Statistical mechanics of general discrete nonlinear Schrödinger models: Localization transition and its relevance for Klein-Gordon lattices

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

Answer requires a *statistical-mechanics* description of the model.

(Rasmussen et al., PRL **84**, 3740 (2000); Rumpf, PRE **69**, 016618 (2004), for 1D DNLS)

Here: Extend to general DNLS models, higher dimensions + connection to Klein-Gordon models

A: 1D General Discrete Nonlinear Schrödinger (DNLS) equation :

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

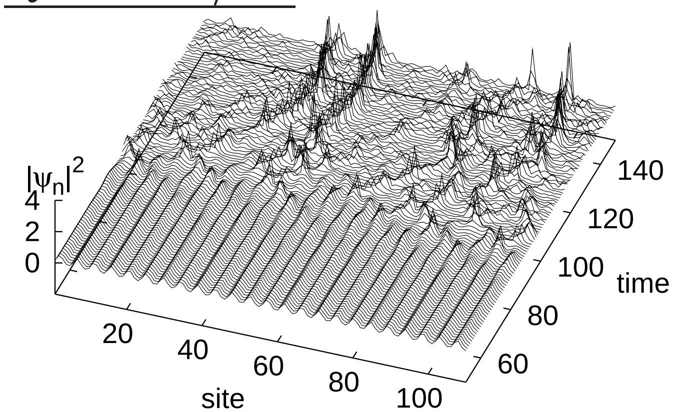
Let $\sigma > 0$ and $C > 0$. ($C < 0 \Leftrightarrow \psi_m \to (-1)^m \psi_m$)

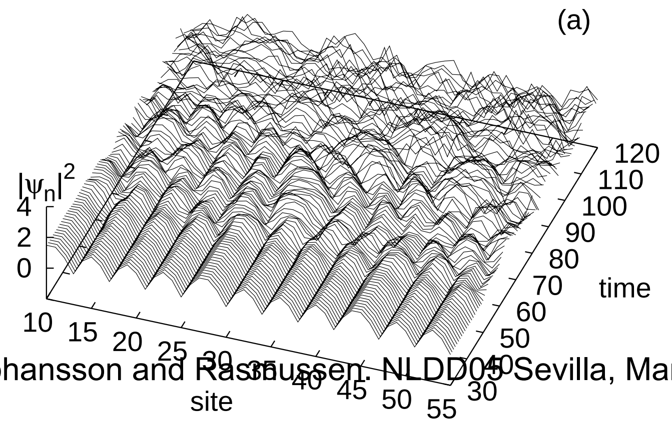
$\sigma = 1$: cubic DNLS with many well-known applications, e.g.:

- Describes *generically* slow small-amplitude dynamics of weakly coupled anharmonic oscillators (e.g. Kivshar, Phys. Lett. **173**, 172 (1993)).
- Nonlinear optics: Discrete spatial solitons in waveguide arrays. (e.g. Sukhorukov et al. IEEE J. Quantum Electron. **39**, 31 (2003))
- Coupled Bose-Einstein condensates (BECs), e.g. in external periodic potentials. (e.g. Smerzi/Trombettoni, Chaos **13**, 766 (2003))

Example: Nonlinear standing-wave phonons in DNLS

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





Two main motivations to study $\sigma \neq 1$:

• Some effects of higher dimensionality captured in 1D models with $\sigma = 2$ or $\sigma = 3$. E.g., there is an *excitation threshold* for creation of localized excitations when $\sigma D \geq 2$. (Flach et al., PRL **78**, 1207 (1997))

• For BECs in optical lattices, 1D DNLS models with $0 < \sigma < 1$ may account for dimensionality of the condensates *in each well*: $\sigma = 2/(2+d)$, for $d = 0, 1, 2,$ or 3. (Smerzi/Trombettoni, Chaos **13**, 766 (2003))

The DNLS equation has 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,...):

$$\mathcal{A} = \sum_m |\psi_m|^2.$$

Canonical transformation $\psi_m = \sqrt{A_m} e^{i\phi_m}$ (action-angle variables) :

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

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

• Staggered ($q=\pi$) stationary plane wave $\psi_m^{(min)} = \sqrt{a}e^{im\pi}e^{i\Lambda t}$ (with $\Lambda = -2C + a^\sigma$) *minimizes h at fixed a* for all σ:
$h^{(min)} = -2Ca + \frac{a^{\sigma+1}}{\sigma+1}$ (Global min for $a^{(min)} = (2C)^{\frac{1}{\sigma}}$.)

To predict macroscopic average values in the thermodynamic limit ($N \to \infty$), we use standard Gibbsian statistical mechanics.

$\mathcal{A} \leftrightarrow$ 'number of particles' in grand-canonical ensemble

Grand-canonical partition function:

$$\mathcal{Z} = \int_0^\infty \int_0^{2\pi} \prod_{m=1}^{N} d\phi_m dA_m e^{-\beta(\mathcal{H}+\mu\mathcal{A})}$$

$\beta \equiv 1/T \leftrightarrow$ 'inverse temperature'

$\mu \leftrightarrow$ 'chemical potential'

Integrating over the phase variables ϕ_m yields

$$\mathcal{Z} = (2\pi)^N \int_0^\infty \prod_m dA_m I_0(2\beta C\sqrt{A_m A_{m+1}})e^{-\beta A_m\left(\frac{A_m^\sigma}{\sigma+1}+\mu\right)},$$

with $I_0(z)$ modified Bessel function of first kind.

Possible to use 'transfer integral operator' to obtain (numerically) thermodynamic quantities for $N \to \infty$, with 1-1 correspondance between a regime in (a, h)-space and well-defined μ and $\beta > 0$.

But this regime is *bounded* by 'infinite-temperature' line $\beta = 0$, and does not cover all phase-space!

Line $\beta = 0$ associated with singularity of partition function, signalling transition into phase of *formation of localized structures*.

(For $\beta < 0$ and finite μ the probability density $e^{-\beta A_m \left(\frac{A_m^\sigma}{\sigma+1}+\mu\right)}$ would favour large A_m. But then integral diverges for $\mathcal{A} \to \infty$...)

We can obtain analytic expressions for thermodynamic expectation values of h and a close to $\beta \to 0^+$ by approximating $I_0 \approx 1$. (equivalent to $C \to 0$; 'thermalized independent units')

Close to limit $\beta \to 0, \mu \to \infty$ with $\beta\mu \equiv \gamma$ constant, we obtain:

$$\frac{1}{N} \ln \mathcal{Z} \simeq \ln(2\pi) - \ln(\beta\mu) - \frac{\beta\Gamma(\sigma+1)}{(\beta\mu)^{\sigma+1}},$$

with $\Gamma(\sigma+1) = \sigma!$ for integer σ;

$$h = \frac{1}{N}\left(\frac{\mu}{\beta}\frac{\partial}{\partial\mu} - \frac{\partial}{\partial\beta}\right)\ln \mathcal{Z} \simeq \frac{\Gamma(\sigma+1)}{(\beta\mu)^{\sigma+1}},\ a = -\frac{1}{N\beta}\frac{\partial \ln \mathcal{Z}}{\partial\mu} \simeq \frac{1}{\beta\mu}$$

$\because h = h^{(c)}(a;\sigma) \equiv \Gamma(\sigma+1)a^{\sigma+1}$ defines relation between energy and number densities at transition-line $\beta = 0$!

Phase diagram for $\sigma = 1$ $(h^{(c)} = a^2)$ (Rasmussen et al, PRL **84**, 3740 (2000))

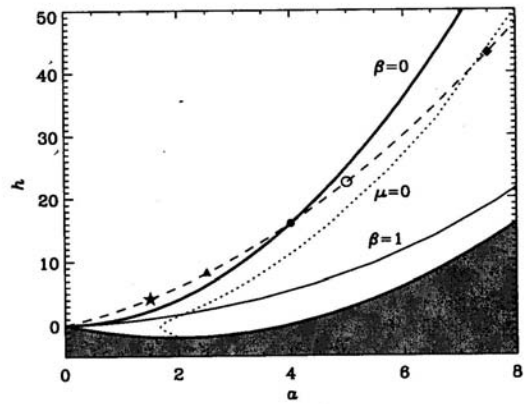


FIG. 1. Parameter space (a, h), where the shaded area is inaccessible. The thick lines represent the $\beta = \infty$ $(T = 0)$ and $\beta = 0$ $(T = \infty)$ lines and thus bound the Gibbsian regime. The dashed line represents the $h = 2a + \frac{\nu}{2}a^2$ line along which the reported numerical simulations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

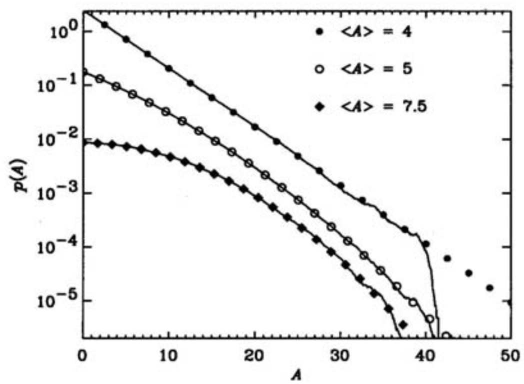


FIG. 2. Distribution of $A = |\psi|^2$ for three cases under (and on) the transition line. The solid lines show the results of simulations and the symbols are given by the transfer operator. Curves are vertically shifted to facilitate visualization.

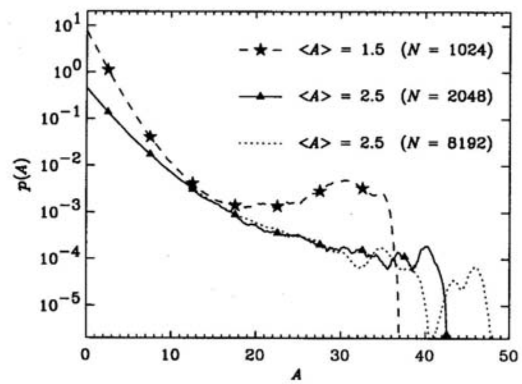


FIG. 3. Distribution of $A = |\psi|^2$ for parameters (h, a) above the transition line (triangles and stars as in Fig. 1. Dotted line indicates random initial condition). Note labels are arranged in order of increasing system size.

• 'Normal' regime $h < h^{(c)}$: Typical initial conditions thermalize according to Gibbsian equilibrium distribution at $\mu, \beta > 0$; $\log p(A_m) \sim -\gamma A_m - \beta A_m^{\sigma+1}/(\sigma+1),\ \beta \to 0$

• 'Anomalous' regime $h > h^{(c)}$: Typical distribution functions $p(A_m)$ for finite systems after long but finite integration times: Positive curvature favours creation of high-amplitude localized excitations!

Heuristic explanation for localization for $h > h^{(c)}$

At *fixed, finite* $\mathcal{A}$, a localized breather uniquely *maximizes* $\mathcal{H}$.

(e.g. Weinstein, Nonlinearity **12**, 673 (1999))

For large $\mathcal{A}$, it localizes essentially at one site, and $\mathcal{H}^{(max)} \simeq \frac{\mathcal{A}^{\sigma+1}}{\sigma+1}$.

In *microcanonical ensemble* (fixed $\mathcal{A}, \mathcal{H}$ and N) entropy (logarithm of number of microstates) is a well-defined function $S(\mathcal{H}, \mathcal{A}, N)$.

Varying $\mathcal{H}$, $S = 0$ for $\mathcal{H} = Nh^{(min)}(\mathcal{A}, N)$, increases towards its maximum when $\mathcal{H} = Nh^{(c)}$ (since $\beta \equiv \frac{\partial S}{\partial \mathcal{H}}|_{\mathcal{A},N} = 0$), and then again decreases towards zero at $\mathcal{H}^{(max)}(\mathcal{A})$.

$\because$ In microcanonical ensemble, temperature $T = \frac{1}{\beta}$ is well-defined, and $T < 0$ for $h > h^{(c)}$.

In grand-canonical ensemble, a part of the system with (microcanonical) $T < 0$ may increase its entropy by decreasing $\mathcal{H}$ at (almost) fixed $\mathcal{A}$. Can transfer superfluous energy into localized breathers, which absorb large $\mathcal{H}$ but only small $\mathcal{A}$!

('overheated' system with $T < 0$ 'cools itself off' by creating breathers as 'hot spots' of localized energy).

Proposed as general mechanism for energy localization in systems with two conserved quantities. (e.g. Rumpf/Newell, Physica D **184**, 162 (2003))

Used to explicitly calculate the thermodynamic properties of the DNLS model in limit of small a. (Rumpf, PRE **69**, 016618 (2004))

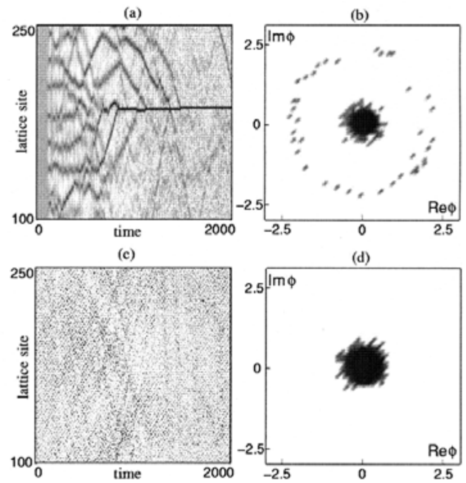


FIG. 1. Numerical integration of the DNLS with 4096 oscillators. The initial conditions are waves with the amplitude $\phi_n = 0.3$ and the wave number $k = 0$ for (a), (b), and with $k = \pi/2$ for (c), (d). (a) and (c) show the spatiotemporal patterns of high-amplitude states (dark gray) in a small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

(Phase space then naturally divides into a small-amplitude 'fluctuation' part and a large-amplitude 'breather' part which only interact weakly).

Yields equilibrium state maximizing total entropy for $h > h^{(c)}$ consisting of one single breather, with rest of the lattice at normal Gibbsian $T = \infty$ distribution.

Argument also valid for large a???

Localization transition for particular families of initial conditions

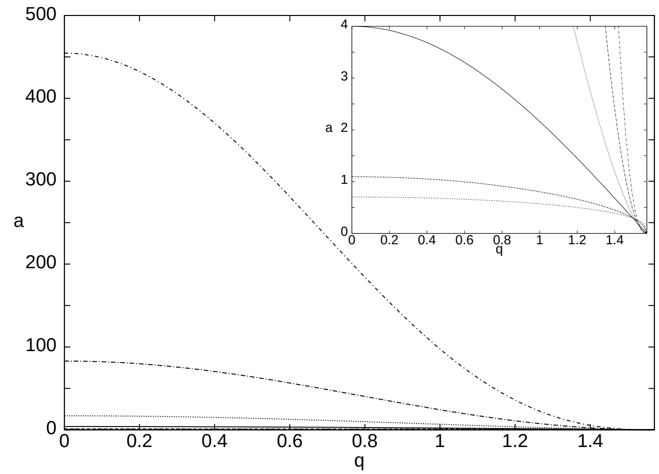
1. Travelling waves: $\psi_m = \sqrt{a} e^{iqm} e^{i\Lambda t}$ (with $\Lambda = 2C \cos q + a^\sigma$);

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

Modulationally unstable for $|q| < \pi/2$ and linearly stable for $\pi/2 < |q| \leq \pi$. (e.g. Smerzi/Trombettoni, Chaos **13**, 766 (2003))

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

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



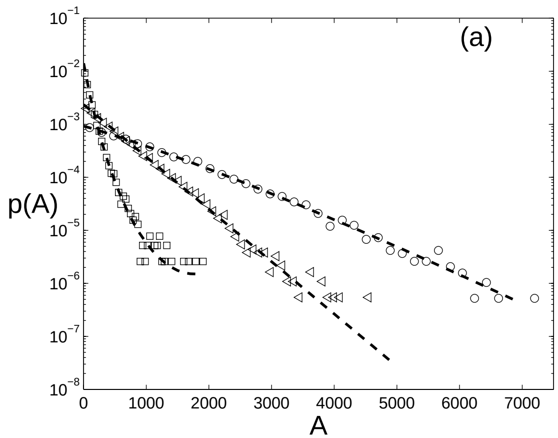
∵ For $|q| < \pi/2$ statistical localization expected for $a < a^{(c)}(q; \sigma)$.

(Evidently, if initial condition is exact no thermalization or localization occurs, but perturbed unstable solutions thermalize rapidly when $a > a^{(c)}$. Even for linearly stable solutions thermalization is expected, but extremely slow through Arnol'd diffusion.)

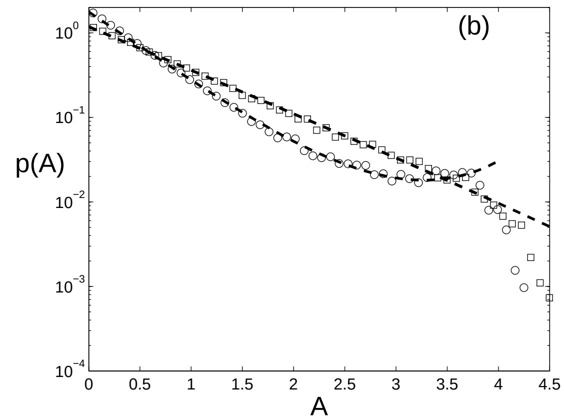
Note: For small σ, localization should occur even for very large a.

Numerics: Distribution functions for $N = 10000$ after $t = 1.1 \cdot 10^6$

$\underline{\sigma = 0.4}$



$\underline{\sigma = 3}$



2. Standing waves (SWs):

Time-periodic *non-propagating* solutions, periodic or quasiperiodic in space with wave vector Q. (e.g. Morgante et al., PRL **85**, 550 (2000))

Particularly interesting are *SWs with* $Q = \frac{\pi}{2}$: ('period-doubled states')

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

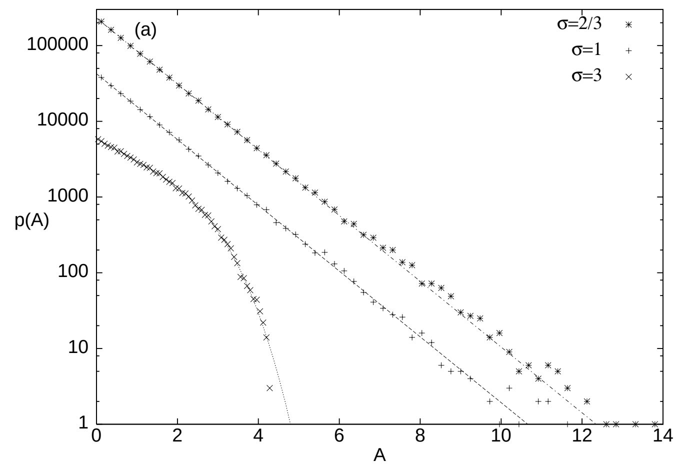
Since $\frac{2^\sigma}{\sigma+1} = \Gamma(\sigma+1)$ if and only if $\sigma = 1$, this solution defines curve of transition into phase of statistical localization only for cubic DNLS.

For $0 < \sigma < 1$ it is always in breather-forming regime, while for $\sigma > 1$ always in normal thermalizing regime.

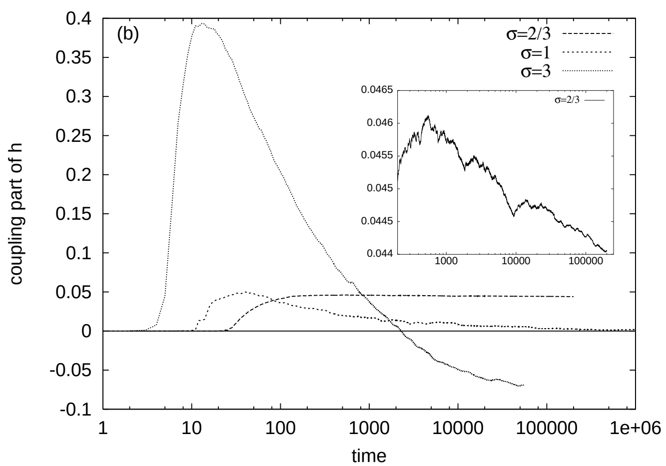
Numerically obtained (time-averaged) distribution functions from (unstable) $\pi/2$ SW initial conditions for $\sigma = \frac{2}{3}, 1, 3$ (a=C=1):

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

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



Extremely slow approach to equilibrium in breather-forming case $\sigma = \frac{2}{3}$:



B: Generalization to higher-dimensional models are immediate!

2D quadratic lattice of N sites: $\mathcal{H} =$

$$\Sigma_{m,n=1}^{\sqrt{N}} \left\{ 2C \left[\sqrt{A_{m,n}A_{m+1,n}} \cos(\phi_{m,n} - \phi_{m+1,n}) + \sqrt{A_m A_{m,n+1}} \cos(\phi_{m,n} - \phi_{m,n+1}) \right] + \frac{1}{\sigma+1} A_{m,n}^{\sigma+1} \right\}$$

Grand-canonical partition function:

$$\mathcal{Z} = (2\pi)^N \int_0^\infty \prod_{m,n=1}^{\sqrt{N}} dA_{m,n} I_0(2\beta C \sqrt{A_{m,n}A_{m+1,n}}) I_0(2\beta C \sqrt{A_{m,n}A_{m,n+1}}) e^{-\beta A_{m,n}\left(\frac{A_{m,n}^{\sigma}}{\sigma+1} + \mu\right)}$$

High-temperature limit $\beta \to 0^+$ again by approximating $I_0 \approx 1$

('thermalized independent units' neglects all interaction terms)

$h^{(c)}(a;\sigma) \equiv \Gamma(\sigma+1)a^{\sigma+1}$ gives transition line in any dimension!

Specific example: 2D plane wave $\psi_{m,n} = \sqrt{a} e^{i(q_x m + q_y n)} e^{i\Lambda t}$

Modulationally unstable if either $|q_x|$ or $|q_y|$ smaller than $\pi/2$.

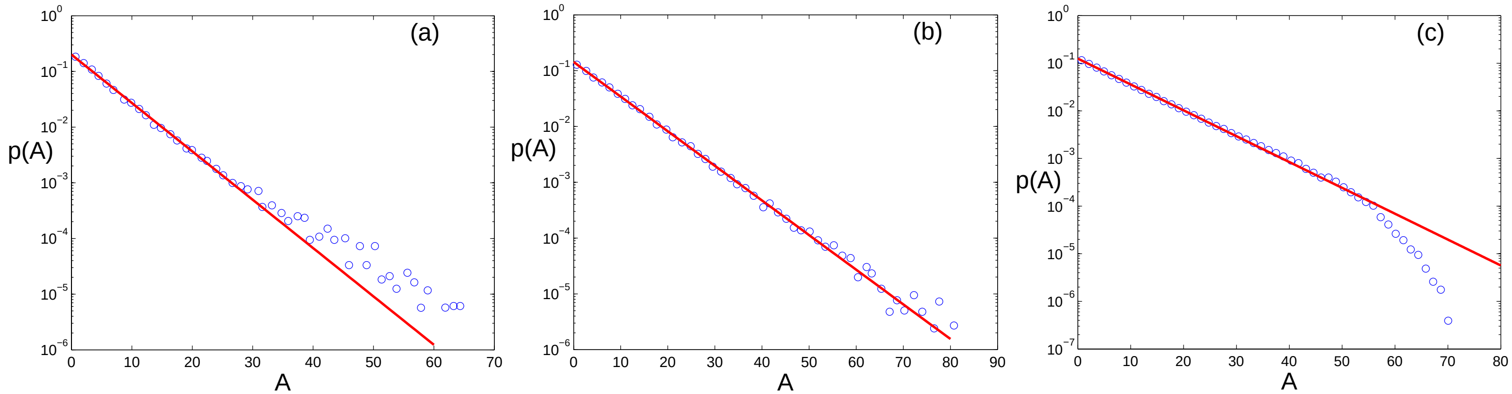
$$h = 2Ca(\cos q_x + \cos q_y) + \frac{a^{\sigma+1}}{\sigma+1} \Rightarrow$$

Statistical localization for $a < a^{(c)}$, with $a^{(c)} = \left[\frac{2(\sigma+1)C(\cos q_x + \cos q_y)}{\Gamma(\sigma+2)-1}\right]^{\frac{1}{\sigma}}$.

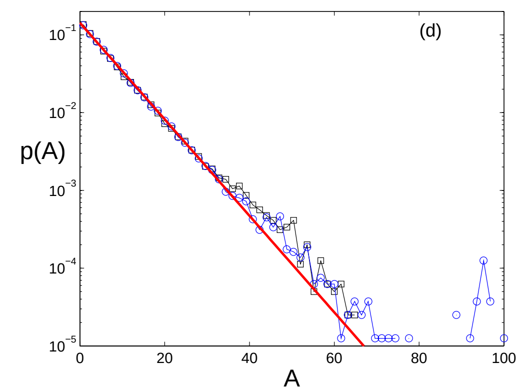
$\because \cos q_x + \cos q_y > 0$ necessary condition for persistent breather formation from 2D travelling waves.

In particular, for constant-amplitude solution ($q_x = q_y = 0$) with $\sigma = 1$, threshold is $a^{(c)} = 8C$ (compare $a^{(c)} = 4C$ in 1D).

Numerically obtained distribution functions ($N = 128 \times 128$):



Time-evolution of distribution at $a = 7$:



- Small t: Smooth curve with positive curvature, negative-temperature behaviour $\beta < 0$.

- Larger t: Discontinuous curve.

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

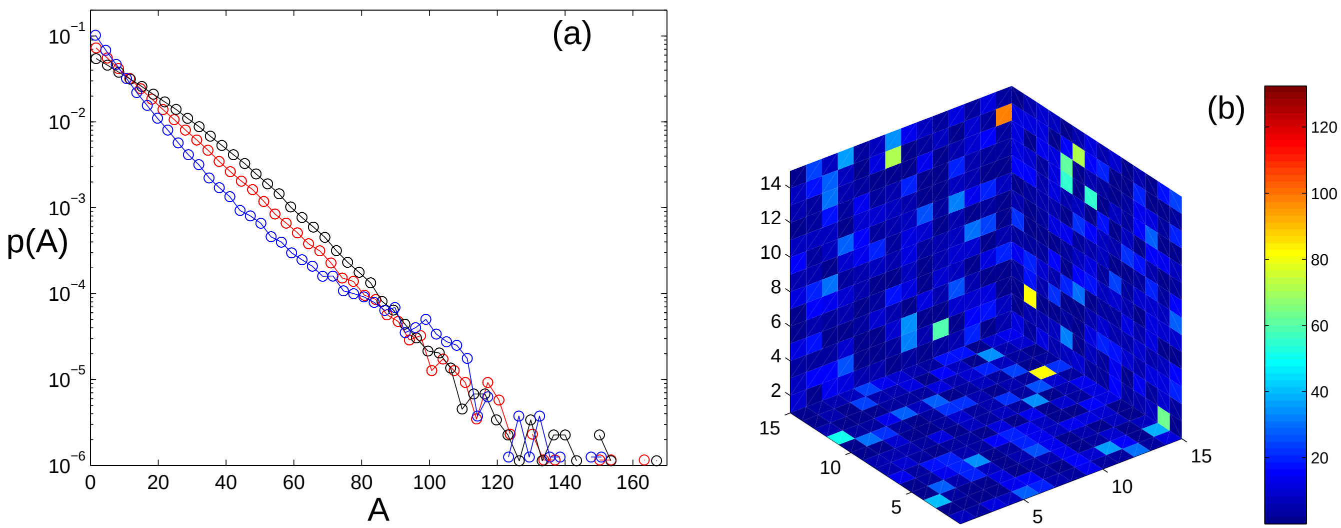
High-amplitude part: breathers with increasing amplitude.

$\because$ Phase space separation also for large a!?

Extension to travelling waves in 3D cubic lattice, $\psi_{m_x,m_y,m_z} = \sqrt{a} e^{i(q_x m_x + q_y m_y + q_z m_z)} e^{i\Lambda t}$, is immediate: just add $\cos q_z$ everywhere!

$\Rightarrow$ For a constant-amplitude solution in 3D with $\sigma = 1$, critical value becomes $a = 12C$.

Numerical integration to $t = 5 \cdot 10^6$ for $N = 64 \times 64 \times 64$:



Klein-Gordon correspondence to DNLS phase transition line

For small amplitudes ϵ and weak coupling C_K, find quantities approximately corresponding to DNLS Hamiltonian and norm!

Use wellknown ideas of expanding over multiple time-scales.

(e.g. Daumont et al., Nonlinearity **10**, 617 (1997); Morgante et al., Physica D **162**, 53 (2002))

KG Hamiltonian H: $H = \sum_{n=1}^{N} \left[\frac{1}{2}\dot{u}_n^2 + V(u_n) + \frac{1}{2}C_K(u_{n+1}-u_n)^2\right]$,

with on-site potential $V(u)$: $V(u) = \frac{1}{2}u^2 + \alpha\frac{u^3}{3} + \beta'\frac{u^4}{4} + \ldots$.

Expand $u_n(t)$ as $u_n(t) = \sum_p a_n^{(p)} e^{ip\omega_b t}$, assume $a_n^{(p)} \sim \epsilon^p$ for $p > 0$, $a_n^{(0)} \sim \epsilon^2$, $C_K \sim \epsilon^2$, and a slow time-dependence $a_n^{(p)}(\epsilon^2 t)$, gives general DNLS equation to $\mathcal{O}(\epsilon^5)$: $(\lambda' \equiv -\frac{10}{3}\alpha^2 + 3\beta')$

$$2i\omega_b\dot{a}_n^{(1)} + (1-\omega_b^2)a_n^{(1)} - C_K(a_{n+1}^{(1)} + a_{n-1}^{(1)} - 2a_n^{(1)}) + \lambda'|a_n^{(1)}|^2 a_n^{(1)} = 0 + \mathcal{O}(\epsilon^5).$$

Its two conserved quantities can be expressed as:

$\mathcal{A} = \frac{|\lambda'|}{C_K}\sum_{n=1}^{N}|a_n^{(1)}|^2$, $\mathcal{H} = \frac{|\lambda'|}{C_K^2}\sum_n \left[C_K(a_{n+1}^{(1)}a_n^{(1)*} + a_{n+1}^{(1)*}a_n^{(1)}) - \frac{\lambda'}{2}|a_n^{(1)}|^4\right]$

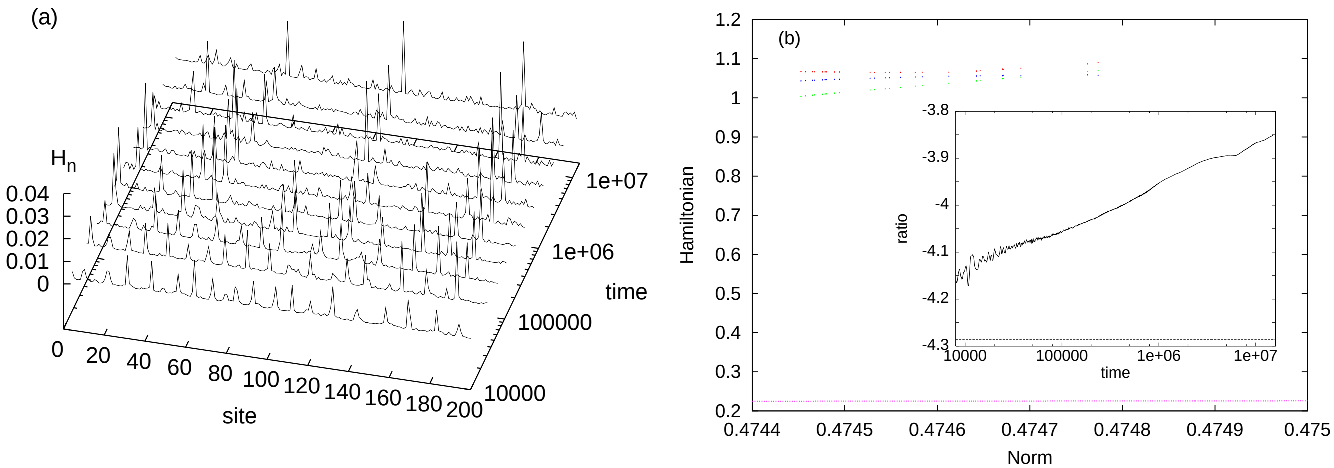
In the KG model, the quantities $\mathcal{A}/N$ and $\mathcal{H}/N$ correspond to quantities of order unity with time variation $\sim f(\epsilon^4 t)$, i.e., two orders of magnitude slower than the typical time scale for $a_n^{(1)}$.

Calculate $\mathcal{A}$ and $\mathcal{H}$ explicitly in terms of time-averages of different contributions to the KG Hamiltonian H:

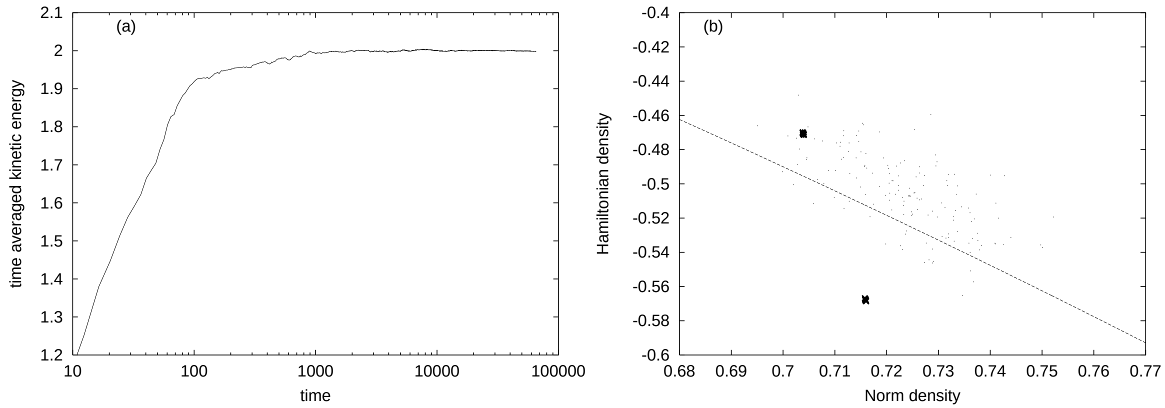
$$\mathcal{A} = \frac{|\lambda'|}{C_K}\left(< \sum_{n=1}^{N} \frac{u_n^2}{2} > + \frac{19}{30} < \sum_n \alpha \frac{u_n^3}{3} >\right) + \mathcal{O}(\epsilon^4);$$

$$\mathcal{H} = -\frac{|\lambda'|}{C_K^2}\left[H - < \sum_n \frac{\dot{u}_n^2}{2} > -(1+2C_K) < \sum_n \frac{u_n^2}{2} > - \frac{1}{2} < \sum_n \frac{\alpha u_n^3}{3} >\right] + \mathcal{O}(\epsilon^2).$$

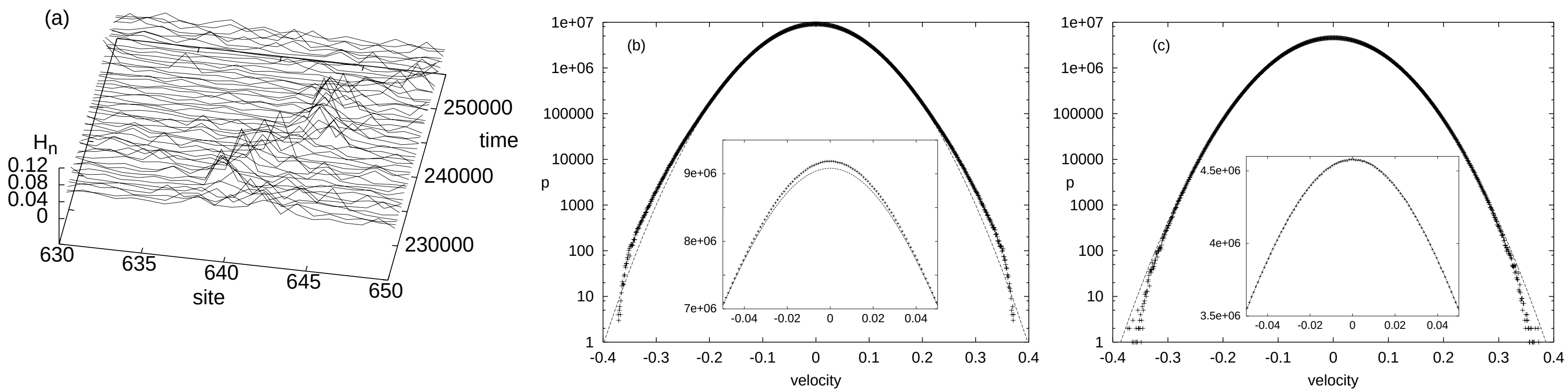
(non-unique expression!)



Numerical integration of KG Morse chain with $C_K = 0.005$, $N = 200$, and randomly perturbed constant-amplitude initial condition $u_n(0) = 0.05$. (a) Time evolution of local energy density (note logarithmic time scale). (b) Main figure: $\mathcal{H}/N$ vs. $\mathcal{A}/N$ for the simulation in (a). Time runs from right to left (i.e. $\mathcal{A}/N$ decreases). Lowest curve is the localization transition line. Inset in (b) shows the ratio of time-averaged cubic to quartic energies versus time, compared to the DNLS prediction (lower line).



Thermalization of a quartic KG chain ($\alpha = 0, \beta' = 1$) with $C_K = 0.01$, $N = 800$, coupled to a thermal bath at temperature $T' = 0.005$ with dissipation constant $\eta = 0.1$. (a) Time-averaged total kinetic energy $< \sum_n \frac{\dot{u}_n^2}{2} >$. (b) $\mathcal{H}/N$ vs. $\mathcal{A}/N$ for the simulation in (a). Each dot represents a time-average over the interval $[t - 100, t]$ at 15382 different times t. Line in (b) is the localization transition line. Larger points in (b) show the locations of the initial conditions used below.



(c) Example of a breather appearing in the microcanonical integration of an initial condition represented by the lower large point in (b). (d),(e) (Non-normalized) velocity distribution functions $p(\dot{u}_n)$ obtained from long-time numerical microcanonical integrations (points) compared to Maxwellian distributions $P(\dot{u}) \sim (2\pi T')^{-1/2} \exp(-\dot{u}^2/2T')$ (lines) at the estimated temperature. In (d) the initial condition is the same as for (c), the temperature is $T' \approx 0.00494$ and the integration time is $1.2 \cdot 10^6$. (e) corresponds to the upper large point at $(0.704, -0.471)$ in (b) with $T' \approx 0.00485$, and integration time $0.6 \cdot 10^6$.

Remarks and perspectives

• The statistical mechanics description yields explicit necessary conditions for formation of persistent localized modes, in terms of average values of the two conserved quantitities $\mathcal{H}$ and $\mathcal{A}$.

• 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.

• 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 a?

•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 $t \sim 10^{60}$...?