Derivation of Hartree theory for generic mean-field Bose gases

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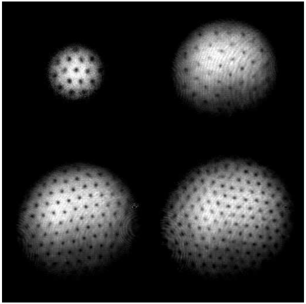
Bose-Einstein condensation (BEC)

▶ Macroscopic number of particles occupy the **same quantum state**

- Very **low temperature**
- **Weak interactions**
- **Symmetry breaking**, e.g. vortices $\Longrightarrow$
- **Superfluidity**, e.g. for Helium-4



W. Ketterle *et al* (MIT)

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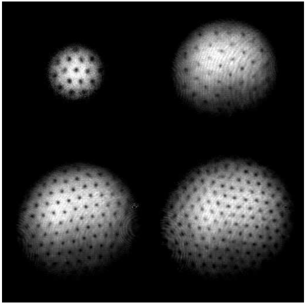

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▶ N interacting bosons in a domain $\Omega \subset \mathbb{R}^d$

$$H_N = \sum_{j=1}^{N} \big(-\Delta_{x_j} + V(x_j) \big) + \lambda \sum_{1 \leq k < \ell \leq N} w(x_k - x_\ell), \qquad \lambda \ll 1$$

on $\mathfrak{H}^N := L^2_s(\Omega^N) = \{\Psi \in L^2(\Omega^N) \text{ symmetric}\}$

Assumptions

$$H_N = \sum_{j=1}^{N} \left(-\Delta_{x_j} + V(x_j) \right) + \frac{1}{N-1} \sum_{1 \leq k < \ell \leq N} w(x_k - x_\ell)$$

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

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

We can deal with much more complicated models, e.g. in $\Omega = \mathbb{R}^d$

$$-\Delta + V(x) \rightsquigarrow \left(m^2 + |A(x) - i\nabla|^2\right)^s - m^{2s} + V(x)$$

Hartree theory

Restrict H_N to uncorrelated functions $\Psi = u(x_1)\cdots u(x_N)$, with $\int_\Omega |u|^2 = 1$:

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

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

Under the previous assumptions on V and w, we have:

$$\lim_{N\to\infty} \frac{\inf \sigma(H_N)}{N} = e_{\rm H} := \inf\left\{\mathcal{E}_{\rm H}^V(u)\ :\ \int_\Omega |u|^2 = 1\right\}$$

Raggio-Werner ('89), Petz-Raggio-Verbeure ('89): confined case
Benguria-Lieb ('83): bosonic atoms; Lieb-Yau ('87): boson stars

Density matrices

- *The many-body wave function Ψ_N is usually* **not** *close to $u^{\otimes N}$ in norm!*

Note that $\langle \Psi, H_N \Psi\rangle = \mathrm{tr}_{\mathfrak{H}^N}\big(H_N|\Psi\rangle\langle\Psi|\big)$.

Definition (Density matrices)

The k-**particle density matrix of** Ψ is the operator $\gamma_\Psi^{(k)}$ acting on $\mathfrak{H}^k$ defined by the partial trace

$$\gamma_\Psi^{(k)} = \mathrm{tr}_{k+1\to N}\,|\Psi\rangle\langle\Psi|.$$

Equivalently

$$\gamma_\Psi^{(k)}(X,X') = \int_{\Omega^{N-k}} \Psi(X,Y)\overline{\Psi(X',Y)}\,dY \quad \text{where } X,X' \in \Omega^k.$$

We have $\gamma_\Psi^{(k)} \geq 0$ and $\mathrm{tr}_{\mathfrak{H}^k}\,\gamma_\Psi^{(k)} = 1$ for all $k \geq 1$.

Hartree state:

$$\gamma_{u^{\otimes N}}^{(k)} = |u^{\otimes k}\rangle\langle u^{\otimes k}|$$

Bose-Einstein condensation: confined case

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:*

$$\lim_{N\to\infty} \gamma^{(k)}_{\Psi_N} = |u_0^{\otimes k}\rangle\langle u_0^{\otimes k}|, \qquad \forall k \geq 1.$$

Similar result at (small) positive temperature
Similar previous results by Raggio-Werner ('89), Petz-Raggio-Verbeure ('89)

Bose-Einstein condensation: unconfined case

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

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

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

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

Example: bosonic atoms

- N charged bosons ("electrons") + 1 nucleus of charge Z, $t = (N-1)/Z$

$$H_N = \sum_{j=1}^N \left(-\Delta_{x_j} - \frac{1}{t|x_j|}\right) + \frac{1}{N-1} \sum_{1\leq k<\ell\leq N} \frac{1}{|x_k - x_\ell|},$$

$$e_{\rm H}(t) := \inf_{\int_{\mathbb{R}^3}|u|^2=1} \left\{\int_{\mathbb{R}^3} |\nabla u|^2 - \frac{|u|^2}{t|x|} + \frac{1}{2}\int_{\mathbb{R}^6} \frac{|u(x)|^2|u(y)|^2}{|x-y|} dx\,dy\right\}$$

$e_{\rm H}(t)$ admits a unique minimizer u_t iff $t \leq t_c \simeq 1.21$

- $t \leq t_c \Rightarrow \gamma^{(k)}_{\Psi_N} \to |u_t^{\otimes k}\rangle\langle u_t^{\otimes k}|$ strongly (Benguria-Lieb '83)
- $t > t_c \Rightarrow \gamma^{(k)}_{\Psi_N} \rightharpoonup_* |\tilde{u}_t^{\otimes k}\rangle\langle \tilde{u}_t^{\otimes k}|$ weakly-$*$, where $\tilde{u}_t = (t_c/t)^{3/2} u_{t_c}(t_c \cdot /t)$

Quantum de Finetti

$\frac{\langle \Psi_N, H_N \Psi_N \rangle}{N} = \frac{1}{2} \operatorname{tr}_{\mathfrak{H}^2} H_2 \gamma^{(2)}_{\Psi_N} \Rightarrow$ what is the set of $\gamma^{(2)}_{\Psi_N}$'s in the limit $N \to \infty$?

Quantum de Finetti

$$\frac{\langle \Psi_N, H_N \Psi_N \rangle}{N} = \frac{1}{2} \operatorname{tr}_{\mathfrak{H}^2} H_2 \gamma^{(2)}_{\Psi_N} \Rightarrow$$ what is the set of $\gamma^{(2)}_{\Psi_N}$'s in the limit $N \to \infty$?

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

Let $\mathfrak{H}$ be any separable Hilbert space and $\mathfrak{H}^k := \bigotimes_s^k \mathfrak{H}$. 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 $\operatorname{tr}_{\mathfrak{H}^k} \gamma^{(k)} = 1$. If the hierarchy is consistent

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

then there exists a Borel probability measure μ on the sphere $S\mathfrak{H}$ of $\mathfrak{H}$ 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 the famous Hewitt-Savage thm, which deals with probability measures instead of trace-class operators.

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**.

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

- **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 □

A weak version of de Finetti

Unconfined case: particles can go to infinity $\Rightarrow \gamma^{(k)}$ not necessarily consistent

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 $u_N \rightharpoonup v \Longrightarrow \mu = \delta_v$

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 (looking at weak limits not sufficient)

The next order

Theorem (Bogoliubov theory [LewNamSerSol-12])

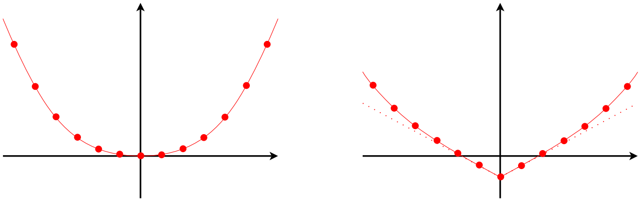
If $e_{\rm H}^V(1)$ *has a* **unique, non-degenerate minimizer** u_0, *then*

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

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 $\Phi^j=(\varphi_n^j)_{n\geq 0}\in\Gamma_s(\mathfrak{H}_+)$ *solves* $\mathbb{H}\,\Phi^j=\lambda_j(\mathbb{H})\,\Phi^j$, *with* $\sum_{n\geq 0}\left\|\varphi_n^j\right\|^2_{\mathfrak{H}^n}=1$.



without interactions *with interactions*