Interacting Brownian Motions and the Gross-Pitaevskii Formula

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Background

Consider a large quantum system of N particles in a trap in $\mathbb{R}^d$ with mutually repellent interaction, described by the Hamilton operator

$$\mathcal{H}_N = -\sum_{i=1}^N \Delta_i + \sum_{i=1}^N W(x_i) + \sum_{1\leq i<j\leq N} v(|x_i - x_j|), \qquad x_1,\dots,x_N \in \mathbb{R}^d.$$

- The kinetic energy term Δ_i acts on the ith particle.
- examples of trap potential: $W(x) = |x|^2$ or $W = \infty \mathbb{1}_\Lambda$ with $\Lambda \subset \mathbb{R}^d$ a box.
- the pair potential $v\colon (0,\infty) \to [0,\infty]$ decays quickly at ∞ and explodes at 0.

Goal: Describe the particle system at zero or very low temperature in the limit $N \to \infty$, coupled with $\Lambda \to \mathbb{R}^d$.
In particular, understand Bose-Einstein condensation (BEC):

> At very low temperature, the wave function of N indistinguishable particles (Bosons) can be described in terms of a one-particle wave function.

In other words, a macroscopic portion of the atoms collaps into the lowest possible energy state. (Theoretically predicted in 1924/25 by A. Einstein and N. Bose, first experimental realisation in 1995, mathphys community has not yet agreed on a mathematical definition of this effect).

Goals

From now on, put $d = 3$.
Replace the trap W by the rescaling

$$W_N(\cdot) = L_n^{-2} W\big(\cdot\ L_N^{-1}\big), \qquad \text{for some } L_N \to \infty$$

and consider the particle density $\rho_N = N L_N^{-3}$.

Long-term goal: Describe the system for $\rho_N \asymp 1$ as $N \to \infty$ at zero or very low temperature.

In this talk: Assume that $\rho_N \asymp N^{-2}$ (dilute system), i.e., $L_N = N$.
By rescaling, we may leave W independent on N and replace v by the rescaling $v_N(\cdot) = N^2 v(\cdot\, N)$. That is, N particles are in a fixed trap with repellence length $\asymp 1/N$.

Hence, we study

$$\mathcal{H}_N = -\sum_{i=1}^N \Delta_i + \sum_{i=1}^N W(x_i) + \frac{1}{N} \sum_{1\le i<j\le N} N^3 v\big(N|x_i - x_j|\big), \qquad x_1, \dots, x_N \in \mathbb{R}^3.$$

Zero temperature

At zero temperature, the system is described by the ground state energy of $\mathcal{H}_N$:

$$
\begin{aligned}
N\chi_N &= \inf_{h\in H^1(\mathbb{R}^{3N}):\ \|h\|_2=1} \langle h, \mathcal{H}_N h\rangle \\
&= \inf_{h\in H^1(\mathbb{R}^{3N}):\ \|h\|_2=1} \Big[\sum_{i=1}^N \big(\|\nabla_i h\|_2^2 + \langle h^2, W(x_i)\rangle\big) \\
&\qquad + \frac{1}{N} \sum_{1\le i<j\le N} \Big\langle h^2, N^3 v\big(N|x_i - x_j|\big)\Big\rangle \Big].
\end{aligned}
$$

Existence and uniqueness of minimisers h_N^* (ground states) is well-known.

reduced density matrix:

$$
\gamma_N(x,y) = \int_{\mathbb{R}^{3(N-1)}} h_N^*(x, x_2, \ldots, x_N) h_N^*(y, x_2, \ldots, x_N)\,\mathrm{d}x_2 \cdots \mathrm{d}x_N
$$

Gross-Pitaevskii formula, scattering length

- Gross-Pitaevskii formula with parameter $\alpha \in (0, \infty)$:

$$\chi^{(\mathrm{GP})}(\alpha) = \inf_{\varphi \in H^1(\mathbb{R}^3)\colon \, \|\varphi\|_2 = 1} \Big[\|\nabla \varphi\|_2^2 + \langle \varphi^2, W \rangle + 4\pi\alpha \|\varphi\|_4^4 \Big].$$

  - The minimiser φ_α is positive and $\mathcal{C}^1$ [Gross 1961], [Pitaevskii 1962].

- Scattering length of the interaction potential v:

$$\alpha(v) = \lim_{r \to \infty} \Big(r - \frac{u(r)}{u'(r)} \Big),$$

where u solves the scattering equation $u'' = \frac{1}{2} uv, \quad u(0) = 0$.

  - If $v = \infty \mathbb{1}_{(0, a^*]}$, then $\alpha(v) = a^*$.
  - The scattering length of $N^2 v(N\,\cdot)$ is $\frac{1}{N}$ times the one of v.

BEC at zero temperature

[Lieb, Seiringer, Yngvason 1999-2002]: If $N\chi_N$ denotes the ground state energy of $\mathcal{H}_N$ and γ_N its reduced density matrix, then

(i) $\lim_{N\to\infty} \chi_N = \chi^{(\mathrm{GP})}(\alpha(v))$,

(ii) $\lim_{N\to\infty} \gamma_N = \varphi_{\alpha(v)} \otimes \varphi_{\alpha(v)}$ in trace norm.

Remarks:

- The proof shows that

$$h_N(x_1,\dots,x_N) \approx \prod_{i=1}^N \frac{\varphi_{\alpha(v)}(x_i)}{\|\varphi_{\alpha(v)}\|_\infty} \prod_{i=1}^N f\big(\min\{|x_i - x_j| \colon j = 1,\dots,i-1\}\big),$$

  where $f(r) = u(r)/r$, and u is the solution to the scattering equation.
- (ii) implies that the reduced density matrix has an eigenvalue of order 1 ($\Longrightarrow$ another indication of BEC).
- The proof is based on some earlier work of Dyson (1962).

Positive temperature

The N-particle system is described by the trace of $\mathrm{e}^{-\beta\mathcal{H}_N}$, where $\beta \in (0,\infty)$ is the inverse temperature. This trace may be written in terms of Brownian bridges:

$$\mathrm{Tr}\big(\mathrm{e}^{-\beta\mathcal{H}_N}\big) = \int_{(\mathbb{R}^d)^N} \mathrm{d}x_1 \dots \mathrm{d}x_N \bigotimes_{i=1}^N \mathbb{E}^\beta_{x_i,x_i}\Big[\mathrm{e}^{-H_{N,\beta}}\Big],$$

where

$$H_{N,\beta} = \sum_{i=1}^N \int_0^\beta W(B_s^{(i)})\,\mathrm{d}s + \frac{1}{N}\sum_{1\le i<j\le N}\int_0^\beta \mathrm{d}s\, N^3 v\big(N|B_s^{(i)} - B_s^{(j)}|\big).$$

The free energy of Bosons is described by the trace of the projection of $\mathrm{e}^{-\beta\mathcal{H}_N}$ on the set of permutation symmetric functions:

$$\mathrm{Tr}_+\big(\mathrm{e}^{-\beta\mathcal{H}_N}\big) = \frac{1}{N!}\sum_\sigma \int_{(\mathbb{R}^d)^N} \mathrm{d}x \bigotimes_{i=1}^N \mathbb{E}^\beta_{x_i,x_{\sigma(i)}}\Big[\mathrm{e}^{-H_{N,\beta}}\Big].$$

Zero-temperature limit: As in [Adams, Bru and K. (2006a)] one can show that

$$\lim_{\beta\to\infty}\frac{1}{\beta N}\log \mathrm{Tr}_+\big(\mathrm{e}^{-\beta\mathcal{H}_N}\big) = \lim_{\beta\to\infty}\frac{1}{\beta N}\log \mathrm{Tr}\big(\mathrm{e}^{-\beta\mathcal{H}_N}\big) = \frac{1}{N}\chi_N.$$

The Hartree model

Replace $H_{N,\beta}$ by

$$K_{N,\beta} = \sum_{i=1}^{N} \int_0^\beta W(B_s^{(i)})\,\mathrm{d}s + \frac{1}{N} \sum_{1\le i<j\le N} \int_0^\beta \mathrm{d}s\, \frac{1}{\beta} \int_0^\beta \mathrm{d}t\, N^3 v\big(N|B_s^{(i)} - B_t^{(j)}|\big),$$

i.e., the pair interaction is not local, but mean-field in time. Actually, this is a path interaction rather than a particle interaction. The arising model is named after the variational formula that appears in the zero-temperature limit:

Theorem [Adams, Bru and K. 2006a]. Put $d \in \{2,3\}$. Then

$$\lim_{\beta\to\infty} \frac{1}{\beta N} \log \mathbb{E}_0\Big[\mathrm{e}^{-K_{N,\beta}}\Big] = \frac{1}{N}\chi_N^{\otimes},$$

where

$$\chi_N^{\otimes} = \inf_{\substack{h_1,\dots,h_N\in H^1(\mathbb{R}^d)\\ \|h_i\|_2=1\,\forall i}} \big\langle \mathcal{H}_N(h_1\otimes\cdots\otimes h_N), h_1\otimes\cdots\otimes h_N\big\rangle.$$

That is, the path-interaction model leads to the ground product-states of $\mathcal{H}_N$.

On the proof

Large-deviation arguments for $\mu_\beta^{(i)} = \frac{1}{\beta}\int_0^\beta \mathrm{d}s\,\delta_{B_s^{(i)}}$ in the spirit of Donsker-Varadhan:

The probability is

$$\mathbb{P}_0\big(\mu_\beta^{(i)}(\mathrm{d}x) \approx h_i^2(x)\,\mathrm{d}x\big) \approx \mathrm{e}^{-\beta\|\nabla h_i\|_2^2},$$

giving the energy term $\sum_{i=1}^N \|\nabla h_i\|_2^2$.

The trap interaction is

$$\sum_{i=1}^N \int_0^\beta W(B_s^{(i)})\,\mathrm{d}s = \beta\sum_{i=1}^N \langle \mu_\beta^{(i)}, W\rangle,$$

giving the trap term $\sum_{i=1}^N \langle h_i^2, W\rangle$.

The pair interaction is

$$\frac{1}{N}\sum_{1\leq i<j\leq N}\int_0^\beta \mathrm{d}s\int_0^\beta \frac{\mathrm{d}t}{\beta}\,N^3 v\big(N|B_s^{(i)}-B_t^{(j)}|\big) \approx \frac{\beta}{N}\sum_{1\leq i<j\leq N}\int_{\mathbb{R}^3}\mathrm{d}x N^3 v(N|x|)\big(\mu_\beta^{(i)}\star\mu_\beta^{(j)}\big)(\mathrm{d}x$$

giving the interaction term $\frac{1}{N}\sum_{1\leq i<j\leq N}\int N^3 v(N|x|)\big(h_i^2\star h_j^2\big)(x)$.

Large-N limit at zero temperature

Like the canonical model, in the large-N limit the Hartree model scales to the Gross-Pitaevskii formula:

Theorem [ADAMS, BRU AND K. 2006A]. Put $d \in \{2,3\}$, assume that $\widetilde{\alpha}(v) = \frac{1}{8\pi}\int v(|x|)\,\mathrm{d}x < \infty$, and replace v by $N^{d-1}v(\,\cdot\,N)$. Then

$$\lim_{N\to\infty} \frac{1}{N}\chi_N^{\otimes} = \chi^{(\mathrm{GP})}\big(\widetilde{\alpha}(v)\big).$$

Furthermore, if $(h_1^*,\dots,h_N^*)$ is any tuple of minimisers, then

$$L^1 - \lim_{N\to\infty} \frac{1}{N}\sum_{i=1}^N (h_i^*)^2 = (\varphi^*_{\widetilde{\alpha}(v)})^2.$$

Methods of proof: standard compactness arguments, potential theory, smoothing techniques, harmonic analysis.

The relation between ground product states and the integral of the interaction potential was phenomenogically discussed since long, like the one between the product states and the scattering length.

Large-N limit at positive temperature

Recall: $d = 3$ and $\widetilde{\alpha}(v) = \frac{1}{8\pi}\int v(|x|)\,\mathrm{d}x < \infty$.

Theorem [ADAMS, BRU AND K. (2006B)]. For any $\beta \in (0,\infty)$,

$$\lim_{N\to\infty}\frac{1}{\beta N}\log\mathbb{E}_0\Big[\mathrm{e}^{-K_{N,\beta}}\Big] = -\chi_\beta\big(\widetilde{\alpha}(v)\big),$$

where

$$\chi_\beta(\alpha) = \inf_{\varphi\in H^1(\mathbb{R}^d)\colon\,\|\varphi\|_2=1}\Big[J_\beta(\varphi^2) + \langle W,\varphi^2\rangle + 4\pi\alpha\|\varphi\|_4^4\Big]$$

and

$$J_\beta(\varphi^2) = \sup_{f\in\mathcal{C}_\mathrm{b}(\mathbb{R}^d)}\Big[\langle f,\varphi^2\rangle - \frac{1}{\beta}\log\mathbb{E}_0\big[\mathrm{e}^{\int_0^\beta f(B_s)\,\mathrm{d}s}\big]\Big].$$

- $J_\beta(\varphi^2)$ is a ‘probabilistic’ energy term and depends on initial and terminal condition of the Brownian motions.
- Conjecture: $\lim_{\beta\to\infty}\chi_\beta(\alpha) = \chi^{(\mathrm{GP})}(\alpha)$.
- The proof uses Cramér’s theorem for $\frac{1}{N}\sum_{i=1}^N\frac{1}{\beta}\int_0^\beta\mathrm{d}s\,\delta_{B_s^{(i)}}$.
- Pair interaction is expressed in terms of Brownian intersection local times.

Heuristics for the proof

Local times of $B^{(i)} - B^{(j)}$, formally defined as

$$L_\beta^{(i,j)}(x) = \frac{1}{\beta^2} \int_0^\beta \mathrm{d}s \int_0^\beta \mathrm{d}t \, \delta_{B_s^{(i)} - B_t^{(j)}}(\mathrm{d}x).$$

Hence,
$$K_{N,\beta} = N\beta \int_{\mathbb{R}^3} \mathrm{d}x \, v(x) \frac{1}{N^2} \sum_{1 \le i < j \le N} L_\beta^{(i,j)}(\tfrac{1}{N}x).$$

[Geman, Horowitz, Rosen (1984)]: $x \mapsto L_\beta^{(i,j)}(x)$ is continuous in $x = 0$, and (formally)

$$L_\beta^{(i,j)}(0) = \int_{\mathbb{R}^3} \mathrm{d}x \, \frac{\mu_\beta^{(i)}(\mathrm{d}x)}{\mathrm{d}x} \frac{\mu_\beta^{(j)}(\mathrm{d}x)}{\mathrm{d}x},$$ Brownian intersection local time.

Hence,

$$K_{N,\beta} \approx N\beta 4\pi \widetilde{\alpha}(v) \frac{2}{N^2} \sum_{1 \le i < j \le N} L_\beta^{(i,j)}(0) \approx N\beta 4\pi \widetilde{\alpha}(v) \left\| \frac{\mathrm{d}\overline{\mu}_{N,\beta}}{\mathrm{d}x} \right\|_2^2,$$

where $\overline{\mu}_{N,\beta} = \frac{1}{N} \sum_{i=1}^N \mu_\beta^{(i)}$.

Cramér's theorem $\Longrightarrow$ $$\mathbb{P}\big(\overline{\mu}_{N,\beta} \approx \varphi^2(x)\,\mathrm{d}x\big) \approx \mathrm{e}^{-N\beta J_\beta(\varphi^2)}.$$

Now substitute $\varphi^2(x)\,\mathrm{d}x = \overline{\mu}_{N,\beta}(\mathrm{d}x)$.

The effect of symmetrisation

So far, we studied the large-N limit for Brownian motions starting at the origin and having a free end. What happens for symmetrised motions? We do this here without pair interaction. Let $\mathfrak{m} \in \mathcal{M}_1(\mathbb{R}^d)$ be an initial distribution and consider the (non-normalised!) symmetrised Brownian bridge measure

$$\mathbb{P}_{\mathfrak{m},\beta}^{(\mathrm{sym},N)} = \frac{1}{N!} \sum_{\sigma} \int_{(\mathbb{R}^d)^N} \mathfrak{m}^{\otimes N}(\mathrm{d}x) \bigotimes_{i=1}^{N} \mathbb{P}_{x_i,x_{\sigma(i)}}^{\beta}$$

(For symmetrised traces, we must replace $\mathfrak{m}$ by Lebesgue measure.) We are interested in the large deviations of

$$\overline{\mu}_{N,\beta} = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{\beta} \int_0^{\beta} \mathrm{d}s \, \delta_{B_s^{(i)}} \in \mathcal{M}_1(\mathbb{R}^d).$$

In other words, we search for a function $I_{\beta,\mathfrak{m}} \colon \mathcal{M}_1(\mathbb{R}^d) \to \mathbb{R}$ such that

$$\mathbb{P}_{\mathfrak{m},\beta}^{(\mathrm{sym},N)} \big(\overline{\mu}_{N,\beta} \in A \big) \approx \mathrm{e}^{-N \inf_A I_{\beta,\mathfrak{m}}}, \qquad A \subset \mathcal{M}_1(\mathbb{R}^d).$$

Large deviations for symmetrised BMs

Theorem [Adams, K. (2006)]. Let $d \in \mathbb{N}$ be arbitrary. Then, as $N \to \infty$, $\overline{\mu}_{N,\beta}$ satisfies under $\mathbb{P}^{(\mathrm{sym},N)}_{\mathfrak{m},\beta}$ a large-deviation principle with rate function

$$I_{\beta,\mathfrak{m}}(\varphi^2) = \inf_{q \in \mathcal{M}_1^{(\mathrm{s})}(\mathbb{R}^d \times \mathbb{R}^d)} \Big[H(q|\overline{q} \otimes \mathfrak{m}) + J_\beta^{(q)}(\varphi^2) \Big],$$

where

$$J_\beta^{(q)}(\varphi^2) = \sup_{f \in \mathcal{C}_\mathrm{b}(\mathbb{R}^d)} \Big[\beta \langle f, \varphi^2 \rangle - \int_{(\mathbb{R}^d)^2} q(\mathrm{d}x\,\mathrm{d}y)\, \log \mathbb{E}^\beta_{x,y}\big[\mathrm{e}^{\int_0^\beta f(B_s)\,\mathrm{d}s} \big] \Big].$$

Here $\overline{q}(A) = q(A \times \mathbb{R}^d) = q(\mathbb{R}^d \times A)$ and $H(q|\overline{q} \otimes \mathfrak{m}) = \int q \, \log \frac{\mathrm{d}q}{\mathrm{d}(\overline{q} \otimes \mathfrak{m})}$.

Explanation:

- For any $U_1, U_2 \subset \mathbb{R}^d$, $Nq(U_1 \times U_2)$ Brownian motions start in U_1 and end in U_2.
- The entropy term $H(q|\overline{q} \otimes \mathfrak{m})$ describes the rate of the number of corresponding permutations.
- The ‘probabilistic’ energy function $J_\beta^{(q)}$ describes the large deviations for the N Brownian motions with the prescribed initial-terminal condition.

The special case of traces

If we want to describe traces, we replace $\mathfrak{m}$ by Lebesgue measure and must add a trap potential W. By an explicit analytical identification of the rate function of the previous theorem, one finds:

Corollary [ADAMS, K. (2006)]. Let $d \in \mathbb{N}$ and let $\mathfrak{m}$ be Lebesgue measure. Then $\mu_{N,\beta}$ satisfies under the measure

$$\exp\Big\{ -\sum_{i=1}^N \int_0^\beta W(B_s^{(i)})\, \mathrm{d}s \Big\}\, \mathrm{d}\mathbb{P}_{\mathfrak{m},\beta}^{(\mathrm{sym},N)}$$

a large deviation principle with rate function $\varphi^2 \mapsto \beta\big[\|\nabla\varphi\|_2^2 + \langle W, \varphi^2\rangle\big]$.

- Hence, the large-N deviations of N symmetrised BM's with time length β are the same as the ones of one single BM with time length β.
- Interpretation: The main contribution comes from those permutations that possess a cycle of length N.
- From this corollary, one can conjecture that, for any $\beta \in (0,\infty)$,

$$\lim_{N\to\infty} \frac{1}{N\beta} \log \mathrm{Tr}_+\big(\mathrm{e}^{-\beta \mathcal{H}_N}\big) = -\chi^{(\mathrm{GP})}(\alpha(v)).$$

Concluding remarks

- Actually, the last statement has been proved in [SEIRINGER (2006)] using his older result and standard, but clever, entropy estimates for the symmetrised trace respectively an eigenvalue expansion.
- The Hartree model is not as ‘physical’ as the canonical model, but is a good test case for rigorous investigations.
- The Hartree model is easier to study than the canonical model and features similar properties.