Weierstrass Institute for
Applied Analysis and Stochastics

Leibniz Association

The free energy of the interacting Bose gas, loops and interlacements

Wolfgang König (WIAS Berlin und TU Berlin)

acknowledging many discussions with Stefan Adams, Guillaume Bellot, Alexander Drewitz, Benedikt Jahnel, Quirin Vogel, and Alexander Zass

SPP2265
Random Geometric Systems

SPP2265
Random Geometric Systems

Summary

- The Bose gas can be presented as a Brownian loop ensemble, a PPP of Brownian loops of various (unbounded!) lengths.
- For describing the thermodynamic limit, methods for level-3 large deviations exist since the early 1990s (GEORGII/ZESSIN, e.g.) in the framework of PPPs in $\mathbb{R}^d$ with marks (=loops).
- However, the (very important) long loops could not be handled in this way yet.
- I am presenting a new approach:
  1. Decompose the large box regularly into mesoscopic boxes.
  2. Cut the long loops (those that do not fit into one of the meso-boxes) into its shreds.
  3. Collect all the small loops and all the shreds in a loop-shred configuration.
  4. Adapt large-deviation arguments for the large box, followed by the limit of large meso-boxes.
- We describe the free energy in terms of a (well-behaved) variational formula with loops and interlacements. This offers new possibilities to understand the Bose gas and its condensation in future.

Hamilton operator for a quantum system of N particles in a box $\Lambda \subset \mathbb{R}^d$ with mutually repellent pair interaction:

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

- The kinetic energy term Δ_i acts on the i-th particle.
- The pair potential $v\colon \mathbb{R}^d \to [0,\infty)$ measurable. (Later assumed to be continuous, bounded, compactly supported and superstable.)

Hamilton operator for a quantum system of N particles in a box $\Lambda \subset \mathbb{R}^d$ with mutually repellent pair interaction:

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

- The kinetic energy term Δ_i acts on the i-th particle.
- The pair potential $v\colon \mathbb{R}^d \to [0,\infty)$ measurable. (Later assumed to be continuous, bounded, compactly supported and superstable.)

We describe Bosons and introduce a symmetrisation at temperature $1/\beta$ in a centred box Λ:

partition function: $$Z_N(\beta,\Lambda) = \mathrm{Tr}_+\big(\exp\{-\beta\mathcal{H}_N^{(\Lambda)}\}\big),$$

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

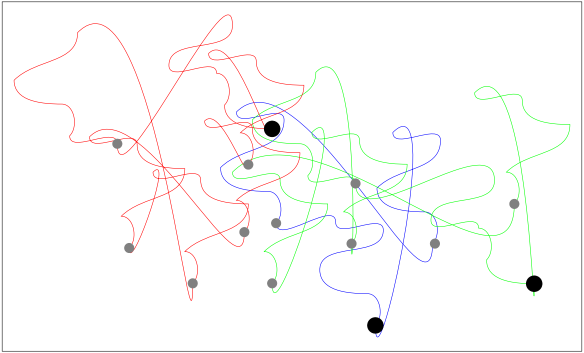
Free energy per volume in the thermodynamic limit:

$$\mathrm{f}(\beta,\rho) = \lim_{N\to\infty} \frac{1}{|\Lambda_N|} \log Z_N(\beta,\Lambda_N), \qquad |\Lambda_N| \sim N/\rho.$$

Purpose of this talk: Derive a formula for $\mathrm{f}(\beta,\rho)$, based on a path-integral representation in terms of the Brownian loop soup.

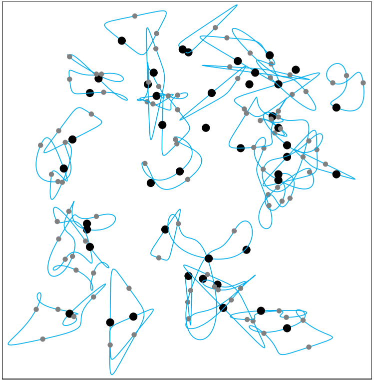
- Unterstanding the conjectured Bose–Einstein condensation (BEC) phase transition is one of the great open problems in mathematical physics.
- Definition of BEC is more tricky than just non-analyticity of $\mathrm{f}(\beta, \cdot)$.
- Connection with Brownian loops goes back to a vaguely formulated idea from [FEYNMAN 1953].
- Mathematical foundation of loop soup representations start with [GINIBRE 1970]; little used in proofs yet in the analysis / mathphys literature on the Bose gas.
- Driving force (not only) for probabilists: Bose–Einstein condensate $\Longleftrightarrow$ long loops?
- We consider periodic boundary condition and Dirichlet zero boundary condition, but suppress this in this talk.

The Bose gas can be written as a random ensemble of Brownian cycles (bridges) $B^{(k,i)}$ of length k, $i = 1, \dots, l_k$, with $N = \sum_{k\in\mathbb{N}} kl_k$ particles.

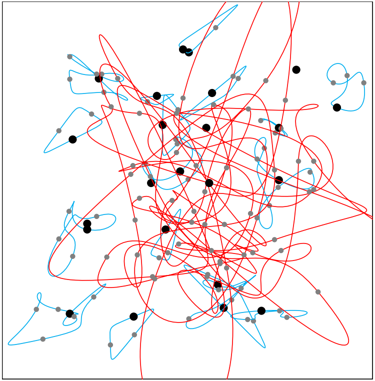


Bose gas consisting of 14 particles, organised in three Brownian cycles, assigned to three Poisson points. The red cycle contains six particles, the green and the blue each four.

The big conjecture is that, for $d \geq 3$ and large enough ρ, in the loop soup a macroscopic part of particles emerge in long loops, the conjectured condensate:



Subcritical (low ρ) Bose gas
without condensate



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

marked point process $\quad \omega = \sum_{x\in\xi} \delta_{(x,f_x)} \in \mathcal{L} = \mathcal{M}_{\mathbb{N}_0}(\mathbb{R}^d \times \mathcal{C}^{(\circlearrowleft)})$

with mark space $\mathcal{C}^{(\circlearrowleft)} = \bigcup_{k\in\mathbb{N}} \mathcal{C}_k^{(\circlearrowleft)}$, where $\mathcal{C}_k = \mathcal{C}([0,\beta k] \to \mathbb{R}^d)$, and $\mathcal{C}_k^{(\circlearrowleft)} = \{f \in \mathcal{C}_k \colon f(\beta\ell(f)) = f(0)\}$ is the set of marks with length = particle number $\ell(f) = k$.

number of particles at points in Λ : $\quad \mathfrak{N}_\Lambda^{(\ell)}(\omega) = \sum_{x\in\Lambda\cap\xi} \ell(f_x).$

interaction: $\quad \Phi_{\Lambda,\Lambda'}(\omega) = \sum_{x\in\xi\cap\Lambda, y\in\xi\cap\Lambda'} T_{x,y}(f_x, f_y),$

where

$$T_{x,y}(f_x,f_y) = \frac{1}{2}\sum_{i=1}^{\ell(f_x)}\sum_{j=1}^{\ell(f_y)} \mathbb{1}\{(x,i)\neq(y,j)\} V(f_{x,i}, f_{y,j}), \qquad x,y\in\xi,\ f_x,f_y\in\mathcal{C}^{(\circlearrowleft)},$$

and $f_{x,i}(\cdot) = f_x((i-1)\beta + \cdot)|_{[0,\beta]}$ is the i-th leg of a function $f_x \in \mathcal{C}^{(\circlearrowleft)}$, and

$$V(f,g) = \int_0^\beta v(f(s) - g(s))\,\mathrm{d}s.$$

Reference PPP $\omega_{\rm P}$ on $\mathbb{R}^d \times \mathcal{C}^{\circlearrowleft}$ with distribution Q and intensity measure

$$\nu_\Lambda(\mathrm{d}x, \mathrm{d}f) = \sum_{k\in\mathbb{N}} \frac{1}{k} \mathrm{Leb}(\mathrm{d}x) \otimes \mu_{x,x}^{(k\beta)}(\mathrm{d}f),$$

where

$$\mu_{x,y}^{(\beta)}(A) = \mathbb{P}_x(B \in A; B_\beta \in \mathrm{d}y)/\mathrm{d}y, \qquad A \subset \mathcal{C}([0,\beta] \to \mathbb{R}^d)$$

is the Brownian bridge measure with generator Δ and time horizon $[0,\beta]$, starting from x and terminating at y. For $x = y$, it has total mass $(4\pi\beta)^{-d/2}$. Hence,

$$\overline{q} = \frac{1}{|\Lambda|} \nu_\Lambda(\Lambda \times \mathcal{C}^{(\circlearrowleft)}) = (4\pi\beta)^{-d/2} \sum_{k\in\mathbb{N}} k^{-1-d/2}.$$

Here is our starting point:

PPP-representation [Adams/Collevecchio/K. 2011]

$$Z_N(\beta,\Lambda) = \mathrm{e}^{|\Lambda|\overline{q}}\, \mathbb{E}\big[\mathrm{e}^{-\Phi_{\Lambda,\Lambda}(\omega_{\rm P})} \mathbb{1}\{\mathfrak{N}_\Lambda^{(\ell)}(\omega_{\rm P}) = N\}\big].$$

Fix a box $W \subset \mathbb{R}^d$. We distinguish loops according to whether their particles are entirely contained in W or not. In the latter case, we shred them into the pieces from entering W till exiting W, but we never cut legs.

projection operator on loops with all the particles in W (W-loop space):

$$\Pi_W^{(\mathcal{L})}(\omega) = \sum_{x\in\xi\colon\, f_x(k\beta)\in W\ \forall k\in[\ell(f_x)]} \delta_{(x,f_x)} \in \mathcal{L}_W, \qquad \text{for } \omega = \sum_{x\in\xi} \delta_{(x,f_x)}.$$

Shredding operator on loops that don't:

$$\Pi_W^{(\mathcal{S})}(\omega) = \sum_{f_x} \sum_{i\in\Gamma_W(f_x)} \delta_{g_i} \in \mathcal{S}_W = \mathcal{M}_{\mathbb{N}_0}(\mathcal{C}_W),$$

where $\Gamma_W(f_x)$ is the set of all W-shreds of f_x, and $\mathcal{C}_W$ is the set of all W-shreds.

Superposed projection operator: $\Pi_W = \Pi_W^{(\mathcal{L})} \oplus \Pi_W^{(\mathcal{S})}$.

boundary-shred operator (collection of entry/exit sites and lengths)

$$\partial\Pi_W^{(\mathcal{S})}(\omega) = \sum_{f_x} \sum_{i\in\Gamma_W(f_x)} \delta_{(g_i(k_1\beta),k_2-k_1,g_i(k_2\beta))} \in \mathcal{T}_W = \mathcal{M}_{\mathbb{N}_0}(W\times\mathbb{N}\times W^{\mathrm{c}}).$$

We aim at a formula of the form (with energy F and entropy I)

$$\mathrm{f}(\beta,\rho)=\overline{q}-\inf\Big\{F(P)+I(P)\colon P\in\mathcal{M}_1^{(\mathrm{s})}(\mathcal{L}\times\mathcal{S}),\langle P,\mathfrak{N}_U^{(\ell)}\rangle=\rho\Big\}.$$

$\mathcal{L}=$ loops space, $\mathcal{S}=$ interlacements space.

For a boundary-shred configuration $\mu=\sum_i\delta_{(x_i,l_i,y_i)}$, denote by $\mathtt{K}_W(\mu,\cdot)=\otimes_i\mu_{x_i,y_i}^{(W,\beta l_i)}$ the canonical extension inside W with l_i-length Brownian bridges in W from x_i to y_i.

Joint specific relative entropy density

The following limit exists for any $P\in\mathcal{M}_1^{(\mathrm{s})}(\mathcal{L}\times\mathcal{S})$ with finite expected particle number in U (with $W=W_R=[-R,R]^d$):

$$\mathrm{h}^{(\mathcal{L},\mathcal{S})}(P)=\lim_{R\to\infty}\frac{1}{|W|}H_{\mathcal{L}_W\times\mathcal{S}_W}\big(\Pi_W(P)\,\big|\,\Pi_W^{(\mathcal{L})}(\mathtt{Q})\otimes[\partial\Pi_W^{(\mathcal{S})}(P)\otimes\mathtt{K}_W]\big).$$

$\mathrm{h}^{(\mathcal{L},\mathcal{S})}$ is lower semi-continuous and affine. Moreover, for any sequence $(K_R)_{R\in\mathbb{N}}$ of compact sets $K_R\subset\mathcal{T}_{W_R}$, the restricted level set is compact for any $c\in\mathbb{R}$:

$$\bigcap_{R\in\mathbb{N}}\{P\in\mathcal{M}_1^{(\mathrm{s})}(\mathcal{L}\times\mathcal{S})\colon\partial\Pi_{W_R}^{(\mathcal{S})}(P)\in K_R,\mathrm{h}^{(\mathcal{L},\mathcal{S})}(P)\le c\}.$$

- Λ_N = centred box with volume $\sim N/\rho$.
- Regular decomposition $\Lambda_N = \bigcup_{z\in Z_{N,R}} z + W_R$, with $Z_{N,R} \subset 2R\mathbb{Z}^d$.
- $\mathfrak{N}^{(\neg R)}_{\Lambda_N}$ = number of particles in loops that have particles only in one of the $z + W_R$.
- $\mathfrak{N}^{(R)}_{\Lambda_N}$ = number of particles in loops that have particles in at least two of the $z + W_R$.
- $F_U(\omega, \varpi)$ = interaction between any particle in $U = [-\frac{1}{2}, \frac{1}{2}]^d$ and all others.
- transformed probability measure

$$\mathrm{d}\widehat{\mathsf{Q}}^{(\Lambda,\mathrm{bc})} = \frac{\mathrm{e}^{-\Phi_{\Lambda,\Lambda}}}{\widehat{Z}^{(\mathrm{bc})}_N(\Lambda)}\,\mathrm{d}\mathsf{Q}^{(\Lambda,\mathrm{bc})}.$$

Constrained free energy

In the limit as $N \to \infty$, followed by $R \to \infty$, the pair $\frac{1}{|\Lambda_N|}(\mathfrak{N}^{(R)}_{\Lambda_N}, \mathfrak{N}^{(\neg R)}_{\Lambda_N})$ satisfies under the measure $\widehat{\mathsf{Q}}^{(\Lambda_N,\mathrm{bc})}$ an LDP on $\{(\rho_1,\rho_2) \in [0,\infty)^2 \colon \rho_1 + \rho_2 = \rho\}$ with continuous and convex rate function $(\rho_1,\rho_2) \mapsto \chi(\rho_1,\rho_2) - \overline{\chi}(\rho)$, where

$$\chi(\rho_1,\rho_2) = \inf\Big\{\mathrm{h}^{(\mathcal{L},\mathcal{S})}(P) + \langle F_U, P\rangle \colon P \in \mathcal{M}^{(\mathrm{s})}_1(\mathcal{L}\times\mathcal{S}),$$
$$\langle \mathfrak{N}^{(\ell,\mathcal{L})}_U, P\rangle = \rho_1, \langle \mathfrak{N}^{(\ell,\mathcal{S})}_U, P\rangle = \rho_2\Big\}.$$

- The number of particles in Λ_N in loops of lengths $\leq L$ and $> L$, respectively, are exponentially equivalent to $(\mathfrak{N}^{(R)}_{\Lambda_N}, \mathfrak{N}^{(\neg R)}_{\Lambda_N})$ in the limit $N \to \infty$, followed by $R \to \infty$, respectively $L \to \infty$. That is, we are on the way to specifying FEYNMAN's vague idea.
- We assumed the interaction potential v to be continuous, bounded and compactly supported, to avoid technicalities. However, we did need super-stability, in order to have a sufficient mutual repellence. This implies nice compactness properties also for the variational formula $\chi(\rho_1, \rho_2)$.
- In [ADAMS, COLLEVECCHIO, K. 2011], only short loops were adequately treated, and only small ρ could be handled.
- In [BELLOT, DEREUDRE, MAÏDA 2024], a Gibbs measure is constructed that might be related to the minimizers of our formula.
- Using some path manipulations, one can show that $\chi(\rho_1 + \rho_2, 0) \leq \chi(\rho_1, \rho_2)$, i.e., every loop-interlacements configuration can be approximated with a loop-configuration.
- Big future goal (non-trivial step towards proving BEC): Prove that, in $d \geq 3$, if ρ is large, then $\chi(\rho, 0)$ has no minimizer.

In the non-interacting case $v = 0$, the "existence of long loops" is "known" since long with critical value

$$\rho_{\rm c} = (4\pi\beta)^{-d/2}\zeta(d/2) = \sum_{k\in\mathbb{N}} k q_k, \qquad \text{with} \qquad q_k = \frac{1}{k}(4\pi\beta k)^{-d/2}.$$

Our formula yields an explicit minimizer as a point process with loops and interlacements of the form

$$P_\rho = \begin{cases} \mathtt{Q}^{(\rho)} \otimes \delta_{\underline{0}}, & \text{if } \rho < \rho_{\rm c}, \\ \mathtt{Q} \otimes \mathtt{R}^{(u_\rho,\beta)}, & \text{if } \rho \geq \rho_{\rm c}, \end{cases}$$

where

- $\underline{0}$ is the empty interlacement point process,
- $\mathtt{R}^{(u,\beta)}$ is essentially SZNITMAN's PPP of Brownian interlacements with particle density $\rho - \rho_{\rm c}$,
- $\mathtt{Q}^{(\rho)}$ is the marked PPP with q_k replaced by some parameter that ensure the particle density $\rho \wedge \rho_{\rm c}$.

Decompose $\Lambda_N = \bigcup_{z\in Z_{N,R}} z + W_R$ regularly into boxes of radius R and register the empirical average of the configurations in the subboxes, distinguished in loops and shreds. More explicitly, define the discrete empirical configuration measure (with $W = W_R = [-R,R]^d$ and $W_z = z + W$)

$$\Xi^{(\omega)}_{N,R} = \frac{1}{\# Z_{N,R}} \sum_{z\in Z_{N,R}} \delta_{(\theta_z(\Pi^{(\mathcal{L})}_{W_z}(\omega)),\theta_z(\Pi^{(\mathcal{S})}_{W_z}(\omega))} \in \mathcal{M}_1(\mathcal{L}_W \times \mathcal{S}_W), \tag{1}$$

where θ_z is the shift-operator such that $\theta_z(z) = 0$.

Strategy:

1. rewrite the partition function $\widehat{Z}_N$ in terms of an integral over $\Xi^{(\omega_{\mathrm{P}})}_{N,R}$ (dropping all interaction between different W_z's),
2. find a large deviation principle for $\Xi^{(\omega_{\mathrm{P}})}_{N,R}$ as $N \to \infty$,
3. use Varadhan's lemma to express the large-N exponential rate of the partition function as a variational formula on the space $\mathcal{M}_1(\mathcal{L}_W \times \mathcal{S}_W)$ with $W = [-R,R]^d$,
4. make $R \to \infty$ in that formula to arrive at χ.