Frozen dynamics in the Discrete Nonlinear Schrödinger equation

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Non-equilibrium behaviour of classical and quantum systems
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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

Negative Temperatures

Thermodynamics and Statistical Mechanics at Negative Absolute Temperatures

Norman F. Ramsey
Harvard University, Cambridge, Massachusetts, and Clarendon Laboratory, Oxford, England
(Received March 26, 1956)

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

Statistical Hydrodynamics. (*)

L. Onsager
New Haven, Conn.
Negative Temperature DNLS

**Discrete Breathers**
- Exponentially localized in the real space
- Internal frequency $\omega_b \notin \text{Lin. Spectr.}$
- Consequence of nonlinearity and spatial discreteness. No role of disorder.
- Static (pinned) or mobile
- Experimental observations
Maximum entropy state


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

\[ \Downarrow \text{Relaxation } \tau \Downarrow \]

\[ |z_n|^2 \]

\[ \text{n} \quad 0 \quad 1024 \]

\[ |z_n|^2 \]

\[ \text{n} \quad 0 \quad 1024 \]

\[ \text{BUT} \]

- The transient \( \tau \) may last for astronomical times

What happens over physically accessible time scales?
Long-time DNLS dynamics
Symplectic numerical integration

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

- 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)

\[
H = \sum_{n=1}^{N} \frac{\nu}{2} |z_n|^4 + (\bar{z}_n^* z_{n+1} + \text{c.c.})
\]

\[
A = \sum_{n=1}^{N} |z_n|^2
\]
Stochastic models (purely entropic effects)

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


Condensation phenomena

- J. Szavits-Nossan, M. Evans, S. N. Majumdar, PRL (2014)
DNLS relaxation dynamics

- 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

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circle size = standard deviation of error on lifetime
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breather lifetime
rate 0.91
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breather lifetime
rate 0.91
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breather lifetime
rate 0.91
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“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)

$\lambda_{min}$ minimum PCA eigenvalue
The quasi-conserved quantity

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

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 $T > 0$. 