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

Wolfgang König

Universität Leipzig

joint work with Stefan Adams (Warwick and Leipzig) and Andrea Collevecchio (Venice)

Background

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

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

- 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.

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 $d \ge 3$.

(More about that later).

Goals

Goal: Describe the symmetrised trace of $\exp\{-\beta \mathcal{H}_N\}$ as $N \to \infty$ at fixed temperature $1/\beta \in (0,\infty)$, that is, the trace of the projection on the set of symmetric (= permutation invariant) wave functions:

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

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)].

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

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

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

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

for some rate function $I\colon \mathcal{X} \to [0, \infty]$.

Varadhan's lemma then implies that

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

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

First Reformulation: Feynman-Kac Formula

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

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

Feynman-Kac formula: 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 $1, \dots, N$.

For a proof, see [Ginibre (1970)], e.g.
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 different cycles and within different parts of a cycle.
- 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 $\xi_{\rm P}$ in $\mathbb{R}^d$.

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 $k \in \mathbb{N}$.

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

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

Lemma.

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

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

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

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

- The equality $\langle \mathfrak{R}_N, N_U^{(\ell)}\rangle = \rho$ is turned into an inequality $\langle P, N_U^{(\ell)}\rangle \le \rho$ 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

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

we find additional estimates to identify the limit:

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

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

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

Corollary 1. For any $\beta,\rho\in(0,\infty)$,

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

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

Corollary 2. If $(\beta,\rho)\in\mathcal{D}_v$, then

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

Cycle Lengths and BEC

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, our two formulas presumably differ.)

Hence, we define

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

This criterion is satisfied for sufficiently large ρ as soon as, for some $C_\beta > 0$,

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

Non-occurence of BEC should be signalled by coincidence of the two variational formulas. Future work will be devoted to a proof of this for $d \geq 3$ and β sufficiently large.