Coupled transport and negative temperature states

Antonio Politi

Department of Physics, University of Aberdeen, UK

Glasgow, 23-24 October 2014

Collaborators

Stefano Iubini (Orleans)

Stefano Lepri (ISC-CNR Florence)

Roberto Livi (Dept. of Physics, Florence)

Gian Luca Oppo (Univ. Strathclyde)

Outline

- DNLS as a reference model & and some known facts

Outline

- DNLS as a reference model & and some known facts
- Coupled transport and steady non-equilibrium states

Outline

- DNLS as a reference model & and some known facts
- Coupled transport and steady non-equilibrium states
- Non monotonous temperature profiles

Outline

- DNLS as a reference model & and some known facts
- Coupled transport and steady non-equilibrium states
- Non monotonous temperature profiles
- Nonequilibrium phase-transitions (zero temperature)

Outline

- DNLS as a reference model & and some known facts
- Coupled transport and steady non-equilibrium states
- Non monotonous temperature profiles
- Nonequilibrium phase-transitions (zero temperature)
- Nonequilibrium phase-transitions (beyond infinite temperature)

The model

$$\mathcal{H} = \sum_j V|\psi_j|^4 - Q\sum_j(\psi_j^*\psi_{j+1} + c.c.)$$

$$i\frac{d\psi_j}{dt} = 2V|\psi_j|^2\psi_j - Q(\psi_{j-1} + \psi_{j+1})$$

PARAMETERS (can be scaled out):

$V > 0$: repulsive atomic interation / self-focusing in waveguides

Q: hopping term [the sign is irrelevant - multiply ψ_j by $\exp(i\pi j)$]

TWO CONSERVATION LAWS

Energy: $\mathcal{H}$ Mass: $A = \sum_j |\psi_j|^2$

h: energy density a: mass density

Operative definition of the relevant thermodynamic observables

$$\frac{1}{T} = \frac{\partial \mathcal{S}}{\partial H} \qquad \frac{\mu}{T} = -\frac{\partial \mathcal{S}}{\partial A}$$

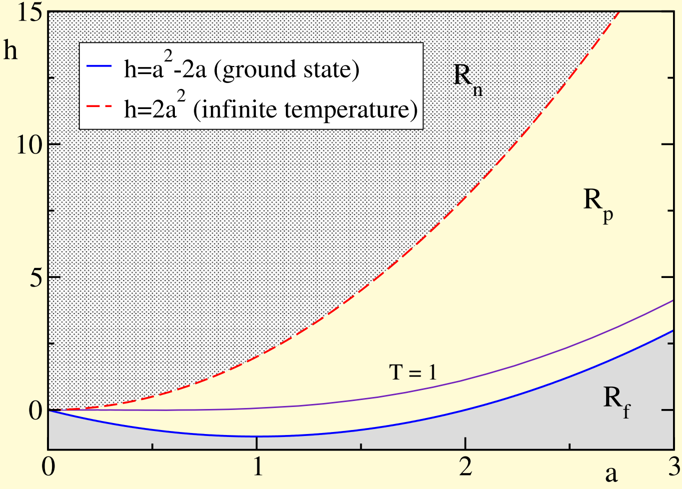
$$\frac{\partial \mathcal{S}}{\partial C_1} = \left\langle \frac{W\|\vec{\xi}\|}{\vec{\nabla} C_1 \cdot \vec{\xi}} \vec{\nabla} \cdot \left(\frac{\vec{\xi}}{\|\vec{\xi}\| W} \right) \right\rangle$$

$$\vec{\xi} = \frac{\vec{\nabla} C_1}{\|\vec{\nabla} C_1\|} - \frac{(\vec{\nabla} C_1 \cdot \vec{\nabla} C_2)\vec{\nabla} C_2}{\|\vec{\nabla} C_1\| \|\vec{\nabla} C_2\|^2} \;;\; W^2 = \sum_{j<k}^{2N} \left[\frac{\partial C_1}{\partial x_j} \frac{\partial C_2}{\partial x_k} - \frac{\partial C_1}{\partial x_k} \frac{\partial C_2}{\partial x_j} \right]^2$$

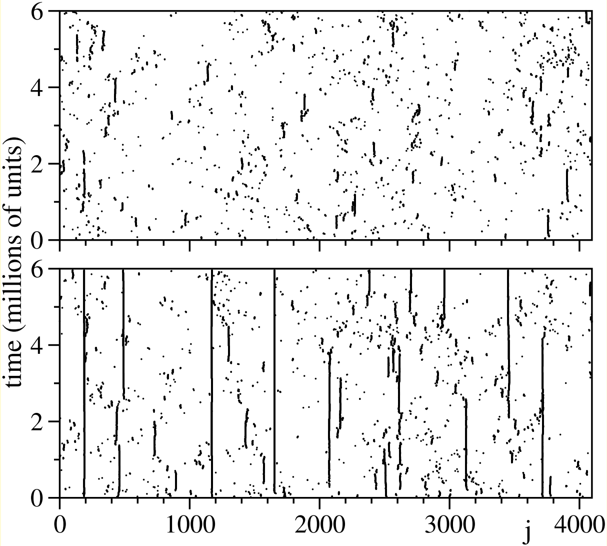
$$C_{1,2} = H, A$$

$\psi_j = x_{2j} + i x_{2j+1}$ (Franzosi 2011, Iubini et al. 2012)

DNLS equilibrium phase diagram (Rasmussen, 2001)

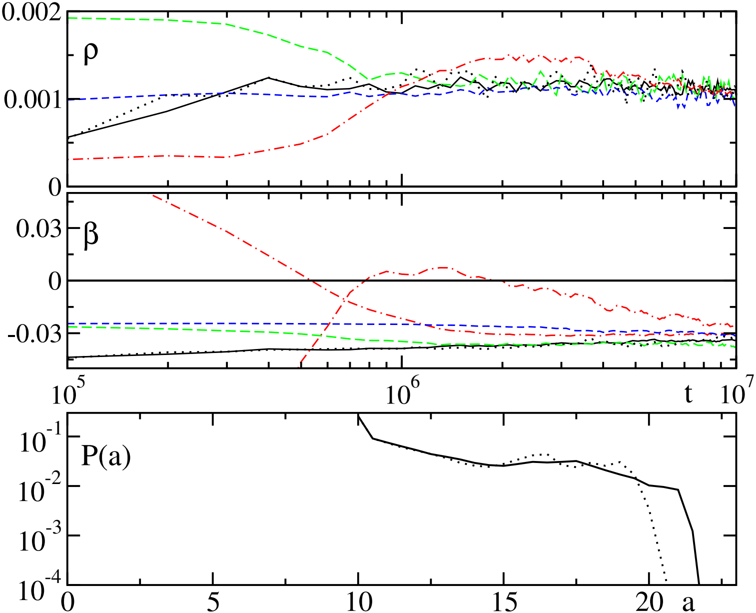


Negative temperatures

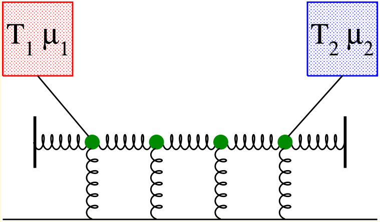


$a = 1$; $h = 2.4$ - 2.8 (upper - lower)

Time evolution



Steady non-equilibrium states: a setup for their analysis



Fluxes

$$J_a(j) = 2\,(p_{j+1}q_j - p_j q_{j+1}) \qquad J_h(j) = -\,(\dot{p}_j p_{j-1} + \dot{q}_j q_{j-1})$$

$$\psi_j = p_j + i q_j$$

Coupled transport: thermoelectric/thermomechanical effects

Seebeck effect: (discovered by Seebeck, correctly interpreted by Oersted)

electromotive force induced by a temperature gradient

Peltier effect: heat generated or removed at the junction of different metals

$$\text{Figure of merit :} \qquad Z = \frac{\sigma S^2}{\kappa}$$

σ electric conductivity

S Seebeck coefficient (thermopower)

κ thermal conductivity

A proper simulation of the interaction with the heat baths: Langevin dynamics

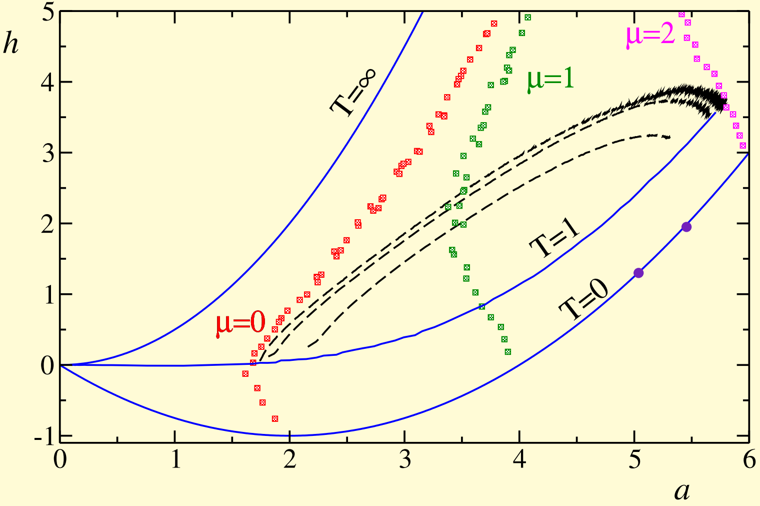
$$i\dot{z}_n = (1+i\gamma)\left[-2|z_n|^2 z_n - z_{n+1} - z_{n-1}\right] + i\gamma\mu z_n + \sqrt{\gamma T}\,\xi_n(t)$$

$\xi_n(t) = \xi_n' + i\xi_n''$

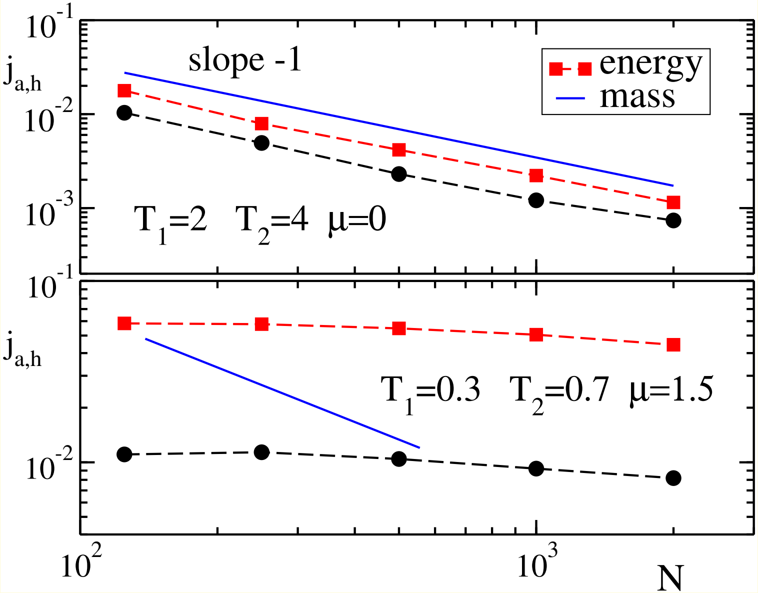
$$\begin{aligned}
\dot{p}_n &= -\frac{\partial H}{\partial q_n} - \gamma\frac{\partial H_\mu}{\partial p_n} + \sqrt{2\gamma T}\xi_n'(t) \\
\dot{q}_n &= \frac{\partial H}{\partial p_n} - \gamma\frac{\partial H_\mu}{\partial q_n} + \sqrt{2\gamma T}\xi_n''(t)
\end{aligned}$$

H_μ is the effective Hamiltonian $H_\mu = H - \mu A$

Nonequilibrium steady states



Scaling of the fluxes



Continuum limit: Onsager matrix

$$j_a = -L_{aa}\frac{d(\beta\mu)}{dy} + L_{ah}\frac{d\beta}{dy}$$

$$j_h = -L_{ha}\frac{d(\beta\mu)}{dy} + L_{hh}\frac{d\beta}{dy}$$

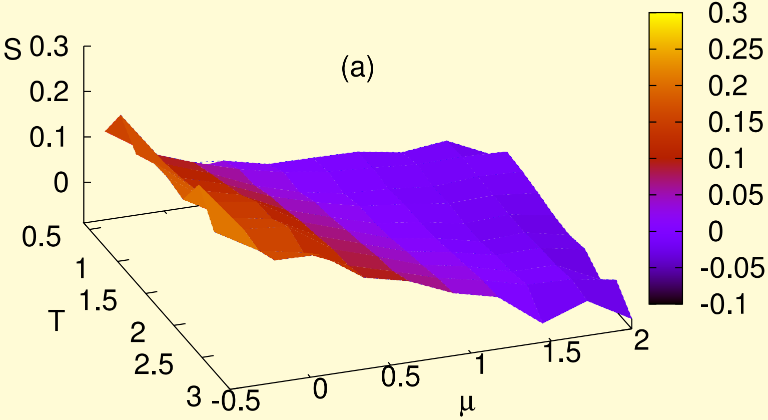
$$y = j/n$$

Particle and thermal conductivity: σ, κ

$$\sigma = \beta L_{aa}; \quad \kappa = \beta^2 \frac{L_{aa}L_{hh} - L_{ha}^2}{L_{aa}}$$

Seebeck coefficient $S = \beta\left(\frac{L_{ha}}{L_{aa}} - \mu\right)$

Seebeck coefficient



The path in μ-T (a, h) plane

$$\mathbf{J} = \mathbf{A}(\mu, T)\frac{d\mathbf{v}}{dy}$$

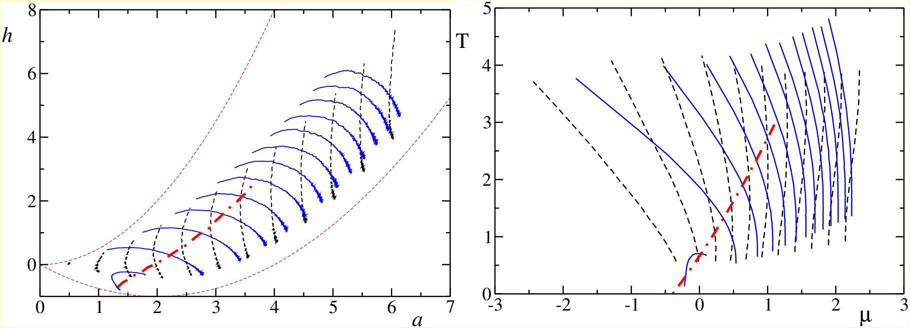
$$\mathbf{J} = (j_a, j_h) \qquad \mathbf{v} = (\mu, T)$$

$\mathbf{A}$ replaces the Onsager matrix

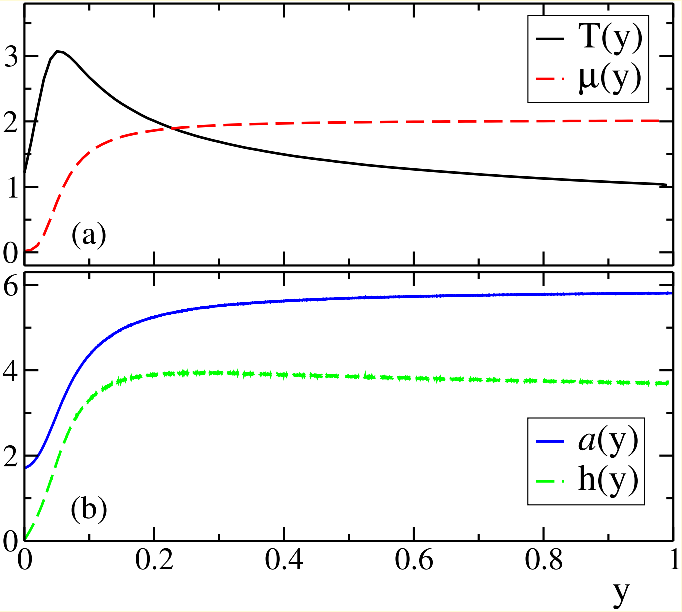
$$\frac{d\mu}{dy} = A^{-1}_{11} j_a + A^{-1}_{12} j_h \qquad \frac{dT}{dy} = A^{-1}_{21} j_a + A^{-1}_{22} j_h$$

$$\frac{dT}{d\mu} = \frac{A^{-1}_{21} + A^{-1}_{22} j_h/j_a}{A^{-1}_{11} + A^{-1}_{12} j_h/j_a}$$

Fix the ratio j_h/j_a and integrate from any point μ, T


h
a
T
μ
0
1
2
3
4
5
6
7
8
-3
-2
-1

Non-monotonous temperature profiles



A simple limit: large mass densities

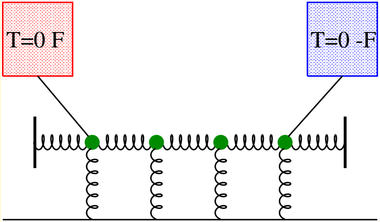
Decompose the variable z_n into λ_n and ϕ_n

$$z_n = \sqrt{a}(1 + \lambda_n/4a)\exp[i(2(a-1)t + \phi_n + n\pi)]$$

$$\begin{aligned} \dot{\phi}_n &= \lambda_n \\ \dot{\lambda}_n &= 4a\left[\sin(\phi_{n+1} - \phi_n) - \sin(\phi_n - \phi_{n-1})\right] - \gamma'(\lambda_n - \delta\mu) + \sqrt{4\gamma T}\xi_n \end{aligned}$$

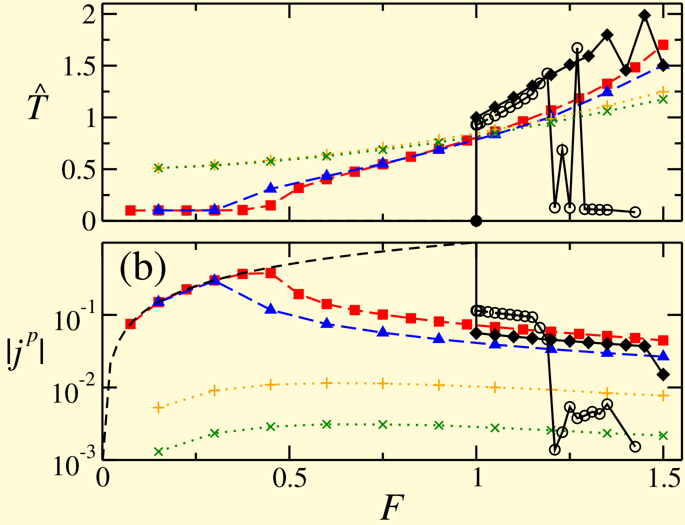
$$\mathcal{H}_{XY} = \sum_n \frac{\lambda_n^2}{2} - \sum_n 4a\cos(\phi_{n+1} - \phi_n)$$

Equivalent problem in a chain of oscillators

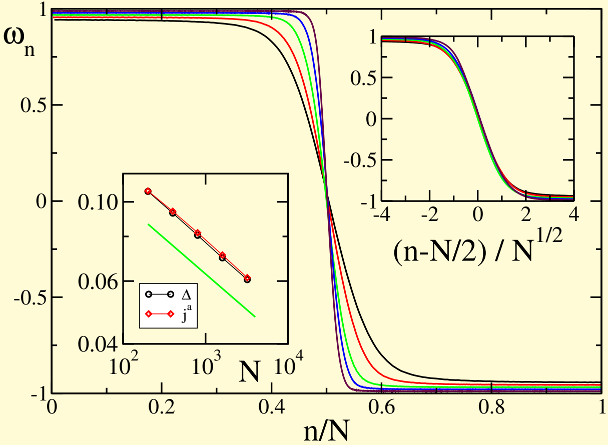


Zero temperature and a fixed torsion

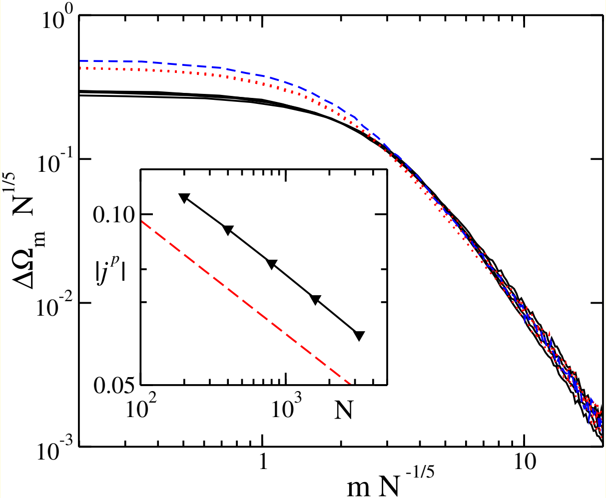
The XY model: a first nonequilibrium phase transition



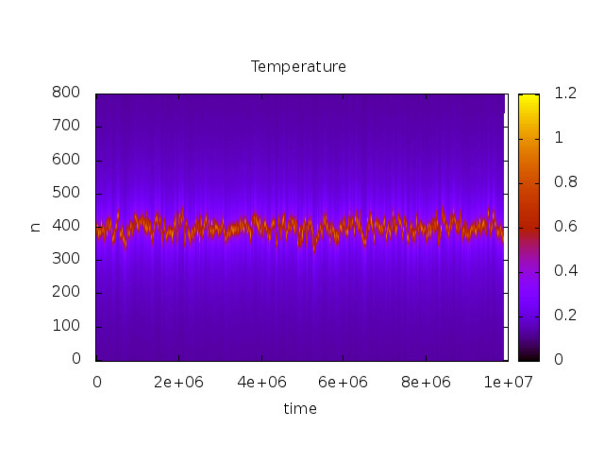
Frequency profile



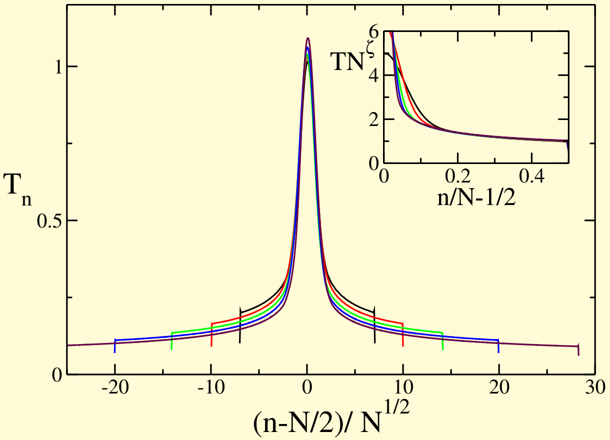
Frequency gradient



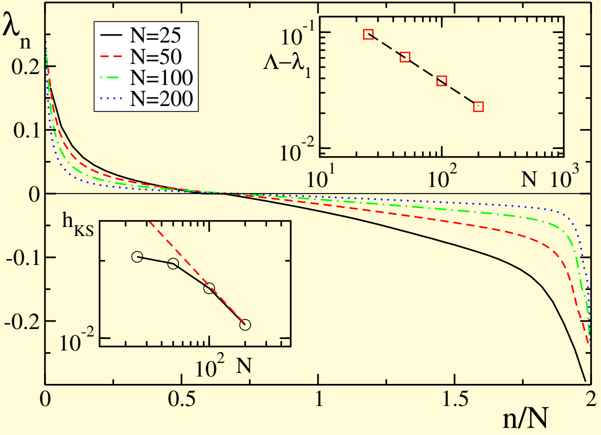
Space-time pattern



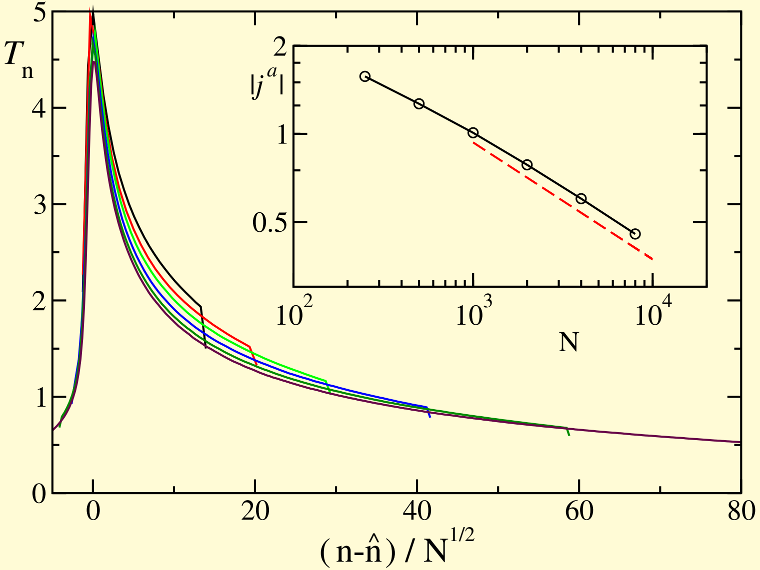
Temperature profile



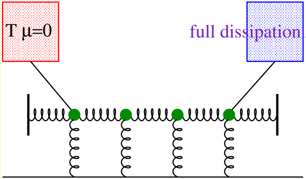
Lyapunov exponents

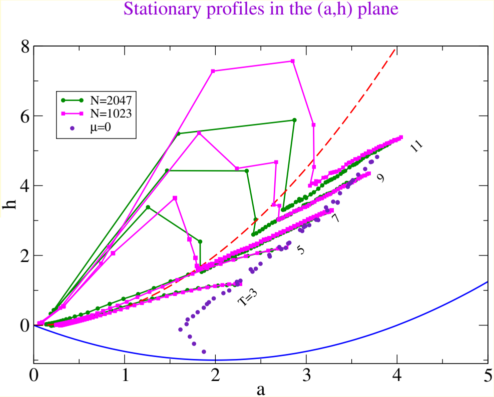


Back to DNLS dynamics

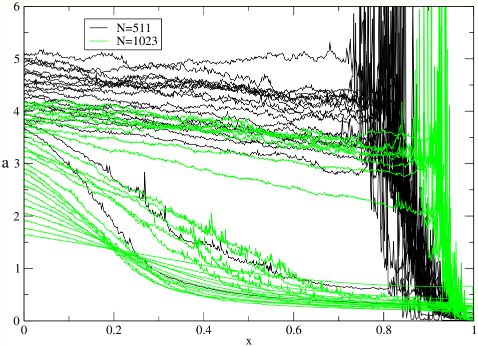


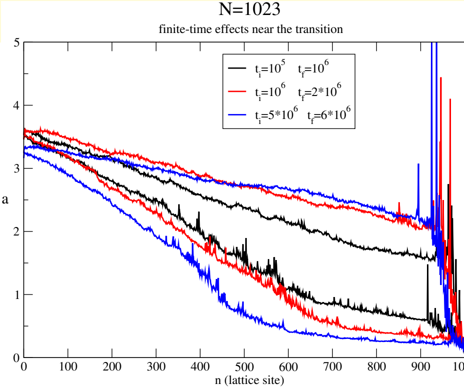
Negative temperatures and a second transition



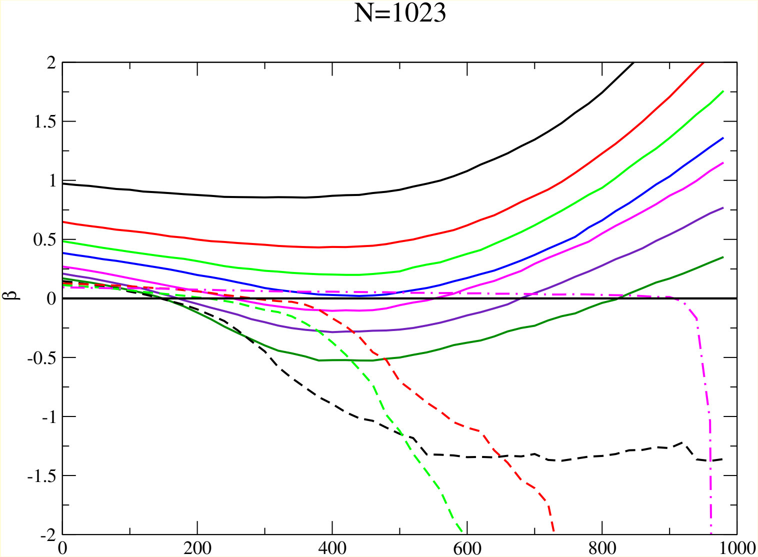


A transition in the transport properties





Inverse temperature profiles



Hysteretic phenomena