Derivation of nonlinear Gibbs measures from quantum mechanics

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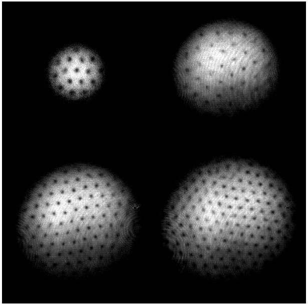
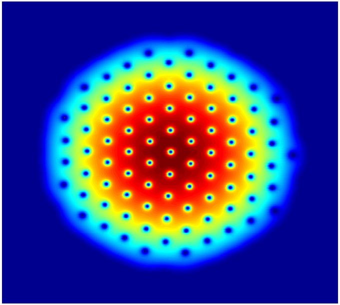
TexAMP, April 2021

Bose-Einstein condensates

- Ultra-cold Bose gases well described by nonlinear Gross-Pitaevskii equation

$$\Big(-\Delta + V(x) + w * |u|^2\Big) = \begin{cases} \lambda u \\ i\partial_t u \end{cases}$$





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 (X. Antoine & R. Duboscq)

Here: associated nonlinear Gibbs measure, describing the formation of the BEC close to the critical temperature

Classical Gibbs measures

- **Classical Hamiltonian** $H(x,p) = |p|^2 + V(x)$

Gibbs (probability) measure

$$\mu(x,p) = Z^{-1} \exp\left(-\frac{H(x,p)}{T}\right) \qquad \text{with} \qquad Z = \iint \exp\left(-\frac{H(x,p)}{T}\right)\, dx\, dp$$

invariant under Hamiltonian flow (Newton's equations)

$$\begin{cases} \dot{x} = \nabla_p H(x,p) \\ \dot{p} = -\nabla_x H(x,p) \end{cases}$$

unique solution to Gibb's variational problem

$$\min_{\substack{f \geq 0 \\ \int f = 1}} \left\{ \int H\, f + T \int f \log f \right\} = -T \log\left(\int e^{-H/T} \right) = -T \log Z$$

Infinite-dimensional Gibbs measures

$$\mathcal{E}(u) = \int_\Omega \left(|\nabla u(x)|^2 + V(x)|u(x)|^2\right)\,dx + \frac{1}{2}\int_\Omega\int_\Omega w(x-y)|u(x)|^2|u(y)|^2\,dx\,dy$$

- $\Omega \subset \mathbb{R}^d$, bounded or not
- V=external potential, confining if Ω unbounded
- w interaction potential

Nonlinear Gibbs measure

$$d\mu(u) = \text{``}Z^{-1}\,e^{-\mathcal{E}(u)}\,du\text{''}$$

formally invariant under Hamiltonian flow ($\Re(u)$ & $\Im(u)$)

$$i\partial_t u = \big(-\Delta + V + |u|^2 * w\big)\,u$$

▶ **Difficulty:** μ singular object, $\mathcal{E}(u) = \infty$ and often $\int_\Omega |u|^2 = \infty$, μ–a.s.

Use of nonlinear measures

$$d\mu(u) = \text{“}Z^{-1}\, e^{-\mathcal{E}(u)}\, du\text{”}$$

- **PDE** to construct solutions to NLS equation, for rough initial data
  Lebowitz-Rose-Speer '88, Bourgain '90s, Burq-Thomann-Tzvetkov '00s,...
- **SPDE** to construct solutions of rough equations (with noise)
  Hairer '10s, ...
- **Euclidean Quantum Field Theory** through a Feyman-Kac type formula
  Glimm-Jaffe '70s, ...
- **Critical phenomena in statistical mechanics** like BEC
  see e.g. books by Zinn-Justin, ...

▶ **Main goal:** Derivation from 'microscopic' (bosonic) Hamiltonian

$$H_{n,\lambda} = \sum_{j=1}^{n} (-\Delta)_{x_j} + V(x_j) + \lambda \sum_{1\leq j<k\leq n} w(x_j - x_k) \qquad \text{acting on } L^2_s(\Omega^n)$$

mean-field limit $\lambda \to 0$ equivalent to zooming at the **BEC phase transition**

Simplification for the talk

Ω =unit cube with periodic boundary conditions and $V \equiv \kappa \geq 0$

μ as an absolutely continuous measure w.r.t. μ_0

Nonlinear term

$$\mathcal{I}(u) := \frac{1}{2}\int_\Omega\int_\Omega |u(x)|^2|u(y)|^2 w(x-y)\,dx\,dy$$

- start with $w \equiv 0$ and define μ relatively to the free measure μ_0

$$d\mu(u) = \frac{e^{-\int_\Omega |\nabla u|^2+\kappa|u|^2-\mathcal{I}(u)}\,du}{\int e^{-\int_\Omega |\nabla u|^2+\kappa|u|^2-\mathcal{I}(u)}\,du}$$

$$= \underbrace{\frac{\int e^{-\int_\Omega |\nabla u|^2+\kappa|u|^2}\,du}{\int e^{-\int_\Omega |\nabla u|^2+\kappa|u|^2-\mathcal{I}(u)}\,du}}_{(z_r)^{-1}} \times e^{-\mathcal{I}(u)} \times \underbrace{\frac{e^{-\int_\Omega |\nabla u|^2+\kappa|u|^2}\,du}{\int e^{-\int_\Omega |\nabla u|^2+\kappa|u|^2}\,du}}_{\substack{:=d\mu_0(u) \\ \textbf{Gaussian (Wiener) measure}}}$$

- $z_r = \int e^{-\mathcal{I}(u)}\,d\mu_0(u) \in [0,1]$ in repulsive case $\mathcal{I}(u) \geq 0$
- $z_r > 0$ iff $\mathcal{I}(u)$ is finite on a set of positive μ_0-measure

Gaussian measures in infinite dimensions

$A > 0$ self-adjoint with compact resolvent on Hilbert space $\mathfrak{H}$, $Av_j = \lambda_j v_j$

Theorem (Gaussian measures)

$$d\nu(u) = \text{“}\frac{e^{-\langle u,Au\rangle}}{\int_{\mathfrak{H}} e^{-\langle u,Au\rangle}\,du}\text{”} = \bigotimes_{j\geq 1}\left(\frac{\lambda_j}{\pi}e^{-\lambda_j|u_j|^2}\,du_j\right), \qquad u_j = \langle v_j, u\rangle \in \mathbb{C}$$

is a well-defined probability measure on $\mathfrak{H} \iff \mathrm{tr}(A^{-1}) = \sum_{j\geq 1}\frac{1}{\lambda_j} < \infty$.

Theorem (Zero-one law for Gaussian measures)

Let $B > 0$ be another self-adj. operator on $\mathfrak{H}$. Then we have

- **either** $\int_{\mathfrak{H}} e^{\varepsilon\langle u,Bu\rangle}\,d\nu(u) < \infty$ *for some* $\varepsilon > 0$*;*
- **or** $\langle u, Bu\rangle = +\infty$ ν*–a.s.*

The two alternatives can be detected by looking at $\int_{\mathfrak{H}} \langle u, Bu\rangle\,d\nu(u) = \mathrm{tr}(BA^{-1})$

Examples: ▶ $B = 1$, ▶ $B = A \Rightarrow \langle u, Au\rangle = +\infty$ ν–a.s.

Skorokhod, *Integration in Hilbert space* (1974). Bogachev, *Gaussian measures* (1998)

Gaussian measures: application to $A = -\Delta + \kappa$

- Since we have **periodic BC**

$$\mathrm{tr}_{L^2(\Omega)}(-\Delta+\kappa)^{-1} = \sum_{k\in 2\pi\mathbb{Z}^d} \frac{1}{|k|^2+\kappa} < \infty \text{ only in 1D}$$

μ_0 well-defined on $L^2(\Omega)$ only in 1D

- For $d \geq 2$, change ambient Hilbert space

$$\langle u, Au\rangle = \left\langle A^{-\frac{\alpha}{2}}u, A^{1+\alpha}A^{-\frac{\alpha}{2}}u\right\rangle := \left\langle u, A^{1+\alpha}u\right\rangle_{H^{-\alpha}}$$

Theorem (Free Gibbs measure)

Gaussian measure μ_0 of $A = -\Delta + \kappa$ is well defined on H^s for all $s < 1 - d/2$ and all $\kappa > 0$. We have $\|u\|_{H^s} = +\infty$ μ_0–almost surely for all $s \geq 1 - d/2$.

- $\displaystyle\int_\Omega |u(x)|^2\,dx = +\infty$ for $d \geq 2$, $\displaystyle\int_\Omega |\nabla u(x)|^2\,dx = +\infty$ for $d \geq 1$

Nonlinear Gibbs measures: 1D case

Nonlinear term

$$\mathcal{I}(u) := \frac{1}{2}\int_\Omega\int_\Omega |u(x)|^2|u(y)|^2 w(x-y)\,dx\,dy$$

- **1D case:** μ_0 concentrated on H^s for all $s < 1/2$, hence on L^p for all $1 \leq p < \infty$

Theorem (1D case)

Let $d = 1$ and $w \in \mathcal{M}^1 + L^\infty$ with $w \geq 0$ or $\widehat{w} \geq 0$ so that $\mathcal{I} \geq 0$. Then $\mu = (z_r)^{-1}e^{-\mathcal{I}}\mu_0$ well defined in 1D. If $w = \lambda\delta$ with $\lambda < \lambda_c$, then $\mu = (z_r)^{-1}e^{+\mathcal{I}}\mu_0$ is also well-defined.

Lebowitz-Rose-Speer, *J. Statist. Phys.*, 1988

- **Dimensions $d \geq 2$:** $\mathcal{I}$ never well defined for $w \neq 0$, renormalization needed

Renormalized mass for $d = 2, 3$

$$\int \|P_N u\|^2 d\mu_0(u) = \int_{P_N\mathfrak{H}} \Big(\sum_{j=1}^N |u_j|^2\Big) \prod_{j=1}^N \frac{\lambda_j e^{-\lambda_j |u_j|^2}}{\pi}\, du_j = \sum_{n=1}^N \frac{1}{\lambda_j} = \mathrm{tr}(P_N A^{-1}) \to +\infty$$

Definition (Renormalized=Wick-ordered mass)

$$\mathcal{M}_N(u) := \|P_N u\|^2 - \int \|P_N u\|^2 d\mu_0(u) = \sum_{j=1}^N \left(|u_j|^2 - \frac{1}{\lambda_j}\right)$$

$$\int \Big(\mathcal{M}_N(u) - \mathcal{M}_K(u)\Big)^2 d\mu_0(u) = (\cdots) = \sum_{j=K+1}^N \frac{1}{(\lambda_j)^2}$$

Theorem (Renormalized mass)

If $\mathrm{tr}(A^{-2}) < \infty$, then $\mathcal{M}_N$ converges strongly in $L^2(H^s, d\mu_0)$ to $\mathcal{M}_{\rm ren}$ called the renormalized mass. We have $\int e^{\beta \mathcal{M}_{\rm ren}(u)}\, d\mu_0(u) < \infty$ for every $\beta < \lambda_1(A)$.

- $\mathrm{tr}(-\Delta + \kappa)^{-2} < \infty$ in dimensions $d = 1, 2, 3$
- Similar renormalization for $\langle u, Bu\rangle$ if $\mathrm{tr}(B^* A^{-1} B A^{-1}) < \infty$

Renormalized interaction for $d = 2, 3$

Theorem (Wick-renormalized interaction)

We assume that $\widehat{w} \geq 0$ *and* $w \in L^p(\mathbb{R}^d)$ *for* $1 < p \leq \infty$ *if* $d = 2$ *and* $3 < p \leq \infty$ *if* $d = 3$. *Then*

$$\mathcal{I}_N(u) := \frac{1}{2} \iint_{\Omega\times\Omega} \left(|P_N u(x)|^2 - \left\langle |P_N u(x)|^2 \right\rangle_{\mu_0} \right) \times \\ \times \left(|P_N u(y)|^2 - \left\langle |P_N u(y)|^2 \right\rangle_{\mu_0} \right) w(x-y)\, dx\, dy \geq 0$$

converges strongly to a limit $\mathcal{I}_{\rm ren}(u) \geq 0$ *in* $L^1(H^s, d\mu_0)$, *with*

$$\int \mathcal{I}_{\rm ren}(u)\, d\mu_0(u) = \frac{1}{2} \iint_{\Omega\times\Omega} w(x-y) |G_\kappa(x,y)|^2\, dx\, dy$$

where G_κ *is the Green's function of* $-\Delta + \kappa$ *on* Ω.

$$d\mu := z_r^{-1} e^{-\mathcal{I}_{\rm ren}(u)} d\mu_0(u), \qquad z_r := \int e^{-\mathcal{I}_{\rm ren}(u)} d\mu_0(u)$$

Rmk. There is a **renormalized time-dependent G-P equation**, well-posed in H^s, for which μ is invariant. Bourgain '94–99

Quantum model and the mean-field limit

- To get μ we have to work in Fock space $\mathcal{F} := \mathbb{C} \oplus \bigoplus_{n\geq 1} L^2_s(\Omega^n)$,

$$\mathbb{H}_\lambda = \bigoplus_{n\geq 0} \underbrace{\left(\sum_{j=1}^n (-\Delta+\kappa)_{x_j} + \lambda \sum_{1\leq j<k\leq n} w(x_j-x_k) \right)}_{H_{n,\lambda}} = \mathbb{H}_0 + \lambda \mathbb{W}$$

$$= \int_\Omega a^\dagger(x)(-\Delta_x+\kappa)a(x)\,dx + \frac{\lambda}{2} \iint_{\Omega\times\Omega} a^\dagger(x)a^\dagger(y)w(x-y)a(x)a(y)\,dx\,dy$$

- **2D/3D:** replace $a^\dagger(x)a(x)$ by $a^\dagger(x)a(x) - \left\langle a^\dagger(x)a(x)\right\rangle_{\text{free}}$ which amounts to

$$H^{\text{ren}}_{n,\lambda} = \sum_{j=1}^n \Big(-\Delta + \kappa - \delta_\kappa(\lambda)\widehat{w}(0) \Big)_{x_j} + \lambda \sum_{1\leq j<k\leq n} w(x_j-x_k) + \frac{\delta_\kappa(\lambda)^2 \widehat{w}(0)}{2\lambda}$$

$$\delta_\kappa(\lambda) := \lambda \sum_{k\in 2\pi\mathbb{Z}^2} \frac{1}{e^{\lambda(|k|^2+\kappa)}-1} \underset{\lambda\to 0}{\sim} \begin{cases} \frac{\log(\lambda^{-1})}{4\pi} & \text{(2D)} \\ \frac{\zeta(3/2)}{8\pi^{\frac32}} \lambda^{-\frac12} & \text{(3D)} \end{cases}$$

Quantum states

$\Gamma_\lambda = e^{-\lambda \mathbb{H}^{\text{ren}}_\lambda}/Z_\lambda$ with $Z_\lambda = \operatorname{tr}_{\mathcal{F}}\left[e^{-\lambda \mathbb{H}^{\text{ren}}_\lambda}\right]$, $\Gamma_0 = Z_0^{-1} e^{-\lambda \mathbb{H}_0}$, $Z_0 = \operatorname{tr}_{\mathcal{F}}\left[e^{-\lambda\mathbb{H}_0}\right]$

- k-particle density matrix: $\Gamma^{(k)}_\lambda = Z_\lambda^{-1} \sum_{n\geq k} \frac{n!}{(n-k)!} \operatorname{tr}_{k+1,\dots,N}\left[e^{-\lambda H_{n,\lambda}}\right]$

Convergence

Theorem (Derivation of μ)

Let $\kappa > 0$, $\widehat{w} \geq 0$ with $w \in \mathcal{M}^1 + L^\infty$ in 1D and $(1+|k|^2)\widehat{w}(k) \in \ell^1$ in 2D/3D.

$$\lim_{\lambda\to 0} \frac{Z_\lambda}{Z_0} = z_r = \int e^{-\mathcal{I}_{\rm ren}(u)}\, d\mu_0(u)$$

$$\lim_{\lambda\to 0} \lambda^k \Gamma_\lambda^{(k)} = \int |u^{\otimes k}\rangle\langle u^{\otimes k}|\, d\mu(u), \qquad \forall k \geq 1$$

in trace (1D) or Hilbert-Schmidt (2D/3D) norm. The moments on the right characterize the measure μ.

- More complicated for other boundary conditions or in a confining potential. Need to use reference Gaussian measure solving nonlinear equation of Hartree type
- **1D case:** M.L., Nam, Rougerie, *J. Éc. polytech. Math.*, 2015
- **1D and 2D/3D with modified quantum state:** Fröhlich, Knowles, Schlein, Sohinger, *Comm. Math. Phys.*, 2017
- **2D case:** LNR, ArXiv 2018
- **2D/3D case:** LNR, *Invent. Math.*, 2021. FKSS, *ArXiV*, 2020
- **1D time-dependent:** FKSS, *Adv. Math.* 2019

Gaussian measures / free Bose gas phase transition

Noninteracting bosons in a large cube $C_L = (-L/2, L/2)^d$ with periodic BC, at temperature T and chemical potential $-\tilde\kappa < 0$

- **Microscopic scale:**
  - grand-canonical one-particle density matrix is $\tilde\gamma_L = \left(e^{\frac{-\Delta_L+\tilde\kappa}{T}} - 1\right)^{-1}$
  - nb of particles per unit volume

$$\frac{1}{L^d}\sum_{k\in 2\pi\mathbb{Z}^d/L}\frac{1}{e^{\frac{|k|^2+\tilde\kappa}{T}}-1} \underset{L\to\infty}{\longrightarrow} \frac{T^{\frac{d}{2}}}{(2\pi)^d}\int_{\mathbb{R}^d}\frac{dk}{e^{k^2+\widetilde\kappa/T}-1}$$

  - critical density $\rho_c(T) = \frac{T^{\frac{d}{2}}}{(2\pi)^d}\int_{\mathbb{R}^d}\frac{dk}{e^{k^2}-1} = \begin{cases} +\infty & d=1,2 \\ \frac{T^{\frac{d}{2}}\zeta\left(\frac{d}{2}\right)}{2^d\pi^{\frac{d}{2}}} < \infty & d\geq 3\end{cases}$
  - **Canonical case:** imposing $\rho > \rho_c(T)$ gives macroscopically occupied mode

$$\tilde\gamma_L^{\rm can} \simeq \underbrace{L^d(\rho-\rho_c(T))|L^{-\frac{d}{2}}\rangle\langle L^{-\frac{d}{2}}|}_{\rm BEC} + \frac{1}{e^{\frac{-\Delta_{\mathbb{R}^d}}{T}}-1}$$

- **Emergence of BEC:** take $\tilde\kappa_L \to 0^+$ and look at macroscopic scale $y = x/L$

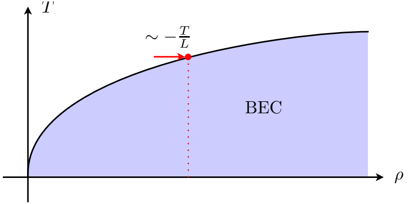
Thirring, Quantum Mathematical Physics

- **Macroscopic scale (in $\Omega = C_1$):** $\gamma_L = \left(e^{\frac{-\Delta_1 + L^2\tilde\kappa_L}{TL^2}} - 1\right)^{-1}$

$$\tilde\kappa_L := \frac{\kappa}{L^2}, \qquad \lambda = \frac{1}{TL^2} \to 0$$

$$\lambda\gamma_L = \frac{\lambda}{e^{\lambda(-\Delta_1+\kappa)} - 1} \underset{L\to\infty}{\longrightarrow} \frac{1}{-\Delta_1 + \kappa} = \int |u\rangle\langle u| \, d\mu_0(u)$$

$$\text{density} = \begin{cases} c_\kappa TL + o(L) & \text{1D} \\ \frac{T}{2\pi}\log(L) + O(1) & \text{2D} \\ \rho_c(T) - c_\kappa \frac{T}{L} + o(L^{-1}) & \text{3D} \end{cases}$$



Conclusion

- Chemical potential of order $-\kappa/L^2$ corresponds to zooming at transition
- Gaussian measure μ_0 with covariance $(-\Delta + \kappa)^{-1}$ on $\Omega = C_1$ describes system at macroscopic scale
- Our result for the interacting system in Ω corresponds to a microscopic interaction $L^{-4}w(x/L)$ living at macro scale but small in intensity

Strategy: variational, based on entropy

$$-\log \operatorname{tr} e^{-A} = \min_{\substack{M\geq 0\\ \operatorname{tr} M=1}} \Big\{ \operatorname{tr}(AM) + \operatorname{tr}(M\log M)\Big\} \qquad \rightsquigarrow M_0 = \frac{e^{-A}}{\operatorname{tr}(e^{-A})}$$

$$-\log \frac{\operatorname{tr} e^{-A-B}}{\operatorname{tr} e^{-A}} = \min_{\substack{M\geq 0\\ \operatorname{tr} M=1}} \Big\{ \underbrace{\mathcal{H}(M,M_0)}_{\operatorname{tr} M(\log M - \log M_0)} + \operatorname{tr}(BM)\Big\} \qquad \rightsquigarrow M = \frac{e^{-A-B}}{\operatorname{tr}(e^{-A-B})}$$

quantum relative entropy

$$-\log z_r = -\log\left(\int e^{-\mathcal{I}_{\rm ren}(u)}\,d\mu_0(u)\right)$$

$$= \min_{\nu \text{ probability measure}} \Big\{ \underbrace{\mathcal{H}_{\rm cl}(\nu,\mu_0)}_{\int \left(\frac{d\nu}{d\mu_0}\right)\log\left(\frac{d\nu}{d\mu_0}\right)d\mu_0} + \int \mathcal{I}_{\rm ren}(u)\,d\nu(u)\Big\} \qquad \rightsquigarrow \mu$$

classical relative entropy

Semi-classical / de Finetti measures

$$\lambda\mathbb{H}_\lambda = \lambda\int_\Omega a^\dagger(x)(-\Delta_x+\kappa)a(x)\,dx + \frac{\lambda^2}{2}\iint_{\Omega\times\Omega} a^\dagger(x)a^\dagger(y)w(x-y)a(x)a(y)\,dx\,dy$$

- **∞-dim. semi-classical analysis = quantum Hewitt-Savage/de Finetti**

A priori bounds on density matrices $\Longrightarrow \exists\nu$ such that

$$\operatorname*{weak\,lim}_{\lambda\to0} \lambda^k\Gamma^{(k)}_\lambda = \int |u^{\otimes k}\rangle\langle u^{\otimes k}|\,d\nu(u) \qquad \forall k\geq 1$$

Ammari-Nier 2008, M.L.-Nam-Rougerie '2014

- Show that ν solves variational problem for μ. Lower bound relies on:
  1. Monotonicity of relative entropy + Berezin-Lieb-type inequalities (any $d\geq1$):

$$\liminf_{\lambda\to0}\mathcal{H}(\Gamma_\lambda,\Gamma_0)\geq\mathcal{H}_{\rm cl}(\nu,\mu_0)$$

M.L.-Nam-Rougerie '2015

  2. Interaction is wlsc

$$\liminf_{\lambda\to0}\lambda^2\,{\rm tr}(\mathbb{W}_{\rm ren}\Gamma_\lambda)\geq\int\mathcal{I}_{\rm ren}(u)\,d\nu(u)$$

In 1D: Fatou since PDM bounded in trace-class and $\mathbb{W}\geq0$
Very difficult in 2D/3D: $\mathbb{W}_{\rm ren}$ contains divergent terms which are supposed to cancel each other

New correlation inequality

Lower bound on interaction energy requires to control high energy two-particle correlations

Lemma (Controlling variance by first moments)

$$\frac{\mathrm{tr}\left(A^2 e^{-H}\right)}{\mathrm{tr}(e^{-H})} \leq \frac{2(1+a^2+\eta^2)}{a}\eta\, e^{a\eta}$$

for all $a > 0$ and all bounded operator A, where

$$\eta := \sup_{\varepsilon\in[-a,a]} \frac{\left|\mathrm{tr}\left(Ae^{-H+\varepsilon A}\right)\right|}{\mathrm{tr}(e^{-H+\varepsilon A})} + a\big\|[[H,A],A]\big\|\sqrt{1+\|A\|^2},$$

- Think of $A \rightsquigarrow A - \dfrac{\mathrm{tr}(Ae^{-H})}{\mathrm{tr}(e^{-H})}$ so that the first term in the sup is small
- We typically apply this to $A = a_k^\dagger a_k$ for large momentum k, which gives us access to the 2-PDM