Gibbs measures of nonlinear Schrödinger equations as limits of many-body quantum states

Vedran Sohinger (University of Warwick)

Joint work with
Jürg Fröhlich (ETH Zürich),
Antti Knowles (University Geneva),
Benjamin Schlein (University of Zürich).

Cergy-Singapore-Warwick
Theoretical and Mathematical Physics workshop.
July 10, 2020.

The nonlinear Schrödinger equation

Consider the spatial domain $\Lambda = \mathbb{T}^d$ for $d = 1, 2, 3$.

- Study the ***nonlinear Schrödinger equation (NLS)***.

$$\begin{cases} \mathrm{i}\partial_t \phi_t(x) = \big(-\Delta/2 + \kappa\big)\phi_t(x) + \int \mathrm{d}y\, w(x-y)\, |\phi_t(y)|^2\, \phi_t(x) \\ \phi_0(x) = \Phi(x) \in H^s(\Lambda)\,. \end{cases}$$

- Parameter: $\kappa > 0$.
- Interaction: $w : \Lambda \to \mathbb{R}$ is of *positive type* $(\hat{w} \geqslant 0)$.
- Sobolev space H^s with norm $\|f\|_{H^s(\Lambda)} := \|(1-\Delta)^{s/2} f\|_{L^2(\Lambda)}$.
- Conserved energy

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

Gibbs measures for the NLS

- The ***Gibbs measure*** $\mathrm{d}\mu$ associated with H is the probability measure on the space of fields $\phi : \Lambda \to \mathbb{C}$

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

  $\mathrm{d}\phi =$ (formally-defined) Lebesgue measure.

- Formally, $\mathrm{d}\mu$ is invariant under the flow of the NLS:

$$(\mathrm{F}_t)_* \mathrm{d}\mu = \mathrm{d}\mu \,,$$

  where $\mathrm{F}_t :=$ flow map of NLS.

Gibbs measures for the NLS: known results

- **Rigorous construction of Gibbs measure:** CQFT literature in the 1970-s (Nelson, Glimm-Jaffe, Simon).
- **Proof of invariance:** Bourgain and Zhidkov (1990s).
  $\rightarrow$ Measure supported on low-regularity Sobolev spaces.
- **Application to PDE:** *Obtain low-regularity solutions of NLS μ-almost surely*.
  Recent advances: Bourgain-Bulut, Burq-Tzvetkov, Burq-Thomann-Tzvetkov, Cacciafesta- de Suzzoni, Deng-Nahmod-Yue, Fan-Ou-Staffilani-Wang, Genovese-Lucà-Valeri, Nahmod-Oh-Rey-Bellet-Staffilani, Nahmod-Rey-Bellet-Sheffield-Staffilani, Oh-Pocovnicu, Oh-Tzvetkov-Wang, Thomann-Tzvetkov, Tzvetkov, ...

Derivation of Gibbs measures: informal statement

NLS is a classical limit of many-body quantum theory.

- On $\mathfrak{H}^{(n)} \equiv L^2_{\mathrm{sym}}(\Lambda^n)$ we consider the n*-body Hamiltonian*

$$H^{(n)} := -\frac{1}{2}\sum_{i=1}^{n}\Delta_i + \frac{1}{n}\sum_{i,j=1}^{n} w(x_i - x_j)\,.$$

- Solve *n-body Schrödinger equation*

$$\mathrm{i}\partial_t \Psi_{n,t} = H^{(n)}\Psi_{n,t}\,.$$

  Obtain that, as $n \to \infty$

$$\Psi_{n,0} \sim \phi_0^{\otimes n} \quad \text{implies} \quad \Psi_{n,t} \sim \phi_t^{\otimes n}\,.$$

  (Hepp (1974), Ginibre-Velo (1979), Spohn (1980), Fröhlich-Tsai-Yau (1998), Fröhlich-Knowles-Pickl (2006), Erdős-Schlein-Yau (2006, 2007), Fröhlich-Graffi-Schwarz (2007), Fröhlich-Knowles-Schwarz (2009), T. Chen-Pavlović (2010), Pickl (2010), Ammari-Nier (2011), . . .).

- **Problem:** Obtain Gibbs measure $\mathrm{d}\mu$ as many-body quantum limit.

The Wiener measure and classical free field

- Let $H_0(\phi) := \int \mathrm{d}x \, (|\nabla\phi(x)|^2/2 + \kappa|\phi(x)|^2)$.
  Define the ***Wiener measure*** $\mathrm{d}\mu_0$

$$\mu_0(\mathrm{d}\phi) := \frac{1}{Z_0} \mathrm{e}^{-H_0(\phi)} \, \mathrm{d}\phi \,, \qquad Z_0 := \int \mathrm{e}^{-H_0(\phi)} \, \mathrm{d}\phi \,.$$

- For $\phi \in \operatorname{supp} \mathrm{d}\mu_0$,

$$\phi \equiv \phi^\omega \sim \sum_{k \in \mathbb{Z}^d} \frac{g_k(\omega)}{(|k|^2 + \kappa)^{1/2}} \, \mathrm{e}^{2\pi i k \cdot x} \,, \quad (g_k) = \text{i.i.d. complex Gaussians.}$$

  $\rightarrow$ ***Classical free field***.

- Series converges almost surely in $H^{1-\frac{d}{2}-\varepsilon}(\Lambda)$.

The classical system and Gibbs measures

- The *classical interaction* is

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

- In $[0, +\infty)$ almost surely if $d = 1$ and $w \in L^\infty(\mathbb{T}^1)$ is *of positive type* (or *pointwise nonnegative*).
- In this case $\mathrm{d}\mu$ is a well-defined probability measure on $H^{1/2-\varepsilon}(\mathbb{T}^1)$ which satisfies

$$\mathrm{d}\mu \ll \mathrm{d}\mu_0 \, .$$

- For $d = 2, 3$, W *is infinite almost surely* even if $w \in L^\infty(\mathbb{T}^d)$.

The classical system and Gibbs measures

- Perform a *renormalisation* in the form of ***Wick ordering***.

$$W^w := \frac{1}{2} \int \mathrm{d}x \, \mathrm{d}y \, \left(|\phi^\omega(x)|^2 - \infty\right) w(x-y) \left(|\phi^\omega(y)|^2 - \infty\right) \geqslant 0 \,.$$

- Classical Gibbs state $\rho(\cdot)$: Given $X \equiv X(\omega)$ a random variable, let

$$\rho(X) := \frac{\int X \, \mathrm{e}^{-W} \, \mathrm{d}\mu_0}{\int \mathrm{e}^{-W} \, \mathrm{d}\mu_0} = \int X \, \mathrm{d}\mu \,.$$

- On $\mathfrak{H}^{(p)} \equiv L^2_{\mathrm{sym}}(\Lambda^p)$ define the ***classical p-particle correlation function*** γ_p by its operator kernel

$$(\gamma_p)_{x_1,\dots,x_p;y_1,\dots,y_p} := \rho\left(\overline{\phi^\omega}(y_1) \cdots \overline{\phi^\omega}(y_p) \phi^\omega(x_1) \cdots \phi^\omega(x_p)\right) .$$

$\rightarrow$ μ is determined by $(\gamma_p)_p$.

The quantum problem

- Consider $d = 1$.
- Given $m > 0$ (mass of particles) and $\lambda > 0$ (coupling constant), we work with

$$H^{(n)} := \frac{1}{m} \sum_{i=1}^{n} \Big(-\frac{\Delta_i}{2} + \kappa\Big) + \frac{\lambda}{2} \sum_{i,j=1}^{n} w(x_i - x_j)\,.$$

- At inverse temperature $\beta \in (0, \infty)$, equilibrium of $H^{(n)}$ is governed by the *Canonical ensemble*

$$\frac{1}{Z_\beta^{(n)}} \mathrm{e}^{-\beta H^{(n)}}\,, \qquad Z_\beta^{(n)} := \operatorname{Tr} \mathrm{e}^{-\beta H^{(n)}}\,.$$

- Henceforth consider $\beta = 1$.
- We take $m = 1/\nu$ and $\lambda \sim \nu^2$ and analyse the regime $\nu \to 0$.
  This can be interpreted as a *mean-field/semiclassical limit*.

The quantum problem

- Work on the *Bosonic Fock space*

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

with *quantum Hamiltonian*

$$\mathbb{H}_\nu \equiv \mathbb{H}_{\nu,w} := \bigoplus_{n \in \mathbb{N}} H_\nu^{(n)} \,,$$

where

$$H_\nu^{(n)} := \nu \sum_{i=1}^{n} \Big(-\frac{\Delta_i}{2} + \kappa\Big) + \frac{\nu^2}{2} \sum_{i,j=1}^{n} w(x_i - x_j)\,.$$

- On $\mathcal{F}$ define the *grand canonical ensemble* by

$$\mathbb{P}_\nu := \frac{1}{Z_\nu} \bigoplus_{n \in \mathbb{N}} \mathrm{e}^{-H_\nu^{(n)}} \,, \qquad \mathrm{Tr}_{\mathcal{F}}\, \mathbb{P}_\nu = 1\,.$$

The quantum Gibbs state

- Work with *quantum fields (operator-valued distributions)* ϕ_ν, ϕ_ν^* on $\mathcal{F}$ that satisfy

$$[\phi_\nu(x), \phi_\nu^*(y)] = \nu\delta(x-y)\,, \quad [\phi_\nu(x), \phi_\nu(y)] = [\phi_\nu^*(x), \phi_\nu^*(y)] = 0\,.$$

Heuristic: $\phi_\nu \longleftrightarrow \phi^\omega$, $\phi_\nu^* \longleftrightarrow \overline{\phi^\omega}$.

- Quantum Gibbs state $\rho_\nu(\cdot)$: Given $\mathcal{A} \in \mathcal{L}(\mathcal{F})$ we define its expectation

$$\rho_\nu(\mathcal{A}) := \mathrm{Tr}_{\mathcal{F}}(\mathcal{A}\mathbb{P}_\nu)\,.$$

On $\mathfrak{H}^{(p)}$ define the ***quantum p-particle correlation function*** $\gamma_{\nu,p}$ by

$$(\gamma_{\nu,p})_{x_1,\ldots,x_p;y_1,\ldots,y_p} = \rho_\nu\big(\phi_\nu^*(y_1)\cdots\phi_\nu^*(y_p)\phi_\nu(x_1)\cdots\phi_\nu(x_p)\big)\,.$$

$\rightarrow \mathbb{P}_\nu$ is determined by $(\gamma_{\nu,p})_p$.

Main result

Theorem: Fröhlich, Knowles, Schlein, S. (Preprint, 2020).

Suppose that w is *continuous* and of *positive type*.

(i) We have $\mathcal{Z}_\nu \to \zeta$ as $\nu \to 0$, where

$$\mathcal{Z}_\nu := \frac{\operatorname{Tr}_{\mathcal{F}} \mathbb{H}_{\nu,w}}{\operatorname{Tr}_{\mathcal{F}} \mathbb{H}_{\nu,0}}, \qquad \zeta := \frac{\int \mathrm{e}^{-H(\phi)}\,\mathrm{d}\phi}{\int \mathrm{e}^{-H_0(\phi)}\,\mathrm{d}\phi}.$$

(ii) For $p \in \mathbb{N}$ we have

$$\gamma_{\nu,p} \xrightarrow{L^r} \gamma_p \quad \text{as} \quad \nu \to 0\,,$$

for optimal r.

$$r \in \begin{cases} [1,\infty]\,, & d=1 \\ [1,\infty)\,, & d=2 \\ [1,3)\,, & d=3\,. \end{cases}$$

Related results

- $1D$ results: previously shown using variational techniques by Lewin, Nam, Rougerie (J. Éc. Polytech. Math., 2015).
Higher dimensions: non local, non translation-invariant interactions.
Extensions in $1D$ in (JMP, 2018).
- Fröhlich, Knowles, Schlein, S. (CMP 2017): Translation-invariant interactions in $2D$ and $3D$ with modified Gibbs state. Perturbative techniques.
- Lewin, Nam, Rougerie (preprint 2018) : $2D$ problem with translation-invariant interaction without modified Gibbs state.
- S. (preprint 2019) : Unbouded interaction potentials in optimal L^p class.
- Lewin, Nam, Rougerie (preprint 2020) : Extension to $3D$.
- Fröhlich, Knowles, Schlein, S. (AIM 2019): time-dependent problem in $1D$. $\rightarrow$ *Corresponds to the invariance of the measure*.

The $\nu \to 0$ limit in the free case

Examine the limit $\nu \to 0$ in the *free case* $w = 0$.

- Define the *rescaled particle number operator* by

$$\mathcal{N}_\nu := \nu \bigoplus_{n \in \mathbb{N}} n \mathrm{I}_{\mathfrak{H}^{(n)}} = \int \mathrm{d}x \, \phi_\nu^*(x) \, \phi_\nu(x) \, .$$

- Compare with

$$\mathcal{N} := \int \mathrm{d}x \, |\phi^\omega(x)|^2 \, .$$

- We have

$$\rho_\nu(\mathcal{N}_\nu) \sim \sum_{k \in \mathbb{Z}^d} \frac{\nu}{\mathrm{e}^{\nu(|k|^2 + \kappa)} - 1} \sim \begin{cases} 1 & \text{if } d = 1 \\ \log \nu^{-1} & \text{if } d = 2 \\ \nu^{-1/2} & \text{if } d = 3 \, . \end{cases}$$

  $\rho_\nu(\cdot)$ has a *natural cut-off* for $|k| \geqslant \nu^{-1/2}$.

$\to$ *Need to renormalise when* $d = 2, 3$.

Idea of proof

Main idea: Use a *functional integral* formulation.
$\rightarrow$ Represent the field theory as a gas of *interacting Brownian loops and paths* : Ginibre (1965), Symanzik (1968).

Setting up the functional integral

(1) Hubbard-Stratonovich transformation: for a real Gaussian measure $\mu_{\mathcal{C}}$ with covariance $\mathcal{C}$ we have

$$\int \mu_{\mathcal{C}}(\mathrm{d}\sigma)\,\mathrm{e}^{\mathrm{i}\langle f,\sigma\rangle} = \mathrm{e}^{-\frac{1}{2}\langle f,\mathcal{C}f\rangle}\,.$$

(2) Feynman-Kac formula. The propagator satisfying

$$\partial_\tau W^{\tau,\tilde{\tau}} = \left(\frac{1}{2}\Delta + V(\tau)\right)W^{\tau,\tilde{\tau}}\,, \qquad W^{\tau,\tau} = 1$$

has operator kernel

$$W^{\tau,\tilde{\tau}}_{x,\tilde{x}} = \int \mathbb{W}^{\tau,\tilde{\tau}}_{x,\tilde{x}}(\mathrm{d}\omega)\,\mathrm{e}^{\int_{\tilde{\tau}}^{\tau}\mathrm{d}s\,V(s,\omega(s))}\,.$$

References and conclusion

References:

(i) J. Fröhlich, A. Knowles, B. Schlein, V. Sohinger, *The mean–field limit of quantum Bose gases at positive temperature*, preprint (2020), `https://arxiv.org/abs/2001.01546`.

(ii) J. Fröhlich, A. Knowles, B. Schlein, V. Sohinger, *A path-integral analysis of interacting Bose gases and loop gases*, preprint (2020), `https://arxiv.org/abs/2001.11714`. To appear in Journal of Statistical Physics.

Thank you for your attention!