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The interacting Bose gas in the semiclassical limit

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A quantum system of N particles in a box $\Lambda \subset \mathbb{R}^d$ with mutually repellent interaction is described by the Hamilton operator

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

- The kinetic energy term Δ_i acts on the i-th particle.
- The trap potential $W\colon \mathbb{R}^d \to [0,\infty]$ satisfies $\lim_{|x|\to\infty} W(x) = \infty$ and $\int_{\mathbb{R}^d} \mathrm{e}^{-\beta W(x)}\,\mathrm{d}x < \infty$ for any $\beta > 0$.
- The pair potential $v\colon \mathbb{R}^d \to [0,\infty)$ is assumed (for simplicity) to be bounded and continuous.

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We concentrate on Bosons and introduce a symmetrisation. The symmetrised trace of $\exp\{-\beta\mathcal{H}^{(\Lambda)}_N\}$ at fixed temperature $1/\beta \in (0,\infty)$ in Λ is the

partition function: $$Z_N(\beta,a,W,v) = \mathrm{Tr}_+\big(\mathrm{e}^{-\beta\mathcal{H}^{(N)}_{a,W,v}}\big) = Z_N(\beta a, 1, \tfrac{1}{a}W, \tfrac{1}{a}v).$$

(the trace of the projection on the set of symmetric ($=$ permutation invariant) wave functions).

In this talk, we consider the semiclassical limit:

$$a = N^{-d/2} \qquad \text{and} \qquad \frac{1}{N}v \text{ instead of } v.$$

Hence, we consider

$$Z_N^{(\mathrm{MFSC})}(\beta) = Z_N(\beta, N^{-2/d}, W, \tfrac{1}{N}v).$$

This regime is sometimes called (mean-field) semiclassical, since the squared Planck constant in the front of the Laplace operator is replaced by $N^{-2/d}$, while the interaction is of mean-field type.

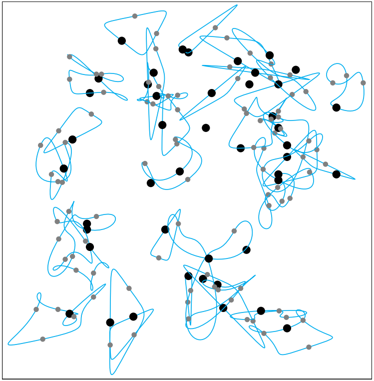
- Every particle interacts with every particle on the same scale one,
- The total interaction of the system is scaled to order N.
- Each of the three energies (kinetic, trap, interaction) contributes on the same scale.
- The N particles are confined in a finite region (not dependent on N).

(The special case $d = 3$, $W(x) = \frac{1}{4}\omega^2|x|^2$, $||\mathrm{Hess}(v)|| \leq \frac{1}{2}\omega$ was handled in [DEUCHERT/SEIRINGER (2021)], see later.)

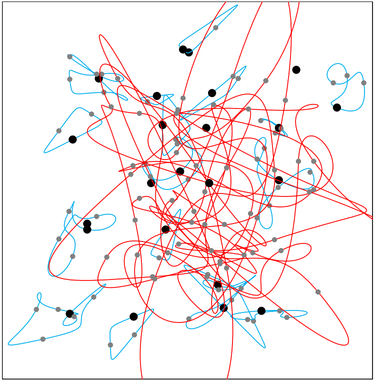
- We derive a variational formula for the free energy in which all parts (condensate and remaining particles) appear with spatial information.
- We want to start from the Feynman–Kac formula, and the variational formula explicitly shows the family of cycles of all lengths and their spatial distribution, and the remaining particles in all long cycles.
- The long cycles come with interaction energy only and have no entropy term .
- This formula will have always minimizers; the term coming from the long cycles might be zero or non-trivial. We want to see a phase transition in β here.
- We want to employ combinatorial and probabilistic arguments (theory of large deviations of sums of i.i.d. random variables).
- The FK formula seems too cumbersome to handle also the *off-diagonal long-range order (ODLRO)* explicitly. However, (work in progress), we will give evidence for the relation

$$\text{long loops} \qquad \Longleftrightarrow \qquad \text{condensate.}$$

Illustration of condensate phase transition



Subcritical (low β) Bose gas
without condensate



Supercritical (large β) Bose gas
with additional condensate (red)

Limiting free energy: $$f_{\mathrm{MFSC}}(\beta) = -\frac{1}{\beta}\lim_{N\to\infty}\frac{1}{N}\log Z_N^{(\mathrm{MFSC})}(\beta).$$

Variational characterisation

$$f_{\mathrm{MFSC}}(\beta) = \inf_{\substack{\mu,\mu_c\in\mathcal{M}(\mathbb{R}^d):\\ \mu+\mu_c\in\mathcal{M}_1(\mathbb{R}^d)}} \Big(\big\langle(\mu+\mu_c), v\star(\mu+\mu_c)\big\rangle + \langle W,\mu+\mu_c\rangle + \frac{1}{\beta}I(\mu)\Big),$$

where

$$I(\mu) = \inf_{\substack{p=(p_k)_{k\in\mathbb{N}}\in[0,1]^{\mathbb{N}}:\\ \sum_k kp_k=\mu(\mathbb{R}^d)}} \Big(\mathcal{S}(p) + \inf_{\substack{(\rho_k)_k\in\mathcal{M}_1(\mathbb{R}^d)^{\mathbb{N}}:\\ \mu=\sum_k kp_k\rho_k}} \sum_{k\in\mathbb{N}} p_k\Big\langle\rho_k, \log\frac{\mathrm{d}\rho_k}{\mathrm{dLeb}}\Big\rangle\Big),$$

and

$$\mathcal{S}(p) = \sum_{k\in\mathbb{N}} p_k \log\Big(\frac{k}{\mathrm{e}}p_k(4\pi\beta k)^{d/2}\Big).$$

Remark: $\langle W,\mu\rangle = \sum_{k\in\mathbb{N}} kp_k\langle W,\rho_k\rangle = -\frac{1}{\beta}\sum_{k\in\mathbb{N}} p_k\langle\rho_k, \log\frac{1}{\mathrm{e}^{-\beta kW}}\rangle$, and an entropy formula can be substituted.

We are based on the Feynman–Kac formula, which writes the partition function in terms of a family of Brownian cycles ($\Longrightarrow$ later).

- $\rho_k =$ spatial density (normalized) of the loops of length k
- $p = (p_k)_{k\in\mathbb{N}} =$ distribution of lengths (normalized by $\sum_k kp_k = \mu(\mathbb{R}^d)$)
- $\mathcal{S}(p) =$ combinatorial entropy
- $\mu =$ spatial distribution (unnormalized) of the short loops
- $\mu_{\rm c} =$ spatial distribution of the long loops, normalized such that $\mu(\mathbb{R}^d) + \mu_{\rm c}(\mathbb{R}^d) = 1$.
- Given μ, the distribution $\mu_{\rm c}$ is an equilibrium measure in the sense that it minimizes $\langle \mu_{\rm c}, v\star\mu_{\rm c}\rangle + \langle \mu_{\rm c}, W + 2v\star\mu\rangle$ subject to having total mass $1-\mu(\mathbb{R}^d)$. In general, such minimizers are highly non-trivial.
- In the free case ($v = 0$), and $W = +\infty 1\!\!1_{Q^{\rm c}}$ with a box Q of volume $1/\rho$,

$$f_{\rm MFSC}(\beta) = \frac{1}{\beta} \inf_{\mu\in\mathcal{M}_{\leq 1}(Q)} I(\mu).$$

  and $\inf_{\rho_k}\langle \rho_k, \log\frac{\rho_k}{{\rm Leb}_Q}\rangle = \log\rho$. Then $I(\mu)$ is the variational formula that appears in the free Bose gas in the thermodynamic limit with ρ equal to the particle density. It shows the famous phase transition at $\rho = \rho_{\rm c}(\beta) = (4\pi\beta)^{-d/2}\sum_k k^{-d/2}$.

We write $\xi_{x,y}^{(\beta)}$ for the canonical Brownian bridge measure from x to y with time interval $[0,\beta]$ and denote the set of integer partitions of N by

$$\mathfrak{P}_N = \Big\{ l = (l_k)_{k\in\mathbb{N}} \in \mathbb{N}_0^{\mathbb{N}} \colon \sum_{k\in\mathbb{N}} k l_k = N \Big\}.$$

Starting point of proof

$$Z_N(\beta,a,W,v) = \sum_{l\in\mathfrak{P}_N} \Big(\prod_{k\in\mathbb{N}} \frac{(4\pi\beta a k)^{-\frac{d}{2}l_k} \gamma_{\beta a k,\frac{1}{a}W}^{l_k}}{l_k!\, k^{l_k}} \Big) \bigotimes_{k\in\mathbb{N}} \big(\overline{\xi}^{(\beta a k,\frac{1}{a}W)}\big)^{\otimes l_k} \Big[\mathrm{e}^{-\beta \mathcal{G}_{\beta a,v}^{(l)}} \Big],$$

where

$$\overline{\xi}^{(\beta,W)}(\mathrm{d}f) = \frac{\int_{\mathbb{R}^d} \mathrm{d}x\, \mathrm{e}^{-\beta \mathcal{W}_\beta(f)}\, \xi_{x,x}^{(\beta)}(\mathrm{d}f)}{(4\pi\beta)^{-d/2}\gamma_{\beta,W}},$$

and $\gamma_{\beta,W}$ is the normalization such that $\overline{\xi}^{(\beta,W)}$ is a probability measure.

- trap interaction: $\mathcal{W}_\beta(f) = \frac{1}{\beta}\int_0^\beta W(f(s))\,\mathrm{d}s.$
- mutual interaction: $\mathcal{V}_\beta(f,g) = \frac{1}{\beta}\int_0^\beta v(f(s)-g(s))\,\mathrm{d}s.$
- All the mutual interactions of the legs of the cycles are summarized in $\mathcal{G}_{\beta a,v}^{(l)}$.

Recall: later $a = N^{-2/d}$, and v is replaced by $\frac{1}{N}v$.

For $v \equiv 0$ and $W = \infty$ outside a box $\Lambda \subset \mathbb{R}^d$ and continuous inside Λ, it was shown in [Adams and K. (2008)] for the case $a = 1$ that

$$\lim_{N\to\infty} \frac{1}{N} \log Z_N(\beta, 1, W, 0) = \beta\lambda(W),$$

where $\lambda(W)$ is the largest L^2-eigenvalue of $\Delta + W$. The r.h.s. is the exponential rate for the contribution from one single Brownian loop of length N (i.e., time interval $[0, \beta]$). This admits the interpretation of 100 percent condensation.

Conjectures:

- This is true for any $a \gg N^{-2/d}$ and many v, since all finite-length cycles are suppressed: all the partition terms $1/l_k!$ with $l_k \asymp N$ cannot be balanced by the term $a^{-\frac{d}{2} l_k} \ll \frac{1}{N}$ that comes from the normalization $(4\pi\beta a k)^{-d/2}$ of the Brownian bridge measure.
- Furthermore, if $a \ll N^{-2/d}$, for the same reason the finite-length cycles give a much larger contribution than all the long loops $\Longrightarrow$ no condensation.

Stirling's formula and elementary computation, putting $l_k \approx Np_k$ and $a = N^{-2/d}$, leads to

$$\prod_{k\in\mathbb{N}} \frac{(4\pi\beta ak)^{-\frac{d}{2}l_k}\gamma_{\beta ak,W/a}^{l_k}}{l_k!\,k^{l_k}} \approx \exp\Big\{-N\Big[\mathcal{S}(p) - \sum_{k\in\mathbb{N}} p_k \log \int_{\mathbb{R}^d} \mathrm{e}^{-\beta kW(x)}\,\mathrm{d}x\Big]\Big\}.$$

Since the time length $\beta N^{-2/d}$ of each leg vanishes, we can approximate

$$\mathcal{V}_{\beta N^{-2/d}}(f,g) \approx v(f(0)-g(0)) \qquad \text{and} \qquad \mathcal{W}_{\beta N^{-2/d}}(f) \approx W(f(0)), \qquad f,g \in \mathcal{C}_{\beta N^{-2/d}}.$$

The particles of the system are at the sites

$$X_j^{(k,i)} = B_j^{(k,i)}(0) = B^{(k,i)}(j\beta N^{-2/d}), \qquad j = 1,\dots,k.$$

Empirical measure of the particles in cycles of length $\leq L$:

$$\mu_N^{(l,\leq L)} = \frac{1}{N}\sum_{k=1}^{L}\sum_{i=1}^{l_k}\sum_{j=1}^{k}\delta_{X_j^{(k,i)}} \approx \sum_{k=1}^{L}\frac{kl_k}{N}\frac{1}{l_k}\sum_{i=1}^{l_k}\delta_{X_0^{(k,i)}}.$$

This is a mixture of independent empirical measures of i.i.d. points.

Sanov's theorem gives the rate $\mu \mapsto \inf_{\substack{\rho_1,\dots,\rho_L\in\mathcal{M}_1(\mathbb{R}^d):\\ \sum_{k=1}^L p_k k\rho_k=\mu}} \sum_{k=1}^L p_k \Big\langle \rho_k, \log\frac{\rho_k}{f_k}\Big\rangle,$

where $f_k(x) = \mathrm{e}^{-\beta k W(x)}/\int_{\mathbb{R}^d}\mathrm{e}^{-\beta k W}$.

$\Big($Hint: $(\overline{\xi}^{(\beta N^{-2/d}k,N^{2/d}W)})^{\otimes l_k}\Big(\frac{1}{l_k}\sum_{i=1}^{l_k}\delta_{X_0^{(k,i)}}\approx\rho_k\Big)\approx \mathrm{e}^{-l_k\langle\rho_k,\log\frac{\rho_k}{f_k}\rangle}, \qquad l_k\to\infty.\Big)$

L-condensate: $\mu_{N,\mathrm{c}}^{(l,>L)} = \frac{1}{N}\sum_{k=L+1}^{\infty}\sum_{i=1}^{l_k}\sum_{j=1}^{k}\delta_{X_j^{(k,i)}}$

Its entropy is of order $\mathrm{e}^{O(N^{1-\frac{2}{d}})}$ (= total time length of underlying Brownian motions)
The interaction is a function of the two empirical measures:

$$\mathcal{G}^{(l)}_{\beta N^{-2/d},vN^{2/d}} \approx \big\langle \mu_N^{(l,\le L)}+\mu_{N,\mathrm{c}}^{(l,>L)}, v\star(\mu_N^{(l,\le L)}+\mu_{N,\mathrm{c}}^{(l,>L)})\big\rangle.$$

The variational formula always has a minimizer (μ, μ_c). (Weak topology of measures, lower semicontinuity, compactness of level sets of entropies)

Critical thresholds:

$$\beta_c^{(1)} = \inf\{\beta \in (0,\infty) \colon \text{there is a minimizer } (\mu,\mu_c) \text{ with } \mu_c \neq 0\}, \quad (1)$$

$$\beta_c^{(2)} = \inf\{\beta \in (0,\infty) \colon \text{every minimizer } (\mu,\mu_c) \text{ has } \mu_c \neq 0\}, \quad (2)$$

Phase transition

1. If $d \geq 3$ and β is large enough, then every minimizer (μ, μ_c) satisfies $\mu_c \neq 0$. In particular, $\beta_c^{(2)} < \infty$.
2. Assume that $d \in \mathbb{N}$ is arbitrary and that $v \in L^p(\mathbb{R}^d)$ for some $p > 1$. Then, if $\beta \in (0, \infty)$ is small enough, then every minimizer (μ, μ_c) satisfies $\mu_c = 0$. In particular, $\beta_c^{(1)} > 0$.

EL–equations for minimizing $((\rho_k)_{k\in\mathbb{N}}, \mu_c)$ with $\mu = \sum_{k\in\mathbb{N}} k\rho_k$:
Define

$$g_k = \frac{\mathrm{d}\rho_k}{\mathrm{d}x} \qquad \text{and} \qquad \Phi(x) = 2v \star (\mu + \mu_c)(x) + W(x), \qquad x \in \mathbb{R}^d,$$

then we have

$$\beta k \Phi(x) + \log g_k(x) + \log\left((4\pi\beta k)^{d/2} k\right) = \beta\lambda k, \qquad x \in \mathbb{R}^d, k \in \mathbb{N},$$

where $\lambda \in \mathbb{R}$ is the Lagrange multiplier, and

$$\Phi \geq \lambda \quad \text{in } \mathbb{R}^d, \qquad \text{and} \qquad \Phi = \lambda \quad \text{on } \mathrm{supp}(\mu_c).$$

(See also semi-classical limit for fermions at zero temperature [FOURNAIS, LEWIN, SOLOVEJ (2018)] and at positive temperature [LEWIN, MADSEN, TRIAY (2019)].)

Special case ([DS 21]):

$$d = 3, \qquad W(x) = \frac{\omega^2}{4} x^2, \qquad ||\mathrm{Hess}(v)|| \le \frac{1}{2}\omega.$$

The latter assumption implies that the condensate is concentrated at 0, i.e., $\mu_c = g\delta_0$.
For $\gamma\colon \mathbb{R}^3 \times \mathbb{R}^3 \to [0,\infty)$ and $g \in [0,1]$, put

$$\mathcal{F}^{(\mathrm{sc})}(\gamma, g) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3\times\mathbb{R}^3} \big(p^2 + W(x)\big)\gamma(p,x)\,\mathrm{d}(p,x) + \frac{1}{2}\langle \rho, v \star \rho\rangle$$
$$+ \frac{1}{\beta}\frac{1}{(2\pi)^3} \int_{\mathbb{R}^3\times\mathbb{R}^3} \big(\gamma \log\gamma - (1+\gamma)\log(1+\gamma)\big)\,\mathrm{d}(p,x),$$

(γ, g) is subject to the normalization (here ρ is the spatial distribution of the particles)

$$\rho \in \mathcal{M}_1(\mathbb{R}^d) \qquad \text{and} \qquad \rho(\mathrm{d}x) = \Big(\frac{1}{(2\pi)^3}\int_{\mathbb{R}^3} \gamma(p,x)\,\mathrm{d}p\Big)\mathrm{d}x + g\delta_0(\mathrm{d}x).$$

Then [DS 21] says that the free energy is equal to the minimum of $\mathcal{F}^{(\mathrm{sc})}(\gamma, g)$ over these γ and g, and ρ is the particle distribution and g the total mass of the condensate.

$\mathcal{F}^{(\mathrm{sc})}$ possesses precisely one minimizing (γ, g) with Euler-Lagrange equation

$$\gamma(p,x) = \frac{1}{\exp\big(\beta\big(p^2 + W(x) + v \star \rho(x) - \mu\big)\big) - 1},$$

for some chemical potential $\mu \le v \star \rho(0)$ with $[\mu - v \star \rho(0)]g = 0$. Replacing v by λv and making $\lambda \in (0,\infty)$ small enough, then Banach's fixed point theorem applies and shows that there is precisely one solution to the crucial fixed point equation

$$h(x) = \beta^{-3/2} \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{1}{\exp\big(p^2 + \beta\big(W(x) + \lambda v \star h(x) - \lambda v \star h(0)\big)\big) - 1}\, \mathrm{d}p.$$

It follows (after showing that there are non-trivial sub- and supercritical phases) that there is $\beta_{\mathrm{c}} \in (0,\infty)$ such that $g = 0$ for $\beta < \beta_{\mathrm{c}}$ and $g > 0$ for $\beta > \beta_{\mathrm{c}}$.

Observation: In this special case, the EL equations of [DS (2021)] for ρ coincide with our EL equations for $\mu + \mu_{\mathrm{c}}$ (expand $\gamma(p,x)$ into a geometric series and use a Gaussian integral to indentify $\rho(x)$), even though we were not able to map their variational problem on ours.
We might be able (work in progress) to carry out analogous arguments for our more general case, at least in $d \ge 5$.

As said before, proof of ODLRO with FK formula seems hard.
Alternately, consider $\varphi\colon \mathbb{R}^d \to [0,\infty)$ with $\|\varphi\|_1 = 1$ and define

$$a^+(\varphi)a(\varphi)|f_1,\dots,f_N\rangle = \sum_{i=1}^N \langle\varphi, f_i\rangle |f_1,\dots,f_{i-1},\varphi,f_{i+1},\dots,f_N\rangle.$$

Then

$$a^+(\varphi)a(\varphi) = \sum_{i=1}^N [(\mathcal{L}_\varphi)_i + \varphi(x_i)],$$

where $(\mathcal{L}_\varphi)_i$ is the restriction to the i-th coordinate of the operator

$$\mathcal{L}_\varphi(f)(x) = \varphi(x)\int_{\mathbb{R}^d} f\varphi(y)[f(y)-f(x)]\,\mathrm{d}y.$$

Plan: Find large-deviations rate function for the process with generator $-N^{-2/d}\sum_{i=1}^N \Delta_i + h\mathcal{L}_\varphi$, with $h>0$, and use that to derive a formula for the free energy in the semiclassical limit for that instead of $-N^{-2/d}\sum_{i=1}^N \Delta_i$. Then show that $\frac{\partial^+}{\partial h}|_{h=0}$ depends only on μ_c.