Gibbs measures of nonlinear Schrödinger equations as limits of quantum many-body states in dimension $d \leqslant 3$.

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Hamiltonian systems

A general ***Hamiltonian system*** is comprised of the following.

(1) Phase space Γ. We denote its elements by ϕ.

(2) Hamilton (energy) function $H \in C^\infty(\Gamma)$.

(3) Poisson bracket $\{\cdot,\cdot\}$ defined on $C^\infty(\Gamma) \times C^\infty(\Gamma)$.

- Antisymmetric : $\{f,g\} = -\{g,f\}$.
- Distributive : $\{f+g,h\} = \{f,h\} + \{g,h\}$.
- Leibniz rule : $\{fg,h\} = \{f,h\}g + f\{g,h\}$.
- Jacobi identity : $\{f,\{g,h\}\} + \{g,\{h,f\}\} + \{h,\{f,g\}\} = 0$.

The ***Hamiltonian flow*** $\phi \mapsto \phi_t$ of H on Γ is determined by the ODE

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

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

NLS as a Hamiltonian system

Fix $\Lambda = \mathbb{R}^d$ or $\Lambda = \mathbb{T}^d$.

(1) Γ is the Sobolev space $H^s(\Lambda)$ with norm $\|f\|_{H^s(\Lambda)} := \|(1+|\xi|)^s \widehat{f}(\xi)\|_{L^2_\xi}$.

(2) Hamilton function is

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

(3) Poisson bracket is

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

Hamiltonian equations of motion are given by the ***nonlinear Hartree equation***

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

If $w = \delta$, this is the ***cubic nonlinear Schrödinger equation (NLS)***.

$$\mathrm{i}\partial_t \phi_t(x) + \Delta\phi_t(x) = |\phi_t(x)|^2 \, \phi_t(x) .$$

Gibbs measures for the NLS

- Fix $\Lambda = \mathbb{T}^d$ for $d = 1, 2, 3$ and $w \geqslant 0$.
- The ***Gibbs measure*** $\mathrm{d}\mu$ associated to 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.

- **Rigorous construction:** CQFT literature in the 1970-s (Nelson, Glimm-Jaffe, Simon), also Lebowitz-Rose-Speer (1988).
- **Proof of invariance:** Bourgain and Zhidkov (1990s).
- **Application to PDE:** *Obtain low-regularity solutions of NLS μ-almost surely*.
  Recent advances: Bourgain-Bulut, Burq-Thomann-Tzvetkov, Cacciafesta-de Suzzoni, Deng, Genovese-Lucà-Valeri, Nahmod-Oh-Rey-Bellet-Staffilani, Nahmod-Rey-Bellet-Sheffield-Staffilani, Oh-Quastel, Thomann-Tzvetkov, Tzvetkov, ...

The Wiener measure

- Define ***Wiener measure*** $\mathrm{d}\mu_0$

$$\mu_0(\mathrm{d}\phi) \;:=\; \frac{1}{Z_0}\mathrm{e}^{-\int \mathrm{d}x\; |\nabla\phi(x)|^2}\,\mathrm{d}\phi\,, \qquad Z_0 \;:=\; \int \mathrm{e}^{-\int \mathrm{d}x\; |\nabla\phi(x)|^2}\,\mathrm{d}\phi\,.$$

- Write $a_k := \widehat{\phi}(k)$ and $\mathrm{d}^2 a_k := \mathrm{d}\,\mathrm{Im} a_k \;\mathrm{d}\,\mathrm{Re} a_k$.

$$\mu_0(\mathrm{d}\phi) \;=\; \prod_{k \in \mathbb{Z}^d} \frac{\mathrm{e}^{-c|k|^2|a_k|^2}\mathrm{d}^2 a_k}{\int \mathrm{e}^{-c|k|^2|a_k|^2}\mathrm{d}^2 a_k}\,.$$

- For $\phi \in \operatorname{supp}\mathrm{d}\mu_0$, $|k|a_k = |k|\widehat{\phi}(k)$ *has a Gaussian distribution*.

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

$\rightarrow$ ***Gaussian free field***.

- Avoid problems with mode $k = 0$. For $\kappa > 0$ replace

$$\Delta \mapsto \Delta - \kappa, \qquad |k| \mapsto \sqrt{|k|^2 + \kappa}\,.$$

The Wiener measure

- **Question:** What is the Sobolev regularity of a typical element in the support of $\mathrm{d}\mu_0$?
- **Equivalent question:** What is the Sobolev regularity of ϕ^ω?
- Compute

$$\mathbb{E}_{\mu_0}\|\phi^\omega\|_{H^s}^2 = \sum_{k\in\mathbb{Z}^d}(|k|^2+1)^s\frac{\mathbb{E}_{\mu_0}\left(|g_k|^2\right)}{|k|^2+\kappa} \sim \sum_{k\in\mathbb{Z}^d}(|k|^2+1)^{s-1}\,.$$

  Finite if and only if $s<1-\frac{d}{2}$.
- One has

$$\mu_0(H^s) = \begin{cases}1 & \text{if} \quad s<1-\frac{d}{2}\\ 0 & \text{otherwise}\,.\end{cases}$$

- If $w \geqslant 0$ we expect Gibbs measure $\mathrm{d}\mu$ to be absolutely continuous with respect to $\mathrm{d}\mu_0$.

The classical system and Gibbs measures

- The *classical interaction* is $W := \frac{1}{2}\int \mathrm{d}x\,\mathrm{d}y\,|\phi^\omega(x)|^2\,w(x-y)\,|\phi^\omega(y)|^2$.
- Finite almost surely if $d=1$ and $w \in L^\infty(\mathbb{T})$.
- For $d=2,3$, W *is infinite almost surely* even if $w \in L^\infty(\mathbb{T}^d)$:
  Perform a *renormalization* in the form of ***Wick ordering***. Formally replace W by the *Wick-ordered classical interaction*

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

- Rigorously defined as limit in $\bigcap_{m\geqslant 1} L^m(\mathrm{d}\mu_0)$ of truncations

$$W_{[K]} := \frac{1}{2}\int \mathrm{d}x\,\mathrm{d}y\,\big(|\phi^\omega_{[K]}(x)|^2 - \varrho_K\big)\,w(x-y)\,\big(|\phi^\omega_{[K]}(y)|^2 - \varrho_K\big)\,,\text{ for}$$

$$\phi^\omega_{[K]}(x) := \sum_{|k|\,\leqslant\,K} \frac{g_k(\omega)}{\sqrt{|k|^2+\kappa}}\,\mathrm{e}^{2\pi i k\cdot x}\,, \qquad \varrho_K(x) := \mathbb{E}_{\mu_0}\,|\phi^\omega_{[K]}(x)|^2\,.$$

The classical system and Gibbs measures

- 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 the space

$$\mathfrak{H}^{(p)} := L^2_{\mathrm{sym}}\big((\mathbb{T}^d)^p\big) \, ,$$

define the ***classical p-particle correlation function*** γ_p by

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

Derivation of Gibbs measures: informal statement

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

- On $\mathfrak{H}^{(n)}$ we consider the n*-particle Hamiltonian*

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

- Solve *many-body Schrödinger equation* $\mathrm{i}\partial_t \Psi_{n,t} = H^{(n)} \Psi_{n,t}$ and obtain

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

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

- At temperature $\tau > 0$, equilibrium of $H^{(n)}$ is governed by the *Gibbs state*

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

- **Goal:** Obtain correlation functions γ_p in limit as $\tau = n \to \infty$.

The quantum problem: $d = 1$

- Consider first $d = 1$.
- Work on the *Bosonic Fock space*

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

with *quantum Hamiltonian*

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

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

$$P_\tau := \mathrm{e}^{-H_\tau} .$$

- Consider the ***p-particle correlation function of P_τ***

$$\gamma_{\tau,p} := \frac{1}{\mathrm{Tr}(P_\tau)} \sum_{n \geqslant p} \frac{n(n-1)\cdots(n-p+1)}{\tau^p} \mathrm{Tr}_{p+1,\ldots,n}\left(\mathrm{e}^{-H^{(n)}/\tau}\right) .$$

($\sim$ Quantum analogue of γ_p obtained from P_τ).

Second quantization

- Rewrite $\gamma_{\tau,p}$ using second-quantized notation.
- Introduce *quantum fields (operator-valued distributions)* ϕ_τ, ϕ_τ^* on $\mathcal{F}$ satisfying

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

- Given $\mathcal{A} \in \mathcal{L}(\mathcal{F})$ we define its expectation

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

- We can write

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

Derivation of Gibbs measures: statement of result

Theorem 1: Fröhlich, Knowles, Schlein, S. (preprint 2016; to appear in CMP).

Fix $w \in L^\infty(\mathbb{T}^d)$ with $w \geqslant 0$.

(i) [After Lewin-Nam-Rougerie (2015)]
Let $d = 1$. Then for all $p \in \mathbb{N}$ we have

$$\gamma_{\tau,p} \to \gamma_p \quad \text{as} \quad \tau \to \infty\,.$$

The convergence is in the trace class.

(ii) Let $d = 2, 3$. The convergence holds in the Hilbert-Schmidt class *after an appropriate renormalization procedure* and with a *slight modification of the grand canonical ensemble P_τ* (needed for technical reasons).

$1D$ result: previously shown using different techniques by Lewin-Nam-Rougerie (J. Éc. Polytech. Math., 2015). In higher dimensions, they consider non local, non translation-invariant interactions.
Lewin-Nam-Rougerie (2017) : $1D$ problem with subharmonic trapping.

The high-temperature limit in the free case

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

- Define the *rescaled particle number operator* by

$$\mathcal{N}_\tau \; := \; \frac{1}{\tau} \bigoplus_{n \in \mathbb{N}} n \mathrm{I}_{\mathfrak{H}^{(n)}} \; = \; \int \mathrm{d}x \, \phi_\tau^*(x) \, \phi_\tau(x) \, .$$

- We have

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

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

Renormalization in the quantum problem

Consider the quantum problem for $d = 2, 3$.

- On $\mathcal{F}$ define the *free quantum Hamiltonian*

$$H_{\tau,0} := \frac{1}{\tau} \bigoplus_{n \in \mathbb{N}} H_0^{(n)} ,$$

  where $H_0^{(n)} := \sum_{i=1}^n (-\Delta_{x_i} + \kappa)$.
- Given $\mathcal{A} \in \mathcal{L}(\mathcal{F})$ let

$$\rho_{\tau,0}(\mathcal{A}) := \frac{\mathrm{Tr}(\mathcal{A}\, \mathrm{e}^{-H_{\tau,0}})}{\mathrm{Tr}(\mathrm{e}^{-H_{\tau,0}})} .$$

- The *Wick-ordered many-body Hamiltonian* is

$$H_\tau := H_{\tau,0} + W_\tau , \quad \text{for}$$

$$W_\tau := \frac{1}{2} \int \mathrm{d}x \, \mathrm{d}y \, \big(\phi_\tau^*(x)\phi_\tau(x) - \varrho_\tau(x)\big) \, w(x-y) \, \big(\phi_\tau^*(y)\phi_\tau(y) - \varrho_\tau(y)\big) .$$

- $\varrho_\tau(x) := \rho_{\tau,0}\big(\phi_\tau^*(x)\phi_\tau(x)\big) = \varrho_\tau(0) \to \infty$ as $\tau \to \infty$.

Idea of the proof: perturbative expansion

- Our proof is based on a *perturbative expansion in the interaction*.
- **Example**: Consider the classical partition function

$$A(z) := \int \mathrm{e}^{-zW} \, \mathrm{d}\mu_0$$

and the quantum partition function

$$A_\tau(z) := \frac{\mathrm{Tr}\left(\mathrm{e}^{-\eta H_{\tau,0}} \, \mathrm{e}^{-(1-2\eta)H_{\tau,0} - zW_\tau} \, \mathrm{e}^{-\eta H_{\tau,0}}\right)}{\mathrm{Tr}(\mathrm{e}^{-H_{\tau,0}})}\,, \qquad \eta \in [0, 1/4]\,.$$

- Our goal is to prove that

$$\lim_{\tau \to \infty} A_\tau(z) = A(z) \text{ for } \mathrm{Re}\, z > 0\,.$$

- **Problem:** The series expansions

$$A(z) = \sum_{m=0}^{M-1} a_m z^m + R_M(z)\,, \quad A_\tau(z) = \sum_{m=0}^{M-1} a_{\tau,m} z^m + R_{\tau,M}(z)$$

have *radius of convergence zero*.

Idea of proof: Borel summation

- Recover $A(z), A_\tau(z)$ from their coefficients by ***Borel summation***.
- Given a formal power series

$$\mathcal{A}(z) \;=\; \sum_{m\geqslant 0} \alpha_m z^m$$

its *Borel transform* is

$$\mathcal{B}(z) \;:=\; \sum_{m\geqslant 0} \frac{\alpha_m}{m!} z^m\,.$$

Formally we have

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

- By a result of Sokal (1980) the method applies provided that

$$\begin{cases} |a_m| + |a_{\tau,m}| \;\leqslant\; C^m m! \\ |R_M(z)| + |R_{\tau,M}(z)| \;\leqslant\; C^M M! |z|^M \text{ for } \operatorname{Re} z \;\geqslant\; 0\,. \end{cases}$$

The quantum Wick theorem

- Compute $a_{\tau,m}$ by repeatedly applying Duhamel's formula.
- Rewrite $a_{\tau,m}$ using the *quantum Wick theorem*

$$\frac{1}{\mathrm{Tr}(\mathrm{e}^{-H_{\tau,0}})} \mathrm{Tr}\Big(\phi_\tau^*(x_1)\cdots\phi_\tau^*(x_k)\phi_\tau(y_1)\cdots\phi_\tau(y_k)\,\mathrm{e}^{-H_{\tau,0}}\Big)$$

$$= \sum_{\pi\in\mathcal{S}^k}\prod_{j=1}^{k}\frac{1}{\mathrm{Tr}(\mathrm{e}^{-H_{\tau,0}})}\mathrm{Tr}\Big(\phi_\tau^*(x_j)\phi_\tau(y_{\pi(j)})\,\mathrm{e}^{-H_{\tau,0}}\Big).$$

- Factors are

$$\frac{1}{\mathrm{Tr}(\mathrm{e}^{-H_{\tau,0}})}\mathrm{Tr}\Big(\phi_\tau^*(x)\phi_\tau(y)\,\mathrm{e}^{-H_{\tau,0}}\Big) = G_\tau(x;y)\,,$$

where

$$G_\tau = \frac{1}{\tau\big(\mathrm{e}^{(-\Delta+\kappa)/\tau}-1\big)}$$

is the *quantum Green function*.

The graph structure: Setup

- Obtain a *graph structure*.
- Each occurrence of $\phi^*_\tau(v)$ and $\phi_\tau(v)$ gives rise to a vertex. Join vertices according to quantum Wick theorem.
- Total number of graphs is at most $(2m)! = \mathcal{O}(C^m m!^2)$.
- Obtain gain of $\frac{1}{m!}$ from the time integral

$$\int_0^1 \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \cdots \int_0^{t_{m-1}} \mathrm{d}t_m = \frac{1}{m!}\,.$$

- Conclude that $|a_{\tau,m}| \leqslant C^m m!$.

The graph structure: Example

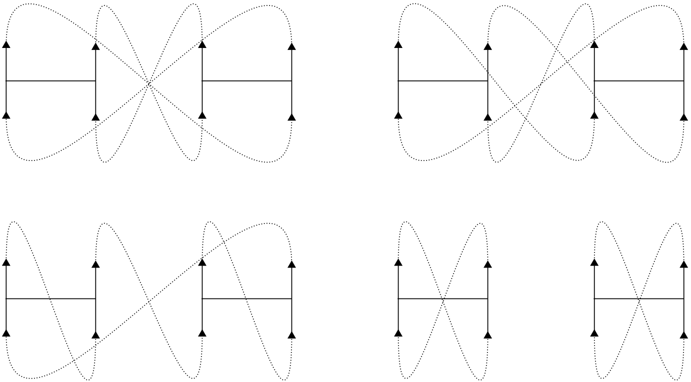

Figure: Some examples of the possible graphs when $m = 2$.

For $d = 2, 3$, no two vertically adjacent vertices are joined due to Wick ordering.

Time-dependent correlations

- Let $(\Gamma, H, \{\cdot,\cdot\})$ be a Hamiltonian system.
- $\mu(\mathrm{d}\phi) \;:=\; \frac{1}{Z}\mathrm{e}^{-H(\phi)}\,\mathrm{d}\phi$, the associated Gibbs measure.
- S_t := flow map of H.
- Given $m \in \mathbb{N}$, observables $X^1, \dots, X^m \in C^\infty(\Gamma)$, and times $t_1, \dots, t_m \in \mathbb{R}$, define the ***$m$-particle time-dependent correlation function***

$$\mathcal{Q}_\mu(X^1, \dots, X^m; t_1, \dots, t_m) \;:=\; \int X^1(S_{t_1}\phi) \cdots X^m(S_{t_m}\phi)\,\mathrm{d}\mu\,.$$

- **Goal:** Obtain a derivation of $\mathcal{Q}_\mu$ from quantum many-body expectation values in the setting where S_t *is the flow of the cubic NLS on* $\mathbb{T}^1$.
- S_t is globally defined on $\Gamma := L^2(\mathbb{T}^1)$ (Bourgain, 1993).

Time-dependent correlations

Given an observable $X \in C^\infty(\Gamma)$, define the *time-evolved observable* $\Psi^t X \in C^\infty(\Gamma)$ according to

$$\Psi^t X(\phi) \; := \; X(S_t \phi)\,.$$

Theorem 2: Fröhlich, Knowles, Schlein, S. (preprint 2017).

Given $m \in \mathbb{N}$, observables $X^j \in C^\infty(\Gamma)$ and times t_j, we have

$$\rho_\tau\Big(\Psi_\tau^{t_1} X_\tau^1 \cdots \Psi_\tau^{t_m} X_\tau^m\Big) \to \rho\Big(\Psi^{t_1} X^1 \cdots \Psi^{t_m} X^m\Big) \quad \text{as} \quad \tau \to \infty\,,$$

with appropriately defined quantum objects.

Theorem 1 in $1D$ corresponds to Theorem 2 with $m = 1$.

Idea of proof

- Use an approximation argument to reduce to showing that

$$\rho_\tau\Big(\Psi_\tau^{t_1} X_\tau^1 \cdots \Psi_\tau^{t_m} X_\tau^m F(\mathcal{N}_\tau)\Big) \to \rho\Big(\Psi^{t_1} X^1 \cdots \Psi^{t_m} X^m F(\mathcal{N})\Big)\,,$$

where $\mathcal{N} := \int \mathrm{d}x\, |\phi^\omega(x)|^2$ and $F \in C_c^\infty(\mathbb{R})$.

- Presence of cut-off F *does not allow direct application of Wick theorem*.
- Use the *Helffer-Sjöstrand formula* to write

$$F(\mathcal{N}_\sharp) \;=\; \frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}\zeta\, \frac{\partial_{\bar\zeta}\big[(f(u)+\mathrm{i}vf'(u))\chi(v)\big]}{\mathcal{N}_\sharp - \zeta}\,,$$

for $\zeta = u + \mathrm{i}v$ and appropriate $\chi \in C_c^\infty(\mathbb{R})$.

- Write for $\operatorname{Re}\zeta < 0$

$$\frac{1}{\mathcal{N}_\sharp - \zeta} \;=\; \int_0^\infty \mathrm{d}\nu\, \mathrm{e}^{\zeta\nu}\, \mathrm{e}^{-\nu\mathcal{N}_\sharp}\,.$$

Reduce to analysis from Theorem 1 with κ replaced by $\kappa + \nu$.

Thank you for your attention!