Mean-field limits for quantum systems and nonlinear Gibbs measures

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Mean-field limit

Linear Schrödinger equation in $\mathbb{R}^{dN}$

$$\left(\sum_{j=1}^{N}\Big(-\Delta_{x_j}+V(x_j)\Big)+\lambda\sum_{1\leq j<k\leq N}w(x_j-x_k)\right)\Psi=E\,\Psi$$

$$\Big\Downarrow \quad \begin{array}{l} N\to\infty \\ N\lambda\to 1\end{array}$$

Nonlinear Schrödinger equation in $\mathbb{R}^{d}$

$$\Big(-\Delta+V+|u|^2*w\Big)\,u=\varepsilon_0\,u$$

Gross-Pitaevskii, Hartree

Main (wrong) idea: $\Psi(x_1,...,x_N)\approx\prod_{j=1}^{N}u(x_j)=:u^{\otimes N}(x_1,...,x_N)$ [I.I.D.]

Mean-field limit II

- **Mean-field models**
  - statistical mechanics (Curie-Weiss for Ising)
  - many-body systems, quantum chemistry
  - biology, social sciences, economy (mean-field games), etc

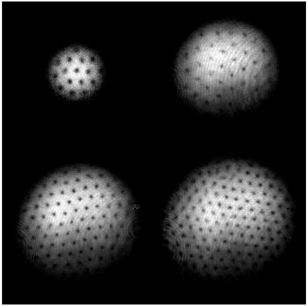
- **Rigorous mean-field limits:**
  - classical/quantum, stationary/time-dependent
  - time-dependent quantum: Hepp, Ginibre-Velo, Spohn, Erdös-Schlein-Yau, ...
  - stationary quantum: **Lieb** with Benguria, Seiringer, Solovej, Yau, Yngvason

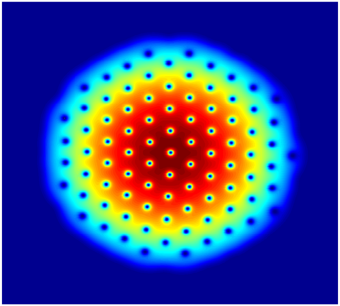
- **This talk:**
  - new method with Phan Thành Nam (Munich) and Nicolas Rougerie (Lyon)
  - (non-commutative) probabilistic tool: quantum de Finetti theorem
  - nonlinear Gibbs measures

Bose-Einstein Condensates

At very low temperature, **condensation** of Bose gases (e.g. ^{4}He, sodium)

Bose '24, Einstein '25





Left: Experimental pictures of fast rotating Bose-Einstein condensates. Ketterle *et al* at MIT in 2001
Right: Simulation of Gross-Pitaevskii equation with software GPELab (Antoine & Duboscq)

- well described by nonlinear Gross-Pitaevskii equation
- crystallization conjecture for vortices
- in experiments, rather dilute regime (Lieb-Seiringer-Yngvason 2000–10)
- nonlinear Gibbs measure = formation of BEC close to critical temperature

X. Blanc, M. Lewin. The Crystallization Conjecture: A Review, *EMS Surv. Math. Sci.* (2015)

Convergence of minimum

$$H_{N,\lambda} = \sum_{j=1}^{N} \Big(-\Delta_{x_j} + V(x_j) \Big) + \lambda \sum_{1\leq j<k\leq N} w(x_j - x_k)$$

$$\mathcal{E}(u) = \int_{\mathbb{R}^d} |\nabla u(x)|^2 \,\mathrm{d}x + \int_{\mathbb{R}^d} V(x)|u(x)|^2 \,\mathrm{d}x + \frac{1}{2} \iint_{\mathbb{R}^{2d}} |u(x)|^2 |u(y)|^2 w(x-y) \,\mathrm{d}x \,\mathrm{d}y$$

$$E(N,\lambda) := \min \sigma(H_{N,\lambda}) = \inf_{\|\Psi\|=1} \langle \Psi, H_{N,\lambda}\Psi\rangle, \qquad e_{\rm GP} := \inf_{\|u\|=1} \mathcal{E}(u)$$

Theorem (convergence of minimum LNR14)

- **(confined case)** *$w, V_- \in (L^p + L^\infty)(\mathbb{R}^d,\mathbb{R})$ with $p=1$ if $d=1$, $p>1$ if $d=2$ and $p=d/2$ if $d\geq 3$, $V_+ \in L^1_{loc}(\mathbb{R}^d,\mathbb{R})$ with $V_+ \to +\infty$;*
- **(unconfined or locally confined case)** *$V, w \in (L^p + L^\infty)(\mathbb{R}^d,\mathbb{R})$ with p as above, and $V, w \to 0$ at infinity*

$$\lim_{\substack{N\to\infty \\ \lambda N \to 1}} \frac{E(N,\lambda)}{N} = e_{\rm GP}.$$

M. Lewin, P. T. Nam, N. Rougerie. Derivation of Hartree's theory for generic mean-field Bose systems, *Adv. Math.* (2014)

Convergence of minimum II

- Many similar results in literature for particular models

Lieb-Benguria '83, Lieb-Yau '87, Lieb-Seiringer-Yngvason '00s

- **Exact upper bound** $E(N,\lambda) \leq N\, e_{\rm GP}$ when $\lambda = \frac{1}{N-1}$

$$E(N,\lambda) \leq \left\langle u^{\otimes N}, H_{N,\lambda} u^{\otimes N}\right\rangle$$
$$= N\left(\int_{\mathbb{R}^d} |\nabla u|^2 + V|u|^2 + \frac{\lambda(N-1)}{2}\iint_{\mathbb{R}^{2d}} |u(x)|^2|u(y)|^2 w(x-y)\,{\rm d}x\,{\rm d}y\right)$$

- **Lower bound** relatively easy if $\widehat{w} \geq 0$

$$\sum_{1\leq j<k\leq N} w(x_j-x_k) = \frac12 \iint_{\mathbb{R}^d} w(x-y)\left(\sum_{j=1}^N \delta_{x_j}-\eta\right)(x)\left(\sum_{j=1}^N \delta_{x_j}-\eta\right)(y)$$
$$+\sum_{j=1}^N w*\eta(x_j) - \frac12\iint_{\mathbb{R}^{2d}} \eta(x)\eta(y)w(x-y)\,{\rm d}x\,{\rm d}y - \frac{N}{2}w(0)$$

"Onsager argument" (1939) $\equiv$ "Linear programming bounds" (Cohn-Kumar, 2007)

- General w: elementary proof in ICM proceedings, following Lieb-Yau '87

Convergence in sense of density matrices

kth "density matrix" on $L^2(\mathbb{R}^{dk})$ of symmetric Ψ

$$\Gamma^{(k)}_\Psi(X,Y) := \frac{N!}{(N-k)!}\int_{(\mathbb{R}^d)^{N-k}} \Psi(X,Z)\overline{\Psi(Y,Z)}\,dZ$$

- $\operatorname{tr}\Gamma^{(k)}_\Psi = \frac{N!}{(N-k)!}$ and $\|\Gamma^{(k)}_\Psi\| \leq \frac{N!}{(N-k)!}$ but usually bounded in large systems
- $\Gamma^{(k)}_{u^{\otimes N}} = \frac{N!}{(N-k)!}|u^{\otimes k}\rangle\langle u^{\otimes k}| \sim N^k |u^{\otimes k}\rangle\langle u^{\otimes k}|$

Theorem (Convergence LNR14)

Assume $\langle \Psi_N, H_{N,\lambda}\Psi_N\rangle = E(N,\lambda) + o(N)$. In the **confined case**, *there exists a probability measure μ on $\mathcal{M} = \{$minimizers for $e_{\rm GP}\}$ such that for a subsequence*

$$(N_j)^{-k}\Gamma^{(k)}_{\Psi_{N_j}} \longrightarrow \int_{\mathcal{M}} |u^{\otimes k}\rangle\langle u^{\otimes k}|\,d\mu(u), \qquad \forall k\geq 1,$$

strongly in trace norm. Same in **unconfined or locally-confined case**, *with weak-$*$ limit and $\mathcal{M} = \{$weak limits of minimizing sequences for $e_{\rm GP}\}$.*

Proof: quantum de Finetti + many-body localization techniques + tools from calculus of variations ($\approx$ concentration-compactness)

Quantum de Finetti

Penrose–Onsager (1956) predicted that $\Gamma_\Psi^{(k)} \sim N^k$ only for with $u^{\otimes k}$

Theorem ('weak' quantum de Finetti LNR14)

Let Ψ_N be any sequence of normalized symmetric functions on $(\mathbb{R}^d)^N$. Assume

$$N^{-k}\Gamma_{\Psi_N}^{(k)} \underset{*}{\rightharpoonup} \Upsilon^{(k)}, \qquad \forall k \geq 1, \quad \textit{weakly-}* \textit{ in trace.}$$

Then there exists a probability measure μ on $\mathcal{B} = \{\|u\|_{L^2} \leq 1\}$ such that

$$\Upsilon^{(k)} = \int_{\mathcal{B}} |u^{\otimes k}\rangle\langle u^{\otimes k}| \, \mathrm{d}\mu(u), \qquad \forall k \geq 1.$$

Convergence holds in trace norm for one (hence all) $k \geq 1$, if and only if μ concentrates on the unit sphere $\mathcal{S} = \{\|u\|_{L^2} = 1\}$.

- non-commutative+weak-limit version of de Finetti '31, Hewitt-Savage '55
- 'strong' version on $\mathcal{S}$ due to Størmer '69, Hudson-Moody '75
- important in quantum information theory
- Ammari-Nier '08: semi-classical analysis in infinite dimension

Convergence of Ψ_N: Bogoliubov theory

Theorem (Bogoliubov's theory LNSS15)

In **confined case**, *assume* $e_{\rm GP}$ *admits a* **unique** *and* **non-degenerate** *minimizer* u_0 *(modulo phase). Then, for any given* $j \geq 1$ *the* j*th eigenvalue (counted with multiplicity) satisfies*

$$\lim_{\substack{N\to\infty \\ \lambda=\frac{1}{N-1}}} \Big(\lambda_j(H_{N,\lambda}) - Ne_{\rm GP}\Big) = \lambda_j(\mathbb{H}_0)$$

where $\mathbb{H}_0$ *is the Bogoliubov Hamiltonian on Fock space* $\mathcal{F} = \bigoplus_{n\geq 0}\bigotimes_s^n\{u_0\}^\perp$, *that is, the second-quantization of* $\mathrm{Hess}_{u_0}\mathcal{E}\big|_{\{u_0\}^\perp}$.
Any corresponding sequence of eigenfunctions (Ψ_N) *satisfies (up to extraction)*

$$\lim_{N\to\infty}\left\|\Psi_N - \sum_{n=0}^N \varphi_n \otimes_s (u_0)^{\otimes N-n}\right\|_{L^2(\mathbb{R}^{dN})} = 0$$

where $\mathbb{H}_0\Phi = \lambda_j(\mathbb{H}_0)\Phi$ *and* $\Phi = (\varphi_n)_{n\geq 0}$, *with* $\varphi_n \in \bigotimes_s^n\{u_0\}^\perp$.

- previous works by Lieb-Solovej '04, Seiringer '11
- impressive recent developments by Fournais-Solovej '20, Schlein *et al* '20

M. Lewin, P. T. Nam, S. Serfaty & J. P. Solovej, Bogoliubov spectrum of interacting Bose gases, *Comm. Pure Appl. Math.* (2015)

Nonlinear (non-Gaussian) Gibbs measures

$$d\mu(u) = \text{``}\, z^{-1} \exp\Big(-\mathcal{E}(u) - \kappa \int_{\mathbb{R}^d} |u|^2 \Big)\, \mathrm{d}u \,\text{''}$$

- **Difficulties:** $\mathcal{E}(u) = \infty$ and often $\int_{\mathbb{R}^d} |u|^2 = \infty$, μ–a.s.

In $d \geq 2$, μ concentrates on singular distributions $\rightsquigarrow$ renormalization

- (more and more) used in different areas of mathematics, e.g.
  - **PDE** to construct solutions to NLS equation, for rough initial data
    Lebowitz-Rose-Speer '88, Bourgain '90s, ...
  - **SPDE** to construct solutions of rough equations (with noise)
    Hairer, Kupiainen, Mourrat-Weber '10s, ...
  - **Euclidean Quantum Field Theory** through a Feyman-Kac type formula
    Symanzik, Glimm-Jaffe-Spencer, Nelson, Guerra-Rosen-Simon '70s, ...
  - **Critical phenomena in statistical mechanics** like BEC

- **Construction of μ:** $\mathcal{E}(u) =$ quadratic $+$ quartic and start with Gaussian part

Gaussian part μ_0 of μ

$$d\mu_0(u) = \text{“}\, z_0^{-1} e^{-\langle u, (-\Delta+V+\kappa)u\rangle} du\, \text{”} = \bigotimes_j \frac{(\lambda_j+\kappa)e^{-(\lambda_j+\kappa)|u_j|^2}}{\pi} du_j$$

with $(-\Delta+V)v_j = \lambda_j v_j$, $u_j = \langle v_j, u\rangle$ and $\kappa > -\lambda_1$

Properties

Assume $C^{-1}|x|^s - C \leq V(x) \leq C(1+|x|^s)$ with $s > 0$, and $\kappa > -\lambda_1$.

- We always have $\int_{\mathbb{R}^d} |\nabla u|^2 = \int_{\mathbb{R}^d} V|u|^2 = +\infty$ μ_0–a.s.
- If $d = 1$, $u \in H^{1/2-}_{\rm loc}(\mathbb{R})$ μ_0–a.s. We have $\int_{\mathbb{R}} |u|^2 < +\infty$ μ_0–a.s. iff $s > 2$
- If $d \geq 2$, μ_0 concentrates on distributions of negative regularity $< 1 - d/2$
- If $d \in \{1,2,3\}$ and $s > \frac{2d}{4-d}$ then, with $P_J =\perp$ proj. on span$(v_1, ..., v_J)$,

$$M_{\rm ren}(u) := \lim_{J\to\infty} \left(\|P_J u\|^2_{L^2(\mathbb{R}^d)} - \left\langle \|P_J u\|^2_{L^2(\mathbb{R}^d)} \right\rangle_{\mu_0} \right) \quad \text{exists in } L^2(d\mu_0), \quad \text{[Wick]}$$

$$\int M_{\rm ren}(u)^2\, d\mu_0(u) = \mathrm{tr}(-\Delta+V)^{-2} < \infty$$

Nelson '66, Glimm-Jaffe '87

(Renormalized) Nonlinear Gibbs measure

Corollary

Assume $C^{-1}|x|^s - C \leq V(x) \leq C(1+|x|^s)$ *with* $s>0$, *and* $\kappa > -\lambda_1$.

- *If* $d=1$, $s>2$ *and* $w \in (L^1+L^\infty)(\mathbb{R}^d,\mathbb{R})$ *with* $w \geq 0$ *or* $\widehat{w} \geq 0$, *then*

$$0 \leq \mathcal{I}(u) := \frac{1}{2}\iint_{\mathbb{R}^{2d}} |u(x)|^2|u(y)|^2 w(x-y)\,\mathrm{d}x\,\mathrm{d}y \in L^1(\mathrm{d}\mu_0)$$

hence $z := \int e^{-\mathcal{I}(u)}\mathrm{d}\mu_0(u) > 0$ *and* $\mathrm{d}\mu := z^{-1}e^{-\mathcal{I}(u)}\mathrm{d}\mu_0$ *is well defined.*

- *If* $d \in \{1,2,3\}$, $s > \frac{2d}{4-d}$ *and* $0 \leq \widehat{w} \in L^1(\mathbb{R}^d,\mathbb{R})$, *then*

$$0 \leq \mathcal{I}_{\mu_0}(u) := \lim_{J\to\infty} \frac{1}{2}\iint_{\mathbb{R}^{2d}} \left(|P_Ju(x)|^2 - \left\langle|P_Ju(x)|^2\right\rangle_{\mu_0}\right) \times \left(|P_Ju(y)|^2 - \left\langle|P_Ju(y)|^2\right\rangle_{\mu_0}\right) w(x-y)\,\mathrm{d}x\,\mathrm{d}y$$

exists in $L^1(\mathrm{d}\mu_0)$, *hence* $\mathrm{d}\mu := z^{-1}e^{-\mathcal{I}_{\mu_0}(u)}\mathrm{d}\mu_0$ *is well defined.*

Nelson '66, Glimm-Jaffe '87, Bourgain '97

Convergence in 1D

Averaged (grand-canonical) kth density matrix

$$\Gamma^{(k)}_{\kappa,\lambda,\beta}(X,Y) := \frac{\displaystyle\sum_{n\geq k} e^{-\beta\kappa n}\frac{n!}{(n-k)!}\int_{(\mathbb{R}^d)^{n-k}} e^{-\beta H_{n,\lambda}}(X,Z;Y,Z)\mathrm{d}Z}{\displaystyle\sum_{n\geq 0} e^{-\beta\kappa n}\int_{(\mathbb{R}^d)^{n}} e^{-\beta H_{n,\lambda}}(Z;Z)\mathrm{d}Z}$$

(same as replacing V by $V+\kappa$)

Theorem (Convergence in 1D, LNR15)

Let $d=1$ and $V\sim|x|^s$ as before with $s>2$. Assume $w\in(L^1+L^\infty)(\mathbb{R}^d)$ with either $w\geq 0$ or $\widehat{w}\geq 0$. We have for any fixed $\kappa>-\lambda_1(-\Delta+V)$

$$\lambda^k\Gamma^{(k)}_{\kappa,\lambda,\beta} \underset{\substack{\lambda\to 0\\ \beta\sim\lambda}}{\longrightarrow} \int_{\mathcal{M}} |u^{\otimes k}\rangle\langle u^{\otimes k}|\,\mathrm{d}\mu(u), \qquad \forall k\geq 1,$$

strongly in the trace-class, where $\mathrm{d}\mu = z^{-1}e^{-\mathcal{I}(u)}\mathrm{d}\mu_0$ with μ_0 the Gaussian measure of covariance $(-\Delta+V+\kappa)^{-1}$.

Extensions by Fröhlich-Knowles-Schlein-Sohinger (incl. time-dependent)

M. Lewin, P. T. Nam & N. Rougerie. Derivation of nonlinear Gibbs measures from many-body quantum mechanics, *J. Éc. polytech. Math.* (2015)

Convergence to renormalized measure in 2D and 3D

Theorem (Convergence in 2D–3D, LNR21/FKSS21)

Let $d \in \{2,3\}$ *and* $V \sim |x|^s$ *as before with* $s > \frac{2d}{4-d}$. *Assume* $\widehat{w}, |k|^2\widehat{w} \in L^1(\mathbb{R}^d)$ *with* $\widehat{w} \geq 0$. *For fixed* κ *large enough we have in Hilbert-Schmidt norm*

$$\lambda^k \Gamma^{(k)}_{\kappa_\lambda,\lambda,\beta} \underset{\substack{\lambda\to 0\\ \beta\sim\lambda}}{\longrightarrow} \int_{\mathcal{M}} |u^{\otimes k}\rangle\langle u^{\otimes k}|\, \mathrm{d}\mu_{\rm ren}(u), \qquad \forall k \geq 1,$$

$$\kappa_\lambda := \begin{cases} \kappa - \dfrac{\log(\kappa\lambda)^{-1}}{4\pi} \int_{\mathbb{R}^d} w & (d=2)\\[2mm] \kappa - \left(\dfrac{\zeta(3/2)}{8\pi^{\frac{3}{2}}\sqrt{\lambda}} - \dfrac{\sqrt{\kappa}}{4\pi}\right)\int_{\mathbb{R}^d} w & (d=3)\end{cases}$$

Here $\mathrm{d}\mu_{\rm ren} = z^{-1}e^{-\mathcal{I}_{\mu_0}(u)}\mathrm{d}\mu_0$ *with* $\mathcal{I}_{\mu_0}$ *the Wick-renormalized interaction and* μ_0 *the Gaussian measure of covariance* $(-\Delta + V_0 + \kappa)^{-1}$, *where* V_0 *is the unique solution to the nonlinear equation*

$$V_0(x) = V(x) + \int_{\mathbb{R}^d} w(x-y)\Big\{(-\Delta + V_0 + \kappa)^{-1} - (-\Delta+\kappa)^{-1}\Big\}(y,y)\,\mathrm{d}y$$

Rmk. $\mathcal{I}_{\mu_0}(u) + \langle u, (-\Delta + V_0 + \kappa)u\rangle = \mathcal{E}(u) + (\kappa - \alpha)\int_{\mathbb{R}^d}|u|^2 + \beta$ with $\alpha, \beta = +\infty$

M. Lewin, P. T. Nam & N. Rougerie. Classical field theory limit of many-body quantum Gibbs states in 2D and 3D, *Invent. Math.* (2021)
J. Fröhlich, A. Knowles, B. Schlein & V. Sohinger, The mean-field limit of quantum Bose gases at positive temperature, *J. Amer. Math. Soc.* (2021)

Strategy & Conclusion

- **Strategy:**
  - variational characterization, for both μ_{ren} and quantum state
  - reduction to finite dim. using strong subadditivity of entropy (Lieb-Ruskai '73)
  - quantum de Finetti in finite dim. with quantitative errors [$\sim$semiclassics]
  - **difficulty:** control interaction [divergent terms compensating each other]
  - new quantum correlation inequalities

- **Conclusion:**
  - **quantum de Finetti** provides new and more conceptual interpretation of condensation
  - **new results for Bose gases** when married with techniques from calculus of variations & PDEs
  - **big open problems:**
    1. Gibbs measures in dilute regime
    2. going outside of mean-field and dilute regimes