Large deviation estimates for weakly interacting bosons

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joint work with
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Bosons in the mean-field regime

We consider N bosons described on $L^2_s(\mathbb{R}^{3N})$ by

$$H_N = \sum_{j=1}^{N} (-\Delta_j) + \frac{1}{N} \sum_{1 \le i < j \le N} v\,(x_i - x_j)$$

Ground state: **Lieb, Seiringer**: ψ_N^{gs} of H_N exhibits BEC , i.e. the one-particle reduced density $\gamma_{\psi_N^{\mathrm{gs}}} = \mathrm{tr}_{2,\dots,N} |\psi_N^{\mathrm{gs}}\rangle\langle\psi_N^{\mathrm{gs}}|$ satisfies

$$\gamma_{\psi_N^{\mathrm{gs}}} \to |\varphi\rangle\langle\varphi| \quad \text{as} \quad N \to \infty$$

where φ denotes the Hartree minimizer. Note that $\psi_N^{\mathrm{gs}} \not\approx \varphi^{\otimes N}$.

Dynamics: We consider the many-body time evolution

$$i\partial_t \psi_{N,t} = H_N \psi_{N,t}, \quad \text{with} \quad \psi_{N,0} = \varphi_0^{\otimes N} \quad (\text{then } \; \gamma_{\psi_{N,0}} = |\varphi_0\rangle\langle\varphi_0|).$$

Erdösz, Fröhlich, Ginibre, Knowles, Lee, Pickl, Pizzo, Rodnianski, Schlein, Yau...:

$$\gamma_{\psi_{N,t}} \to |\varphi_t\rangle\langle\varphi_t| \quad \text{as} \quad N \to \infty$$

and $i\partial_t \varphi_t = (-\Delta + (v * |\varphi_t|^2))\varphi_t$ solves the Hartree equation, but $\psi_{N,t} \not\approx \varphi_t^{\otimes N}$.

Probabilistic Description

For a self-adjoint one-particle operator O on $L^2(\mathbb{R}^3)$ we define the random variable $O^{(i)} = 1 \otimes \cdots \otimes 1 \otimes O \otimes 1 \otimes \cdots \otimes 1$ with probability distribution

$$\mathbb{P}_{\psi_N}\left[O^{(i)} \in A\right] = \langle \psi_N, \chi_A\left(O^{(i)}\right)\psi_N\rangle, \quad \text{where } \psi_N \in L^2_s(\mathbb{R}^{3N})$$

and χ_A denotes the characteristic function of the set $A \subset \mathbb{R}$.

Question: Characterization $\mathbb{P}_{\psi_N}$ through principles of classical probability theory.

Factorized states: $\psi_{N,0} = \varphi_0^{\otimes N}$, correspond to **i.i.d.** random variables. They satisfy a **law of large numbers**, i.e. for $\delta > 0$

$$\mathbb{P}_{\varphi_0^{\otimes N}}\left[\, \Big| \frac{1}{N}\sum_{j=1}^{N} O^{(i)} - \langle \varphi_0,\ O\varphi_0\rangle \Big| > \delta \right] \to 0 \quad \text{as} \quad N \to \infty.$$

Does a LLN hold for $\psi_{N,t}$?

Law of large numbers

Let $\psi_{N,t}$ denote the solution to $i\partial_t \psi_{N,t} = H_N \psi_{N,t}$ with factorized initial data $\psi_{N,0} = \varphi_0^{\otimes N}$.

Ben Arous-Kirkpatrick-Schlein (2013): Let $\delta > 0$, then

$$\lim_{N\to\infty} \mathbb{P}_{\psi_{N,t}} \left[\Big| \frac{1}{N} \sum_{i=1}^{N} \left(O^{(i)} - \langle \varphi_t, O\varphi_t \rangle \right) \Big| > \delta \right] = 0$$

- Correlations of the particles do not affect the law of large numbers
- Law of large numbers is a consequence of BEC
- Similar statement holds for the ground state ψ_N^{gs}: for any $\delta > 0$

$$\lim_{N\to\infty} \mathbb{P}_{\psi_N^{\mathrm{gs}}} \left[\Big| \frac{1}{N} \sum_{i=1}^{N} \left(O^{(i)} - \langle \varphi, O\varphi \rangle \right) \Big| > \delta \right] = 0$$

PROOF:

$$\begin{aligned}
&\mathbb{P}_{\psi_{N,t}}\left[\Big|\frac{1}{N}\sum_{i=1}^{N}\big(O^{(i)}-\langle\varphi_t, O\varphi_t\rangle\big)\Big|>\delta\right]\\
=&\mathbb{P}_{\psi_{N,t}}\left[\Big|\frac{1}{\delta N}\sum_{i=1}^{N}\widetilde{O}^{(i)}\Big|>1\right]\\
\leq&\frac{1}{N^2\delta^2}\mathbb{E}_{\psi_{N,t}}\Big|\sum_{i=1}^{N}\widetilde{O}^{(i)}\Big|^2=\frac{1}{N^2\delta^2}\mathbb{E}_{\psi_{N,t}}\sum_{i,j=1}^{N}\widetilde{O}^{(i)}\widetilde{O}^{(j)}\\
\leq&\frac{CN(N-1)}{\delta^2N^2}\mathrm{tr}\gamma^{(2)}_{\psi_{N,t}}\left(\widetilde{O}\otimes\widetilde{O}\right)+\frac{N}{N^2\delta^2}\mathrm{tr}\gamma_{\psi_{N,t}}\widetilde{O}^2\to 0\quad\text{as}\quad N\to\infty.\qquad\square
\end{aligned}$$

Central limit theorem

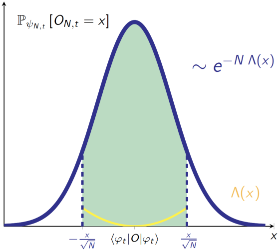
Ben Arous-Kirkpatrick-Schlein, Buchholz-Saffirio-Schlein:

$$\lim_{N\to\infty} \mathbb{P}_{\psi_{N,t}} \left[\Big| \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \left(O^{(i)} - \langle \varphi_t, O\varphi_t \rangle \right) \Big| < x \right] = \frac{1}{\sqrt{2\pi}\sigma_t} \int_{-\infty}^{x} e^{-r^2/2\sigma_t^2} dr$$

- The variance $\sigma_t^2 = \|f_{0;t}\|_2^2$ is determined by $f_{s;t}$ satisfying for $s \in [0, t]$

$$i\partial_s f_{s;t} = \left(h_H(s) + \widetilde{K}_{1,s} + J\widetilde{K}_{2,s} \right) f_{s;t},$$

  with $f_{t;t} = q_t O\varphi_t = O\varphi_t - \langle \varphi_t, O\varphi_t \rangle$ and
  $h_H(t) = -\Delta + (v * |\varphi_t|^2)$,
  $K_{1,t}(x;y) = v(x-y)\varphi_t(x)\overline{\varphi}_t(y)$, $\widetilde{K}_{1,s} = q_s K_{1,s} q_s$,
  $K_{2,t}(x;y) = v(x-y)\varphi_t(x)\varphi_t(y)$, $\widetilde{K}_{1,s} = q_s K_{1,s} q_s$.
- Similar results in more singular scaling regimes **(R.)** and the ground state, too **(R.-Schlein)**



Large deviation estimates

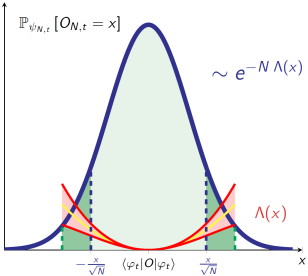
The large deviation regime is characterized by the rate function, if it exists, given by

$$\Lambda_{\psi_{N,t}}(x) := \lim_{N\to\infty} \frac{1}{N} \log \mathbb{P}_{\psi_{N,t}} \left[\Big| \frac{1}{N} \sum_{i=1}^{N} \big(O^{(i)} - \langle \varphi_t, O\varphi_t \rangle \big) \Big| > x \right]$$

Kirkpatrick-R.-Schlein, R.-Seiringer: If $\Lambda_{\psi_{N,t}}$ exists, we have

$$\Lambda_{\psi_{N,t}}(x) = -\frac{x^2}{2\sigma_t^2} + O(x^3) \quad \text{for all} \quad 0 < x \leq e^{-e^{C|t|}} / |||O||| \ .$$

- We assume $v \leq C(1-\Delta)$ and O s.t. $|||O||| = \|\Delta O(1-\Delta)^{-1}\|_{\text{op}} < \infty$
- The variance is explictely given by $\sigma_t^2 = \|f_{0;t}\|_2^2$



Cumulant generating function

Cramer's theorem shows that for i.i.d. random variables, the rate function is given through the Legendre tansform

$$\Lambda_{\varphi_0^{\otimes N}}(x) = \inf_{\lambda} \left[\lambda x - \Lambda^*_{\varphi_0^{\otimes N}}(\lambda) \right]$$

with $\Lambda^*_{\varphi_0^{\otimes N}}(\lambda) = \log \langle \varphi, e^{\lambda(O^{(1)} - \langle \varphi, O\varphi \rangle)} \varphi \rangle$ the cumulant generating function.

Kirkpatrick-R.-Schlein, R.-Seiringer: For all $0 \leq \lambda \leq e^{-e^{Ct}} / |||O|||$, we have

$$e^{N\left(\frac{\lambda^2}{2}\sigma_t^2 - C_t\lambda^3\right) - C\lambda} \leq \mathbb{E}_{\psi_{N,t}} \left[e^{\lambda\left(\sum_{j=1}^N (O^{(j)} - \langle \varphi_t, O\varphi_t \rangle)\right)} \right] \leq e^{N\left(\frac{\lambda^2}{2}\sigma_t^2 + C_t\lambda^3\right) + C\lambda}$$

The previous theorem on the rate function follows from a generalization of Cramer's theorem:

- upper bound follows from Markov's inequality
- lower bound generalizes ideas from Cramer's theorem

Fluctuations around Hartree dynamics

We describe the system on the bosonic Fock space $\mathcal{F} = \bigoplus_{n\geq 0} L^2_s\left(\mathbb{R}^{3n}\right)$ with creation and annihilation operators $a^*(f), a(f)$ and the vacuum Ω.

Fock space of excitations **(Lewin-Nam-Serfaty-Solovej)**: Any $\psi_N \in L^2_s(\mathbb{R}^{3N})$ can be decomposed as

$$\psi_N = \eta_0 \varphi_t^{\otimes N} + \eta_1 \varphi_t^{\otimes (N-1)} + \cdots + \eta_N, \quad \text{where} \quad \eta_j \in L^2_{\perp \varphi_t}(\mathbb{R}^3)^{\otimes j}$$

We define the unitary $\mathcal{U}_t : L^2_s\left(\mathbb{R}^{3N}\right) \to \mathcal{F}^{\leq N}_{\perp \varphi_t} = \bigoplus_{j\geq 0}^N L^2_{\perp \varphi_t}\left(\mathbb{R}^{3j}\right)$ by

$$\mathcal{U}_t \psi_N = \{\eta_0, \cdots, \eta_N\}.$$

For $f, g \in L^2_{\perp \varphi_t}(\mathbb{R}^3)$, the unitary satisfies the following properties

$$\begin{aligned}
\mathcal{U}_t \; a^*(\varphi_t) a(\varphi_t) \, \mathcal{U}_t^* &= N - \mathcal{N}_+(t), \quad \mathcal{U}_t \; a^*(f) a(g) \, \mathcal{U}_t^* = a^*(f) a(g) \\
\mathcal{U}_t \; a^*(f) a(\varphi_t) \, \mathcal{U}_t^* &= a^*(f) \sqrt{N - \mathcal{N}_+(t)} = \sqrt{N} b^*(f) \\
\mathcal{U}_t \; a^*(\varphi_t) a(f) \, \mathcal{U}_t^* &= \sqrt{N - \mathcal{N}_+(t)} a(f) = \sqrt{N} b(f).
\end{aligned}$$

The modified creation and annihilation operators $b^*(f), b(f)$ satisfy

$$[b(g), b(f)] = [b^*(g), b^*(f)] = 0, \quad [b(g), b^*(f)] = \langle g, f \rangle \left(1 - \frac{\mathcal{N}_+}{N}\right) - \frac{1}{N} a^*(f) a(g).$$

We write $\psi_{N,t} = e^{-iH_N t}\varphi_0^{\otimes N} = e^{-iH_N t}\mathcal{U}_0^*\Omega = \mathcal{U}_t^*\left(\mathcal{U}_t e^{-iH_N t}\mathcal{U}_0^*\right)\Omega$ and define the FLUCTUATION DYNAMICS $\mathcal{W}_N(t;s)$

$$i\partial_t \mathcal{W}_N(t;s) = \mathcal{L}_N(t)\mathcal{W}_N(t;s)$$

with $\mathcal{L}_N(t) = (i\partial_t\mathcal{U}_t)\mathcal{U}_t^* + \mathcal{U}_t^* H_N \mathcal{U}_t$, given for $\xi_1, \xi_2 \in \mathcal{F}_{\perp\varphi_t}^{\leq N}$ by

$$\begin{aligned}
\langle \xi_1, \mathcal{L}_N(t)\xi_2\rangle = \langle \xi_1, d\Gamma(h_H(t) + K_{1,t})\xi_2\rangle + \mathrm{Re}\int dxdy\; K_{2,t}(x;y)\,\langle \xi_1, b_x^* b_y^* \xi_2\rangle \\
- \frac{1}{2N}\langle \xi_1, d\Gamma(v * |\varphi_t|^2 + K_{1,t} - \mu_t)(\mathcal{N}_+(t) - 1)\xi_2\rangle \\
+ \frac{2}{\sqrt{N}}\mathrm{Re}\,\langle \xi_1, \mathcal{N}_+ b((v * |\varphi_t|^2)\varphi_t)\xi_2\rangle \\
+ \frac{2}{\sqrt{N}}\int dxdy\; v(x-y)\mathrm{Re}\,\varphi_t(x)\langle \xi_1, a_y^* a_{x'} b_{y'}\xi_2\rangle \\
+ \frac{1}{2N}\int dxdy\; v(x-y)\langle \xi_1, a_x^* a_y^* a_x a_y \xi_2\rangle
\end{aligned}$$

Here $h_H(t) = -\Delta + (v * |\varphi_t|^2)$, $K_{1,t}(x;y) = v(x-y)\varphi_t(x)\overline{\varphi}_t(y)$, $K_{2,t}(x;y) = v(x-y)\varphi_t(x)\varphi_t(y)$, $2\mu_t = \int dxdy\; v(x-y)|\varphi_t(x)|^2|\varphi_t(y)|^2$.

Bogoliubov dynamics

The limiting dynamics $\mathcal{W}_\infty(t;s)$ on $\mathcal{F}_{\perp\varphi_t}$with generator

$$\langle \xi_1, \mathcal{L}_\infty(t)\xi_2\rangle = \langle \xi_1, d\Gamma(h_H(t) + K_{1,t})\xi_2\rangle + \mathrm{Re}\int dxdy\ K_{2,t}(x;y)\,\langle \xi_1, a_x^* a_y^* \xi_2\rangle$$

gives rise to a Bogoliubov transform: Let $A(f;g) = a(f) + a^*(\overline{g})$ for $f \in L^2_{\perp\varphi_{t_2}}$ and $g \in JL^2_{\perp\varphi_{t_2}}$ where $Jg = \overline{g}$. Then,

$$\mathcal{W}_\infty^*(t;s)A(f;g)\mathcal{W}_\infty(t;s) = A\left(\Theta(t;s)(f;g)\right),$$

for a two-parameter family of operators $\Theta(t;s)$. **Ben Arous-Kirkpatrick - Schlein** show

$$i\partial_t\Theta(t;s) = \mathcal{A}(t)\Theta(t;s)$$

where

$$\mathcal{A}(t) = \begin{pmatrix} h_H(t) + K_{1,t} & -JK_{2,t}J \\ K_{2,t} & -J\left(h_H(t) + K_{1,t}\right)J \end{pmatrix}.$$

Ref.: **Boßman, Chen, Grillakis, Hepp, Lewin, Machedon, Margetis, Nam, Napirkowski, Pavlović, Petrat, Pickl, Schlein, Soffer, ...**

Idea of the proof (upper bound)

We consider

$$\mathbb{E}_{\psi_{N,t}}\, e^{\lambda\left[\sum_{j=1}^{N}(O^{(j)}-\langle\varphi_t,O\varphi_t\rangle)\right]} = \langle\psi_{N,t},\, e^{\lambda\left[\sum_{j=1}^{N}(O^{(j)}-\langle\varphi_t,O\varphi_t\rangle)\right]}\psi_{N,t}\rangle$$
$$= \left\langle\Omega, \mathcal{W}_N^*(t;0)e^{\lambda d\Gamma(q_t\widetilde{O}_tq_t)+\lambda\sqrt{N}\phi_+(q_tO\varphi_t)}\mathcal{W}_N(t;0)\Omega\right\rangle$$

with $\phi_+(f) = b^*(f) + b(f)$ and $\widetilde{O} = O - \langle\varphi_t, O\varphi_t\rangle$.

Step 1: There exist constants $C, c > 0$ such that for sufficiently small λ

$$\left\langle\Omega, \mathcal{W}_N^*(t;0)e^{\lambda d\Gamma(q_t\widetilde{O}_tq_t)+\lambda\sqrt{N}\phi_+(q_tO\varphi_t)}\mathcal{W}_N(t;0)\Omega\right\rangle$$
$$\leq e^{CN\|O\|^3\lambda^3+C\lambda}\left\langle\Omega, \mathcal{W}_N^*(t;0)e^{\lambda\sqrt{N}\phi_+(q_tO\varphi_t)/2}e^{c\lambda\|O\|\mathcal{N}_+(t)}e^{\lambda\sqrt{N}\phi_+(q_tO\varphi_t)/2}\mathcal{W}_N(t;0)\Omega\right\rangle$$

STEP 2: For given $c > 0$ there exists a constant $C > 0$ such that for an appropriately chosen κ_t and sufficiently small λ

$$\left\langle \Omega, \mathcal{W}_N^*(t;0) e^{\lambda\sqrt{N}\phi_+(q_t O\varphi_t)/2} e^{c\|O\|\mathcal{N}_+(t)} e^{\lambda\sqrt{N}\phi_+(q_t O\varphi_t)/2} \mathcal{W}_N(t;0)\Omega \right\rangle$$
$$\leq e^{C_t N\lambda^3 |||O|||^3 + C_t\lambda} \left\langle \Omega, e^{\lambda\sqrt{N}\phi_+(f_{0;t})/2} e^{\lambda\kappa_t\mathcal{N}_+(0)} e^{\lambda\sqrt{N}\phi_+(f_{0;t})/2}\Omega \right\rangle$$

STEP 3: There exists $C > 0$ such that for sufficiently small λ

$$\left\langle \Omega, e^{\lambda\sqrt{N}\phi_+(f_{0;t})/2} e^{\lambda\kappa_t\mathcal{N}_+(0)} e^{\lambda\sqrt{N}\phi_+(f_{0;t})/2}\Omega \right\rangle \leq e^{\lambda^2 N\|f_{0;t}\|^2/2} e^{C_t N\lambda^3 |||O|||^3}$$

STEP 4: Summarizing, we have shown

$$\mathbb{E}_{\psi_{N,t}}\, e^{\lambda\left[\sum_{j=1}^N (O^{(j)} - \langle\varphi_t, O\varphi_t\rangle)\right]} \leq e^{\lambda^2 N\|f_{0;t}\|^2/2} e^{C_t N\lambda^3 |||O|||^3 + C_t\lambda}.$$

Summary

- For the evolution of factorized initial data in the mean-field regime, fluctuations of bounded one-particle observables satisfy a large deviation estimates
- The rate function is up to quadratic order determined through the limiting Bogoliubov dynamics

Thanks for your attention.