# Nonlinear Gibbs measures and their derivation from many-body quantum mechanics

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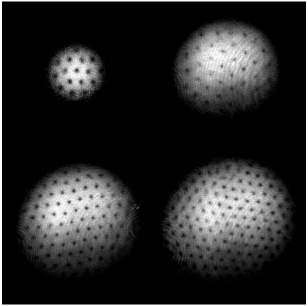
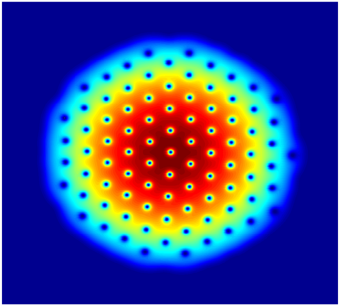
# Bose-Einstein condensates

- Ultra-cold BEC 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 and their derivation

# 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

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

- $\Omega =$ bounded domain $\subset \mathbb{R}^d$, boundary conditions
- $V$=external potential, here often $V \equiv \kappa$
- $w \geq 0$, e.g. $w = \delta_0 \rightsquigarrow$ defocusing NLS

**Nonlinear Gibbs measure**

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

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

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

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

# Bibliography

- **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, ...

▶ Derivation of Hartree from the many-particle (bosonic) Hamiltonian

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

- **Time-Dependent Hartree** from $i\dot{\Psi} = H_{n,\lambda}\Psi$
  Hepp '77, Ginibre-Velo '79, Spohn '80, Erdos-Schlein-Yau '00s, ...
- **Hartree minimizers** from 1st eigenvalue of $H_{n,\lambda}$
  Benguria-Lieb '83, Lieb-Yau '87, Petz-Raggio-Verbeure-Werner '90s, Lieb-Seiringer-Yngvason '00s, Lewin-Nam-Rougerie '14, ...
- **Gibbs measures** from quantum Gibbs states of $H_{n,\lambda}$
  Lewin-Nam-Rougerie '15–18, Fröhlich-Knowles-Schlein-Sohinger '16–17...

| | **Canonical** | **Grand-canonical** |
|---|---|---|
| Mean-field limit: | $n \to \infty$ | average over $n$, then $\langle n \rangle \to \infty$ |
| | $\lambda \sim 1/n$ | $\lambda \sim 1/\langle n \rangle$ |

# $\mu$ as an absolutely continuous measure w.r.t. $\mu_0$

## 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 $\mu$ relatively to the free measure $\mu_0$

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

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

**Gaussian (Wiener) measure**

- $z_r = \int e^{-\mathcal{I}(u)}\,d\mu_0(u) \in [0,1]$ since $w \geq 0$
- $z_r > 0$ iff $\mathcal{I}(u)$ is finite on a set of positive $\mu_0$-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** $\langle u, Bu\rangle = +\infty$ *$\nu$–a.s.*

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

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

Bogachev, *Gaussian measures*, no. 62, Amer. Math. Soc., 1998

# Gaussian measures: application to $A = -\Delta$

For simplicity, we take $V(x) \equiv \kappa$ chosen such that $-\Delta + V > 0$ on $\Omega$

## Periodic BC

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

finite only for $d = 1$ $\rightsquigarrow$ $\mu_0$ well-defined on $\mathfrak{H} = L^2(\Omega)$

- For $d \geq 2$, change ambient Hilbert space $\langle u, (-\Delta+\kappa)u\rangle = \left\langle (-\Delta+\kappa)^{-\frac{\alpha}{2}}u, (-\Delta+\kappa)^{1+\alpha}(-\Delta+\kappa)^{-\frac{\alpha}{2}}u\right\rangle := \left\langle u, (-\Delta+\kappa)^{1+\alpha}u\right\rangle_{H^{-\alpha}}$

## Theorem (Free Gibbs measure)

*For any self-adjoint boundary condition, the Gaussian measure $\mu_0$ of $A = -\Delta + \kappa$ is well defined on $H^s$ for all $s < 1 - d/2$ and all $\kappa > -\lambda_1(-\Delta)$. We have $\|u\|_{H^s} = +\infty$ $\mu_0$–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:** $\mu_0$ concentrated on $H^s$ for all $s < 1/2$, hence on $L^p$ for all $1 \leq p < \infty$

**Theorem (1D case)**

*$\mu = (z_r)^{-1}e^{-\mathcal{I}}\mu_0$ well defined in 1D for all $0 \leq w \in \mathcal{M}^1 + L^\infty$.*

*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, Statistical mechanics of the nonlinear Schrödinger equation, *J. Statist. Phys.*, 1988

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

# 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)

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

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

## 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 $d = 1, 2, 3$ on $\Omega$
- Can similarly renormalize any $\langle u, Bu\rangle$ for $\mathrm{tr}(B^* A^{-1} B A^{-1}) < \infty$

# Renormalized interaction for $d = 2, 3$

**Theorem (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* $G_\kappa$ *is the Green's function of* $-\Delta + \kappa$ *on* $\Omega$.

- In 2D one can also handle $w = \delta$ with slightly different coefficients
- There is a "renormalized" time-dep G-P equation which is well-posed in $H^s$ and for which $\mu$ is invariant. Bourgain '94–99

# Quantum model and the mean-field limit

- Many-particle Hamiltonian:

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

- Grand-canonical quantum partition function

$$Z_\lambda(T) := \sum_{n \ge 0} \operatorname{tr}_{L^2_s(\Omega)} \exp\left( -\frac{H_{n,\lambda}}{T} \right)$$

**Theorem (Derivation of $\mu$ in 1D)**

*Assume that* $0 \le w \in \mathcal{M}^1 + L^\infty$ *and* $d = 1$. *Then*

(*i*)
$$\lim_{\substack{T \to \infty \\ \lambda T \to 1}} \frac{Z_\lambda(T)}{Z_0(T)} = z_r = \int_{L^2(\Omega)} e^{-\mathcal{I}(u)} \, d\mu_0(u)$$

(*ii*)
$$\lim_{\substack{T \to \infty \\ \lambda T \to 1}} \frac{1}{T^k Z_\lambda(T)} \sum_{n \ge k} \frac{n!}{(n-k)!} \underbrace{\operatorname{tr}_{k+1,\dots,N} \left[ e^{-\frac{H_{\lambda,n}}{T}} \right]}_{\text{reduced density matrix}} = \int_{L^2(\Omega)} |u^{\otimes k}\rangle\langle u^{\otimes k}| \, d\mu(u)$$

*strongly in the trace class, for every* $k \ge 1$.

M.L., Nam, Rougerie, Derivation of nonlinear Gibbs measures from many-body quantum mechanics, *J. Éc. polytech. Math.*, 2015

▶ Many-particle renormalized Hamiltonian:

$$H^{\rm ren}_{n,\lambda} = \sum_{j=1}^{n} \Big( -\Delta + \kappa - 2\pi\lambda\rho_0(T)\widehat{w}(0) \Big)_{x_j} + \lambda \sum_{1\le j<k\le n} w(x_j - x_k) + \rho_0(T)^2 \lambda\pi\widehat{w}(0)$$

where $\rho_0(T) := \dfrac{1}{4\pi^2} \displaystyle\sum_{k\in 2\pi\mathbb{Z}^2} \frac{1}{e^{\frac{|k|^2+\kappa}{T}} - 1}$ $\Longleftrightarrow$ renormalization of $\kappa$

## Theorem (Derivation of $\mu$ in 2D)

*Periodic boundary conditions, $\Omega$ =unit cube. Assume that $0 \le (1+|k|)\widehat{w}(k) \in \ell^1$ and $d = 2$. Then*

(*i*)
$$\lim_{\substack{T\to\infty \\ \lambda T \to 1}} \frac{Z^{\rm ren}_\lambda(T)}{Z_0(T)} = z_r = \int e^{-\mathcal{I}_{\rm ren}(u)}\, d\mu_0(u)$$

(*ii*)
$$\lim_{\substack{T\to\infty \\ \lambda T \to 1}} \frac{1}{T^k Z^{\rm ren}_\lambda(T)} \sum_{n\ge k} \frac{n!}{(n-k)!} \underbrace{{\rm tr}_{k+1,\dots,N}\left[ e^{-\frac{H^{\rm ren}_{\lambda,n}}{T}} \right]}_{\text{reduced density matrix}} = \int |u^{\otimes k}\rangle\langle u^{\otimes k}|\, d\mu(u)$$

*strongly in Schatten spaces $p > 1$, for every $k \ge 1$.*

Fröhlich-Knowles-Schlein-Sohinger '17: similar for $d = 2, 3$ but with modified quantum Gibbs measure
M.L., Nam, Rougerie, *in preparation*, 2018

# Strategy: variational, based on entropy

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

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

**relative entropy**

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

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

**classical relative entropy**

- Fock space $\mathcal{F} := \mathbb{C} \oplus \bigoplus_{n\geq 1} L^2_s(\Omega^n)$, Hamiltonian $\mathbb{H}_\lambda = \bigoplus_{n\geq 0} H_{n,\lambda} = \mathbb{H}_0 + \lambda\mathbb{W}$

$$Z_\lambda(T) = \sum_{n\geq 0} \operatorname{tr}_{L^2_s(\Omega^n)} \exp\left(-\frac{H_{n,\lambda}}{T}\right) = \operatorname{tr}_{\mathcal{F}}\left[e^{-\mathbb{H}_\lambda/T}\right]$$

# Main steps in 1D

- **$\infty$-dim. semi-classical analysis = quantum Hewitt-Savage/de Finetti**

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

$$\operatorname*{weak\,lim}_{\substack{T\to\infty\\ \lambda T\to 1}} \frac{1}{T^k Z_\lambda^{\rm ren}(T)} \sum_{n\geq k} \frac{n!}{(n-k)!} \underbrace{\operatorname{tr}_{k+1,\dots,N}\left[e^{-\frac{H^{\rm ren}_{\lambda,n}}{T}}\right]}_{\text{reduced density matrix}} = \int |u^{\otimes k}\rangle\langle u^{\otimes k}|\, d\nu(u)$$

- **lower bound**

$$-\log\frac{Z_\lambda(T)}{Z_0(T)} = \min_\Gamma \left\{\mathcal{H}(\Gamma,\Gamma_{0,T}) + \operatorname{tr}(\mathbb{W}\Gamma)\right\}$$

$$\underset{\substack{T\to\infty\\ \lambda T\to 1}}{\gtrsim} \mathcal{H}_{\rm cl}(\nu,\mu_0) + \int \mathcal{I}(u)\,d\nu(u) \geq \min_\nu\left\{\mathcal{H}_{\rm cl}(\nu,\mu_0) + \int \mathcal{I}(\nu)\,d\nu(u)\right\} = -\log z_r$$

- **Upper bound:** construction of appropriate trial state

# Conclusion

- nonlinear Gibbs measures play important role in (S)PDE, QFT, etc
- concentrated on distribution spaces
- renormalization necessary in dimensions $d = 2, 3$
- can be derived from many-body quantum mechanics in mean-field limit