Frozen dynamics in the Discrete Nonlinear Schrödinger equation

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Non-equilibrium behaviour of classical and quantum systems
SISSA, 10 - 13 September 2018

In collaboration with

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The role of nonlinearity in determining thermodynamic equilibrium and nonequilibrium properties of a Hamiltonian system, the Discrete Nonlinear Schrödinger (DNLS) equation

Outlook

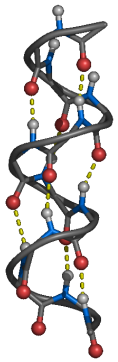
- A slow process involving negative-temperature states and energy localization
- Ergodicity breaking
- A quasi-conserved quantity

The model

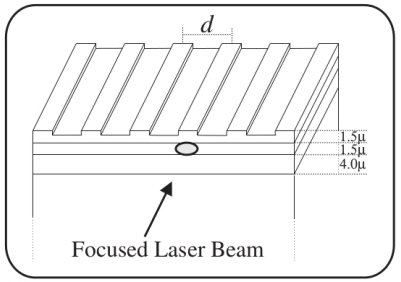
The 1D Discrete Nonlinear Schrödinger (DNLS) Equation

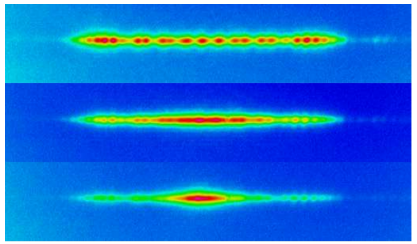
$$i\dot{z}_n = -z_{n+1} - z_{n-1} - \nu|z_n|^2 z_n$$

Davydov theory of protein vibrations

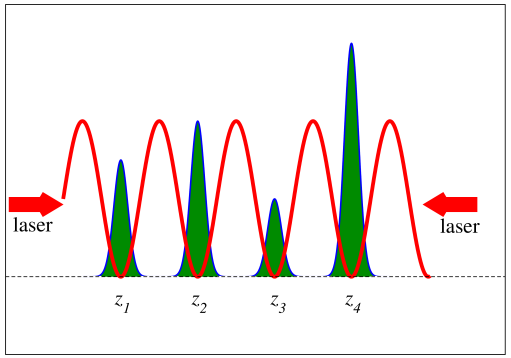


Arrays of optical waveguides with Kerr nonlinearity





Bose-Einstein condensates in optical lattices



The model
The Discrete Nonlinear Schrödinger (DNLS) Equation

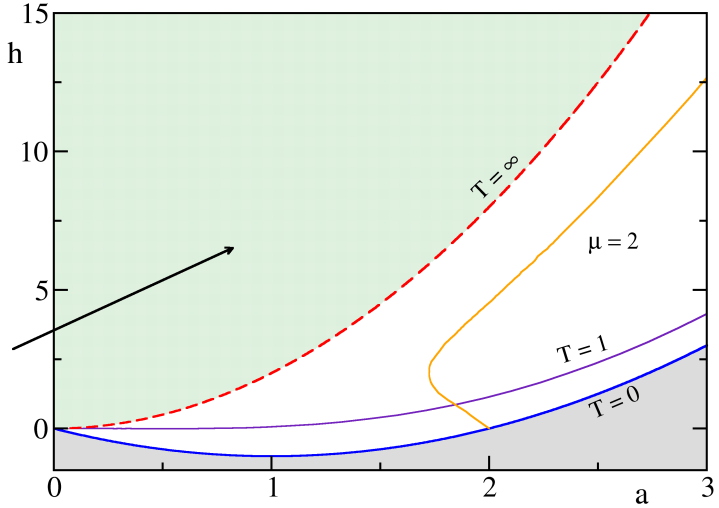
$$i\dot{z}_n = -z_{n+1} - z_{n-1} - \nu|z_n|^2 z_n$$

Two conserved quantities:
Energy & Norm

$$H = \sum_{j=1}^{N} \frac{\nu}{2}|z_j|^4 + (z_j^* z_{j+1} + c.c)$$

$$A = \sum_{j=1}^{N} |z_j|^2$$

Phase diagram



K. Ø. Rasmussen, *Phys. Rev. Lett.*, **84** (2000) 3740

Negative Temperatures

PHYSICAL REVIEW VOLUME 103, NUMBER 1 JULY 1, 1956

Thermodynamics and Statistical Mechanics at Negative Absolute Temperatures

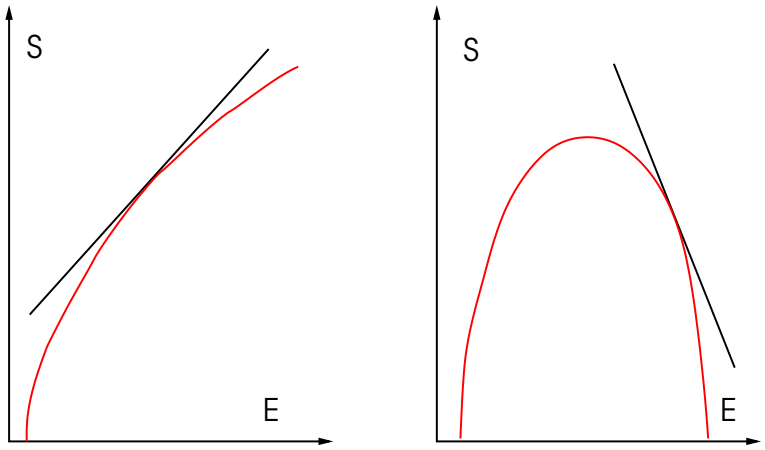
NORMAN F. RAMSEY*
Harvard University, Cambridge, Massachusetts, and Clarendon Laboratory, Oxford, England
(Received March 26, 1956)

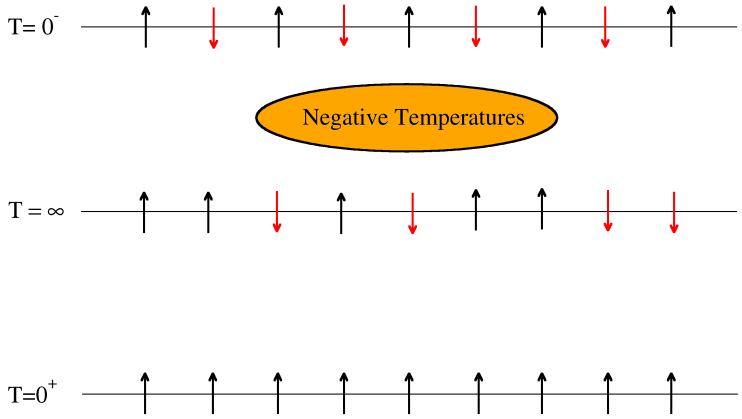
$$\frac{1}{T} = \left.\frac{\partial S}{\partial E}\right|_{A=const}$$

SUPPLEMENTO AL VOLUME VI, SERIE IX DEL NUOVO CIMENTO N. 2, 1949

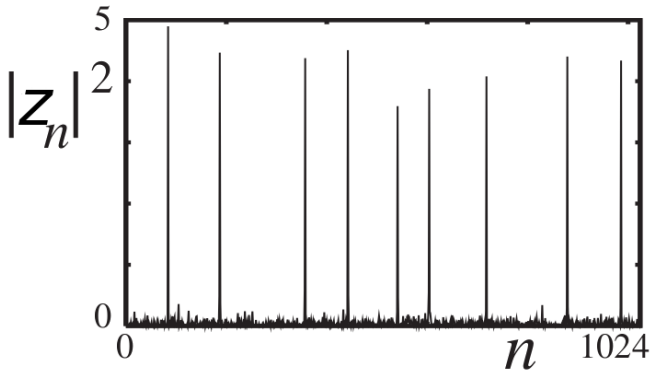
Statistical Hydrodynamics. (*)

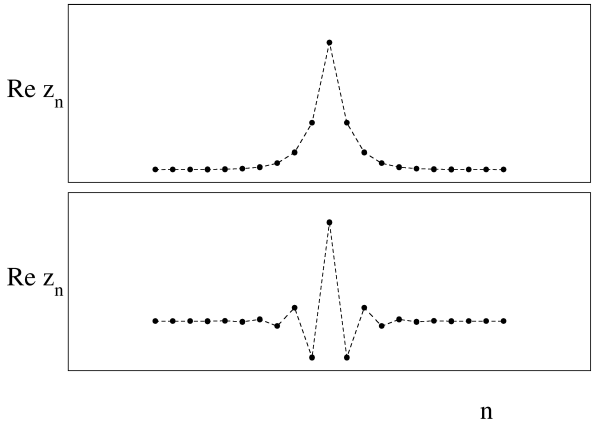
L. ONSAGER
New Haven, Conn.





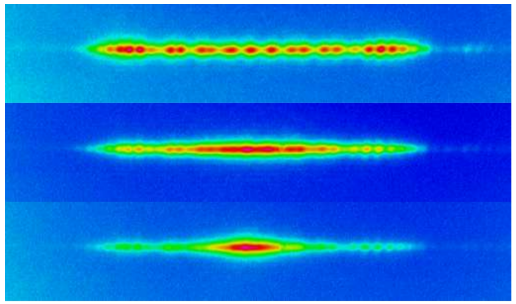
Negative Temperature DNLS



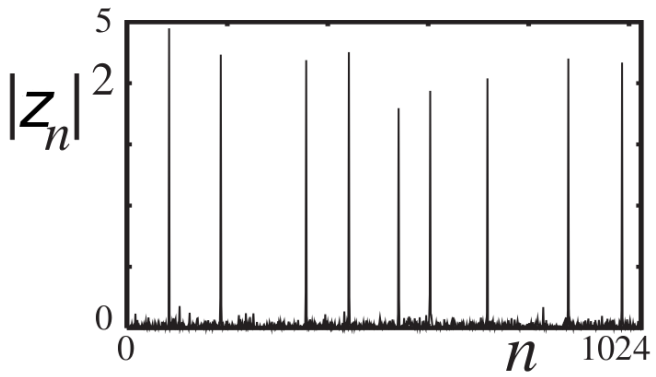


Discrete Breathers

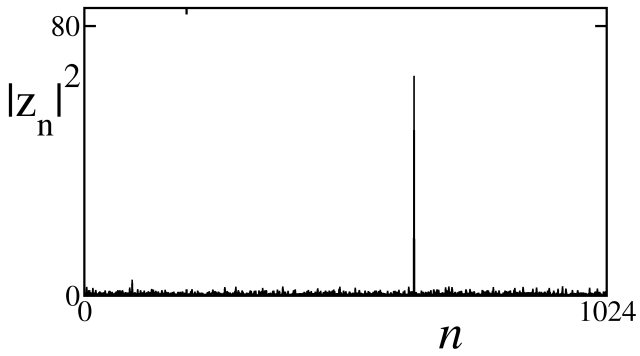
- Exponentially localized in the real space
- Internal frequency $\omega_b \notin$ Lin. Spectr.
- Consequence of nonlinearity and spatial discreteness. No role of disorder.
- Static (pinned) or mobile
- Experimental observations



Maximum entropy state



$\Downarrow$ Relaxation τ $\Downarrow$



B. Rumpf, Phys. Rev. E **69**, 016618 (2004)

- Infinite temperature background superposed to a single breather collecting the excess energy
- No negative temperatures!

BUT

- The transient τ may last for astronomical times

What happens over physically accessible time scales?

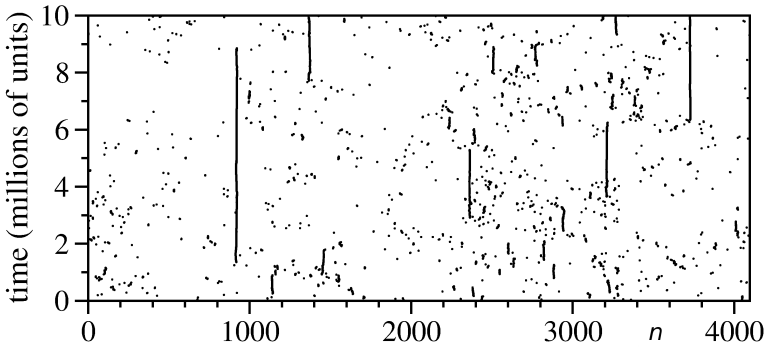
Long-time DNLS dynamics

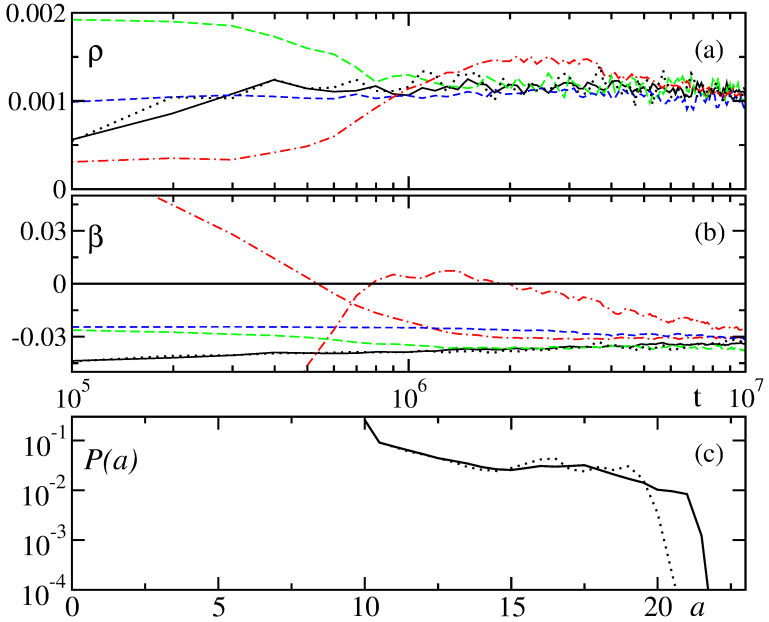
Symplectic numerical integration

$$H = \sum_{n=1}^{N} \frac{\nu}{2}|z_n|^4 + (z_n^* z_{n+1} + c.c.)$$

- Spontaneous birth and death of breathers
- *Finite* density of breathers
- Negative temperature
- Breathers are prevented from becoming "too large"
- Possibility of experimental investigations (boundary cooling / free expansion)

Iubini et al. *New Journal of Physics* 2013





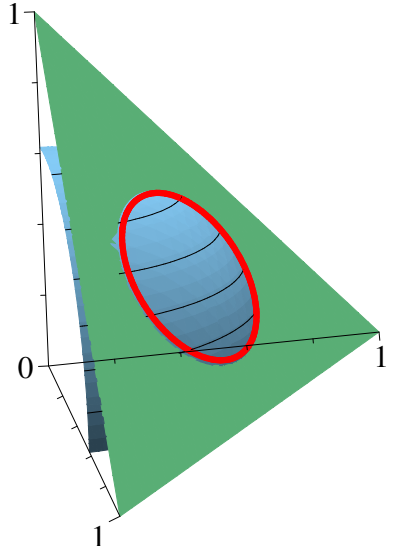
Stochastic dynamics

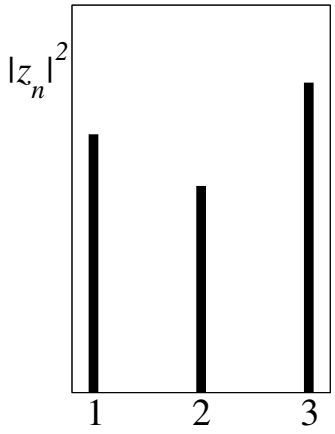
Microcanonical Monte-Carlo algorithm

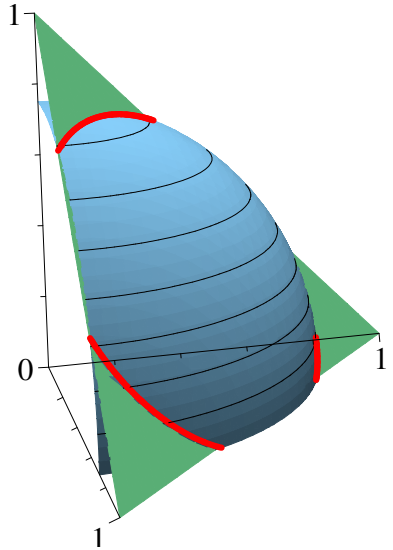
- Investigation of entropic effects during relaxation
- Local conservation of energy and mass
- Weak coupling approximation (large mass densities)

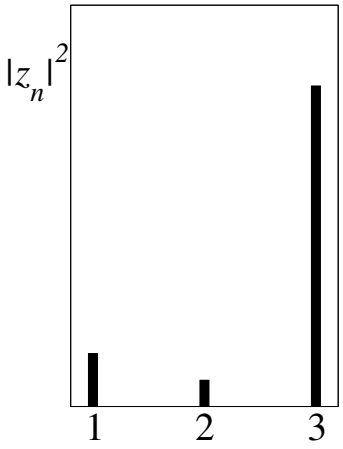
$$H = \sum_{n=1}^{N} \frac{\nu}{2} |z_n|^4 \cancel{+ (z_n^* z_{n+1} + c.c.)}$$

$$A = \sum_{n=1}^{N} |z_n|^2$$





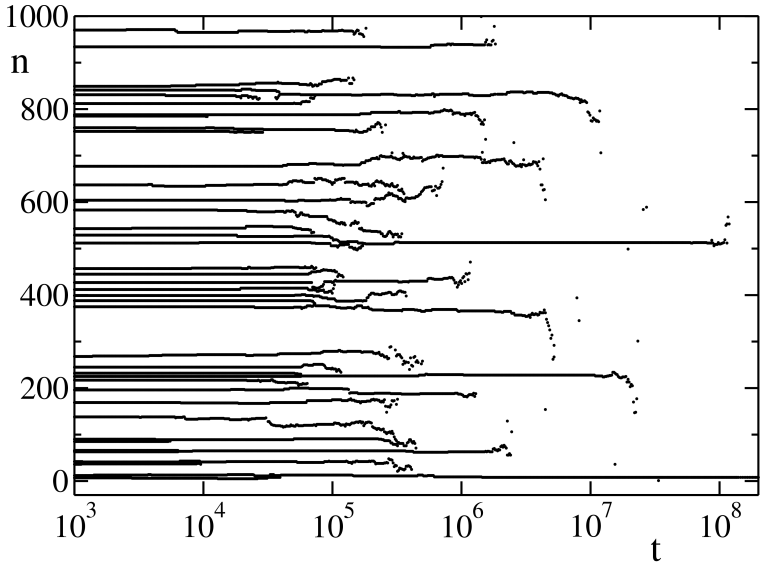


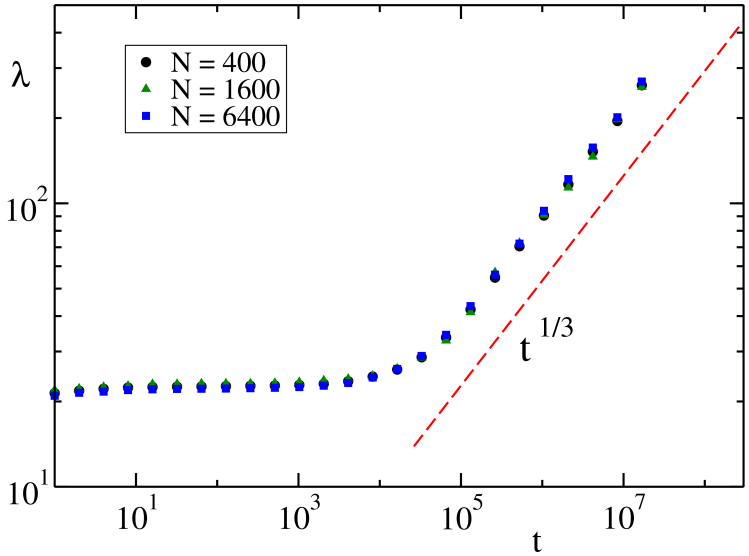


Stochastic models (purely entropic effects)

Coarsening dynamics: breather distance $\lambda(t) \sim t^{1/3}$

- S.I., A. Politi, P. Politi *J. Stat. Phys.* (2013), JSTAT(2017)





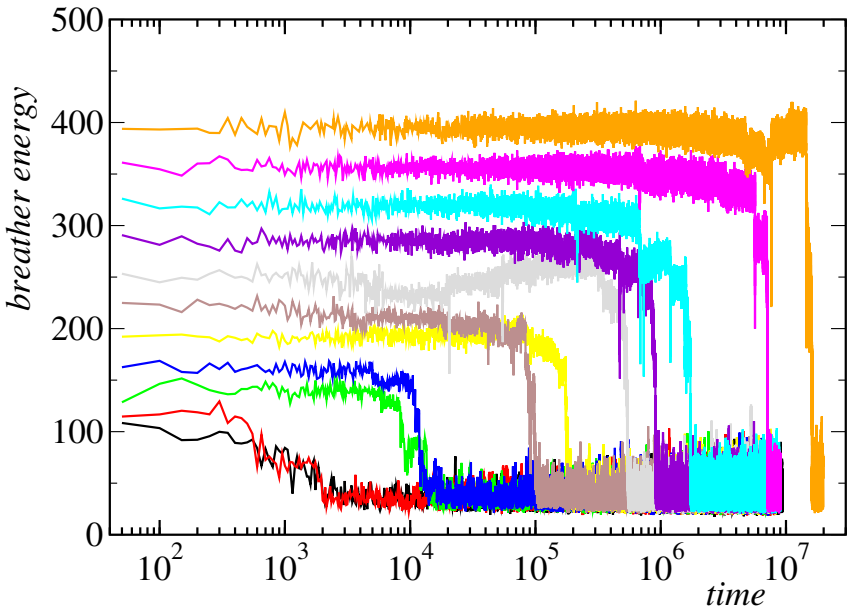
Condensation phenomena

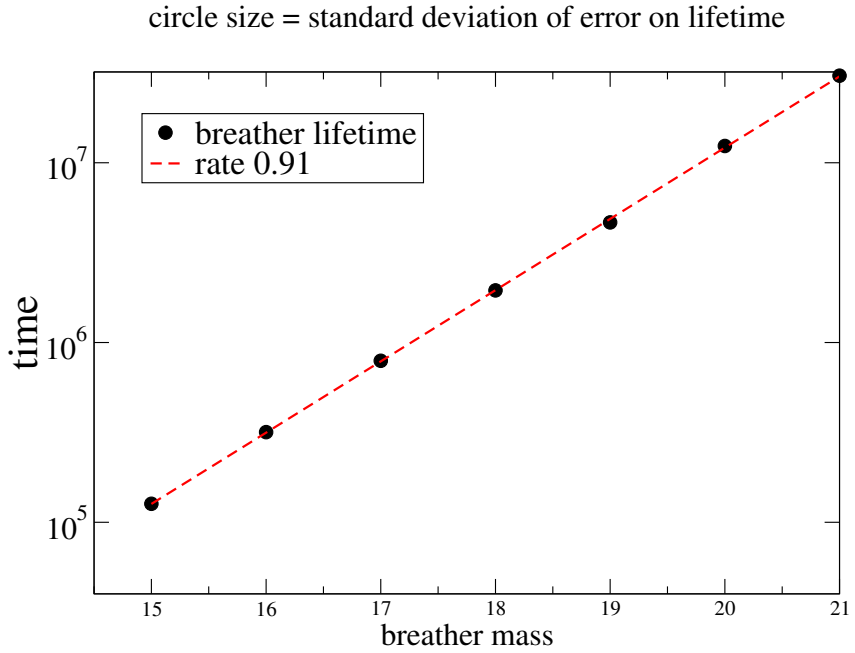
- J. Szavits-Nossan, M. Evans, S. N. Majumdar, PRL (2014)
- J. Szavits-Nossan, M. Evans, and S. N. Majumdar, Journal of Physics A: Mathematical and Theoretical (2014)
- J. Barré, and L. Mangeolle, JSTAT (2018)

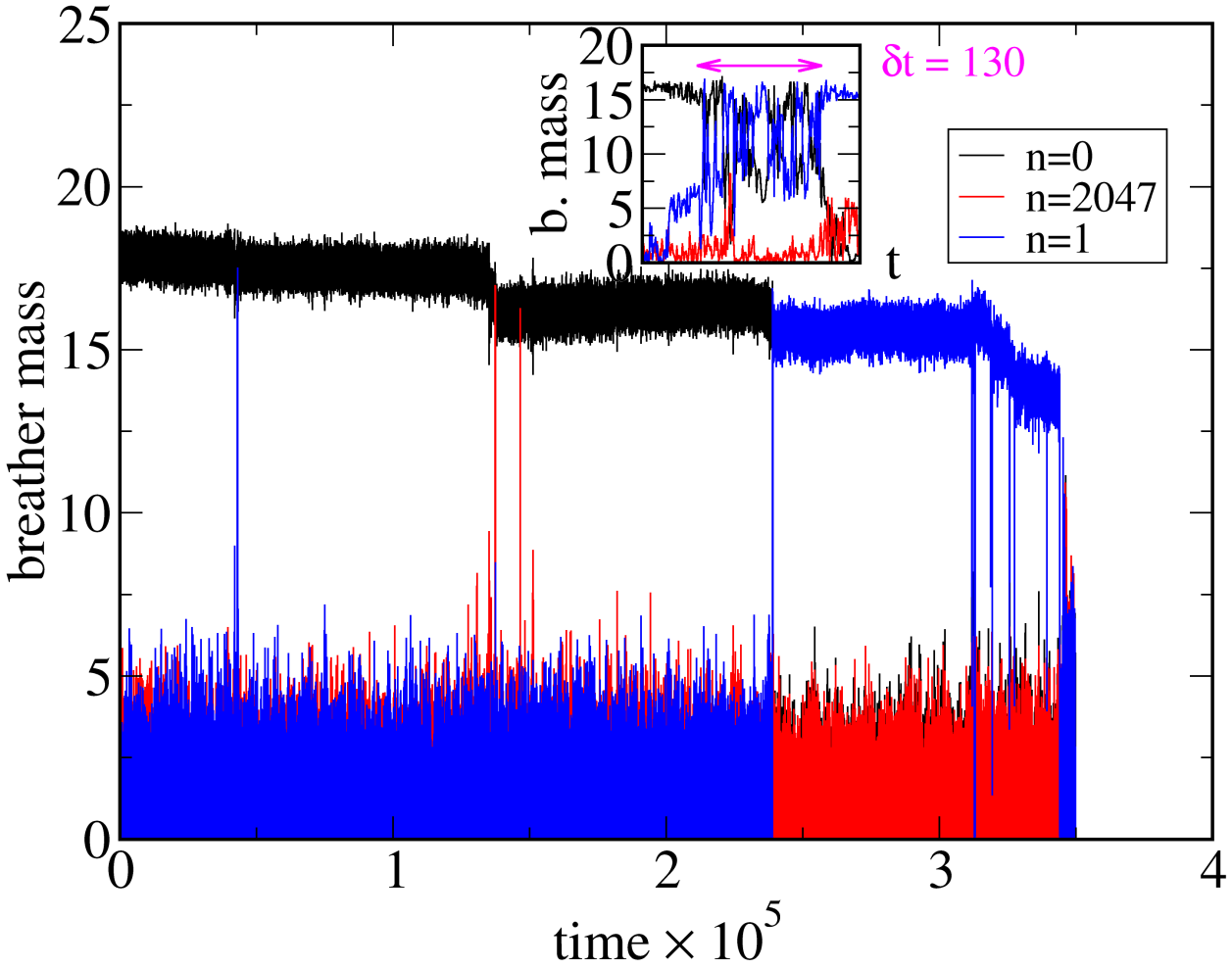
DNLS relaxation dynamics

S.I. , P. Politi, A. Politi, L. Chirondojan, G.L. Oppo - in preparation

- Slow breather dynamics also appears in the positive temperature regime
- Relaxation of a breather on a positive temperature background
- The destruction timescale increases exponentially with the breather amplitude

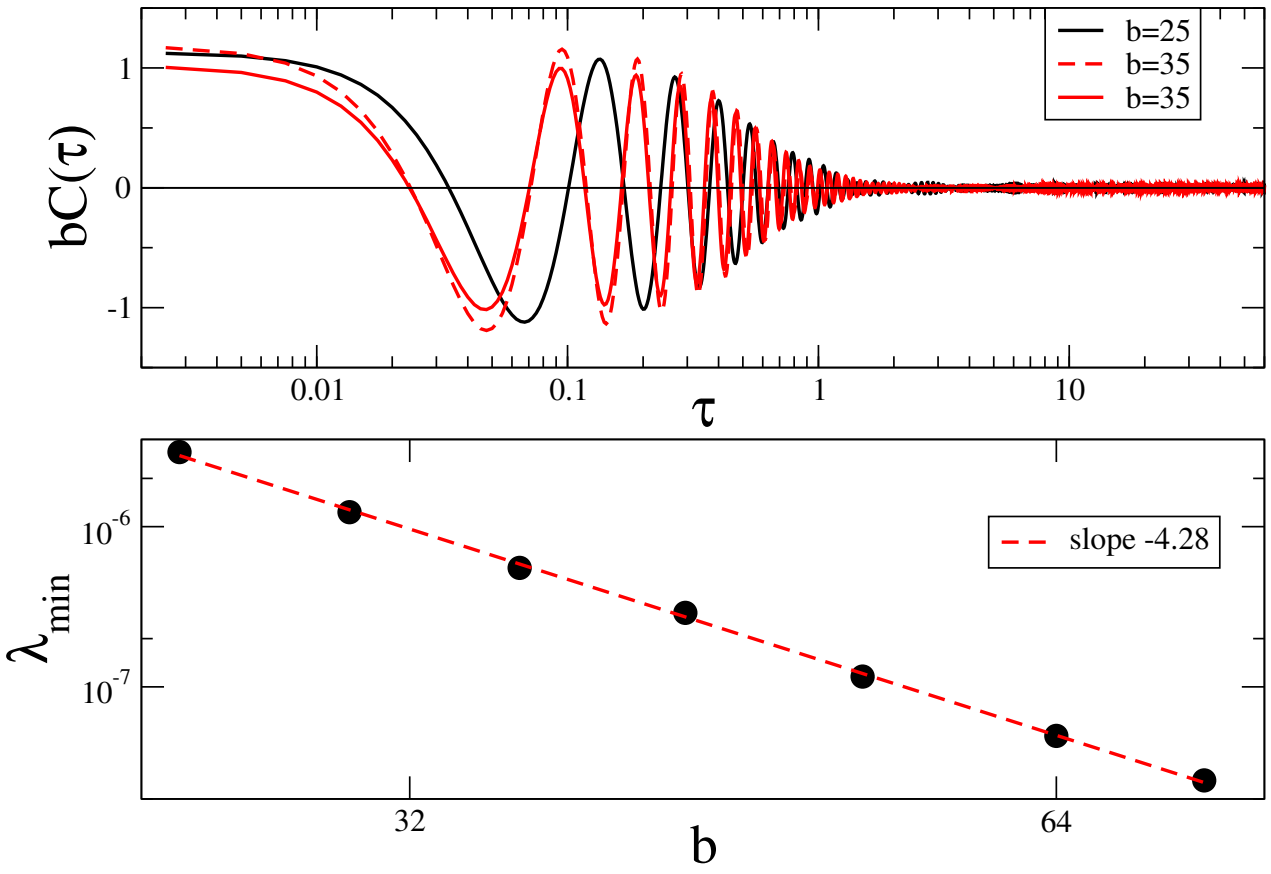





breather mass
time × 10^5
b. mass
t
δt = 130
n=0
n=2047
n=1

“Laminar periods”

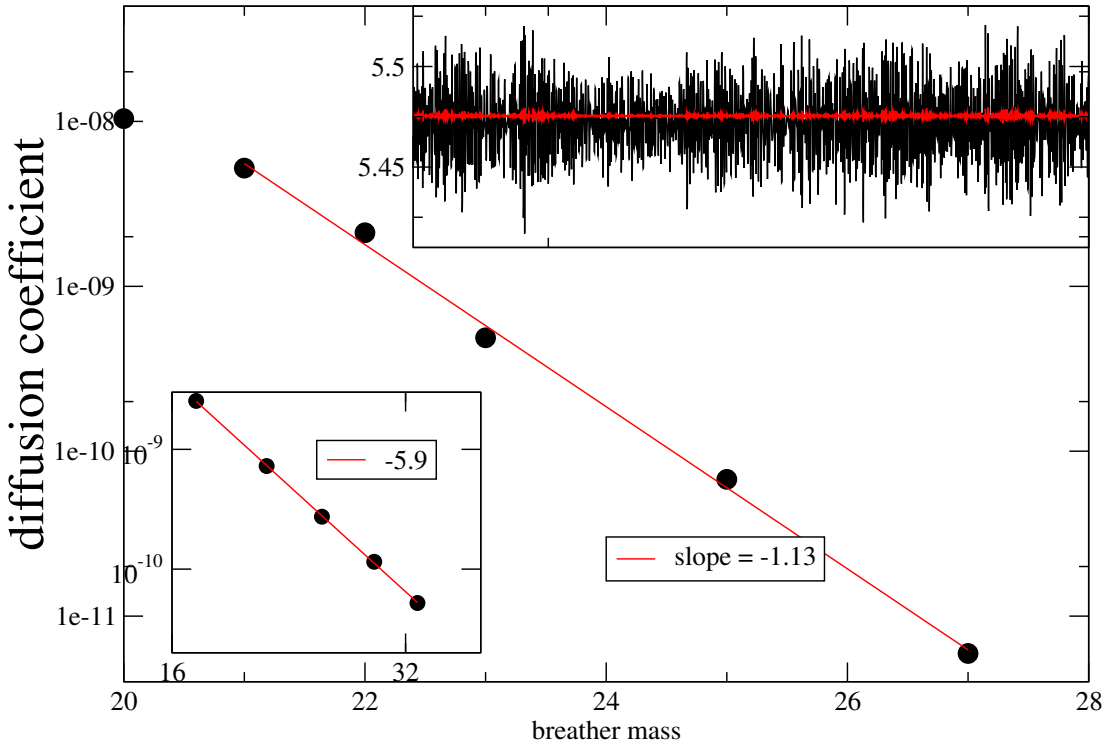
Mass correlation function $C(\tau) = \langle b(t+\tau)b(t)\rangle - \langle b(t)\rangle^2$



Principal Component Analysis on $[z_{-1}, z_0, z_1]$ (five real variables)
λ_{min} minimum PCA eigenvalue

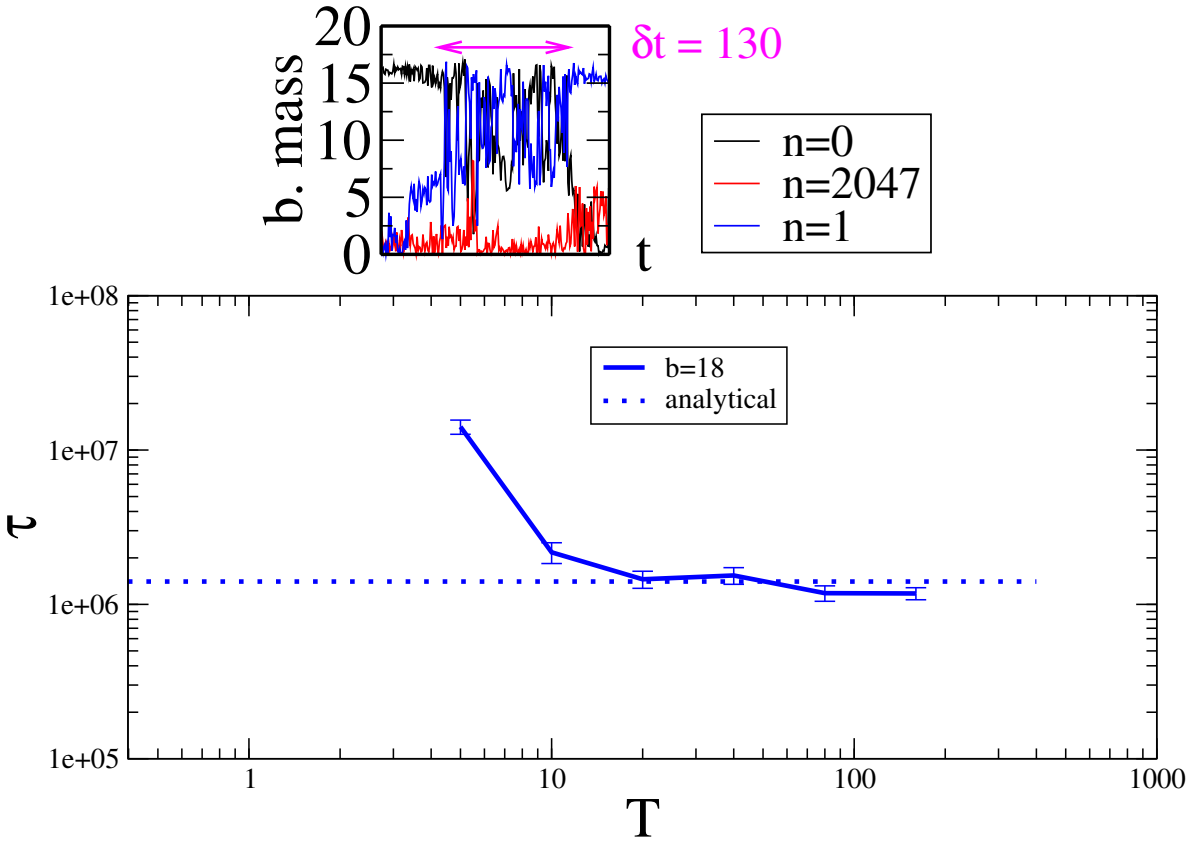
The quasi-conserved quantity

$$Q_1 = A_0 + c[A_{-1}\cos(\phi_{-1} - \phi_0) + A_1\cos(\phi_1 - \phi_0)] \quad \left(z_j = A_j e^{i\phi_j}\right)$$



From perturbative calculations $1/c = 2A_0^2 \simeq \omega$

Sporadic jumps



- Threshold for the creation of a dimer state: $a > (\sqrt{b} - \sqrt{2})^2$
- Given a breather with mass b, the probability of creating a dimer state scales as $P(b) \sim e^{-kb}$

Altogether:

- Evidence of a freezing process of purely dynamical origin (traced back to the existence of the quasi conserved quantity Q_1)
- Energy diffusion is suppressed
- Breather relaxation occurs through rare and sudden mass exchanges triggered by the creation of bound states.
- This mechanism prevents the convergence towards the maximum entropy state for $T < 0$ but also relaxation for $T > 0$.