Probabilistic methods for discrete nonlinear Schrödinger equations

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The cubic nonlinear Schrödinger equation

- Linear Schrödinger equation:

$$\mathrm{i}\partial_t \psi = -\Delta \psi,$$

  where $\psi : \mathbb{R}^d \times \mathbb{R} \to \mathbb{C}$.

- Cubic nonlinear Schrödinger equation:

$$\mathrm{i}\partial_t \psi = -\Delta \psi + \kappa |\psi|^2 \psi.$$

- κ can be $+1$ (defocusing equation) or -1 (focusing equation).
- In this talk, we will concentrate on the focusing equation, that is, $\kappa = -1$.
- Crucial to understanding a variety of physical phenomena:
  - Bose-Einstein condensation
  - Langmuir waves in plasmas
  - Nonlinear optics
  - Envelopes of water waves
  - etc...

The Gibbs measure

- The cubic NLS is a Hamiltonian system, with Hamiltonian

$$H(\psi) = 2 \int |\nabla \psi|^2 dx + \kappa \int |\psi|^4 dx.$$

- One method of studying the behavior of Hamiltonian systems is through invariant measures for the dynamics.
- Gibbs measures, i.e. measures that have density of the form

$$e^{-\beta H(\psi)}$$

  are (formally) invariant by Liouville's theorem.
- Here β is a parameter, sometimes called the 'inverse temperature'.

The mass cut-off

- The Gibbs measure for the focusing NLS has infinite mass (even in 1D) and hence cannot be normalized to give a probability measure.
- This necessitates a mass cut-off: consider densities of the form
$$e^{-\beta H(\psi)} 1_{\{N(\psi)\le B\}}$$
where B is another parameter and $N(\psi) = \int |\psi|^2 dx$.
- Even after mass cut-off, it is not obvious that everything makes sense.
- Following the pioneering work of Lebowitz-Rose-Speer, the approach was given a rigorous foundation through the works of McKean-Vaninsky, Bourgain and Rider.
- Most of the work till now in 1D. Bourgain and Tzvetkov did the 2D defocusing case. Brydges-Slade found some problems in defining the Gibbs measure in the 2D focusing case.
- Analysis of Gibbs measures can lead to conclusions about well-posedness (Bourgain).

3D and higher

- It is not clear (and probably not true) that Gibbs measures for the focusing NLS can be defined analogously in dimensions 3 and higher.
- Our approach: work with a discretized system without worrying about taking continuum limits. Gibbs measures can always be defined for discrete systems.
- Try to understand the fine properties of the system and make inferences about the dynamics.
- One long-term motivation: the soliton resolution conjecture.

The soliton resolution conjecture

- The linear Schrödinger is a dispersive system: while $\int_{\mathbb{R}^d} |\psi|^2 dx$ is conserved over time, for any compact set K,

$$\lim_{t\to\infty} \int_K |\psi|^2 dx = 0.$$

- In its simplest form, the soliton conjecture for the nonlinear NLS says that there is a compact set K such that the above equation does not hold for K, but [see below].
- One can find initial data that disperses even for the nonlinear NLS. But this is the worst-case scenario.
- The conjecture says that complete dispersion does not happen in the typical case, although it is not clear what 'typical' means. [Readable reference: Terry Tao's blog on this.]
- The conjecture has been proved in 1D (cubic), where the system is completely integrable. All other cases are unknown.

Formulation via the invariant measure approach

- One way to quantify 'typical': a set of probability 1 under an invariant probability measure whose support is the space of all initial data with a given mass and energy (say).
- Characteristics of a random pick from the invariant measure do not change as it evolves over time according to the NLS flow.
- Implication: If the random initial data has positive mass in a neighborhood of the origin with probability 1, then it will continue to have this characteristic for all time, satisfying the soliton resolution conjecture.
- Difficulty: We do not know such invariant measures for the continuum system (focusing cubic) in 3D and higher.
- Note: The existence of soliton solutions, e.g. ground state solitons, is known. The difficulty is in proving that such behavior is typical.

The discrete cubic NLS

- Since we cannot handle the continuum system, one alternative is to discretize space.
- Let $G = (V, E)$ be the lattice approximation of the d-dimensional unit torus $[0,1]^d$, where $V = \{0, 1/L, 2/L, \ldots, (L-1)/L\}^d$ and E consists of nearest-neighbor edges.
- Let $h = 1/L$ denote the lattice spacing. Let $n = L^d$ be the size of the graph.
- The discrete nearest-neighbor Laplacian on G is defined as

$$\widetilde{\Delta} f(x) := \frac{1}{h^2} \sum_{y \colon (x,y) \in E} (f(y) - f(x)).$$

- The discrete cubic NLS on G is a family of coupled ODEs with $f_x(t) := f(x,t)$, satisfying for all $x \in V$

$$\mathrm{i} \frac{d}{dt} f_x = -\widetilde{\Delta} f_x + \kappa |f_x|^2 f_x.$$

The discrete Gibbs measure

- The discrete Hamiltonian associated with the focusing NLS is:

$$\widetilde{H}(f) := \frac{2}{n} \sum_{(x,y)\in E} \left| \frac{f_x - f_y}{h} \right|^2 - \frac{1}{n} \sum_{x \in V} |f_x|^4.$$

- Note analogy with continuum Hamiltonian:

$$H(f) = 2 \int |\nabla f|^2 dx - \int |f|^4 dx.$$

- Let $\widetilde{N}(f) = \frac{1}{n} \sum_{x \in V} |f_x|^2$ denote the mass.
- Given $\beta, B > 0$, the probability measure $\tilde{\mu}$ on $\mathbb{C}^n$ defined as

$$d\tilde{\mu} := \frac{1}{Z} e^{-\beta \widetilde{H}(f)} 1_{\{\widetilde{N}(f) \le B\}} \prod_{x \in V} df_x$$

is an invariant probability measure for the discrete focusing cubic NLS. Here $Z = Z(\beta, B)$ is the normalizing constant.

The limiting free energy

- Let $m : [2, \infty) \to \mathbb{R}$ be the function

$$m(\theta) := \frac{\theta}{2} - \frac{1}{2} + \frac{\theta}{2}\sqrt{1 - \frac{2}{\theta}} + \log\left(\frac{1}{2} - \frac{1}{2}\sqrt{1 - \frac{2}{\theta}}\right).$$

- Let θ_c be the unique real zero of m. Numerically, $\theta_c \approx 2.455407$.

Theorem (Chatterjee & Kirkpatrick, 2010)

Suppose $d \geq 3$. As the lattice size $n \to \infty$ (and hence the lattice spacing $h \to 0$),

$$\frac{\log Z(\beta, B)}{n} \to \begin{cases} \log(B\pi e) & \text{if } \beta B^2 \leq \theta_c, \\ \log(B\pi e) + m(\beta B^2) & \text{if } \beta B^2 > \theta_c. \end{cases}$$

Features of the Gibbs measure

- Let ψ be a random initial data from the Gibbs measure.
- Let $M_1(\psi)$ and $M_2(\psi)$ denote the largest and second largest components of the vector $(|\psi_x|^2)_{x\in V}$.
- When $\beta B^2 > \theta_c$, there is high probability that $M_1(\psi) \approx an$ and $M_2(\psi) = o(n)$, where

$$a = a(\beta, B) := \frac{B}{2} + \frac{B}{2}\sqrt{1 - \frac{2}{\beta B^2}}.$$

- Moreover, $\sum_x |\psi_x|^2 \approx Bn$ with high probability.
- Largest component carries more than half of the total mass:

$$\max_x \frac{|\psi_x|^2}{\sum_y |\psi_y|^2} \approx \frac{a}{B} > \frac{1}{2}.$$

- On the other hand, when $\beta B^2 < \theta_c$, then $M_1(\psi) = o(n)$ and $\max_x |\psi_x|^2 / \sum_y |\psi_y|^2 \approx 0$.

Fraction of mass at the heaviest site

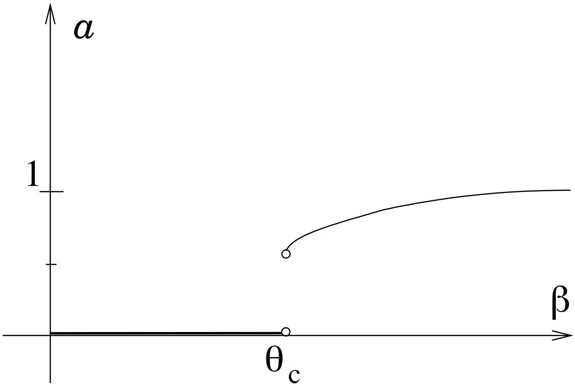

Figure: The fraction of mass at the heaviest site jumps from roughly zero for small inverse temperature, to roughly .71 at the critical threshold. (Here $B = 1$.)

Typicality of soliton-like solutions

Theorem (Chatterjee & Kirkpatrick, 2010)

Suppose $\beta B^2 > \theta_c$ and $d \geq 3$. Suppose $\psi(x,t)$ is a solution of the discrete cubic NLS on lattice of size n with random initial data $\psi(\cdot, 0)$ from the Gibbs measure $\tilde{\mu}$. Then for any $q \in (0,1)$ that is sufficiently close to 1, with probability at least $1 - \exp(-n^q)$ there is a point x_0 such that for all $t \in [0, \exp(n^q)]$,

$$\left| \frac{|\psi(x_0, t)|^2}{n} - a(\beta, B) \right| \leq n^{-(1-q)/4}$$

and

$$\frac{\max_{x \neq x_0} |\psi(x,t)|^2}{n} \leq n^{-(1-q)}.$$

Stability of the soliton: proof sketch

- If $\beta B^2 > \theta_c$, we show that with high probability, there is a single point with abnormally large value of the wave function at $t = 0$.
- As time progresses, the invariance of the Gibbs measure implies that the above picture must hold for all but a very small proportion of times.
- We use estimates related to the NLS flow to show that if the soliton has to jump from one site to another, that cannot happen in a time period as small as allowed by the preceding estimate. Hence the soliton cannot jump.
- The above argument is a simple combination of probabilistic and PDE methods.

Analysis of the Gibbs measure

- Simplifying step: in $d \geq 3$, the interaction term in the Hamiltonian has almost no effect if n is large. In other words, the problem attains a mean-field character. Not obvious *a priori*. Not true in $d = 1$ or 2.
- Upon ignoring the interaction term, the problem boils down to analyzing the uniform probability distribution on subsets of $\mathbb{C}^n$ like

$$\Gamma_{a,b} = \left\{ f \in \mathbb{C}^n : \sum_{x \in V} |f_x|^2 \approx bn, \ \sum_{x \in V} |f_x|^4 \approx a^2 n^2 \right\}.$$

  Here $\approx$ means equal up to error of order smaller than the main term.
- To show: A uniformly chosen point from $\Gamma_{a,b}$ has exactly one abnormally large component with high probability.
- Also, need to compute the volume of $\Gamma_{a,b}$ to connect uniform distributions with Gibbs measures.

A simple problem

- Suppose Z_1, Z_2 are i.i.d. complex Gaussian random variables, and we are given that $|Z_1|^4 + |Z_2|^4 \approx n$, where n is a large number.
- What can you say about the pair (Z_1, Z_2), conditional on this event?
- Conditionally, (Z_1, Z_2) is distributed on the L^4 annulus $\{(z_1, z_2) : |z_1|^4 + |z_2|^4 \approx n\}$ with probability density function proportional to $\exp(-|z_1|^2 - |z_2|^2)$.
- Thus, the conditional distribution must concentrate on the part of the annulus where $|z_1|^2 + |z_2|^2$ is minimized. This happens where the L^4 and L^2 balls touch.
- This implies that with high probability, either $|Z_1|^4 \approx n$ or $|Z_2|^4 \approx n$.

A slightly more complex problem

- The above logic continues to hold if we replace (Z_1, Z_2) by $(Z_1, \ldots, Z_k)$, as long as k is sufficiently small compared to n.
- Precisely, if $k \ll n/\log n$, then the same argument shows that conditional on $|Z_1|^4 + \cdots + |Z_k|^4 \approx n$, we can say that with high probability, there is exactly one i such that $|Z_i|^4 \approx n$.
- However, we are interested in the case where k is of the same order as n. The previous argument breaks down because volumes compete with densities.
- But the result is still true, with a small modification.

An even more complex problem

- Suppose $Z_1, \ldots, Z_n$ are i.i.d. standard complex Gaussian random variables.
- Let A be the event $|Z_1|^4 + \cdots |Z_n|^4 \approx bn$ where b is a constant greater than $\mathbb{E}|Z_1|^4 = 8$ and $\approx$ has some appropriate meaning.
- What does the vector $(Z_1, \ldots, Z_n)$ look like, conditional on A?

Analysis of the complex problem

- Note that

$$\begin{aligned}\mathbb{P}(A) &\geq \mathbb{P}(|Z_1|^4 \approx (b-8)n)\mathbb{P}(|Z_2|^4 + \cdots + |Z_n|^4 \approx 8n)\\ &\approx e^{-c\sqrt{n}},\end{aligned}$$

  where c denotes a constant depending on b.
- On the other hand, if B denotes the event that the histogram of the data $\{|Z_1|^2, \ldots, |Z_n|^2\}$ deviates significantly from its expected shape, then $\mathbb{P}(B) \leq e^{-dn}$, where d is a constant depending on the deviation.
- Thus, $\mathbb{P}(B|A) \leq \mathbb{P}(B)/\mathbb{P}(A) =$ very small.
- Together, this implies that given A, there must exist a relatively small set $S \subseteq \{1, \ldots, n\}$ such that $\sum_{i \in S} |Z_i|^4 \approx (b-8)n$.
- The argument for the simpler problem can be now applied to show that there is exactly one i such that $|Z_i|^2 \approx (b-8)n$.

From Gaussian measures to Gibbs measures

- When the standard Gaussian distribution is restricted to a subset of a thin L^2 annulus (e.g. intersection of L^2 and L^4 annuli), it becomes the uniform distribution on this set.
- The Gibbs measures are approximately convex combinations of uniform distributions on an infinite collection of intersections of L^2 and L^4 annuli.
- Thus, our analysis proceeds as: Gaussian $\rightarrow$ Uniform $\rightarrow$ Gibbs.

Continuum limit

- Unfortunately, the Gibbs measures do not tend to a continuum limit at the grid size goes to zero.
- The reason is the energy levels attained by the Gibbs measure are too low to admit good behavior in the limit.
- In fact, we have a theorem proving convergence to white noise plus one exceptional point.
- Future goal: to develop a continuum version. Requires new ideas in addition to the existing ones.