Dynamical properties of the DNLS

A brief account of some earlier works related to NTS

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Main focus of this talk:

For which kinds of initial spatially *extended states* can we expect spontaneous formation of *persistent localized modes* in a Hamiltonian lattice after long times?

Answer connected to *statistical-mechanics* description of the model and "negative-temperature-like" behaviour (at least transient).

Disclaimer: This talk is a minor update of talks from **2001-2006**, many contributions from the last decade are certainly missing! Hopefully provided by other speakers!

The Discrete Nonlinear Schrödinger (DNLS) equation:

(1D, general power-law nonlinearity)

$$i\dot{\psi}_m + C(\psi_{m+1} + \psi_{m-1}) + |\psi_m|^{2\sigma}\psi_m = 0.$$

Assume $\sigma > 0$ and $C > 0$. ($C < 0 \Leftrightarrow \psi_m \to (-1)^m \psi_m$)

$\sigma = 1$: cubic DNLS with many well-known applications, e.g.:

- Describes *generically* small-amplitude dynamics of weakly coupled anharmonic oscillators ("Klein-Gordon lattice")
- Nonlinear optics: Discrete spatial solitons in waveguide arrays
- Bose-Einstein condensates (BECs) in optical lattices

Two motivations for studying $\sigma \neq 1$:

- There is an excitation threshold for creation of localized excitations when $\sigma D \geq 2$.
  (Flach et al, PRL 78, 1207 (1997))
- Modelling BECs in optical lattices, $0 < \sigma < 1$ may account for dimensionality of the condensates *in each well*.
  (Smerzi/Trombettoni, Chaos **13**, 766 (2003); Anker et al., PRL **94**, 020403 (2005))

Some basic properties of the DNLS equation

2 conserved quantities:

- Hamiltonian (energy): $\mathcal{H} = \sum_m \left[C(\psi_m \psi_{m+1}^* + \psi_m^* \psi_{m+1}) + \frac{|\psi_m|^{2\sigma+2}}{\sigma+1} \right]$

- Excitation number (norm, power, number of particles,...): $\mathcal{A} = \sum_m |\psi_m|^2$

In action-angle variables, $\psi_m = \sqrt{A_m} e^{i\phi_m}$:

$$\mathcal{H} = \sum_{m=1}^{N} \left(2C\sqrt{A_m A_{m+1}} \cos(\phi_m - \phi_{m+1}) + \frac{A_m^{\sigma+1}}{\sigma+1} \right), \mathcal{A} = \sum_{m=1}^{N} A_m .$$

For extended solutions, use intensive quantities: $h = \frac{\mathcal{H}}{N}; a = \frac{\mathcal{A}}{N}$

- One can prove, that a staggered ($q = \pi$) stationary plane wave:

$\psi_m^{(min)} = \sqrt{a} e^{im\pi} e^{i\Lambda t}$ minimizes h at fixed a: $h^{(min)} = -2Ca + \frac{a^{\sigma+1}}{\sigma+1}$

(Global min for $a^{(min)} = (2C)^{\frac{1}{\sigma}}$)

Trivial remark:
The Hamiltonian could equally well be defined with opposite sign, turning the min into a max...

Few words about DNLS statistics

(expect more from next speaker(s)!)

Treating $\mathcal{A}$ as particle number in grand canonical ensemble and using equilibrium Gibbsian statistical mechanics leads to a division of available (h, a)-space into two parts:

(Rasmussen et al., PRL **84**, 3740 (2000), Johansson/Rasmussen, PRE**70**, 066610 (2004))

- 'Normal' regime $h < h^{(c)}$: Typical initial conditions

expected to thermalize with Gibbsian distribution at temperature $T = 1/\beta$ and chemical potential μ.

Exponentially small probabilities for large-amplitude excitations.

- 'Anomalous' regime $h > h^{(c)}$:

Formation of localized structures!

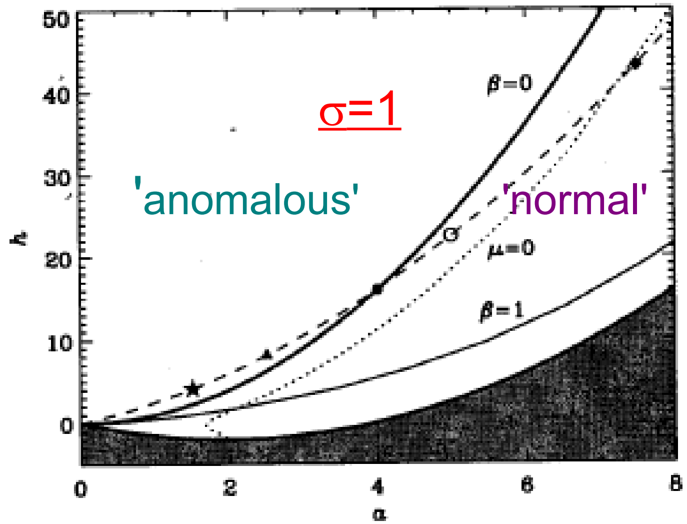


FIG. 1. Parameter space (a, h), where the shaded area is inaccessible. The thick lines represent the $\beta = \infty$ $(T = 0)$ and $\beta = 0$ $(T = \infty)$ lines and thus bound the Gibbsian regime. The dashed line represents the $h = 2a + \frac{\nu}{2}a^2$ line along which the reported numerical simulations are performed (pointed by the symbols).

Transition line can be calculated exactly as infinite-temperature line $\beta = 0$: $h = h^{(c)}(a;\sigma) \equiv \Gamma(\sigma+1)a^{\sigma+1}$

Connection between 'anomalous' regime and negative temperatures:
In *microcanonical ensemble* (fixed $\mathcal{A}$), a localized stationary 'breather' uniquely *maximizes* $\mathcal{H}$.
Localizes essentially at one site for large $\mathcal{A}$, with $\mathcal{H}^{(max)} \simeq \frac{\mathcal{A}^{\sigma+1}}{\sigma+1}$ (Weinstein, Nonlinearity **12**, 673 (1999))

Entropy decrease ↔ Negative T (but not trivial to extend to grand canonical ensemble!)

Examples of dynamics in the different regimes

1. Homogeneous travelling waves: $\psi_m = \sqrt{a}e^{iqm}e^{i\Lambda t}$

$$\Rightarrow \quad h = 2Ca\cos q + \frac{a^{\sigma+1}}{\sigma+1}.$$

Modulationally unstable for $|q| < \pi/2$

(e.g. Smerzi/Trombettoni, Chaos **13**, 766 (2003))

Transition at $h = h^{(c)}$ yields critical amplitude:

$$a^{(c)} = \left[\frac{2(\sigma+1)C\cos q}{\Gamma(\sigma+2)-1}\right]^{\frac{1}{\sigma}}$$

Formation of persistent localized modes expected when

$$|q| < \pi/2 \quad \text{and} \quad a < a^{(c)}(q;\sigma).$$

σ=1, a=0.09

q=0:

$q=\pi/2$

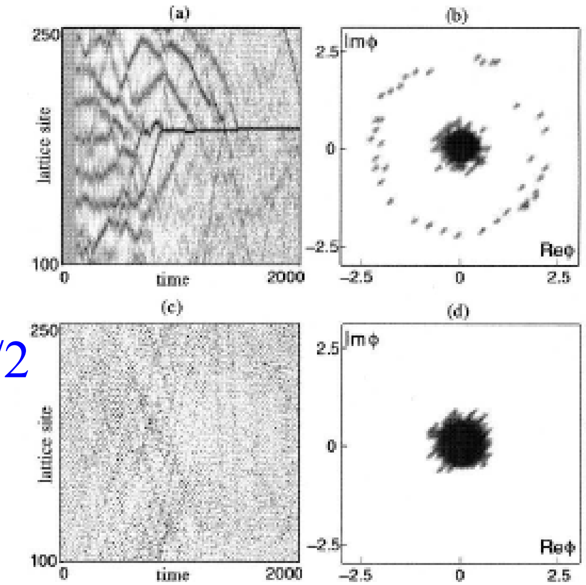


FIG. 1. Numerical integration of the DNLS with 4096 oscillators. The initial conditions are waves with the amplitude $\phi_n=0.3$ and the wave number $k=0$ for (a), (b), and with $k=\pi/2$ for (c), (d). (a) and (c) show the spatiotemporal patterns of high-amplitude states (dark gray) in a small sector of the chain for the first 2000 time steps. (b) and (d) show the distributions of ϕ after 2×10^5 time steps.

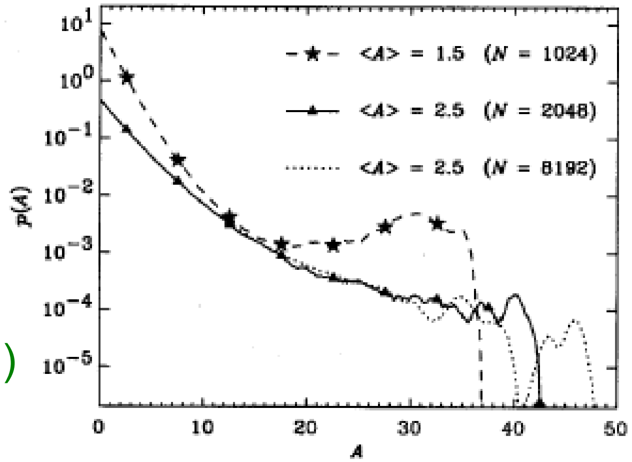
(Rumpf, PRE **69**, 016618 (2004))

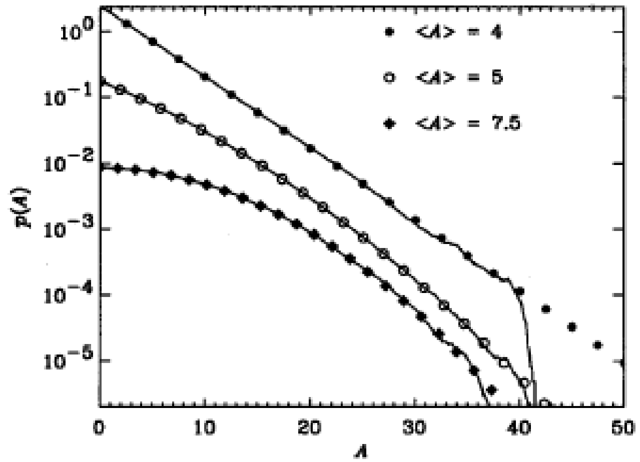
Note separation into small-amplitude 'fluctuations' and large-amplitude 'breathers' for small a and q.

Amplitude distributions for increasing a: $(q = 0,\ \sigma = 1)$

Note change from positive to negative curvature when entering 'normal' regime!

Rasmussen et al, PRL **84**, 3740 (2000)

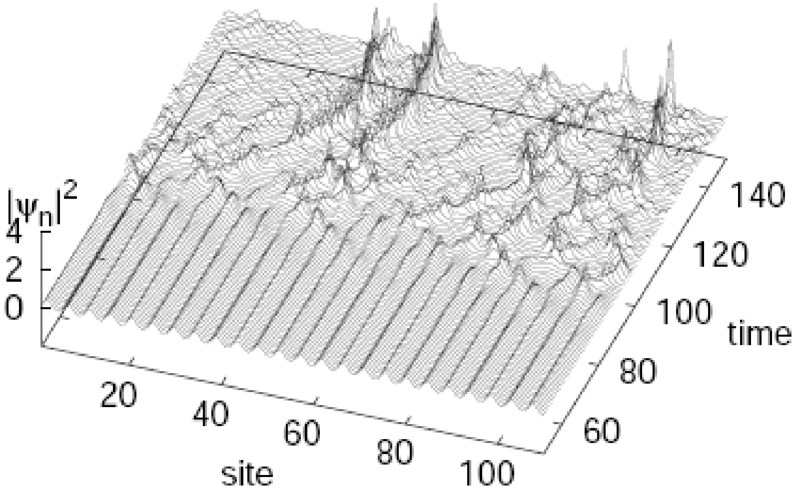


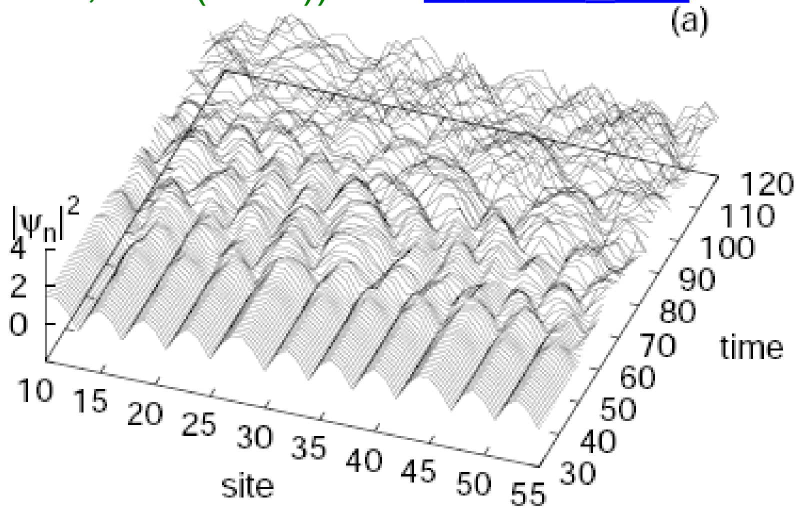


More examples of dynamics from specific initial conditions

2. Non-homogeneous *standing* waves: Time-periodic *non-propagating* exact solutions, periodic or quasiperiodic in space with wave vector Q. (Morgante et al., PRL **85**, 550 (2000))

$\sigma = 1$: $Q = 12\pi/55$ (Johansson et al., EPJ B **29**, 279 (2002)) $Q = 68\pi/89$





Specifically: Simple expression for $Q=\pi/2$: ('period-doubled states')

$$\psi_{2n+1} = 0, \psi_{2n+2} = (-1)^n \sqrt{2a} e^{i(2a)^\sigma t}; \qquad h = \frac{2^\sigma}{\sigma+1} a^{\sigma+1}$$

$\sigma = 1$: Solution family coincides with transition line from 'normal' to 'anomalous' regime!

$0 < \sigma < 1$: Always in 'anomalous' regime

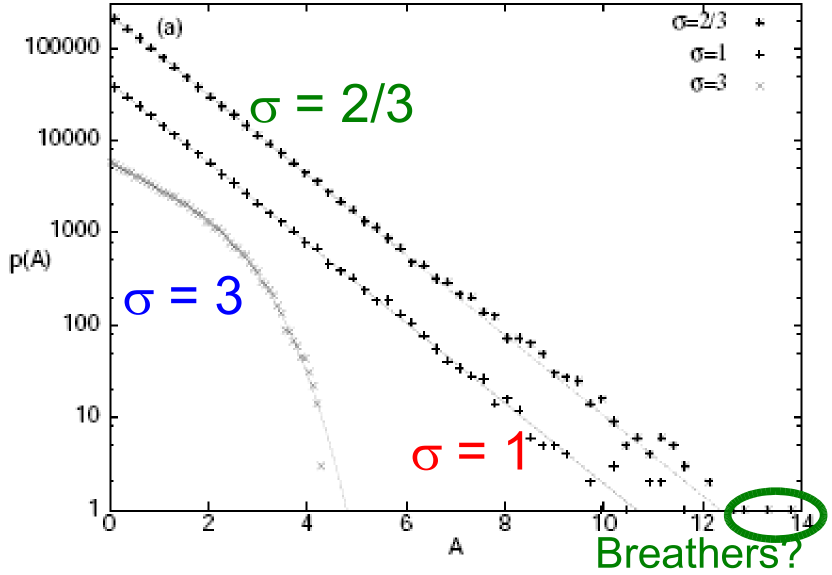
$\sigma > 1$: Always in 'normal' regime

Numerical integration of unstable $Q=\pi/2$ standing waves

Large-temperature predictions for equilibrium amplitude distribution:

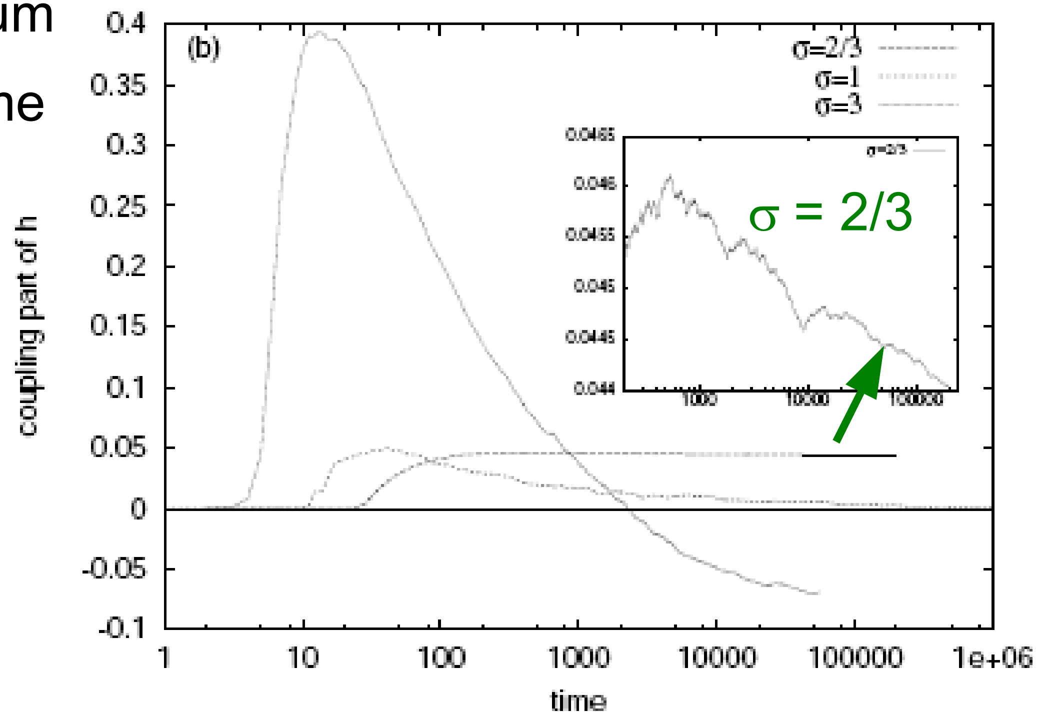
$$T < \infty: \log p(A) \sim -\gamma A - \beta \frac{A^{\sigma+1}}{\sigma+1}$$

$$T = \infty: \log p(A) \sim -\frac{A}{a}$$



Note that the approach to a (possible) equilibrium state is extremely slow in the 'anomalous' regime

$$\langle 2C\sqrt{A_m A_{m+1}} \cos(\phi_m - \phi_{m+1}) \rangle$$



(Johansson/Rasmussen, PRE **70**, 066610 (2004))

Generalizations: higher D

Ex. Plane wave in 2D:

$$a^{(c)} = \left[\frac{2(\sigma+1)C(\cos q_x + \cos q_y)}{\Gamma(\sigma+2)-1}\right]^{\frac{1}{\sigma}}$$

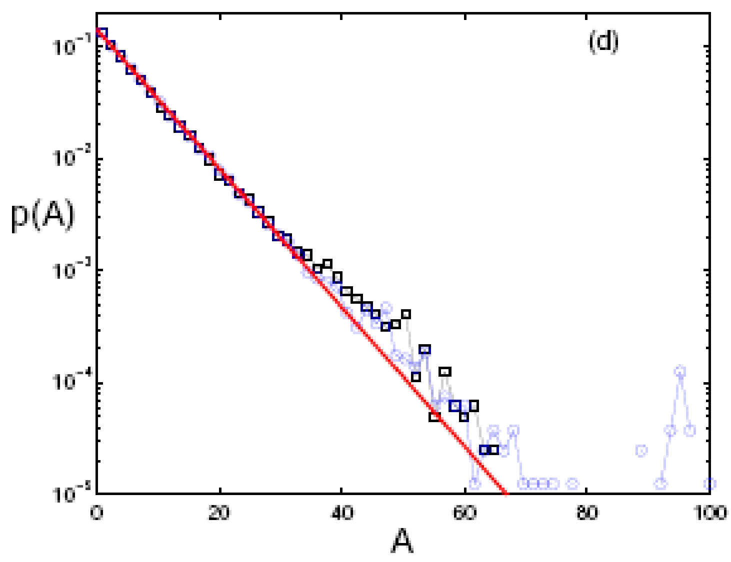
$q = 0,\ \sigma = 1:\quad a^{(c)} = 8C$

$a = 7$ (in 'anomalous regime'):

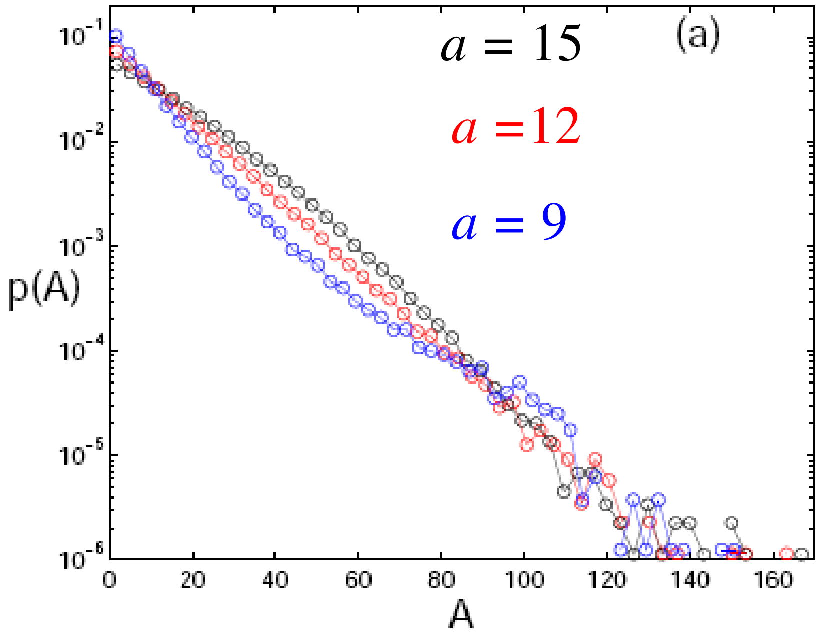
Again discontinuous distribution after 'long enough' times!

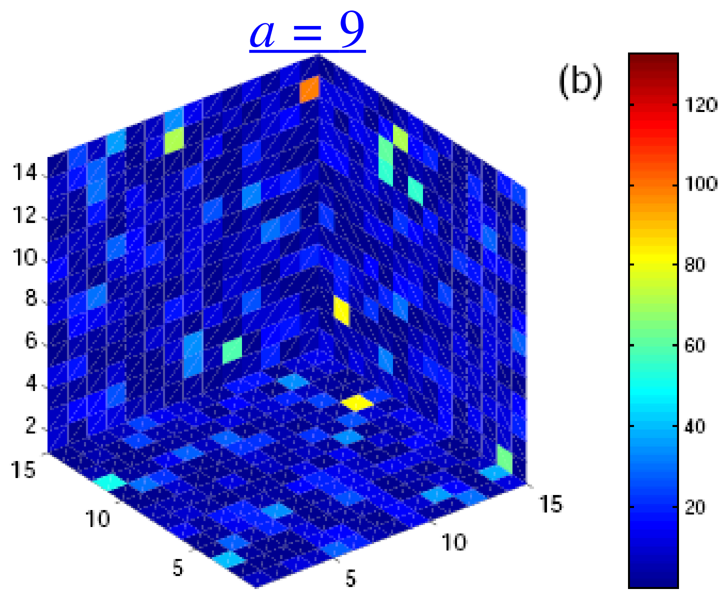
Low-amplitude part: phonon bath at $T = \infty$

High-amplitude part: breathers with increasing amplitude



Ex. Constant-amplitude state in 3D: Critical amplitude $a = 12C$



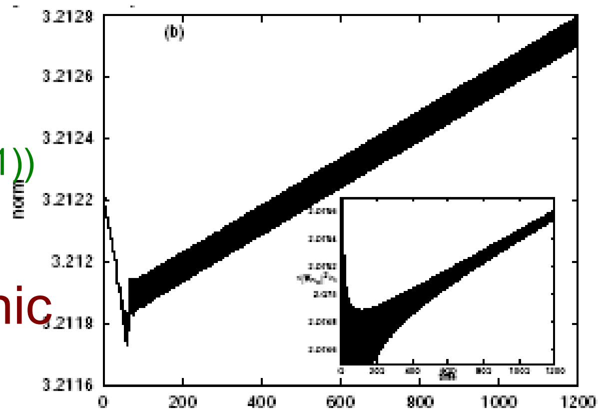


(Johansson/Rasmussen, PRE **70**, 066610 (2004))

Few words about breather-phonon interactions (1D, $\sigma = 1$)

Observation: Pinned breathers seemingly grow only to a certain limit size! Why...?

Possible answer from analysis of fundamental inelastic breather-phonon scattering processes to 2nd order in phonon amplitude.

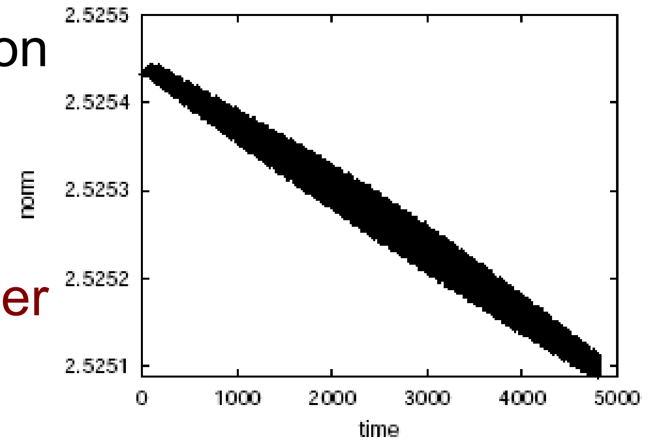


(Breathers are linearly stable, and 1st order scattering is always elastic)

Main results: (Johansson/Aubry, PRE **61,** 5864 (2000), Johansson, PRE **63**, 037601 (2001))

(i) Interaction with single phonon mode may only yield breather growth, and only for wavevectors $q < q_c$ when also second-harmonic is inside phonon band!

(ii) Breather decay requires simultaneous excitation of two phonon modes, with frequency difference inside phonon band.



Interpretation: Scattering towards higher frequencies decreases the energy $\mathcal{H}$ in phonon part, and surplus is absorbed by breather growth (correspondingly decay for lower frequencies)

Important remark: All 2nd order inelastic processes vanish for large breathers ($q_c \to 0$)

$\Rightarrow$ Only higher-order interactions may affect breathers larger than a threshold, corresponding to a peak power $|\psi_{n_0}|^2 \gtrsim 5.\dot{6}\dot{5}$.

More generalizations: inter-site nonlinearities

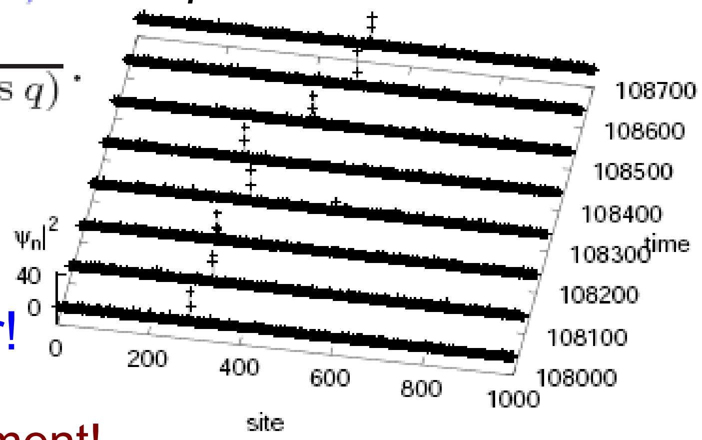
$$
\begin{aligned}
&\mathrm{i}\dot{\psi}_n + C(\psi_{n+1}+\psi_{n-1}) + |\psi_n|^2\psi_n \\
&+Q\left[2\psi_n(|\psi_{n+1}|^2+|\psi_{n-1}|^2) + \psi_n^*(\psi_{n+1}^2+\psi_{n-1}^2) + 2|\psi_n|^2(\psi_{n+1}+\psi_{n-1})\right. \\
&\left. +\psi_n^2(\psi_{n+1}^*+\psi_{n-1}^*) + |\psi_{n+1}|^2\psi_{n+1} + |\psi_{n-1}|^2\psi_{n-1}\right] = 0.
\end{aligned}
$$

(several motivations for 'peculiar' inter-site part: 'rotating-wave' approximation for FPU-chain, optical waveguides embedded in nonlinear medium, correlated tunneling of bosons,...)
(Johansson, Physica D **216**, 62 (2006))

Parameter Q, $0 \le Q \le 1/2$, measures relative strength of intersite anharmonicity.

Only minor changes in phase diagram: $h^{(c)}(a;Q) \equiv (2Q+1)a^2$ for β=0 line

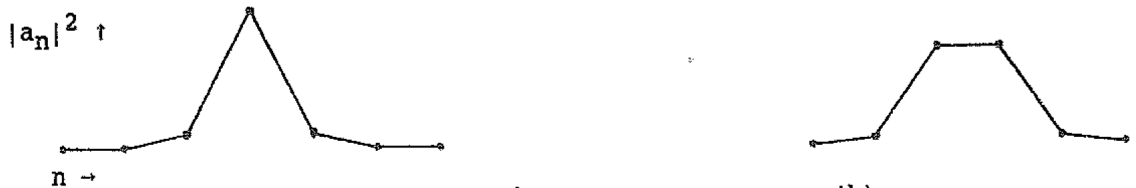
Critical amplitude for plane wave: $a^{(c)} \equiv \frac{4C\cos q}{1+2Q(1-2\cos^2 q-4\cos q)}$.



Major change in the resulting dynamics in the 'anomalous' regime for larger Q: (Q = 0.5 here)

Single remaining, randomly *moving* large-amplitude breather!

Inter-site nonlinearities decrease 'Peierls-Nabarro' barrier for movement!



(a) Fig. 4. (b)

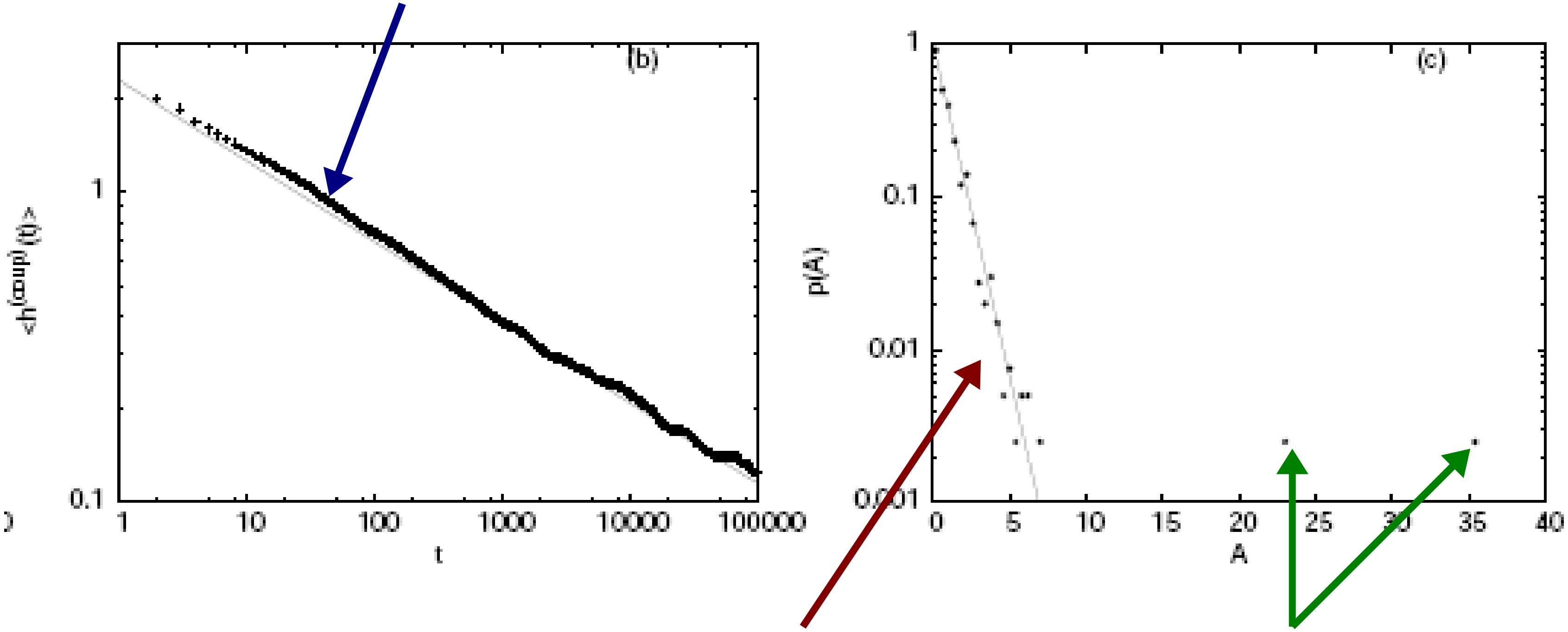
Minimum energy needed for translation one lattice-site. (J.C. Eilbeck, 1986)

Inter-site nonlinearities, continued

Effect: Evolution towards equilibrium in 'anomalous' regime much faster!

$\langle 2C\sqrt{A_m A_{m+1}}\cos(\phi_m - \phi_{m+1})\rangle \rightarrow 0$:

no phase-correlations between sites in infinite-temperature phonon bath.

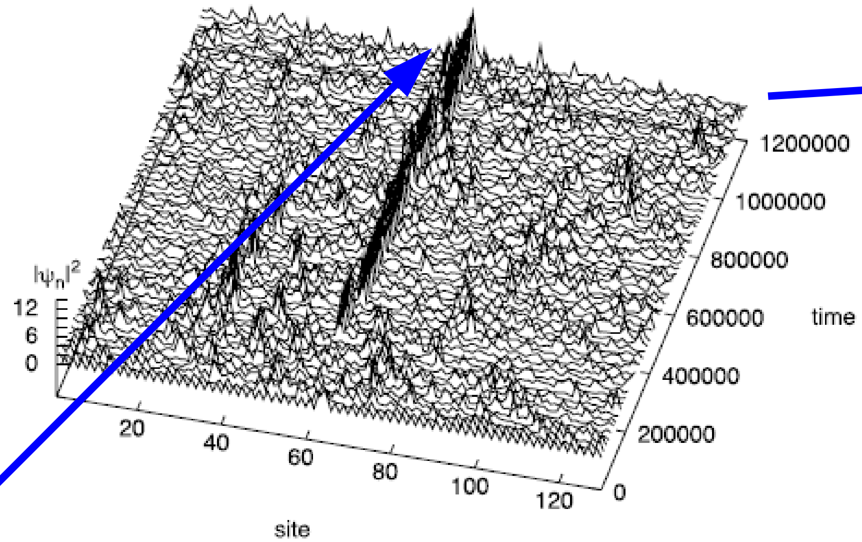


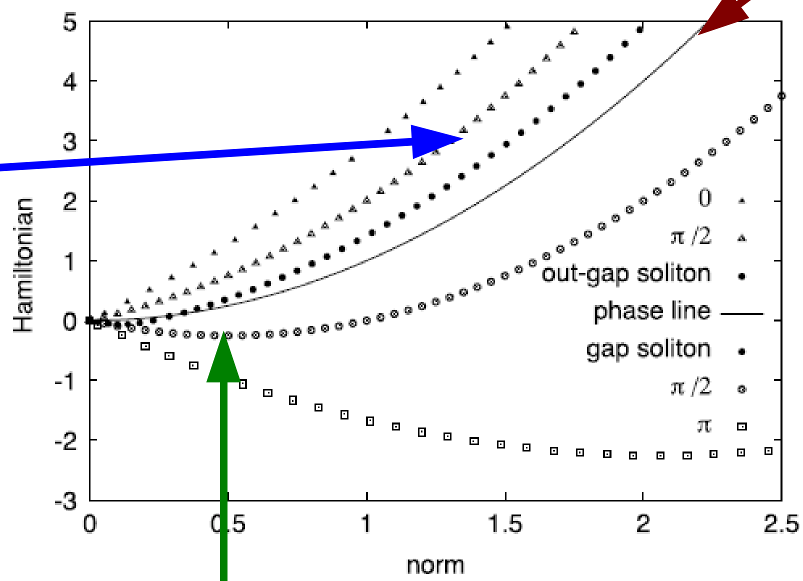
Amplitude distribution separates: $T = \infty$ prediction; 2 neighboring breather sites

...and one more generalization: Binary modulated on-site potential

$$i\frac{d\psi_n}{dt} = V_n\psi_n - \varepsilon(\psi_{n+1} + \psi_{n-1}) - |\psi_n|^2\psi_n$$

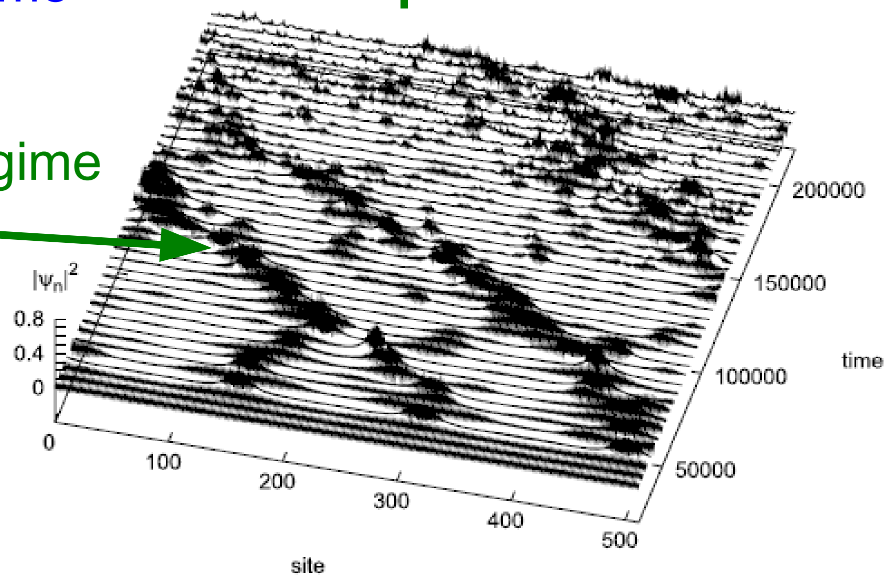
$T = \infty$ line





Persistent breather created in 'anomalous' regime

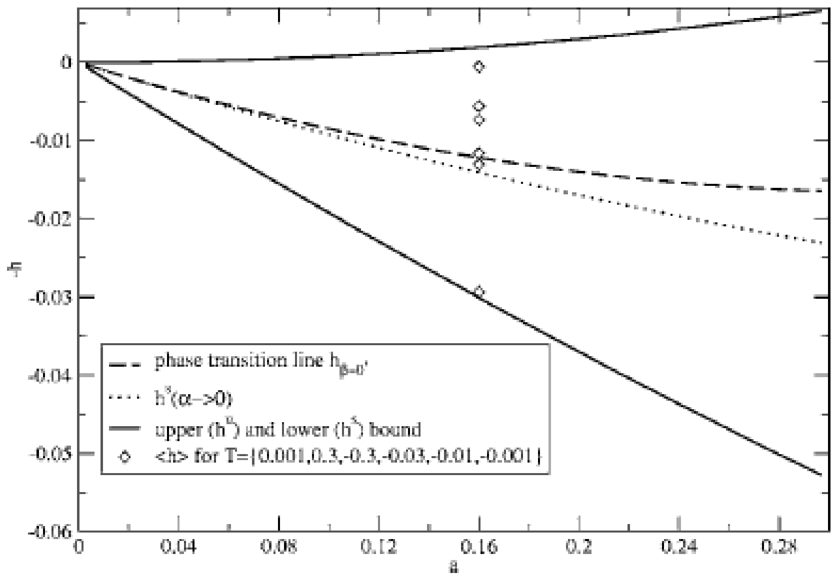
Metastable 'gap solitons' created in 'normal' regime

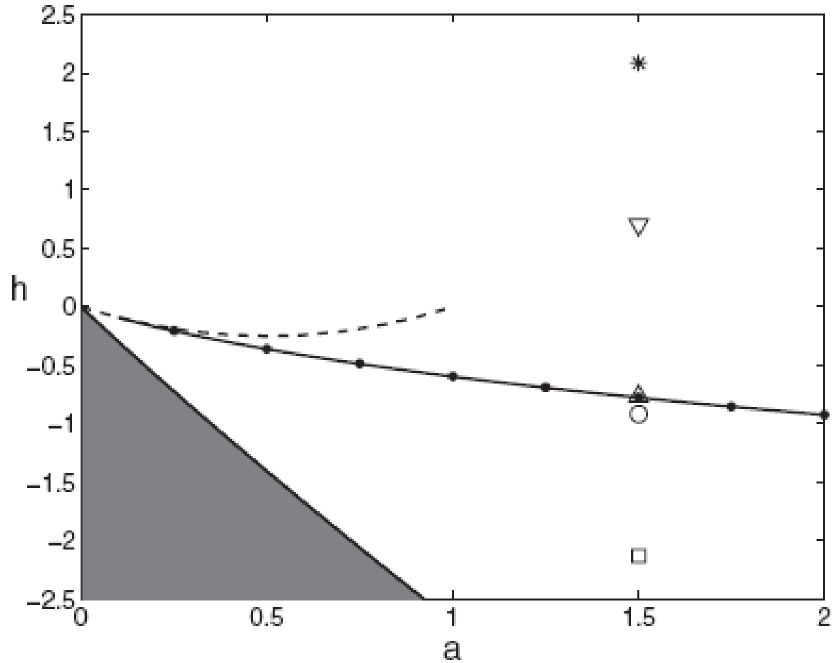


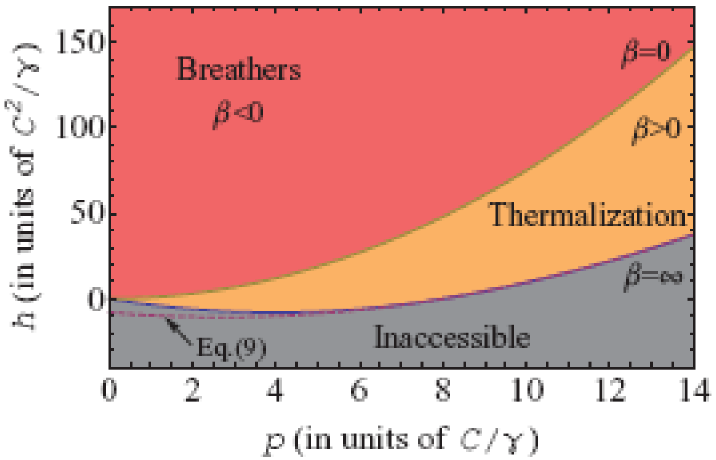
(Kroon et al. Physica D **239**, 269 (2010))

...and just mentioning few other generalizations I am aware of...

- Brunhuber et al., PRE **73**, 056610 (2006): **Long-range** dispersive interactions
- Samuelsen et al., PRE **87**, 049901 (2013): **Saturable** nonlinearity;
- Derevyanko, PRA **88**, 033851 (2013): Two coupled fields with **four-wave mixing**







Concluding remarks and perspectives (as of 2004-2006!):

- The statistical mechanics description yields explicit necessary conditions for formation of persistent localized modes, in terms of average values of the two conserved quantities Hamiltonian and Norm.

- The approach approximately describes situations with non-conserved but slowly varying quantities, e.g. explains formation of long-lived breathers from thermal equilibrium in weakly coupled Klein-Gordon chains.

- In contrast to the condition for existence of an energy threshold for creation of a single breather, σ and D work in opposite directions for the statistical localization transition. The energy threshold affects the approach to equilibrium, not the nature of the equilibrium state.

- For pure on-site nonlinearities the created localized excitations are typically pinned to particular lattice sites, while for significant inter-site nonlinearities they become mobile and merge into one.

Some open(?) issues (as of 2004-2006!):

- Can localization transition be experimentally observed with BEC's in optical lattices, or with optical waveguide arrays??

- Can the hypothesis of separation of phase space in low-amplitude 'fluctuations' and high-amplitude 'breathers' in the equilibrium state be put on more rigorous ground, also for large α?

- What determines the time-scales for approach to equilibrium in breather-forming regime? Are equilibrium states physically relevant, if they can only be reached after t $\sim 10^{60}$...?