Weierstraß-Institut für
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A Variational Formula for the Free Energy of a Many-Boson System

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

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

- The kinetic energy term Δ_i acts on the i-th particle.
- the pair potential $v\colon (0,\infty) \to [0,\infty]$ decays quickly at ∞ and explodes at 0.
- we consider some boundary condition $\mathrm{bc} \in \{\mathrm{Dir}, \mathrm{per}\}$ in the centred box $\Lambda = \Lambda_N \subset \mathbb{R}^d$ with volume N/ρ, where $\rho \in (0,\infty)$ is the fixed particle density.

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Goal of this talk: Describe the particle system at positive temperature in the limit $N \to \infty$, at fixed positive particle density.

We shall concentrate on Bosons and introduce a symmetrisation.

Long-term goal: Understand Bose-Einstein condensation (BEC), a celebrated phase transition at very low temperature in $d \geq 3$.
(More about that later).

Goals

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$$Z_N^{(\mathrm{bc})}(\beta,\Lambda_N) = \mathrm{Tr}_+^{(\mathrm{bc})}\big(\exp\{-\beta\mathcal{H}_N\}\big).$$

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Our starting point ist the existence of the limiting free energy:

Theorem A:

For $\mathrm{bc}\in\{\mathrm{Dir},\mathrm{per}\}$, any $d\in\mathbb{N}$ and any $\beta,\rho\in(0,\infty)$, the following limit exists:

$$f^{(\mathrm{bc})}(\beta,\rho)=-\lim_{N\to\infty}\frac{1}{\beta|\Lambda_N|}\log Z_N^{(\mathrm{bc})}(\beta,\Lambda_N).$$

- The existence of the thermodynamic limit may be also shown by standard methods, see [RUELLE (1969)], e.g.
- We have $f^{(\mathrm{Dir})}=f^{(\mathrm{per})}$, see e.g. [ANGELESCU/NENCI (1973)], in combination with estimates from [BRATTELI/ROBINSON (1997)].

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In the following, we identify the limit, which is the main purpose of this talk. We first restrict to empty boundary condition and write $Z_N = Z_N^{(\emptyset)}$.

Main Strategy (1)

Our overall goal is to make the partition function $Z_N(\beta, \Lambda_N)$ amenable to a large-deviation analysis by rewriting it in a form like

$$Z_N(\beta, \Lambda_N) = \mathbb{E}\Big[\mathrm{e}^{-|\Lambda_N| F(\mathfrak{R}_N)} \mathbb{1}_{\{G(\mathfrak{R}_N)=c\}}\Big],$$

where $c \in \mathbb{R}$, and F and G are continuous and bounded functions on some nice state space $\mathcal{X}$,

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where $c \in \mathbb{R}$, and F and G are continuous and bounded functions on some nice state space $\mathcal{X}$, and $(\mathfrak{R}_N)_{N\in\mathbb{N}}$ is an $\mathcal{X}$-valued sequence of random variables that satisfy a large-deviation principle:

$$\lim_{N\to\infty} \frac{1}{|\Lambda_N|} \log \mathbb{P}(\mathfrak{R}_N \in A) = -\inf_A I, \qquad A \subset \mathcal{X},$$

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Varadhan's lemma then implies that

$$\lim_{N\to\infty} \frac{1}{|\Lambda_N|} \log \mathbb{E}\Big[\mathrm{e}^{-|\Lambda_N| F(\mathfrak{R}_N)} \mathbb{1}_{\{G(\mathfrak{R}_N)=c\}}\Big] = -\inf\Big\{F(R) + I(R) : R \in \mathcal{X}, G(R) = c\Big\}.$$

(If G is only lower semi-continuous, one should have '$G(R) \leq c$' in the formula, and we have *a priori* only '$\leq$' instead of '$=$'.)

Main Strategy (2)

We need three main reformulation steps:

- Feynman-Kac formula: N interacting Brownian bridges with symmetrised initial-terminal condition,
- Cycle expansion: Reorganisation in terms of the cycle lengths of the concatenated Brownian bridges,
- Marked random point fields: Rewrite in terms of Poisson random fields with the cycles attached as marks.

The stationary empirical field of the marked Poisson process, $\mathfrak{R}_N$, will turn out to be the above mentioned large-deviation reference process.

The first step is classic, the second well-known, and the third is new in this context.

N Brownian bridges $B^{(1)}, \dots, B^{(N)}$ in Λ_N with generator Δ and time horizon $[0, \beta]$, starting from x and terminating at y under $\mu_{x,y}^{(\beta)}$.

The total mass of $\mu_{x,x}^{(\beta)}$ is $(4\pi\beta)^{-d/2}$.

The pair interaction is

$$\mathcal{G}_N(\beta) = \sum_{1 \leq i < j \leq N} \int_0^\beta \mathrm{d}s \, v\big(|B_s^{(i)} - B_s^{(j)}|\big).$$

Feynman-Kac formula [GINIBRE (1970)]:

For $\mathrm{bc} \in \{\mathrm{Dir}, \mathrm{per}\}$, any $N \in \mathbb{N}$ and any measurable bounded set Λ,

$$Z_N^{(\mathrm{bc})}(\beta, \Lambda) = \frac{1}{N!} \sum_{\sigma \in \mathfrak{S}_N} \int_{\Lambda^N} \mathrm{d}x_1 \cdots \mathrm{d}x_N \bigotimes_{i=1}^N \mathbb{E}_{x_i, x_{\sigma(i)}}^{(\beta, \mathrm{bc})} \Big[\mathrm{e}^{-\mathcal{G}_N(\beta)} \Big],$$

where $\mathfrak{S}_N$ is the set of permutations of $1, \dots, N$.

We now take empty boundary condition, where $\mu_{x,x}^{(\beta,\mathrm{bc})} = \mu_{x,x}^{(\beta)}$.

Second Reformulation: Cycle Expansion

Every permutation σ with the same cycle structure gives the same contribution: concatenate the Brownian bridges along every cycle and carry out the integrals over the corresponding $x_i \in \Lambda_N$. We obtain a random number of cycles of motions with a random length, with total length equal to N.

Cycle expansion:

For any $N \in \mathbb{N}$ and any measurable bounded set Λ,

$$Z_N(\beta, \Lambda) = \sum_{\substack{\lambda_1, \lambda_2, \dots \in \mathbb{N} \\ \sum_k k\lambda_k = N}} \bigotimes_{k \in \mathbb{N}} \left(\mathbb{E}_\Lambda^{(\beta k)}\right)^{\otimes \lambda_k} \left[\mathrm{e}^{-\mathcal{G}_{N,\beta}} \right] \prod_{k \in \mathbb{N}} \frac{(4\pi\beta k)^{-d\lambda_k/2} |\Lambda|^{\lambda_k}}{\lambda_k! k^{\lambda_k}},$$

where $\mathbb{E}_\Lambda^{(\beta k)}$ is the (normalised) expectation w.r.t. a Brownian bridge from x to x, and x is uniformly distributed over Λ.

- λ_k is the number of cycles of length k, that is, the number of Brownian bridges with time horizon $[0, \beta k]$.
- $\mathcal{G}_{N,\beta}$ summarizes all the interaction between any two different parts of any cycle(s).
- The last term summarizes the combinatorics (number of permutations with given cycle structure) and the normalisations.

The Marked Poisson Point Process

There are $m = \sum_k \lambda_k$ independent Brownian cycles in the box Λ.

Their initial-terminal sites are uniformly distributed over Λ. We consider them as the points of a Poisson point process ξ_{P} in $\mathbb{R}^d$.

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The Brownian cycle B_x starting and ending at the Poisson point $x \in \xi_{\rm P}$ is conceived as the mark attached to x. The marked Poisson point process

$$\omega_{\rm P} = \sum_{x \in \xi_{\rm P}} \delta_{(x, B_x)}$$

is a Poisson process on $\mathbb{R}^d \times E$, where $E = \bigcup_{k \in \mathbb{N}} \mathcal{C}_k$ is the mark space,
and $\mathcal{C}_k = \mathcal{C}([0, \beta k] \to \mathbb{R}^d)$ is the set of marks of length k.
We choose its intensity measure as $\frac{1}{k} {\rm Leb}({\rm d}x) \otimes \mu_{x,x}^{(k\beta)}$ on $\mathcal{C}_k$ for any $k \in \mathbb{N}$.

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Alternatively, the intensity measure of $\xi_{\rm P}$ is equal to $q{\rm Leb}$, where

$$q = (4\pi\beta)^{-d/2} \sum_{k \in \mathbb{N}} k^{-1-d/2}.$$

Given $\xi_{\rm P}$, the marks B_x with $x \in \xi_{\rm P}$ are independent with law $\mu_{x,x}^{(k\beta)}/(4\pi k\beta)^{-d/2}$ on $\mathcal{C}_k$.

The Stationary Empirical Field

For a configuration $\omega \in \Omega$, let $\omega^{(N)}$ be the Λ_N-periodic continuation of the restriction of ω to Λ_N. The stationary empirical field is defined as

$$\mathfrak{R}_N = \frac{1}{|\Lambda_N|} \int_{\Lambda_N} \mathrm{d}y \, \delta_{\theta_y \omega_{\mathrm{P}}^{(N)}} \qquad \text{(with } \theta_y = \text{shift operator.)}$$

Then $\mathfrak{R}_N$ is a random element of the set $\mathcal{P}_\theta$ of stationary marked random point fields.

Theorem. [GEORGII/ZESSIN (1994)]

$(\mathfrak{R}_N)_{N\in\mathbb{N}}$ satisfies a large-deviation principle with rate function

$$I(P) = \lim_{N\to\infty} \frac{1}{|\Lambda_N|} H\big(P_{\Lambda_N} \,\big|\, \omega_{\mathrm{P}}|_{\Lambda_N}\big).$$

I is affine, lower semicontinuous and has compact level sets.

Third Rewrite: Marked Random Point Fields

Introduce U = unit box in $\mathbb{R}^d$ and, for configurations $\omega = \sum_{x\in\xi} \delta_{(x,f_x)}$,

$$N_U(\omega) = |U \cap \xi| \qquad \text{and} \qquad N_U^{(\ell)}(\omega) = \sum_{x\in U\cap\xi} \ell(f_x),$$

where $\ell(f_x)$ is the length (= time horizon) of the cycle f_x. The interaction is expressed as

$$\Phi(\omega) = \frac{1}{2} \sum_{x\in U\cap\xi} \sum_{y\in\xi} \sum_{i=0}^{\ell(f_x)-1} \sum_{j=0}^{\ell(f_y)-1} \mathbb{1}_{\{(x,i)\neq(y,j)\}} \int_0^\beta \mathrm{d}s\, v\big(|f_x(i\beta+s)+x-f_y(j\beta+s)-y|\big).$$

Lemma.

$$Z_N(\beta,\Lambda_N) = \mathrm{e}^{|\Lambda_N|q}\mathbb{E}\Big[\mathrm{e}^{-|\Lambda_N|\langle \mathfrak{R}_N,\Phi\rangle}\, \mathrm{e}^{\Psi_N(\omega_{\mathrm{P}})} \mathbb{1}_{\{\langle \mathfrak{R}_N, N_U^{(\ell)}\rangle=\rho\}}\Big],$$

where $q = (4\pi\beta)^{-d/2}\sum_{k=1}^\infty k^{-1-d/2}$, and the term $\Psi_N(\omega_{\mathrm{P}})$ summarises interaction between the configuration inside and outside Λ_N.

- One of the two sums over $x, y \in \Lambda_N$ goes into the definition of $\mathfrak{R}_N$, hence the x-sum in $\Phi(\omega)$ is only over U.
- The term $\Psi_N(\omega_{\mathrm{P}})$ will turn out to be negligible.
- The condition $\langle \mathfrak{R}_N, N_U^{(\ell)}\rangle = \rho$ says that the total length of all cycles in U is equal to N.

Identification of the Limiting Free Energy

Assume that $\int v(|x|)\,\mathrm{d}x < \infty$ and that $\limsup_{r\to\infty} v(r)r^h < \infty$ for some $h > d$.

Theorem B:

For any $\beta, \rho \in (0,\infty)$,

$$\limsup_{N\to\infty} \frac{1}{|\Lambda_N|} \log Z_N(\beta,\Lambda_N) \leq q - \inf\Big\{I(P) + \langle P,\Phi\rangle : P \in \mathcal{P}_\theta, \langle P, N_U^{(\ell)}\rangle \leq \rho\Big\},$$

$$\liminf_{N\to\infty} \frac{1}{|\Lambda_N|} \log Z_N(\beta,\Lambda_N) \geq q - \inf\Big\{I(P) + \langle P,\Phi\rangle : P \in \mathcal{P}_\theta, \langle P, N_U^{(\ell)}\rangle = \rho\Big\}.$$

- The equality $\langle \mathfrak{R}_N, N_U^{(\ell)}\rangle = \rho$ is turned into an inequality $\langle P, N_U^{(\ell)}\rangle \leq \rho$ in the limit superior (in accordance with Fatou's lemma), but not in the limit inferior.
- P stands for a stationary marked random point field $\sum_{x\in\xi} \delta_{(x,f_x)}$. Its mark f_x at x is a random continuous function $[0,\beta\ell(f_x)] \to \mathbb{R}^d$, starting at ending at x.
- The expected total length $\langle P, N_U^{(\ell)}\rangle$ of all the points in the unit box U is not larger than ρ (this is the only dependence on the particle density).
- $\langle P,\Phi\rangle$ is the expected interaction in the configuration.
- $I(P)$ measures how probable P is by comparison to the above marked Poisson process as a reference process.

High-Temperature Phase

In the phase

$$\mathcal{D}_v = \Big\{(\beta,\rho)\in(0,\infty)^2 \colon (4\pi\beta)^{-d/2} \ge \rho \mathrm{e}^{\beta\rho\int v(|x|)\,\mathrm{d}x}\Big\}$$

we find additional estimates to identify the limit:

Lemma.

For any $N\in\mathbb{N}$ and any measurable bounded Λ,

$$\frac{Z_{N+1}(\beta,\Lambda)}{Z_N(\beta,\Lambda)} \ge (4\pi\beta)^{-d/2}\frac{|\Lambda|}{N+1}\mathrm{e}^{-N\beta\int v(|x|)\,\mathrm{d}x/|\Lambda|}.$$

This yields an upper bound for the free energy ...

Corollary 1.

For any $\beta,\rho\in(0,\infty)$,

$$f(\beta,\rho) \le \frac{\rho}{\beta}\log\Big(\rho(4\pi\beta)^{d/2}\Big) + \rho^2\int v(|x|)\,\mathrm{d}x.$$

... and enables us to close the gap in Theorem B:

Corollary 2.

If $(\beta,\rho)\in\mathcal{D}_v$, then

$$\liminf_{N\to\infty}\frac{1}{|\Lambda_N|}\log Z_N(\beta,\Lambda_N) \ge q - \inf\Big\{I(P)+\langle P,\Phi\rangle \colon P\in\mathcal{P}_\theta, \langle P, N_U^{(\ell)}\rangle \le \rho\Big\}.$$

Our variational formulae only register finite cycle lengths.

The total mass of 'infinite' cycle lengths (i.e., those that are unbounded in N) is registered as the number $\rho - \langle P, N_U^{(\ell)} \rangle$.

According to [SÜTŐ (1993)], [SÜTŐ (2002)], the occurence of BEC is signalled by the appearance of infinite cycles, i.e., by the fact that the total mass of infinite cycles gives a non-trivial contribution. In this case, presumably neither of our bounds are sharp.

Conjecture:

BEC occurs $\iff$ Every minimiser P of $I(\cdot) + \langle \cdot, \Phi \rangle$ satisfies $\langle P, N_U^{(\ell)} \rangle < \rho$.

The r.h.s. is satisfied for sufficiently large ρ as soon as, for some $C_\beta > 0$,

Every P minimising $I(P) + \langle P, \Phi \rangle$ satisfies $\langle P, N_U^{(\ell)} \rangle \leq C_\beta$.

Non-occurence of BEC should be signalled by coincidence of the two variational formulas.