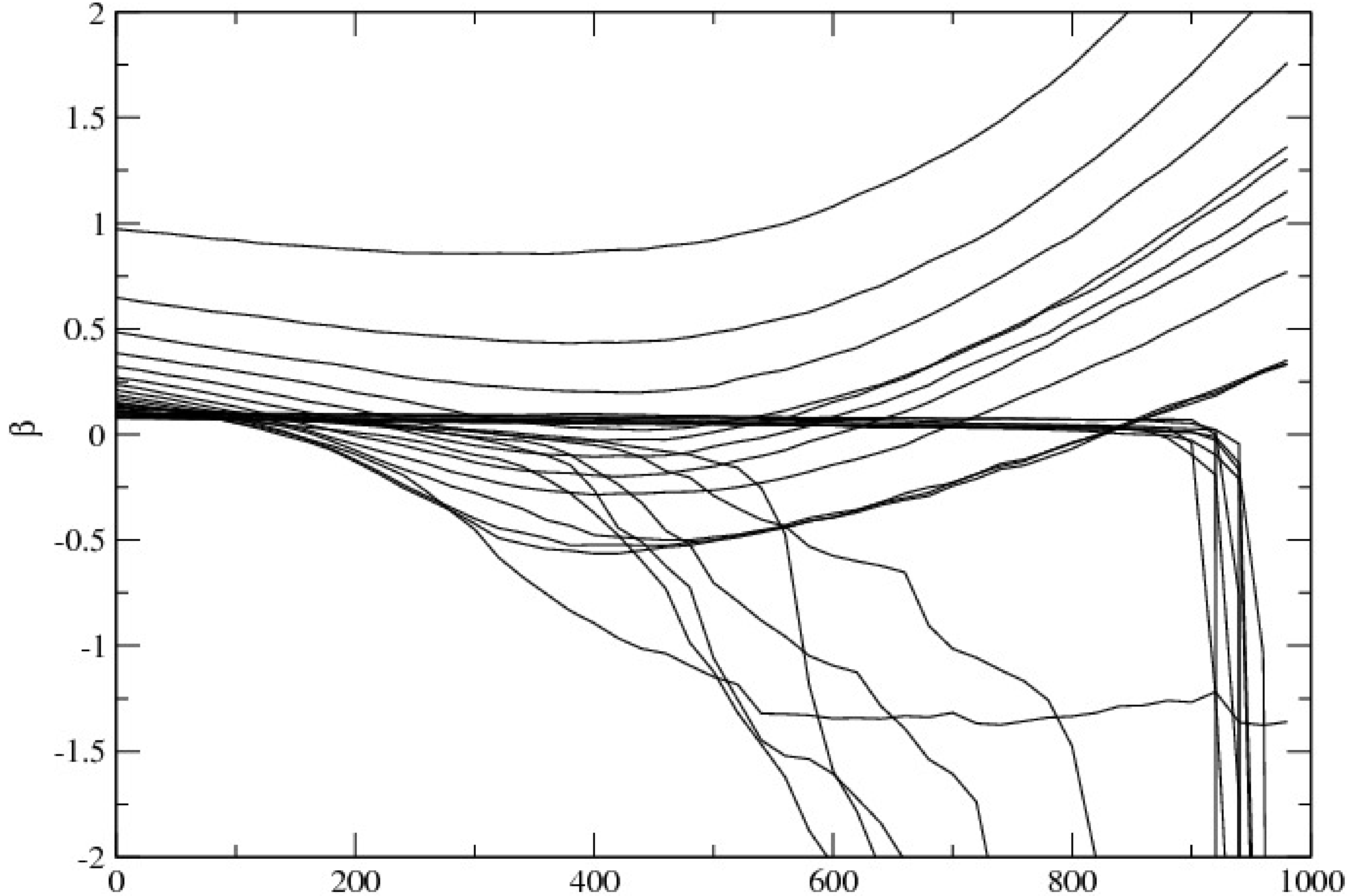
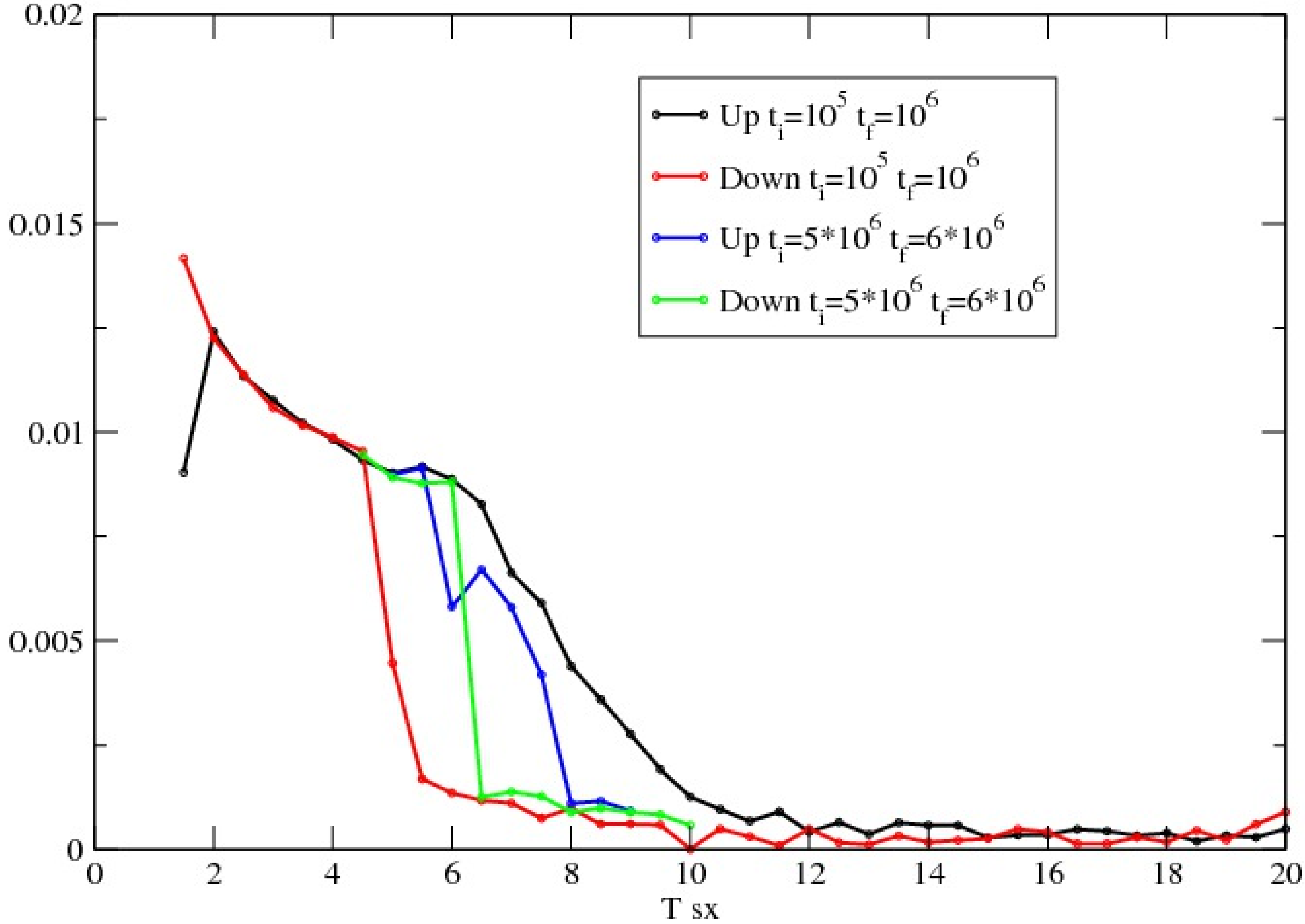
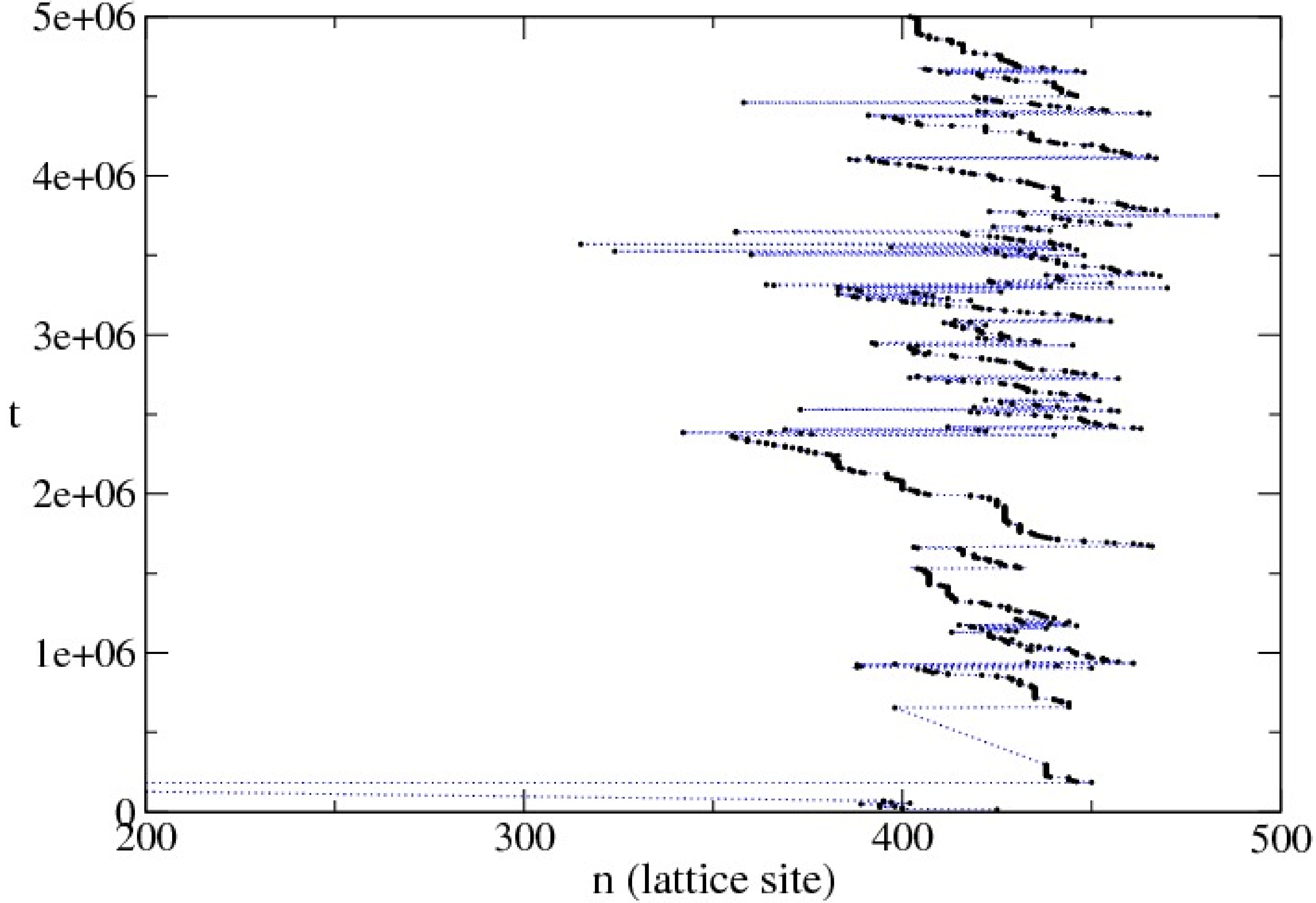
Up long N1023



Mass flux


0.02
0.015
0.01
0.005
0
0 2 4 6 8 10 12 14 16 18 20
T sx
Up $t_i=10^5$ $t_f=10^6$
Down $t_i=10^5$ $t_f=10^6$
Up $t_i=5*10^6$ $t_f=6*10^6$
Down $t_i=5*10^6$ $t_f=6*10^6$



5e+06
4e+06
3e+06
2e+06
1e+06
0
t
200
300
400
500
n (lattice site)

Conclusions and Perspectives

Metastable Negative Temperature states in the DNLSE chain are characterized by the presence of breathers.

Their lifetime is several orders of magnitude longer than the typical time scales of the DNLSE model: the approach to equilibrium (“black hole” state) occurs over an astronomical time scale, even for moderate system size.

Dissipation coupled with nonlinearity may yield nontrivial effects, like the localization of single breather states or the formation of segregation Barriers, yielding a sort of conductor/insulator transition.

An interesing example of ergodicity breaking that affects equilibrium as well as out-of-equilibrium thermodynamic properties.