Derivation of Hartree and Bogoliubov theories for generic mean-field Bose gases

Mathieu LEWIN

Mathieu.Lewin@math.cnrs.fr

(CNRS & Université de Cergy-Pontoise)

joint works with P.T. Nam (Cergy), N. Rougerie (Grenoble), S. Serfaty (Paris) & J.P. Solovej (Copenhagen)

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Main result

$$H_N = \sum_{j=1}^N \big(-\Delta_{x_j} + V(x_j) \big) + \frac{1}{N-1} \sum_{1\leq k<\ell\leq N} w(x_k - x_\ell) \quad \text{on } L^2_s(\Omega^N)$$

- $w = w_1 + w_2$ and $V = V_1 + V_2 + V_+$, $V_+ \geq 0$, $V_+ \in L^{d/2}_{\rm loc}$
- $w_i, V_i \in L^{p_i}$ with $\max(1, d/2) < p_i < \infty$ or $p_i = \infty$ but $\to 0$ at ∞
- works as well for fractional Laplacians, magnetic fields, etc

Confined case: Ω is bounded (with chosen b.c.), or $V_+ \to \infty$ at ∞
Unconfined case: $\Omega = \mathbb{R}^d$ and $V_+ \equiv 0$

▶ **Main result:**

$$\lambda_j(H_N) = \underbrace{N\, e_{\rm H}}_{\text{Hartree (BEC)}} + \underbrace{\lambda_j(\mathbb{H})}_{\text{Bogoliubov}} + o(1)_{N\to\infty}$$

[LewNamSerSol-12] M.L., P.T. Nam, S. Serfaty & J.P. Solovej, *Comm. Pure Applied Math.*, in press.
[LewNamRou-13] M.L., P.T. Nam & N. Rougerie, `arXiv:1303.0981`.

History

- **Time-dependent case:** many results starting with Hepp, Ginibre-Velo, etc.

- **Hartree and Bose-Einstein condensation:**
  - easy for $\widehat{w} \geq 0$ smooth
  - Benguria-Lieb ('83): *bosonic atoms, w=Coulomb*
  - Lieb-Yau ('87): *boson stars, w=Newton* (translation-invariant)
  - Raggio-Werner ('89), Petz-Raggio-Verbeure ('89): *general confined case*
  - Lieb-Seiringer-Yngvason ('00–13): *Gross-Pitaevskii with $w \geq 0$*

- **Bogoliubov:**
  - Girardeau ('60), Lieb-Liniger ('63), etc: 1D completely integrable systems
  - Lieb-Solovej ('01–06): one and two-component charged Bose gases
  - Erdös-Schlein-Yau ('08), Giuliani-Seiringer ('09), Yau-Yin ('09): Lee-Huang-Yang formula for dilute gases
  - Cornean-Derezinski-Jin ('09), Seiringer ('11), Grech-Seiringer ('12), Derezinski-Napiórkowski ('13), *confined case with $\widehat{w} \geq 0$*

Hartree theory

Restrict to uncorrelated functions $\Psi = u^{\otimes N}$, with $\int_\Omega |u|^2 = 1$:

$$\frac{\left\langle u^{\otimes N}, H_N u^{\otimes N}\right\rangle}{N} = \int_\Omega \left(|\nabla u(x)|^2 + V(x)|u(x)|^2\right) dx + \frac{1}{2}\int_\Omega\int_\Omega w(x-y)|u(x)|^2|u(y)|^2 dx\, dy := \mathcal{E}_{\rm H}^V(u)$$

$$e_{\rm H} := \inf\left\{\mathcal{E}_{\rm H}^V(u)\ :\ \int_\Omega |u|^2 = 1\right\}$$

When it exists, a minimizer satisfies $\Big(-\Delta + V + |u_0|^2 * w\Big) u_0 = \varepsilon_0 u_0$

Theorem (Validity of Hartree theory [LewNamRou-13])

Under the previous assumptions on V and w, we have for any fixed j:

$$\lim_{N\to\infty} \frac{\lambda_j(H_N)}{N} = e_{\rm H}$$

Benguria-Lieb ('83): bosonic atoms. Lieb-Yau ('87): boson stars

Bose-Einstein condensation: confined case

k-particle density matrix: $\gamma_\Psi^{(k)} = \mathrm{tr}_{k+1\to N}\, |\Psi\rangle\langle\Psi|$

Theorem (Bose-Einstein condensation [LewNamRou-13])

Consider any sequence (Ψ_N) such that $\langle \Psi_N, H_N \Psi_N\rangle = N\, e_{\rm H} + o(N)$.

In the **confined case**, *there exists a subsequence N_j and a Borel probability measure μ on the unit sphere $S\mathfrak{H}$ of $\mathfrak{H} = L^2(\Omega)$, supported on the set $\mathcal{M}$ of minimizers for $e_{\rm H}$, such that*

$$\lim_{j\to\infty} \gamma^{(k)}_{\Psi_{N_j}} = \int_{\mathcal{M}} d\mu(u)\, |u^{\otimes k}\rangle\langle u^{\otimes k}|$$

strongly in the trace-class for any fixed k.

In particular, if $e_{\rm H}$ admits a unique minimizer u_0 (up to a phase factor), then there is **complete Bose-Einstein condensation** *on u_0:*

$$\lim_{N\to\infty} \gamma^{(k)}_{\Psi_N} = |u_0^{\otimes k}\rangle\langle u_0^{\otimes k}|.$$

Similar previous results by Raggio-Werner '89, Petz-Raggio-Verbeure '89.

Bose-Einstein condensation: unconfined case

Particles can escape to infinity: $e_{\rm H}^V(\lambda) := \inf\left\{\mathcal{E}_{\rm H}^V(u)\ :\ \int_{\mathbb{R}^d}|u|^2=\lambda\right\}$

Theorem (Bose-Einstein condensation [LewNamRou-13])

Consider any sequence (Ψ_N) such that $\langle \Psi_N, H_N\Psi_N\rangle = N\,e_{\rm H} + o(N)$.

In the **unconfined case**, *there exists a subsequence N_j and a Borel probability measure μ on the* **unit ball** *$B\mathfrak{H}$ of $\mathfrak{H}=L^2(\mathbb{R}^d)$, supported on the set*

$$\mathcal{M}=\left\{u\in B\mathfrak{H}\ :\ \mathcal{E}_{\rm H}^V(u)=e_{\rm H}^V(\|u\|^2)=e_{\rm H}^V(1)-e_{\rm H}^0(1-\|u\|^2)\right\},$$

such that

$$\gamma^{(k)}_{\Psi_{N_j}} \rightharpoonup_* \int_{\mathcal{M}} d\mu(u)\,|u^{\otimes k}\rangle\langle u^{\otimes k}|$$

weakly-$*$ in the trace-class for any fixed k.

If furthermore

$$e_{\rm H}^V(1) < e_{\rm H}^V(\lambda)+e_{\rm H}^0(1-\lambda),\qquad \forall 0\le\lambda<1,$$

then supp$(\mu)\subset\mathcal{M}\subset S\mathfrak{H}$ and the limit for $\gamma^{(k)}_{N_j}$ is strong in the trace-class.

Using density matrices

We can write

$$\left\langle \Psi_N, \left(\sum_{j=1}^N \left(-\Delta_{x_j} + V(x_j) \right) \right) \Psi_N \right\rangle = N \operatorname{tr}_{\mathfrak{H}} \left[(-\Delta + V) \gamma^{(1)}_{\Psi_N} \right]$$

$$\left\langle \Psi_N, \left(\sum_{1 \leq k < \ell \leq N} w(x_k - x_\ell) \right) \Psi_N \right\rangle = \frac{N(N-1)}{2} \operatorname{tr}_{\mathfrak{H}^2} \left[w \, \gamma^{(2)}_{\Psi_N} \right]$$

$$\frac{\langle \Psi_N, H_N \Psi_N \rangle}{N} = \frac{1}{2} \operatorname{tr}_{\mathfrak{H}^2} H_2 \gamma^{(2)}_{\Psi_N}$$

Reformulation in terms of density matrices

$$\frac{\lambda_1(H_N)}{N} = \inf \left\{ \frac{1}{2} \operatorname{tr}_{\mathfrak{H}^2} H_2 \gamma^{(2)} \ : \ \gamma^{(2)} \in \mathcal{P}^{(2)}_N \right\}$$

$$\mathcal{P}^{(2)}_N = \{ \gamma^{(2)}_{\Psi_N} \ : \ \Psi_N \in \mathfrak{H}^N, \ \|\Psi_N\| = 1 \}$$

- What is the limit of $\mathcal{P}^{(k)}_N$ as $N \to \infty$?

Quantum De Finetti

Theorem (Quantum de Finetti [Størmer-69, Hudson-Moody-75])

Let $\mathfrak{H}$ be any separable Hilbert space and denote by $\mathfrak{H}^k := \bigotimes_s^k \mathfrak{H}$ the corresponding bosonic k-particle space. Consider a hierarchy $\{\gamma^{(k)}\}_{k=0}^\infty$ of non-negative self-adjoint operators, where each $\gamma^{(k)}$ acts on $\mathfrak{H}^k$ and satisfies $\mathrm{tr}_{\mathfrak{H}^k}\,\gamma^{(k)} = 1$. *We assume that the hierarchy is consistent in the sense that*

$$\mathrm{tr}_{k+1}\,\gamma^{(k+1)} = \gamma^{(k)}, \qquad \forall k \geq 0.$$

Then there exists a Borel probability measure μ on the sphere $S\mathfrak{H}$ of $\mathfrak{H}$, invariant under the group action of S^1, such that, for all $k \geq 1$,

$$\gamma^{(k)} = \int_{S\mathfrak{H}} |u^{\otimes k}\rangle\langle u^{\otimes k}|\, d\mu(u).$$

Quantum equivalent of Hewitt-Savage (probability measures)

Christandl-König-Mitchison-Renner ('07): simple quantitative estimate in **finite-dimension**, similar in spirit to Diaconis-Freedman ('80) in classical case

Idea of the proof in the confined case

- **Step 1: extraction of limits**.
  - may assume $\gamma^{(k)}_{\Psi_N} \rightharpoonup_* \gamma^{(k)}$, $\forall k \geq 1$
  - system is confined $\Rightarrow$ strong CV $\Rightarrow$ consistent hierarchy

- **Step 2: de Finetti**.

  $\gamma^{(k)} = \int_{S\mathfrak{H}} |u^{\otimes k}\rangle\langle u^{\otimes k}|\, d\mu(u)$, $\forall k \geq 1$, for some Borel probability measure μ

- **Step 3: Conclusion**.

$$\liminf_{N\to\infty} \frac{\langle \Psi_N, H_N \Psi_N\rangle}{N} = \liminf_{N\to\infty} \frac{\mathrm{tr}(H_2 \gamma^{(2)}_{\Psi_N})}{2}$$
$$\geq \frac{1}{2}\,\mathrm{tr}(H_2\gamma^{(2)}) = \frac{1}{2}\int_{S\mathfrak{H}} \left\langle u^{\otimes 2}, H_2 u^{\otimes 2}\right\rangle d\mu(u) = \int_{S\mathfrak{H}} \mathcal{E}^V_{\mathrm{H}}(u)\, d\mu(u) \geq e_{\mathrm{H}}$$

Since $\lambda_1(H_N) \leq N\, e_{\mathrm{H}}$, this concludes the proof $\square$

A weak version of de Finetti

Theorem (Weak quantum de Finetti [LewNamRou-13])

Consider a sequence $\Psi_N \in \mathfrak{H}^N$ of normalized states, such that (for a subsequence)

$$\gamma^{(k)}_{\Psi_{N_j}} \rightharpoonup_* \gamma^{(k)}, \qquad \forall k \geq 0.$$

Then there exists a Borel probability measure μ on the unit ball $B\mathfrak{H}$ of $\mathfrak{H}$ such that, for all $k \geq 1$,

$$\gamma^{(k)} = \int_{B\mathfrak{H}} |u^{\otimes k}\rangle\langle u^{\otimes k}| \, d\mu(u).$$

Ex. $\Psi_N = (u_N)^{\otimes N}$ with $u_N \rightharpoonup v \Longrightarrow \mu = \delta_v$

Ammari-Nier ('08): weak de Finetti measure $\simeq$ ∞-dimensional Wigner measure

Proof of weak de Finetti: "geometric localization" in Fock space

Proof of main thm:

- $w \geq 0$ (e.g. bosonic atoms): same lines as before
- general case much more involved (weak limits not sufficient)

The next order

Theorem (Bogoliubov theory [LewNamSerSol-12])

If $e_{\rm H}^V(1)$ *has a* **unique, non-degenerate minimizer** u_0, *then*

$$\lim_{N\to\infty}\left(\lambda_j(H_N)-N\,e_{\rm H}\right)=\lambda_j(\mathbb{H})$$

where $\mathbb{H}$ *is the* **second-quantization** *of Hess* $\mathcal{E}_{\rm H}^V(u_0)/2$ *on the* **bosonic Fock space** $\Gamma_s(\mathfrak{H}_+)$ *built on* $\mathfrak{H}_+=\{u_0\}^\perp$. *Furthermore,*

$$\left\|\Psi_N^j-\sum_{n=0}^N u^{\otimes(N-n)}\otimes_s\varphi_n^j\right\|_{\mathfrak{H}^N}\to 0$$

where $\Phi^j=(\varphi_n^j)_{n\geq0}\in\Gamma_s(\mathfrak{H}_+)$ *solves* $\mathbb{H}\,\Phi^j=\lambda_j(\mathbb{H})\,\Phi^j$, *with* $\sum_{n\geq0}\left\|\varphi_n^j\right\|_{\mathfrak{H}^n}^2=1$.

Confined case with $\widehat{w}\geq0$: Seiringer ('11), Grech-Seiringer ('12), Derezinski-Napiórkowski ('13)

$$\text{Hess}\ \mathcal{E}_{\rm H}^V(u_0)(v,v)=\left\langle\begin{pmatrix}v\\ \overline{v}\end{pmatrix},\begin{pmatrix}h+K & K\\ K & h+K\end{pmatrix}\begin{pmatrix}v\\ \overline{v}\end{pmatrix}\right\rangle_{\mathfrak{H}_+\oplus\mathfrak{H}_+}$$

where $h=-\Delta+V+|u_0|^2*w-\varepsilon_0$, $K(x,y)=u_0(x)u_0(y)w(x-y)$

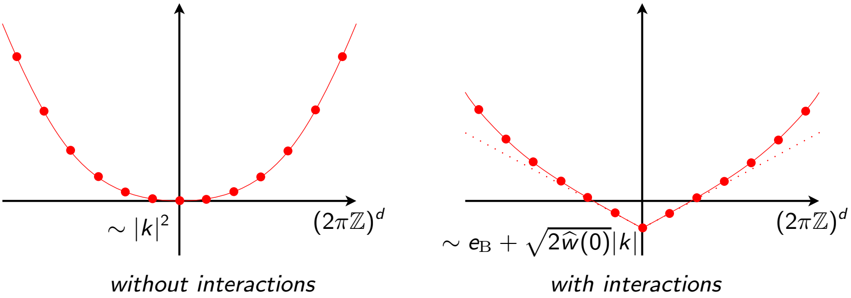
Bogoliubov's theory

$\mathbb{H}$ = **quadratic Hamiltonian**, can be diagonalized explicitly, Bogoliubov ('47)

Example: $\Omega = (0,1)^d$ with periodic b.c., $V \equiv 0$.

$$\lambda_k(\mathbb{H}) = e_{\rm B} + \sqrt{|k|^4 + 2\widehat{w}(k)|k|^2}, \qquad k \in (2\pi\mathbb{Z})^d,$$

where $e_{\rm B} = -\sum_{k\in(2\pi\mathbb{Z})^d\setminus\{0\}} \left(|k|^2 + \widehat{w}(k) - \sqrt{|k|^4 + 2\widehat{w}(k)|k|^2}\right)$



Describing fluctuations around u_0

Any $\Psi \in \mathfrak{H}^N$ can be written in a unique way as

$$\Psi = \underbrace{\psi_0}_{\in\mathbb{C}}\, u_0^{\otimes N} + \underbrace{\psi_1}_{\in\mathfrak{H}_+} \otimes_s u_0^{\otimes N-1} + \underbrace{\psi_2}_{\in\mathfrak{H}_+^2} \otimes_s u_0^{\otimes N-2} + \cdots + \underbrace{\psi_N}_{\in\mathfrak{H}_+^N}$$

and the following map is a unitary operator:

$$\begin{array}{rccl} U_N: & \mathfrak{H}^N & \longrightarrow & \mathbb{C}\oplus\mathfrak{H}_+\oplus\cdots\oplus\mathfrak{H}_+^N := \mathcal{F}_+^{\leq N} \subset \mathcal{F}_+ := \bigoplus_{k\geq 0}\mathfrak{H}_+^k \\ & \Psi & \longmapsto & \psi_0\oplus\psi_1\oplus\cdots\oplus\psi_N \end{array}$$

Theorem (Weak convergence towards $\mathbb{H}$ [LewNamSerSol-12])

Under the previous assumptions, we have

$$\lim_{N\to\infty}\left\langle \Phi, U_N\big(H_N - N\, e_{\rm H}\big)U_N^*\Phi'\right\rangle_{\mathcal{F}_+} = \langle \Phi, \mathbb{H}\Phi'\rangle_{\mathcal{F}_+}$$

for all fixed $\Phi, \Phi' \in \mathcal{F}_+$ (in the q.f. domain of $\mathbb{H}$). Here U_N^* is extended by 0 outside of $\mathcal{F}_+^{\leq N}$.

Conclusion

- Validity of Hartree and Bose-Einstein condensation for generic Bose gases in mean-field regime

- Only has to do with structure of density matrices in the limit $N \to \infty$, as shown by quantum de Finetti theorem

- If Hartree minimizer is unique and non-degenerate, one can expand the energy to the next order $\Rightarrow$ Bogoliubov's theory

- **Open problems:**
  - Quantitative bounds for BEC
  - Gross-Pitaevskii regime (cf Lieb-Seiringer-Yngvason for $w \geq 0$)
  - Bogoliubov for non-degenerate but not necessarily unique Hartree minimizers