Weierstrass Institute for
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Self-repellent Brownian bridges in the interacting Bose gas

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Joint work in progress with Erwin Bolthausen and Chiranjib Mukherjee

We study random (geometric) permutations, that is, a probability measure on the set

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

of all integer partitions, of the form

$$\mathtt{P}_N(l) = \frac{1}{Z_N} \prod_{k\in\mathbb{N}} \frac{[\theta_k^{(N)}]^{l_k}}{l_k!\, k^{l_k}}, \qquad l = (l_k)_{k\in\mathbb{N}} \in \mathfrak{P}_N.$$

For various choices of $\theta_k^{(N)} = \theta_k$, such models have been studied by Betz, Ueltschi, Zeindler and others (starting in 2009 and continuing). Motivation was the interacting Bose gas after severe simplifications, like interchanging logarithm and integral at a decisive point.

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In this work, we start from the interacting Bose gas and simplify it by dropping all interactions between different cycles in the thermodynamic limit. This leads to the choice

$$\theta_k^{(N)} = N(\gamma_k + o(1)), \qquad N \to \infty, k \in \mathbb{N},$$

with some $\gamma_k \in (0,\infty)$. The main point is that all the remaining self-interactions of a cycle in the Bose gas is in the spirit of the famous self-avoiding random walk. Using extensions of recent progress in the study of these processes (using the lace expansion), we prove the Bose–Einstein phase transition for this simplified model in special cases.

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

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

- The kinetic energy term Δ_i acts on the i-th particle.
- The pair potential $v\colon [0,\infty) \to [0,\infty)$ is (for simplicity) continuous and compactly supported.

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

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

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

We will be working in the thermodynamic limit and will take a centred box Λ_N with volume N/ρ with $\rho \in (0,\infty)$ the particle density.

A Brownian bridge B in Λ_N with generator Δ and time horizon $[0, \beta]$, starting from x and terminating at y under $\mu_{x,y}^{(\beta)}$:

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

The operator $\mathrm{e}^{\beta\Delta}$ has density $\mu_{x,y}^{(\beta)}$ in the sense that

$$\mathrm{e}^{\beta\Delta}(f)(x,y) \text{``}=\text{''} \mu_{x,y}^{(\beta)}(\mathrm{d}f), \qquad f \in \mathcal{C}([0,\beta] \to \mathbb{R}^d).$$

The total mass of $\mu_{x,x}^{(\beta)}$ is $(4\pi\beta)^{-d/2}$.
In $\mathcal{H}_N$, we have N independent Brownian bridges $B^{(1)}, \dots, B^{(N)} \in \mathcal{C}([0,\beta] \to \mathbb{R}^d)$. The symmetrisation is expressed by a sum over all permutations σ of $1, \dots, N$ with the condition $B_\beta^{(i)} = B_0^{(\sigma(i))}$.
The pair interaction is

$$\mathcal{G}_N = \sum_{1 \le i < j \le N} V(B_s^{(i)}, B_s^{(j)}),$$

where

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

Feynman-Kac formula [GINIBRE (1970)]:

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

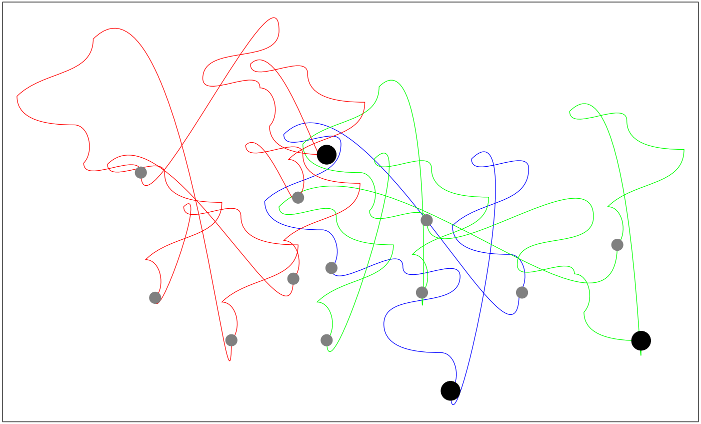
$$Z_N^{(\mathrm{bc})}(\beta, \Lambda) = \frac{1}{N!} \sum_{\sigma \in \mathfrak{S}_N} \int_{\Lambda^N} \mathrm{d}x_1 \cdots \mathrm{d}x_N \bigotimes_{i=1}^{N} \mu_{x_i, x_{\sigma(i)}}^{(\beta,\mathrm{bc})} \Big[\mathrm{e}^{-\mathcal{G}_N(\beta)} \Big],$$

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

Every permutation σ with the same cycle structure gives the same contribution. Indeed, concatenate the Brownian bridges along every cycle and carry out the integrals over the corresponding $x_i \in \Lambda_N$. By the Markov property,

$$\int_{\mathbb{R}^d} \mu_{x,y}^{(\beta)}(\mathrm{d}f_1) \mu_{y,z}^{(\beta)}(\mathrm{d}f_2)\, \mathrm{d}y = \mu_{x,z}^{(2\beta)}(\mathrm{d}(f_1 \diamond f_2)), \qquad f_1, f_2 \in \mathcal{C}([0,\beta] \to \mathbb{R}^d),$$

where $f_1 \diamond f_2 \in \mathcal{C}([0, 2\beta] \to \mathbb{R}^d)$ is the concatenation of f_1 and f_2.
We obtain a random number of cycles of motions with random lengths, with total sum of lengths equal to N.



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.

Every permutation can be decomposed into cycles, i.e., can be represented by a member of the set of *partitions*. We decompose $(B^{(i)})_{i\in\{1,\dots,N\}}$ into the β-legs $B_j = (B_j(s))_{s\in[0,\beta]} = (B((j-1)\beta+s))_{s\in[0,\beta]}$ of the cycles and obtain a family

$$(B_j^{(k,i)})_{k,i,j} \qquad \text{for} \qquad k\in\{1,\dots,N\}, i\in\{1,\dots,l_k\}, \quad \text{and } j\in\{1,\dots,k\}.$$

Then

$$\mathcal{G}_N = \sum_{(k_1,i_1,j_1)\neq(k_2,i_2,j_2)} V\big(B_{j_1}^{(k_1,i_1)}, B_{j_2}^{(k_2,i_2)}\big).$$

Now we change the model: We drop all interactions between different cycles. That is, instead of $\mathcal{G}_N$, we take

$$G_N = \sum_{k=1}^{N}\sum_{i=1}^{l_k}\sum_{1\leq j_1<j_2\leq k} V\big(B_{j_1}^{(k,i)}, B_{j_2}^{(k,i)}\big).$$

Free energy and self-repellent Brownian bridge

Now the partition function decomposes into

$$Z_N^{(\mathrm{bc})}(\beta,) := \sum_{l \in \mathfrak{P}_N} \prod_{k \in \mathbb{N}} \frac{\left[|\Lambda| \Gamma_{\Lambda,k}^{(\mathrm{bc})}\right]^{l_k}}{l_k! \, k^{l_k}},$$

where

$$\Gamma_{\Lambda,k}^{(\mathrm{bc})} = \frac{1}{|\Lambda|} \int_\Lambda \mathrm{d}x \, \mu_{x,x}^{(\mathrm{bc},k\beta)} \left[\mathrm{e}^{-\sum_{1 \le i < j \le k} V(B_i, B_j)} \right].$$

We are interested in the limiting free energy (with $|\Lambda_N| = N/\rho$)

$$f(\beta, \rho) := - \lim_{N \to \infty} \frac{1}{|\Lambda_N|} \log Z_N^{(\mathrm{bc})}(\beta, {}_N), \qquad \beta, \rho \in (0, \infty).$$

We need to introduce the self-repellent Brownian bridge

$$\Gamma_k = \mu_{0,0}^{(k\beta)} \left[\mathrm{e}^{-\sum_{1 \le i < j \le k} V(B_i, B_j)} \right],$$

and its connective constant (convergence radius of power series with coefficients Γ_k)

$$\lambda_{\mathrm{c}}(\beta) = \lim_{k \to \infty} \Gamma_k^{-1/k} \in (0, \infty).$$

Furthermore, denote

$$I(p) = \sum_{k \in \mathbb{N}} p_k \log \frac{p_k k}{\Gamma_k \mathrm{e}}, \qquad p = (p_k)_{k \in \mathbb{N}} \in [0, \infty)^{\mathbb{N}}.$$

Limit of the model

Assume either periodic or zero or free (empty) boundary condition. Then

$$f(\beta,\rho)=\inf_{p\in[0,\infty)^{\mathbb{N}}\colon\ \sum_k kp_k\le\rho}\Big[I(p)+\Big(\rho-\sum_{k\in\mathbb{N}}kp_k\Big)\log\lambda_{\rm c}(\beta)\Big].$$

The normalized cycle-length distribution satisfies a large-deviations principle (LDP) on the set $\{p\in[0,\infty)^{\mathbb{N}}\colon\ \sum_{k\in\mathbb{N}}kp_k\in[0,\rho]\}$ on the scale $|\Lambda_N|$ with rate function

$$J(p)=I(p)+\Big(\rho-\sum_{k\in\mathbb{N}}kp_k\Big)\log\lambda_{\rm c}(\beta)-f(\beta,\rho).$$

A minimizer $p^{(\rho)}$ always exists. If the critical density

$$\rho_{\rm c}(\beta)=\sum_{k\in\mathbb{N}}\lambda_{\rm c}(\beta)^k\Gamma_k\in[0,\infty]$$

is finite, then $f(\beta,\cdot)$ has a phase transition in $\rho_{\rm c}(\beta)$, since $\sum_{k\in\mathbb{N}}kp_k^{(\rho)}=\rho\wedge\rho_{\rm c}(\beta)$.

- We took the cycle weights $\theta_k^{(N)} = N(\gamma_k + o(1))$ for $N \to \infty$ with $\gamma_k = \frac{1}{\rho}\Gamma_k$. For the free Bose gas, $\gamma_k = \frac{1}{\rho}(4\pi\beta k)^{-d/2}$.
- Proof is standard if $\Gamma_{\Lambda_N,k}^{(\mathrm{Dir})}$ respectively $\Gamma_{\Lambda_N,k}^{(\mathrm{per})}$ are replaced by Γ_k (which satisfies empty boundary condition)
- Actually, one would like to have $\theta_k^{(N)} = N(\gamma_k + o(1))$ *uniformly in* k, but this is not true. As far as I have seen the literature, this has not been noticed nor handled for zero and periodic b.c. for the free Bose gas.
- We show that $\Gamma_{\Lambda_N,k}^{(\mathrm{Dir})} \geq \Gamma_k(1-\varepsilon)^k$ for any $\varepsilon > 0$ and all sufficiently large N and all $k \ll N^{1/d}$. (Opposite estimate is clear.) Similar for periodic b.c., but upper bound not yet clear to us.

The free Bose gas (i.e, $v = 0$) condensates in $d \geq 3$. For the interacting Bose gas, one expects it, but is far away from a mathematical understanding. In our model, we can prove:

Phase transition

In $d \geq 5$, the critical density $\rho_c(\beta)$ is finite for any small $\beta > 0$.

- More precisely, the BM in Γ_k behaves like a Gaussian, like the self-repellent random walk.
- Using the conjectural values in $d \leq 4$, we conjecture condensation in $d \geq 2$(!!).
- The proof uses the lace expansion.
- Proofs like that exist since the early 1990s by HARA, SLADE.
- The lace expansion needs a small parameter, usually β, sometimes $1/d$.
- This method can only work if there one can expand around a simple model, often the simple random walk. This can work only in $d \geq 5$.
- More recent proof strategies, starting from the lace expansion, use induction [BOLTHAUSEN, RITZMANN 2015] or clever recursive equations for bounding the Green's function [BOLTHAUSEN, V.D. HOFSTAD, KOZMA 2018]. This was able to handle Gaussian random walks. Our current work extends this.
- Big technical problem: no exact self-intersections, but only approximate ones.

Introduce the SRBM Green's function

$$G_\lambda(x) = \sum_{k=0}^{\infty} \lambda^k \mathbb{E}_0\Big[\mathrm{e}^{-\sum_{1\le i<j\le k} V(B_i,B_j)}\, \mathbb{1}\{B(k\beta)\in \mathrm{d}x\}\Big]\Big/\mathrm{d}x$$

Then $\rho_{\mathrm{c}}(\rho) = G_{\lambda_{\mathrm{c}}(\rho)}(0)$. The finiteness of this is in $d \ge 5$ in the spirit of the CLT (which we will not prove)

$$\mathbb{E}_0\Big[\mathrm{e}^{-\sum_{1\le i<j\le k} V(B_i,B_j)}\, \mathbb{1}\{B(k\beta)\in \mathrm{d}x\}\Big]\Big/\mathrm{d}x \sim \widetilde{C}\lambda_{\mathrm{c}}(\rho)^{-k} k^{-d\xi_d} \mathrm{e}^{-C|x|^2}, \qquad k\to\infty,$$

with the critical exponent $\xi_d = \frac{1}{2}$. That is, for the SRBM the endpoint $B_{k\beta}k^{-1/2}$ is asymptotically Gaussian (some amendment close to the origin). The critical behaviour $B_{k\beta} \asymp k^{\xi_d}$ is conjectured to be

$$\xi_1 = 1, \qquad \xi_2 = \frac{3}{4}, \qquad \xi_3 \approx .598, \qquad \xi_4 = \frac{1}{2}+$$

Since $d\xi_d > 1$ for $d \in \{2,3,4\}$, we conjecture finiteness of the Green's function (including $d = 2$!!).

The generally acknowledged definition of BEC is via the convolution operator $T^{(\mathrm{bc}),\beta}_{N,\Lambda_N}$ on $L^2(\Lambda_N)$ with kernel γ_{N,Λ_N} defined by

$$\gamma_{N,\Lambda}(x,y) = \int_{\Lambda^{2(N-1)}} \mathrm{d}x_2 \dots \mathrm{d}x_N \mathrm{d}y_2 \dots \mathrm{d}y_N \, V^{(\mathrm{bc}),\beta}_{N,\Lambda}(x, x_2, \dots, x_N; y, y_2, \dots, y_N),$$

where $V^{(\mathrm{bc}),\beta}_{N,\Lambda_N}$ is the density of the symmetrization of $\frac{1}{Z^{(\mathrm{bc})}_N(\beta,\Lambda)} \mathrm{e}^{-\beta \mathcal{H}^{(\Lambda)}_N}$.

Definition

We say the model shows ODLRO if the largest eigenvalue of $T^{(\mathrm{bc}),\beta}_{N,\Lambda_N}$ is of order N.
In this case, we say that the model shows Bose–Einstein condensation.

Checking this needs more precision in the asymptotics of $\Gamma^{(\mathrm{bc})}_{\Lambda_N,k}$. The FK-formula for the free Bose gas reads

$$\gamma_{N,\Lambda}(x,y) = \sum_{r=1}^{N} g_{r\beta}(x,y) \frac{Z^{(\mathrm{bc})}_{N-r}(\beta,\Lambda)}{Z^{(\mathrm{bc})}_N(\beta,\Lambda)}.$$

I do not know any proof for ODLRO for periodic of Dirichlet bc for the free Bose gas.