The Discrete Nonlinear Schrödinger Equation: an example of inequivalence between ensembles

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Outline

- The DNLSE model: generalities
- Hamiltonian and μ-canonical Monte Carlo dynamics of the DNLSE
- Thermodynamics of the DNLSE
- Ensemble inequivalence
- Large deviation calculation of the μ-canonical partition function
- Dynamical 1st order phase transition and its order parameter
- Existence of negative temperatures in the condensed phase

Generalities

- The DNLSE is a nonintegrable Hamiltonian on a 1d lattice

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

- $z_n = \frac{1}{\sqrt{2}}(p_n + iq_n)$ is a complex field
- It models various physical problems, e.g. electronic transport in biomolecules, semiclassical description of Bose-Einstein condensates in optical lattices, effects of nonlinearity in Anderson's localization, etc.

Generalities

- DNLSE Dynamics

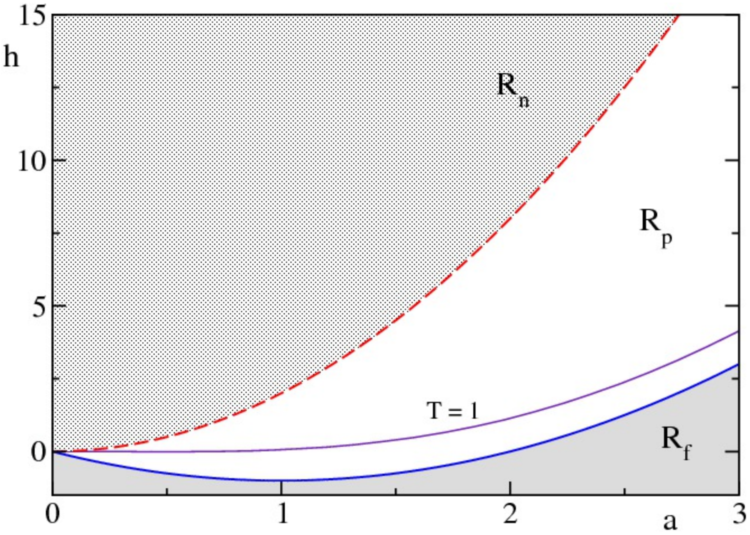
$$i\dot{z}_n = -\frac{\partial \mathcal{H}}{\partial z_n^*} = -(z_{n+1} + z_{n-1}) - \nu |z_n|^2 z_n$$

- Additional conserved quantity : "total mass"

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

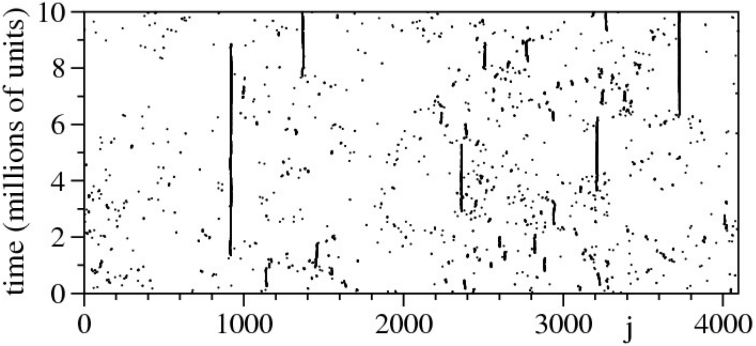
- Interesting phase diagram in the plane $\left(h = \frac{\mathcal{H}}{N}, a = \frac{\mathcal{A}}{N}\right)$

The phase diagram



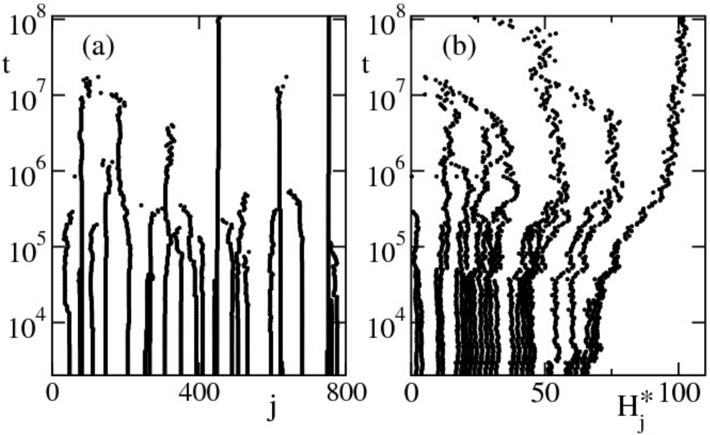
K.Ø. Rasmussen et al. PRL **84**, 3740 (2000)

Hamiltonian Dynamics in R_n



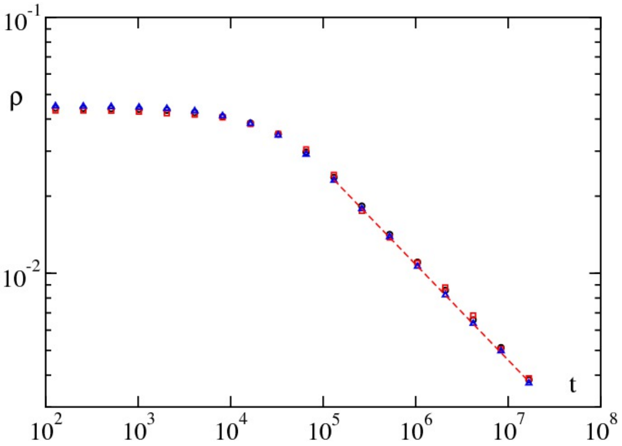
Multibreather state lasting over "astronomical" times: breather lifetime increasing exponentially with its amplitude.

MC Dynamics in R_n



Monte Carlo dynamics conserving $\mathcal{H}$ and $\mathcal{A}$ in the high temperature limit $\equiv$ null hopping.

MC Dynamics in R_n



Coarsening process : density of sites with "mass" larger than a threshold value (10 for $\nu = 1$) $\rho(t) = \rho_0\, t^{-\alpha}$ with $\alpha \simeq 1/3$.

Dynamics in R_n

- Both MC and Hamiltonian dynamics yield a condensed phase in R_n
- The μ-canonical temperature

$$T = \left(\frac{\partial S}{\partial E}\right)^{-1}$$

  is negative in R_n
- Conjecture : negative temperature states are not compatible with "true" thermodynamics and the condensed phase is just a transient towards an asymptotic state at $T = \infty$ with the energy excess stored in a single breather.
- In this seminar we prove that this (contradictory) conjecture is WRONG.

Thermodynamics in R_n

- μ-canonical partition function $\Omega(A, E)$ in the high-T limit

$$(2\pi)^N \int_0^\infty \prod_{n=1}^{N} d\rho_n \, \delta\left(A - \sum_{n=1}^{N} \rho_n^2\right) \, \delta\left(E - \sum_{n=1}^{N} \rho_n^4\right)$$

where $z_n = \rho_n e^{i\phi_n}$, $\mathcal{H} = E$ and $\mathcal{A} = A$.

- G-canonical partition function is its Laplace Transform

$$\mathcal{Z}(\beta, \mu) = \int_0^\infty dA \, dE \, e^{-\beta E - \mu A} \, \Omega(A, E)$$

Thermodynamics in R_n

- The inverse Laplace Transform

$$\Omega(A, E) = \int_{\mu - i\infty}^{\mu + i\infty} d\mu \int_{\beta - i\infty}^{\beta + i\infty} d\beta \; e^{\mu A + \beta E + \log[\mathcal{Z}(\beta,\mu)]}$$

  can be computed at some real positive saddle-point values β_0 and μ_0.

- Thermodynamic potential

$$h(\mu, \beta) = \mu A + \beta E + \log \mathcal{Z}_N(\mu, \beta)$$

Thermodynamics in R_n

- Saddle point equations

$$\frac{\partial h}{\partial \beta} = 0 \implies E = -\frac{1}{\mathcal{Z}_N(\mu,\beta)}\frac{\partial \mathcal{Z}_N(\mu,\beta)}{\partial \beta}$$

$$\frac{\partial h}{\partial \mu} = 0 \implies A = -\frac{1}{\mathcal{Z}_N(\mu,\beta)}\frac{\partial \mathcal{Z}_N(\mu,\beta)}{\partial \mu}$$

- Equivalence between ensembles holds if these equations are solved for real positive values $\beta = \beta_0$ and $\mu = \mu_0$

- But in R_n only the second saddle-point equation can be solved for $\mu_0 = 1/a$
- Inequivalence of Statistical Ensembles (Ruelle)

Thermodynamics in R_n

- The μ-canonical partition function $\Omega(A, E)$ can be computed by large-deviation formalism starting from its L.T. with respect to A

$$\Gamma(\mu, E) = (2\pi)^N \int_0^\infty \prod_{n=1} d\rho_n \;\; e^{-\mu \sum_{n=1}^N \rho_n^2} \;\; \delta\left(E - \sum_{n=1}^N \rho_n^4\right)$$

- change of variable $m_n = \rho_n^4$

$$\Gamma(\mu, E) = \pi^{3N/2} e^{-\frac{N}{2}\log(\mu)} \mathcal{Z}_\mu(E)$$

- where

$$\mathcal{Z}_\mu(E) = \int_0^\infty \mathcal{D}m \;\; \prod_{n=1}^N p_\mu(m_n) \;\; \delta\left(E - \sum_{n=1}^N m_n\right)$$

Thermodynamics in R_n

- with

$$p_\mu(m) = \frac{1}{2}\sqrt{\frac{\mu}{\pi}}\frac{1}{m^{3/4}} \exp\left(-\mu\sqrt{m}\right)$$

- $\mathcal{Z}_\mu(E)$ can be computed by its L.T.

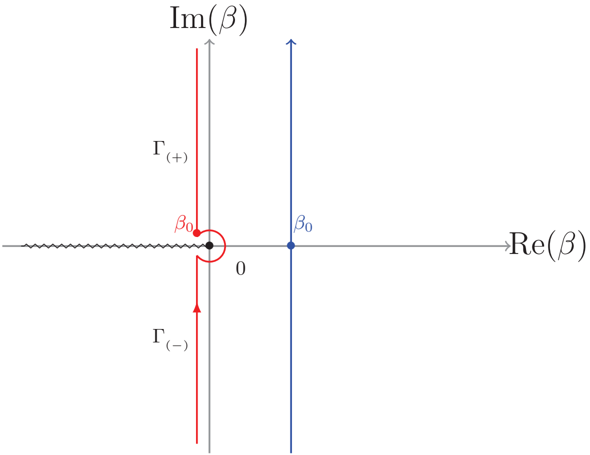
$$\int_0^\infty dE\ e^{-\beta E}\ \mathcal{Z}_\mu(E) = \exp\left\{N \log[g(\beta,\mu)]\right\},$$

- where

$$g(\beta,\mu) = \frac{1}{2}\frac{\mu}{\sqrt{\pi}}\ \frac{\exp\left(\frac{\mu^2}{8\beta}\right)}{\sqrt{\beta}}\ K_{-\frac{1}{4}}\left(\frac{\mu^2}{8\beta}\right)$$

- where $K_s(z)$ is the modified Bessel function of the second kind with a branchcut on the negative semiaxis of z

Thermodynamics in R_n



Thermodynamics in R_n

- We can write

$$\mathcal{Z}_\mu(E) = \int_{\beta_0 - i\infty}^{\beta_0 + i\infty} d\beta \;\exp\left\{\beta E + N \log[g(\beta,\mu)]\right\}$$

- Ensemble inequivalence $\rightarrow$ no real positive solution for the saddle point equation

$$\frac{E}{N} = \mathcal{F}(\beta,\mu) = -\frac{1}{g(\beta,\mu)}\frac{\partial g(\beta,\mu)}{\partial\beta}$$

- Making use of the deformed Bromwich contour and large deviation formalism one can finally compute the μ-canonical partition function $\Omega(A, E)$

Thermodynamics in R_n

Summary of the main results

I. First order dynamical phase transition along the line $\beta = 0$ (or at $E = E_{th}(A)$) from a thermalized to a condensed phase.

II. For any finite N there are three regimes:
Gaussian $E - E_{th} \sim \sqrt{N}$ thermalized phase
Matching $E - E_{th} \sim N^{\frac{2}{3}}$ around the transition
Large-deviation $E - E_{th} \sim N$ condensed phase

III. In the condensed phase the μ-canonical entropy is subextensive and the temperature is negative.

IV. For finite N and $E_{th} < E < E_c$ there are delocalized states with negative temperature

Thermodynamics in R_n

Some relevant details

- The "reduced" partition function in the three regimes

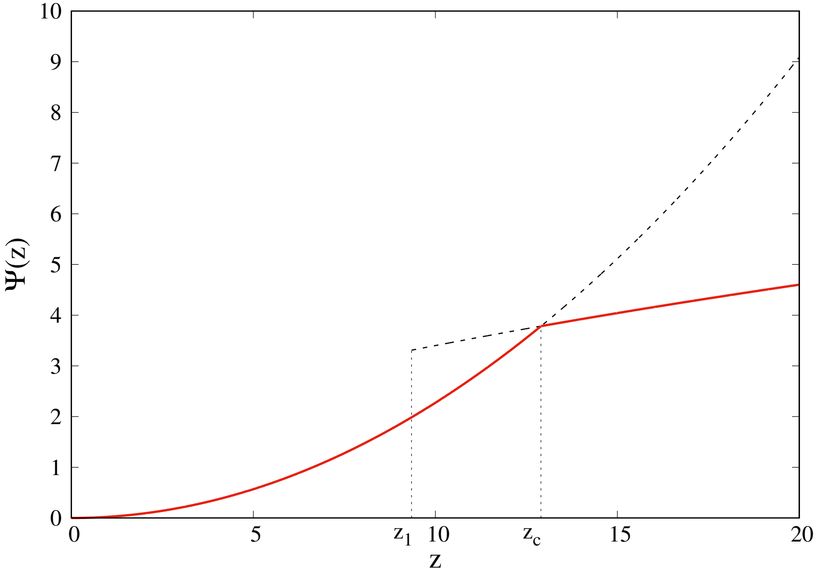
$$\mathcal{Z}_\mu(E) \approx \begin{cases} e^{-(E-E_{\rm th})^2/(2N\sigma_\mu^2)} & \text{for} \quad (E - E_{\rm th}) \sim N^{1/2} \\ e^{-N^{1/3}\Psi(z)} & \text{for} \quad (E - E_{\rm th}) \sim N^{2/3} \\ e^{-(E-E_{\rm th})^{1/2}} & \text{for} \quad (E - E_{\rm th}) \sim N \end{cases}$$

- where

$$z = (E - E_{th})/N^{2/3} \qquad \Psi(z) = \min\left[\frac{z^2}{2\sigma^2}, \chi(z)\right]$$

- $\chi(z)$ can be computed exactly by LDs

Thermodynamics in R_n



Thermodynamics in R_n

Some relevant details

- The μ-canonical partition function in the three regimes

$$\Omega_N(E,A) \approx \begin{cases} \exp\left[-N\left(-3a^2/4\right)^2/(12a^2)\right] \\ \exp\left[-N^{1/3}\Psi(z)\right] \\ \exp\left[-N^{1/2}\sqrt{-3a^2/4}\right] \end{cases}$$

- The order parameter: Participation Ratio

$$Y_2 = \left\langle \frac{\sum_{i=1}^N m_i^2}{\left(\sum_{i=1}^N m_i\right)^2} \right\rangle$$

Thermodynamics in R_n

Some relevant details

- For $E < E_{th}$

$$Y_2 \sim \frac{1}{N}$$

- For $E - E_{th} \sim N^{1/2}$

$$Y_2 \sim \exp\left(-N^{1/4}\right)$$

- For $E > E_c$

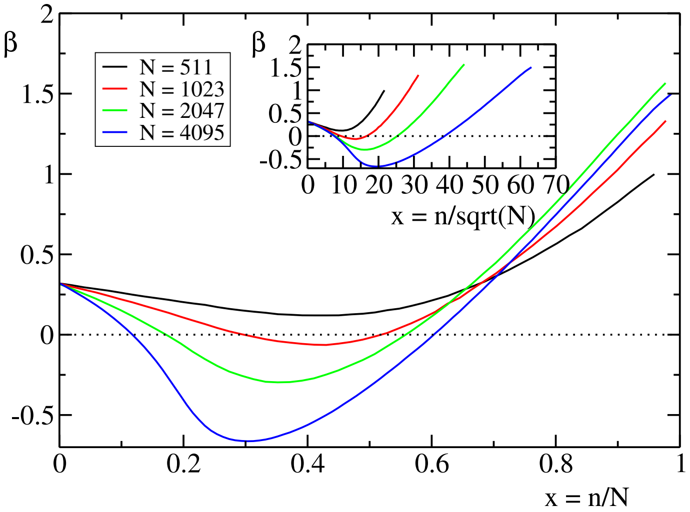
$$Y_2 \sim constant$$

Remarks

- An example of ensemble inequivalence in a short-range interaction model
- Negative temperature states do exist in the condensed phase
- They can be experimentally tested in the "matching regime" for finite N
- Positive and negative temperature states, i.e. the thermalized and the condensed phase, do coexist in out-of-equilibrium conditions

Out of equilibrium states

Positive temperature heat reservoirs at different temperatures acting at the boundaries of the DNLS chain



Thank you for your attention

Some useful references

G. Gradenigo, S. Majumdar, ArXiv1812.07819v1

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