

Gibbs measures of nonlinear Schrödinger equations and many-body quantum mechanics

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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, Leibnitz rule in both arguments, Jacobi identity.)

Classical dynamics is given by **Hamiltonian flow** $\phi \mapsto S^t \phi$ on Γ defined by the ODE

$$\frac{d}{dt} f(S^t \phi) = \{H, f\}(S^t \phi)$$

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

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

The Gibbs measure at temperature β is

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

\mathbb{P} is invariant under the flow S^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 $\{\phi : \mathbb{T}^d \rightarrow \mathbb{C}\}$.
- Hamilton function

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

where $\kappa > 0$.

- Poisson bracket

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

Hamiltonian flow given by **time-dependent nonlinear Schrödinger equation**

$$i\partial_t \phi(x) = (\kappa - \Delta)\phi(x) + \int dy w(x-y)|\phi(y)|^2 \phi(x).$$

Time-dependent nonlinear Schrödinger equation

$$i\partial_t\phi(x) = (\kappa - \Delta)\phi(x) + \int dy w(x-y)|\phi(y)|^2\phi(x). \quad (1)$$

Gibbs measure of nonlinear Schrödinger equation is formally

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

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.

Goal

Analyse \mathbb{P} and (S^t) through

- the **moments** of \mathbb{P} (which determine \mathbb{P}),
- the **time-dependent correlation functions**

$$\int X^1(S^{t_1}\phi) \cdots X^m(S^{t_m}\phi) d\mathbb{P}(\phi),$$

for $X^i \in C^\infty(\Gamma)$ and $t_i \in \mathbb{R}$.

Derivation as a (high-temperature) limit of a microscopic n -body quantum theory of bosons.

Rigorous construction of Gibbs measure

Spectral decomposition

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

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 $\|\phi\|_{\mathcal{H}^s} := \|(\kappa - \Delta)^{s/2} \phi\|_{L^2}$ 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,

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

Under μ_0 , $\phi = \sum_{k \in \mathbb{N}} \frac{\omega_k}{\sqrt{\lambda_k}} u_k$ is a Gaussian free field with covariance $(\kappa - \Delta)^{-1}$:

$$\mathbb{E}^{\mu_0} \langle f, \phi \rangle \langle \phi, g \rangle = \langle f, (\kappa - \Delta)^{-1} g \rangle .$$

We find that

$$\mu_0[\phi \in \mathcal{H}^0] = \begin{cases} 1 & \text{if } d = 1 \\ 0 & \text{if } d > 1 . \end{cases}$$

Define the measure

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

μ is well-defined for instance if

$$d = 1, \quad w \in L^\infty, \quad w \text{ positive definite},$$

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

(Then \mathbb{P} is defined as $\phi_* \mu$.)

Quantum many-body theory

Define the **one-particle space** $\mathfrak{H} := L^2(\mathbb{T}^d; \mathbb{C})$ and the **n -particle space**

$$\mathfrak{H}^{(n)} := \mathfrak{H}^{\otimes_{\text{sym}} n} = L^2_{\text{sym}}((\mathbb{T}^d)^n).$$

Hamilton operator

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

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

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

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

What happens as $n \rightarrow \infty$?

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 and Fock space

Define the **Fock space** $\mathcal{F} := \bigoplus_{n \in \mathbb{N}} \mathfrak{H}^{(n)}$ and the **grand canonical thermal state**

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

Rescaled **particle number** operator $\mathcal{N}_\tau := \frac{1}{\tau} \bigoplus_{n \in \mathbb{N}} nI$. **Expectation** of an observable $A \in \mathfrak{B}(\mathcal{F})$ is

$$\rho_\tau(A) := \frac{\text{Tr}(AP_\tau)}{\text{Tr}(P_\tau)}.$$

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

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

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

Second quantization

Let b, b^* be the bosonic annihilation and creation operators on \mathcal{F} and set $\phi := \tau^{-1/2}b$. Hence,

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

Thus, we can write $H_\tau = H_{\tau,0} + W$, where

$$H_{\tau,0} = \int dx \phi_\tau^*(x) (\kappa - \Delta) \phi_\tau(x),$$
$$W_\tau = \frac{1}{2} \int dx dy \phi_\tau^*(x) \phi_\tau(x) w(x - y) \phi_\tau^*(y) \phi_\tau(y),$$

as well as $P_\tau = e^{-H_\tau}$, $\rho_\tau(A) = \frac{\text{Tr}(AP_\tau)}{\text{Tr}(P_\tau)}$.

High-temperature limit for $d = 1$

Define the p -particle reduced density matrix

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

Analogously, we define the classical p -particle correlation function

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

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 $\gamma_{\tau,p} \rightarrow \gamma_p$ in trace class as $\tau \rightarrow \infty$.

Time-dependent correlations

Introduce Hamiltonian **time evolution**:

(Cl) for a random variable $X \equiv X(\phi)$ set $\Psi^t X(\phi) := X(S^t \phi)$;

(Qu) for an operator \mathbf{X} on \mathcal{F} set $\Psi_\tau^t \mathbf{X} := e^{it\tau H_\tau} \mathbf{X} e^{-it\tau H_\tau}$.

For a p -particle operator ξ on $\mathfrak{H}^{(p)}$ introduce the observables

$$\begin{aligned} \text{(Cl)} \quad \Theta(\xi) &:= \int dx_1 \cdots dx_p dy_1 \cdots dy_p \xi(x_1, \dots, x_p; y_1, \dots, y_p) \\ &\quad \times \bar{\phi}(x_1) \cdots \bar{\phi}(x_p) \phi(y_1) \cdots \phi(y_p); \end{aligned}$$

$$\begin{aligned} \text{(Qu)} \quad \Theta_\tau(\xi) &:= \int dx_1 \cdots dx_p dy_1 \cdots dy_p \xi(x_1, \dots, x_p; y_1, \dots, y_p) \\ &\quad \times \phi_\tau^*(x_1) \cdots \phi_\tau^*(x_p) \phi_\tau(y_1) \cdots \phi_\tau(y_p). \end{aligned}$$

Theorem [Fröhlich-K-Schlein-Sohinger, 2017]. Let $d = 1$ and $w \in L^\infty$ be pointwise positive. Given $m \in \mathbb{N}$, $p_1, \dots, p_m \in \mathbb{N}$, $\xi^1 \in \mathcal{L}(\mathfrak{H}^{(p_1)}), \dots, \xi^m \in \mathcal{L}(\mathfrak{H}^{(p_m)})$ and $t_1, \dots, t_m \in \mathbb{R}$, we have

$$\lim_{\tau \rightarrow \infty} \rho_\tau(\Psi_\tau^{t_1} \Theta_\tau(\xi^1) \cdots \Psi_\tau^{t_m} \Theta_\tau(\xi^m)) = \mathbb{E}^\mu(\Psi^{t_1} \Theta(\xi^1) \cdots \Psi^{t_m} \Theta(\xi^m)).$$

Remarks:

- Also works on \mathbb{R} instead of \mathbb{T} , with sufficiently confining potential v in free Hamiltonian $\kappa - \Delta + v(x)$.
- We also prove that there exists a null sequence $\varepsilon = \varepsilon_\tau$ such that, with a quantum two-body potential $\frac{1}{\varepsilon} w\left(\frac{x}{\varepsilon}\right)$ the limit is that of the cubic NLS with local nonlinearity, $w = \delta$.

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:

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

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

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

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

as $\tau \rightarrow \infty$. 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

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

Rigorously, introduce truncated field and density

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

Then

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

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

Use this W in definition of μ .

Similarly, we need to renormalize the quantum interaction. The quantum Gibbs state is defined by the **renormalized many-body Hamiltonian** $H_\tau = H_{\tau,0} + W_\tau$, where

$$W_\tau := \frac{1}{2} \int dx dy (\phi_\tau^*(x)\phi_\tau(x) - \varrho_\tau(x)) w(x-y) (\phi_\tau^*(y)\phi_\tau(y) - \varrho_\tau(y)),$$

where the **quantum density at x** $\varrho_\tau(x)$ is defined as

$$\varrho_\tau(x) := \rho_{\tau,0}(\phi_\tau^*(x)\phi_\tau(x)).$$

Convergence of moments for $d = 2, 3$

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

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

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

Recent developments:

- [Sohinger, 2019] optimal integrability conditions [Bourgain, 1997] on w :
 $w \in L^1$ ($d = 1$), $w \in L^{1+}$ ($d = 2$), $w \in L^{3+}$ ($d = 3$).
- [Lewin-Nam-Rougerie, 2018] $\eta = 0$ for smooth w and $d = 2$.

Counterterm problem

Also works on \mathbb{R}^d with sufficiently confining potential V . Relation between original and renormalized problems is **nontrivial**. True Hamiltonian

$$\begin{aligned}\tilde{H}_\tau := & \int dx dy \phi_\tau^*(x) (\nu - \Delta + V)(x; y) \phi_\tau(y) \\ & + \frac{1}{2} \int dx dy \phi_\tau^*(x) \phi_\tau^*(y) w(x - y) \phi_\tau(x) \phi_\tau(y)\end{aligned}$$

compared with renormalized Hamiltonian (from above),

$$\begin{aligned}H_\tau = & \int dx \phi_\tau^*(x) (\kappa - \Delta + v_\tau) \phi_\tau(x) \\ & + \frac{1}{2} \int dx dy (\phi_\tau^*(x) \phi_\tau(x) - \varrho_\tau(x)) w(x - y) (\phi_\tau^*(y) \phi_\tau(y) - \varrho_\tau(y))\end{aligned}$$

Essentially, \tilde{H}_τ and H_τ are related by a shift in a diverging chemical potential, provided that one chooses the bare one-body potential v_τ appropriately (depending on τ).

More precisely, for any constant $\bar{\varrho}_\tau \in \mathbb{R}$ we have

$$\tilde{H}_\tau = H_\tau + \left[\bar{\varrho}_\tau \hat{w}(0) - \frac{1}{2\tau} w(0) + \nu - \kappa \right] \mathcal{N}_\tau - \frac{1}{2} \int dx dy \varrho_\tau(x) w(x-y) \varrho_\tau(y),$$

provided that v_τ solves the **counterterm problem**

$$v_\tau = V + w * (\varrho_\tau^{v_\tau} - \bar{\varrho}_\tau). \quad (2)$$

For $\varrho_\tau^{v_\tau} - \bar{\varrho}_\tau$ to remain bounded, we need $\lim_{\tau \rightarrow \infty} \bar{\varrho}_\tau = \infty$, and hence (for bracket to vanish) $\lim_{\tau \rightarrow \infty} \nu = -\infty$. (Compensates **large repulsive interaction energy**.)

The counterterm problem (2) is solved in [FKSS, 2016], where we also show that the solution v_τ converges (in a suitable space) to some $v =$ the correct **renormalized external potential**.

Morsels of proof

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

Toy problem:

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

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

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

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

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. Starting point for algebra is Wick's theorem for the free states.

For time-dependent problem, we perform an expansion of $\Psi_\tau^t \Theta_\tau(\xi) = e^{it\tau H_\tau} \Theta_\tau(\xi) e^{-it\tau H_\tau}$ in powers of the interaction potential w .

The expansion is controlled graphically, **tree graphs** sum up precisely to the quantization of $\Psi^t \Theta(\xi)$.

Problem: expansion is only convergent on sector of \mathcal{F} where \mathcal{N}_τ is bounded.

Introduce cutoff in rescaled number of particles \mathcal{N}_τ . Need to show that for $f \in C_c^\infty(\mathbb{R})$ we have

$$\lim_{\tau \rightarrow \infty} \rho_\tau(\Theta_\tau(\xi) f(\mathcal{N}_\tau)) = \mathbb{E}^\mu(\Theta(\xi) f(\mathcal{N})) \quad (3)$$

Problem: cutoff breaks Gaussianity, and Wick's theorem does not apply to (3).

Idea: using complex analysis, it suffices to analyse $\rho_\tau(\Theta_\tau(\xi) e^{-\nu \mathcal{N}_\tau})$ for fixed $\nu > 0$.