Gibbs measures of nonlinear Schrödinger equations and interacting quantum particles at high temperature

Antti Knowles

ETH Zürich

Institute Henri Poincaré, Paris, 28 June 2016

With Jürg Fröhlich, Benjamin Schlein, and Vedran Sohinger

Classical mechanics and Gibbs measures

A Hamiltonian system consists of the following ingredients.

- Linear phase space $\Gamma \ni \phi$.
- Hamilton (or energy) function $H \in C^\infty(\Gamma)$.
- Poisson bracket $\{\cdot\,,\cdot\}$ on $C^\infty(\Gamma) \times C^\infty(\Gamma)$.

  (Properties: antisymmetric, bilinear, Leibniz rule in both arguments, Jacobi identity.)

Classical dynamics is given by Hamiltonian flow $\phi \mapsto \phi_t$ on Γ defined by the ODE

$$\frac{\mathrm{d}}{\mathrm{d}t} f(\phi_t) = \{H, f\}(\phi_t)$$

for any $f \in C^\infty(\Gamma)$.

Standard example: classical system of n degrees of freedom.

- Phase space $\Gamma = \mathbb{R}^{2n} \ni (p, q)$.
- Hamilton function $H(p,q) = \sum_{i=1}^{n} \frac{p_i^2}{2m_i} + V(q)$.
- Poisson bracket $\{f, g\} = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} - \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} \right)$.

Hamiltonian flow reads

$$\frac{\mathrm{d}}{\mathrm{d}t} p_i = -\frac{\partial H}{\partial q_i} = -\partial_i V(q)\,, \qquad \frac{\mathrm{d}}{\mathrm{d}t} q_i = \frac{\partial H}{\partial p_i} = \frac{p_i}{m_i}\,.$$

The Gibbs measure at temperature β is

$$\mathbb{P}(\mathrm{d}\phi) := \frac{1}{Z} \mathrm{e}^{-\beta H(\phi)}\,\mathrm{d}\phi\,, \qquad Z := \int \mathrm{e}^{-\beta H(\phi)}\,\mathrm{d}\phi\,.$$

$\mathbb{P}$ is invariant under the flow $\phi \mapsto \phi_t$.

Nonlinear Schrödinger equations

Let $\mathbb{T}^d = \mathbb{R}^d/\mathbb{Z}^d$ be the d-dimensional torus.

- Phase space Γ is some appropriate subspace of $\{\phi : \mathbb{T}^d \to \mathbb{C}\}$.
- Hamilton function

  $$H(\phi) = \int \mathrm{d}x\, \bar{\phi}(x)(\kappa - \Delta)\phi(x) + \frac{1}{2}\int \mathrm{d}x\, \mathrm{d}y\, w(x-y)|\phi(x)|^2|\phi(y)|^2\,,$$

  where $\kappa > 0$.
- Poisson bracket

  $$\{\phi(x), \bar{\phi}(y)\} = \mathrm{i}\delta(x-y)\,, \qquad \{\phi(x), \phi(y)\} = \{\bar{\phi}(x), \bar{\phi}(y)\} = 0\,.$$

Hamiltonian flow given by time-dependent nonlinear Schrödinger equation

$$\mathrm{i}\partial_t \phi(x) = (\kappa - \Delta)\phi(x) + \int \mathrm{d}y\, w(x-y)|\phi(y)|^2\phi(x)\,.$$

Time-dependent nonlinear Schrödinger equation

$$\mathrm{i}\partial_t \phi(x) = (\kappa - \Delta)\phi(x) + \int \mathrm{d}y\, w(x-y)|\phi(y)|^2 \phi(x)\,. \tag{1}$$

Gibbs measure of nonlinear Schrödinger equation is formally

$$\mathbb{P}(\mathrm{d}\phi) = \frac{1}{Z}\mathrm{e}^{-H(\phi)}\mathrm{d}\phi\,.$$

Formally, $\mathbb{P}$ is invariant under the flow generated by (1).

Rigorous results: Lebowitz–Rose–Speer, Bourgain, Bourgain–Bulut, Tzvetkov, Thomann–Tzvetkov, Nahmod–Oh–Rey-Bellet–Staffilani, Oh–Quastel, Deng–Tzvetkov–Visciglia, Cacciafesta–de Suzzoni, Genovese–Lucá–Valeri, ...

Important application: $\mathbb{P}$-almost sure well-posedness of (1) for rough initial data.

Rigorous construction of Gibbs measure

Spectral decomposition

$$\kappa - \Delta = \sum_{k \in \mathbb{N}} \lambda_k u_k u_k^* \,, \qquad \lambda_k > 0 \,, \qquad \|u_k\|_{L^2} = 1 \,.$$

Let $\omega = (\omega_k)_{k \in \mathbb{N}} \in \mathbb{C}^{\mathbb{N}}$ be i.i.d. $\mathcal{N}_{\mathbb{C}}(0,1)$ random variables with joint law μ_0.

Define the Gaussian free field

$$\phi^\omega \equiv \phi := \sum_{k \in \mathbb{N}} \frac{\omega_k}{\sqrt{\lambda_k}} u_k \,.$$

The sum converges in $\|\phi\|_{H^s} := \|(\kappa - \Delta)^{s/2} \phi\|_{L^2}$ in the sense of $L^p(\mu_0)$ for all $p \in (1, \infty)$, provided that

$$\sum_{k \in \mathbb{N}} \lambda_k^{s-1} < \infty \,.$$

For example,

$$\mathbb{E}^{\mu_0} \|\phi\|_{H^s}^2 = \sum_{k \in \mathbb{N}} \mathbb{E}^{\mu_0} |\omega_k|^2 \frac{\lambda_k^s}{\lambda_k} = \sum_{k \in \mathbb{N}} \lambda_k^{s-1} \,.$$

$\phi = \sum_{k \in \mathbb{N}} \frac{\omega_k}{\sqrt{\lambda_k}} u_k$ is the Gaussian free field with covariance $(\kappa - \Delta)^{-1}$:

$$\int \mathrm{d}\mu \, \langle f \,, \phi \rangle \langle \phi \,, g \rangle = \langle f \,, (\kappa - \Delta)^{-1} g \rangle \,.$$

We find that

$$\mu_0(H^0) = \begin{cases} 1 & \text{if } d = 1 \\ 0 & \text{if } d > 1 \,. \end{cases}$$

Define the measure

$$\mu(\mathrm{d}\omega) := \frac{1}{Z} \mathrm{e}^{-W(\phi^\omega)} \mu_0(\mathrm{d}\omega) \,, \qquad W(\phi) = \frac{1}{2} \int \mathrm{d}x \, \mathrm{d}y \, w(x - y) |\phi(x)|^2 |\phi(y)|^2 \,.$$

μ is well-defined for instance if:

- $d = 1$,
- $w \in L^\infty$,
- w positive definite,

since then $0 \leqslant W(\phi) < \infty$ μ_0-a.s.

Quantum many-body theory

Quantum (bosonic) n-particle system is formulated on Hilbert space

$$\mathfrak{H}^{(n)} := L^2_{\mathsf{sym}}\big((\mathbb{T}^d)^n\big)$$

consisting of wave functions $\Psi^{(n)}(x_1, \ldots, x_n)$ symmetric in their arguments.

Hamilton operator

$$H^{(n)} := H_0^{(n)} + \lambda \sum_{1 \leqslant i < j \leqslant n} w(x_i - x_j)\,, \qquad H_0^{(n)} := \sum_{i=1}^{n} (\kappa - \Delta_{x_i})$$

Canonical thermal state at temperature $\tau > 0$ is $P_\tau^{(n)} := \mathrm{e}^{-H^{(n)}/\tau}$.

Expectation of an observable $A \in \mathfrak{B}(\mathfrak{H}^{(n)})$ is

$$\rho_\tau^{(n)}(A) := \frac{\mathrm{Tr}(A P_\tau^{(n)})}{\mathrm{Tr}(P_\tau^{(n)})}\,.$$

What happens as $n \to \infty$?

In order to obtain a nontrivial limit, we set $\lambda = 1/n$.

Theorem [Lewin-Nam-Serfaty-Solovej, 2012; Lewin-Nam-Rougerie, 2013]. For $\lambda = 1/n$ and τ fixed, the state $\rho_\tau^{(n)}(\cdot)$ converges to the atomic measure δ_Φ in the sense of p-particle correlation functions (see later), where Φ is the minimizer of the energy function H.

Complete Bose-Einstein condensation for fixed τ.

In order to obtain the Gibbs measure μ, we need to let

- τ grow with n (high-temperature limit),
- n fluctuate. (n/τ will correspond to $\|\phi\|_2^2$.)

High-temperature limit for $d = 1$

Define the Fock space

$$\mathcal{F} := \bigoplus_{n \in \mathbb{N}} \mathfrak{H}^{(n)}$$

and the grand canonical thermal state

$$P_\tau := \bigoplus_{n \in \mathbb{N}} P_\tau^{(n)} = \mathrm{e}^{-H_\tau}\,, \qquad H_\tau := \frac{1}{\tau} \bigoplus_{n \in \mathbb{N}} H^{(n)}\,.$$

Rescaled particle number operator

$$\mathcal{N}_\tau := \frac{1}{\tau} \bigoplus_{n \in \mathbb{N}} n I\,.$$

Expectation of an observable $A \in \mathfrak{B}(\mathcal{F})$ is

$$\rho_\tau(A) := \frac{\mathrm{Tr}(A P_\tau)}{\mathrm{Tr}(P_\tau)}\,.$$

Explicit computation for $d = 1$ and $\lambda = 0$:

$$\lim_{\tau \to \infty} \rho_\tau(\mathcal{N}_\tau^k) = \mathbb{E}^\mu \|\phi\|_{L^2}^{2k}, \qquad k = 1, 2, \dots .$$

Number of particles is of order τ. Thus, set $\lambda := \tau^{-1}$ to obtain nontrivial interacting limit.

Limit of $\rho_\tau(\cdot)$ stated using p-particle correlation functions of P_τ,

$$\gamma_{\tau,p} := \frac{1}{\operatorname{Tr}(P_\tau)} \sum_{n \geqslant p} \frac{n(n-1)\cdots(n-p+1)}{\tau^p} \operatorname{Tr}_{p+1,\dots,n}(P_\tau^{(n)}) .$$

Note: in second-quantized notation we can introduce a quantum field (i.e. operator-valued distribution) ϕ_τ satisfying the canonical commutation relations

$$[\phi_\tau(x), \phi_\tau^*(y)] = \frac{1}{\tau}\delta(x-y), \qquad [\phi_\tau(x), \phi_\tau(y)] = [\phi_\tau^*(x), \phi_\tau^*(y)] = 0,$$

such that

$$\gamma_{\tau,p}(x_1, \dots, x_p; y_1, \dots, y_p) \ := \ \rho_\tau\big(\phi_\tau^*(y_1)\cdots\phi_\tau^*(y_p)\phi_\tau(x_1)\cdots\phi_\tau(x_p)\big) .$$

Analogously, we define the classical p-particle correlation function

$$\gamma_p(x_1, \dots, x_p; y_1, \dots, y_p) \ := \ \mathbb{E}^{\mu}\big(\bar{\phi}(y_1) \cdots \bar{\phi}(y_p)\phi(x_1) \cdots \phi(x_p)\big) \, .$$

The family $(\gamma_p)_{p \in \mathbb{N}}$ completely determines all moments of the field ϕ.

Theorem [Lewin-Nam-Rougerie, 2015]. For $d = 1$ and w positive definite, for any $p \in \mathbb{N}$ we have $\gamma_{\tau,p} \to \gamma_p$ in trace class as $\tau \to \infty$.

Higher dimensions

If $d > 1$ then ϕ has μ_0-a.s. negative regularity, $\phi \notin L^2$, since $\sum_{k \in \mathbb{N}} \lambda_k^{-1} = \infty$.

Consequences:

- $W(\phi) = \frac{1}{2} \int \mathrm{d}x \, \mathrm{d}y \, w(x-y) |\phi(x)|^2 |\phi(y)|^2$ ill-defined even for $w \in L^\infty$.
- p-particle correlation functions γ_p are not in trace class, since

$$\mathrm{Tr}(\gamma_1) = \mathbb{E}^\mu \|\phi\|_{L^2}^2 = \infty \,.$$

- On the quantum side, rescaled number of particles $\mathcal{N}_\tau$ is no longer bounded. Explicit computation for noninteracting case $w = 0$:

$$\rho_\tau(\mathcal{N}_\tau) = \sum_{k \in \mathbb{N}} \frac{1}{\tau} \frac{1}{\mathrm{e}^{\lambda_k/\tau} - 1} \to \infty$$

  as $\tau \to \infty$. Quantum model has intrinsic cutoff at energies $\lambda_k \approx \tau$.

Heuristics:

Singularity of classical field $\iff$ Rapid growth of number of particles.

Renormalization

Renormalize interaction W by Wick ordering. Formally, take

$$W(\phi) = \frac{1}{2} \int \mathrm{d}x \, \mathrm{d}y \, w(x-y)(|\phi(x)|^2 - \infty)(|\phi(y)|^2 - \infty) \,.$$

Rigorously, introduce truncated field and density

$$\phi_{[K]} := \sum_{k=0}^{K} \frac{\omega_k}{\sqrt{\lambda_k}} u_k \,, \qquad \varrho_{[K]} := \mathbb{E}^{\mu_0} |\phi_{[K]}(x)|^2 \,.$$

Then

$$W_{[K]} := \frac{1}{2} \int \mathrm{d}x \, \mathrm{d}y \, w(x-y) \big(|\phi_{[K]}(x)|^2 - \varrho_{[K]} \big) \big(|\phi_{[K]}(x)|^2 - \varrho_{[K]} \big)$$

has a limit in $\bigcap_{p<\infty} L^p(\mu_0)$ as $K \to \infty$, denoted by W.

Use this W in definition of μ.

Similarly, we need to renormalize quantum interaction

$$\frac{1}{\tau} \sum_{1 \leqslant i < j \leqslant n} w(x_i - x_j)$$

to

$$W_\tau^{(n)} := \frac{1}{\tau} \sum_{1 \leqslant i < j \leqslant n} w(x_i - x_j) + \int w(x) \, \mathrm{d}x \left(-\varrho_\tau n + \frac{\tau}{2} \varrho_\tau^2 \right) I \,,$$

where

$$\varrho_\tau := \rho_\tau |_{w=0}(\mathcal{N}_\tau) = \sum_{k \in \mathbb{N}} \frac{1}{\tau} \frac{1}{\mathrm{e}^{\lambda_k / \tau} - 1}$$

is the quantum density. Note that $\varrho_\tau \to \infty$ as $\tau \to \infty$ for $d > 1$.

This gives the renormalized Hamilton operator

$$H_{\tau,0} + W_\tau = \frac{1}{\tau} \bigoplus_{n \geqslant 0} H_0^{(n)} + \frac{1}{\tau} \bigoplus_{n \geqslant 0} W_\tau^{(n)}$$

on Fock space $\mathcal{F}$.

Main result

For technical reasons, instead of $P_\tau = \mathrm{e}^{-H_{\tau,0} - W_\tau}$, we consider a family of modified thermal quantum states

$$P_\tau^\eta \;:=\; \mathrm{e}^{-\eta H_{\tau,0}} \mathrm{e}^{-(1-2\eta) H_{\tau,0} - W_\tau} \mathrm{e}^{-\eta H_{\tau,0}}\,, \qquad \eta \in [0,1)\,.$$

Theorem [Fröhlich-K-Schlein-Sohinger, 2016]. Let $d = 2, 3$, $w \in L^\infty$ positive definite, $\eta > 0$, and $p \in \mathbb{N}$. Then $\gamma_{\tau,p}^\eta \to \gamma_p$ in Hilbert-Schmidt as $\tau \to \infty$.

Remarks:

- Also works on $\mathbb{R}^d$ instead of $\mathbb{T}^d$, with sufficiently confining potential v in free Hamiltonian $\kappa - \Delta + v(x)$.

  On $\mathbb{R}^d$ the relation between original and renormalized problems is nontrivial and governed by counterterm problem, solved in [FKSS, 2016].

- Method works also for $d = 1$ and all $\eta \geqslant 0$: we recover result of Lewin-Nam-Rougerie by a completely different method.

Morsel of proof

Basic approach: perturbative expansion of partition functions $\mathbb{E}^{\mu_0}\mathrm{e}^{-zW}$ and $\mathrm{Tr}(\mathrm{e}^{-H_{\tau,0}-zW_\tau})$ in powers of z. Well-defined for $\mathrm{Re}\, z \geqslant 0$ but ill-defined for $\mathrm{Re}\, z < 0$: zero radius of convergence around $z = 0$.

Toy problem:

$$A(z) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{d}x\, \mathrm{e}^{-x^2/2}\, \mathrm{e}^{-zx^4}\,;$$

analytic for $\mathrm{Re}\, z > 0$ but zero radius of convergence, with Taylor coefficient $a_m = A^{(m)}(0)/m! \sim m!$.

However, Taylor series $\sum_{m\geqslant 0} a_m z^m$ has Borel transform $B(z) := \sum_{m\geqslant 0} \frac{a_m}{m!} z^m$ with positive radius of convergence. Formally, we can recover A from

$$A(z) = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-t} B(tz)\,.$$

Works provided we can prove good enough bounds on Taylor coefficients and remainder term of A (Sokal, 1980).

Main work: control of the coefficients and remainder of quantum many-body problem.