Weierstrass Institute for
Applied Analysis and Stochastics

Leibniz
Association

Off-diagonal long-range order for the free Bose gas via the Feynman–Kac formula

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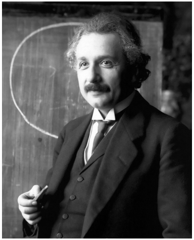
A prediction of 1924

- In 1924, the unknown young physicist SATYENDRA NATH BOSE asked the famous ALBERT EINSTEIN to help him publishing his latest achievement in *Zeitschrift für Physik*.
- Einstein translated the manuscript into German and had published it there for Bose.
- He stressed that the new method is suitable for explaining the quantum mechanics of the ideal gas. He extended the idea to atoms in a second paper: he predicted the existence of a previously unknown state of matter, now known as the Bose–Einstein condensate.



ALBERT EINSTEIN (1879-1955) in 1921

SATYENDRA NATH BOSE (1894-1974) in 1925

- An experimental realisation had to wait until 1995, where some ten thousands of atoms appeared in that condensate at a temperature of 10^{-9} K. $\Longrightarrow$ Nobel Prize in 2001

- Description of the Bose gas in terms of the trace of the negative exponential of an N-particle Hamilton operator in a box
- Bosons need symmetrization.
- Feynman–Kac formula turns the trace into an ensemble of Brownian loops (Feynman cycles) with various lengths ($=$ particle numbers) with a total of N particles.
- Vague idea [FEYNMAN (1953)]: the cycles and their lengths might be a physically relevant quantity? Is the macroscopic appearance of long loops a signal for Bose–Einstein condensation (BEC)? ($\Longrightarrow$ driving force for probabilists!).

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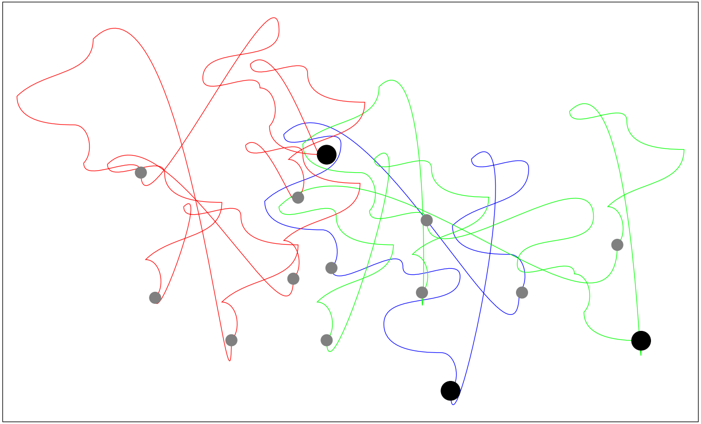
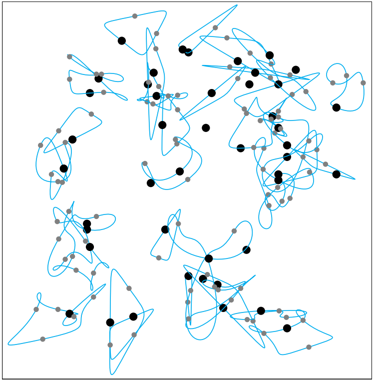
- Vague idea [FEYNMAN (1953)]: the cycles and their lengths might be a physically relevant quantity? Is the macroscopic appearance of long loops a signal for Bose–Einstein condensation (BEC)? ($\Longrightarrow$ driving force for probabilists!).
- Definition of BEC: reduced density matrix of the symmetrized trace operator has an eigenvalue $\asymp N$. This property is called off-diagonal long-range order (ODLRO). One is far away from proving this. It is conjectured to hold true only in $d \geq 3$ ($\Longrightarrow$ famous open problem!)
- Surprisingly, even in the free ($=$ non-interacting) case, the mathematical literature does not have explicit proofs for that for any of the relevant boundary conditions!

Plan of this work: Provide a probabilistic proof in the framework of Feynman cycles.

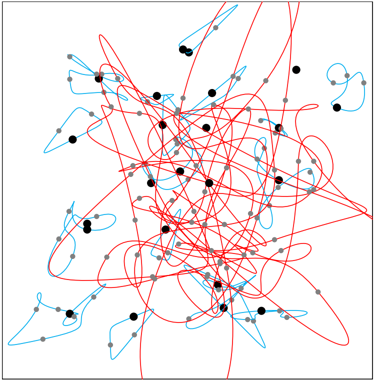


Bose gas consisting of 14 particles, organised in three Brownian cycles, assigned to three Poisson points. The red cycle contains six particles, the green and the blue each four.

Illustration of condensate phase transition



Subcritical (low ρ) Bose gas
without condensate



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

- Popular definition of BEC: a positive fraction of the bosons are in the lowest energy state.
- For the free gas often the non-trivial occupation of the zero Fourier mode is taken as a criterion for BEC (i.e., a positive fraction of the particles occupies the state of zero momentum) [PENROSE/ONSAGER 1956].
- ODLRO as an alternative criterion in the same paper, first only for periodic b.c., later also [GIRARDEAU 1965] for other b.c.'s
- We were not able to find a proof for occurrence of ODLRO (other than via the Fourier mode ansatz) for all reasonable b.c.'s.
- Also in the mathematical literature, only periodic b.c.'s are considered. Often the appearance of long cycles in the FK-formula (in whatever sense) is (wrongly) claimed to be BEC.
- ODLRO ansatz with FK-formula known [GINIBRE (1971)] and discussed [UELTSCHI 2006], [CHEVALIER/KRAUTH (2007], but no proofs.
- Distribution of long loops for several variants found [BETZ/UELTSCHI 2008-11]; no ODLRO.
- Connections with Brownian interlacements for description of long loops [VOGEL 2023], [ARMENDARIZ, FERRARI, YUHJTMAN 2021].

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

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

- The kinetic energy term Δ_i acts on the i-th particle.
- The pair potential $v\colon \mathbb{R}^d \to [0,\infty)$ is rotation symmetric and satisfies ... .

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

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

(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. We fix bc as periodic, Dirichlet zero or von Neumann boundary condition. From now on, $v \equiv 0$.

Free energy per volume:

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

Critical particle density threshold: $\rho_{\mathrm{c}} = \sum_{k\in\mathbb{N}} (4\pi k\beta)^{-d/2} \begin{cases} = \infty & \text{in } d \leq 2, \\ < \infty & \text{in } d \geq 3\,, \end{cases}$

Indeed, f is analytic in $(0,\rho_{\mathrm{c}})$ and constant in $[\rho_{\mathrm{c}},\infty)$.

1-particle-reduced density matrix: the kernel $\gamma_N^{(\Lambda,\mathrm{bc})}\colon \Lambda\times\Lambda \to [0,\infty)$ of the partial trace over $N-1$ variables:

$$\Gamma_N^{(\Lambda,\mathrm{bc})} = \frac{N}{Z_N^{(\Lambda,\mathrm{bc})}} \mathrm{Tr}_{N-1}\Big(\Pi_+ \circ \mathrm{e}^{-\beta\mathcal{H}_N^{(\Lambda,\mathrm{bc})}}\Big)\,.$$

The operator $\Gamma_N^{(\Lambda,\mathrm{bc})}$ acts on $L^2(\Lambda)$.

Its principal eigenvalue: $\sigma_N^{(\Lambda,\mathrm{bc})} = \sup_{f\in L^2(\Lambda)\colon \|f\|_{L^2(\Lambda)}=1} \langle f, \Gamma_N^{(\Lambda,\mathrm{bc})}(f)\rangle.$

Definition of ODLRO

We say that the system exhibits off-diagonal long-range order if $\sigma_N^{(\Lambda_N,\mathrm{bc})} \asymp N$ in the thermodynamic limit at some density ρ.

ODLRO for the free Bose gas with boundary conditions

Fix $d \in \mathbb{N}$ and $\beta, \rho > 0$, let $\Lambda_N = L_N U = L_n[-\frac{1}{2}, \frac{1}{2}]^d$ with volume $L_N^d = N/\rho$. Then

(i) If $d \geq 3$ and $\rho > \rho_c$, then, uniformly in $x, y \in \Lambda_N$, as $N \to \infty$,

$$\gamma_N^{(\Lambda_N,\mathrm{bc})}(x,y) = (\rho - \rho_c + o(1))\phi_1^{(\mathrm{bc})}(\tfrac{x}{L_N})\phi_1^{(\mathrm{bc})}(\tfrac{y}{L_N}) + \psi(|x-y|) + o(1),$$

where $\phi_1^{(\mathrm{bc})}$ is the positive principal eigenfunction of $\Delta^{(U,\mathrm{bc})}$, and $\psi(r) \leq Cr^{2-d}$ as $r \to \infty$ for some $C > 0$. Hence, $\sigma_N^{(\Lambda_N,\mathrm{bc})} \sim (\rho - \rho_c)\,|\Lambda_N|$.

(ii) If $\rho \leq \rho_c$, then, for some $c > 0$ and all $x, y \in \Lambda_N$, as $N \to \infty$,

$$\gamma_N^{(\Lambda_N,\mathrm{bc})}(x,y) = \mathcal{O}\left(\mathrm{e}^{-c|x-y|}\right).$$

As a consequence, $\sigma_N^{(\Lambda_N,\mathrm{bc})} \leq \mathcal{O}(1)$.

$$g_\beta^{(\Lambda,\mathrm{bc})}\colon \Lambda\times\Lambda\to[0,\infty):$$ fundamental solution to $\partial_\beta g_\beta(x,y)=\Delta^{(\Lambda,\mathrm{bc})}g_\beta(x,\cdot)(y)$.

(For free boundary condition: $g_\beta^{(\Lambda,\mathrm{free})}(x,y)=(4\pi\beta)^{-d/2}\mathrm{e}^{-|x-y|^2/4\beta}$.)

Trace of convolution operator with kernel $g_{k\beta}^{(\Lambda,\mathrm{bc})}$: $\quad \mathrm{t}_k^{(\Lambda,\mathrm{bc})}=\int_\Lambda g_{k\beta}^{(\Lambda,\mathrm{bc})}(x,x)\,\mathrm{d}x.$

Feynman–Kac formula + partition representation, goes back to [GINIBRE 1970]

$$Z_N^{(\Lambda,\mathrm{bc})}=\sum_{m\in\mathfrak{P}_N}\prod_{k\in\mathbb{N}}\frac{(\mathrm{t}_k^{(\Lambda,\mathrm{bc})})^{m_k}}{k^{m_k}m_k!}$$ and $$\gamma_N^{(\Lambda,\mathrm{bc})}(x,y)=\sum_{r=1}^N g_{r\beta}^{(\Lambda,\mathrm{bc})}(x,y)\frac{Z_{N-r}^{(\Lambda,\mathrm{bc})}}{Z_N^{(\Lambda,\mathrm{bc})}}.$$

Here $\mathfrak{P}_N=\{m=(m_k)_{k\in\mathbb{N}}\in\mathbb{N}_0^{\mathbb{N}}\colon \sum_k km_k=N\}$ = set of partitions of N.

$N_\Lambda = \sum_{k=1}^N kX_k$ particle number of a PPP $(X_k)_{k\in\{1,\dots,N\}}$ on $\mathbb{N}$ with intensity measure

$$\nu_\Lambda^{(\mathrm{bc},N)} = \sum_{k=1}^N \frac{1}{k}\mathrm{t}_k^{(\Lambda,\mathrm{bc})}\delta_k\,. \qquad (1)$$

X_k = number of loops of length k in the box Λ.

(The X_k are independent Poisson variables with parameter $\frac{1}{k}\mathrm{t}_k^{(\Lambda,\mathrm{bc})}$.)

Put $p_\Lambda^{(\mathrm{bc},N)} = \sum_{k=1}^N \frac{1}{k}\mathrm{t}_k^{(\Lambda,\mathrm{bc})}$.

PPP representation

$$\begin{aligned} Z_N^{(\Lambda,\mathrm{bc})} &= \mathrm{e}^{|\Lambda| p_\Lambda^{(\mathrm{bc},N)}}\,\mathtt{P}_\Lambda^{(\mathrm{bc},N)}(N_\Lambda = N),\\ \gamma_N^{(\Lambda,\mathrm{bc})}(x,y) &= \sum_{r=1}^N g_{r\beta}^{(\Lambda,\mathrm{bc})}(x,y)\frac{\mathtt{P}_\Lambda^{(\mathrm{bc},N)}(N_\Lambda = N-r)}{\mathtt{P}_\Lambda^{(\mathrm{bc},N)}(N_\Lambda = N)}. \end{aligned}$$

Advantage: Main exponential term is isolated and drops out. Description is now based on independent Poisson variables and the Gaussian kernel.

Threshold between short and long loops: $T_N = \lceil L_N^2 \log^{1/2}(N) \rceil \approx N^{2/d}, \qquad N \in \mathbb{N}.$

Number of particles in short and in long loops:

$$\mathrm{N}_\Lambda^{(\mathrm{short})} = \mathrm{N}_\Lambda^{[1,T_N]} = \sum_{k=1}^{T_N} kX_k \qquad \text{and} \qquad \mathrm{N}_\Lambda^{(\mathrm{long})} = \mathrm{N}_\Lambda^{[T_N+1,N]} = \sum_{k=1+T_N}^{N} kX_k\,.$$

- Later, we will see that 100percent of the short loops are even of length $O(1)$ and practically all long ones are of length $\asymp N$.
- $\mathrm{N}_\Lambda^{(\mathrm{short})}$ will be shown to be highly concentrated around its expectation $\rho_{\mathrm{c}}|\Lambda_N|$ with stretched-exponential decay of the probabilities of the deviations. The remaining $\approx N - \rho_{\mathrm{c}}|\Lambda_N| = (\rho - \rho_{\mathrm{c}})|\Lambda_N|$ particles are in long loops.
- The asymptotics of the probability for having k particles in long loops (on mixed polynomial/stretched exponential order!) will be handled using a sophisticated result in the framework of partitions.

The Poisson–Dirichlet distribution

PD$_1$ is the distribution of $(Y_n \prod_{k=1}^{n-1}(1-Y_k))_{n\in\mathbb{N}}$, where $(Y_n)_{n\in\mathbb{N}}$ is an i.i.d. sequence of $\mathrm{Beta}(1,1)$-distributed random variables (i.e., uniformly over $[0,1]$ distributed).

Note that the sum of the elements of a PD$_1$-distributed sequence is equal to one, i.e., this distribution is in fact a random partition. It is well-known in asymptotics for random permutations: As the joint distribution of the lengths of all the cycles of a uniformly picked random permutation of $1,\dots,N$, ordered according to their sizes and normalized by a factor $1/N$, converges weakly to PD$_1$.

Let $L_i^{(N)}$ denote the length of the i-th longest loop in the PPP (counted with multiplicity).

Lengths of long loops

Fix $\rho\in(\rho_{\mathrm{c}},\infty)$ and consider the centred box Λ_N with volume N/ρ. Then, under $\mathrm{P}_\Lambda^{(\mathrm{bc},N)}$, conditional on $\{\mathrm{N}_{\Lambda_N}=N\}$, as $N\to\infty$,

$$\frac{(L_i^{(N)})_{i\in\mathbb{N}}}{|\Lambda_N|(\rho-\rho_{\mathrm{c}})} \Longrightarrow \mathrm{PD}_1.$$

Eigenvalue expansion $\implies$ $$g_{\beta r}^{(\Lambda)}(x,y) \sim \frac{1}{|\Lambda|} \mathrm{e}^{-\lambda_1 \beta r |\Lambda|^{-\frac{2}{d}}} \phi_1\big(\tfrac{x}{L}\big)\phi_1\big(\tfrac{y}{L}\big)\,,$$

where

eigenvalues of $-\frac{1}{2}\Delta^{(U)}$: $$\lambda_1^{(\mathrm{Dir})} = \frac{\pi^2}{2} d, \quad \lambda_1^{(\mathrm{per})} = 0 = \lambda_1^{(\mathrm{Neu})}\,,$$

and

eigenfunctions: $$\phi_1^{(\mathrm{Dir})}(x) = 2^{d/2} \prod_{i=1}^{d} \cos\big(\pi x_i\big), \quad \phi_1^{(\mathrm{per})}(x) = 1 = \phi_1^{(\mathrm{Neu})}(x)\,.$$

Furthermore, by convolution,

$$\mathrm{P}_\Lambda\left(\mathrm{N}_\Lambda = N - r\right) = \sum_k \mathrm{P}_\Lambda\left(\mathrm{N}_{\Lambda_N}^{(\mathrm{short})} = k\right) \mathrm{P}_\Lambda\left(\mathrm{N}_{\Lambda_N}^{(\mathrm{long})} = N - r - k\right)\,.$$

On the other hand, for large N and $N - r - k$, for some constant $\gamma \in (0,\infty)$,

$$\mathrm{P}_\Lambda\left(\mathrm{N}_{\Lambda_N}^{(\mathrm{long})} = N - r - k\right) \sim \frac{\mathrm{e}^{\gamma}}{T_N} \mathrm{e}^{-\lambda_1 \beta (N-k-r) |\Lambda|_N^{-\frac{2}{d}}}$$

Eigenvalue expansion $\Longrightarrow$ $$g^{(\Lambda)}_{\beta r}(x,y) \sim \frac{1}{|\Lambda|} \mathrm{e}^{-\lambda_1 \beta r |\Lambda|^{-\frac{2}{d}}} \phi_1(\tfrac{x}{L})\phi_1(\tfrac{y}{L})\,,$$

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$$\sim \mathrm{P}_\Lambda\left(\mathrm{N}^{(\mathrm{long})}_{\Lambda_N} = N - k\right) \mathrm{e}^{\lambda_1 \beta r |\Lambda|_N^{-\frac{2}{d}}}\,.$$

The last term cancels precisely the eigenvalue term in the expansion! Indeed,

$$\gamma_N(x,y) = \sum_{r=1}^{N} g_{r\beta}(x,y) \frac{\mathtt{P}_{\Lambda_N}\left(\mathrm{N}_{\Lambda_N} = N - r\right)}{\mathtt{P}_{\Lambda_N}\left(\mathrm{N}_{\Lambda_N} = N\right)}$$

$$\sim \sum_{r=1}^{(\rho-\rho_c)|\Lambda_N|} \frac{1}{|\Lambda_N|} \phi_1\left(\tfrac{x}{L_N}\right)\phi_1\left(\tfrac{y}{L_N}\right) \mathrm{e}^{-\lambda_1 \beta r |\Lambda_N|^{-\frac{2}{d}}}$$

$$\times \sum_{k \approx \rho_c |\Lambda_N|} \mathtt{P}_{\Lambda_N}\left(\mathrm{N}_{\Lambda_N}^{(\mathrm{short})} = k\right) \frac{\mathtt{P}_{\Lambda_N}\left(\mathrm{N}_{\Lambda_N}^{(\mathrm{long})} = N - k\right)}{\mathtt{P}_{\Lambda_N}\left(\mathrm{N}_{\Lambda_N} = N\right)} \mathrm{e}^{\lambda_1 \beta r |\Lambda_N|^{-\frac{2}{d}}}$$

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Deviations of the particle number in short loops

For any $\varepsilon > 0$ and for any $\kappa > 0$, we have, for all large $N \in \mathbb{N}$,

$$\mathrm{P}_{\Lambda_N}^{(\mathrm{bc},N)}\Big(\Big|\frac{1}{|\Lambda_N|}\mathrm{N}_{\Lambda_N}^{(\mathrm{short})} - \rho_{\mathrm{c}}\Big| > \varepsilon\Big) \leq \mathrm{e}^{-\kappa|\Lambda_N|^{1-2/d}}.$$

Proof relatively standard with exponential Chebyshev inequality and some careful analysis.

Lower bound for the denominator

Fix $\rho \in (\rho_{\mathrm{c}}, \infty)$. Then

$$\mathrm{P}_{\Lambda_N}^{(\mathrm{bc},N)}(\mathrm{N}_{\Lambda_N} = N) \geq \begin{cases} \mathrm{e}^{-(\rho-\rho_{\mathrm{c}})\beta\lambda_1|\Lambda_N|^{1-\frac{2}{d}}(1+o(1))} & \text{if } \lambda_1 > 0, \\ |\Lambda_N|^{-2-\frac{2}{d}-\varepsilon} & \text{if } \lambda_1 = 0, \end{cases}$$

Proof by picking the optimal size of a long loop $(\rho - \rho_{\mathrm{c}})|\Lambda_N|$ and the typical value of $\frac{1}{|\Lambda_N|}\mathrm{N}_{\Lambda_N}^{(\mathrm{short})}$, namely ρ_c, then using the Poisson properties and the above lemma.

Distribution of the number of particles in long loops

Fix $\rho \in (\rho_c, \infty)$. Then, in the limit as $N \to \infty$, uniformly in $N^{2/d} \log^2(N) \leq k \leq N$,

$$\mathrm{P}_{\Lambda_N}^{(\mathrm{bc},N)}\Big(\mathrm{N}_{\Lambda_N}^{(\mathrm{long})} = k\Big) \sim \mathrm{e}^{-\gamma} \mathrm{e}^{-\beta \lambda_1 k |\Lambda_N|^{-\frac{2}{d}}} \times \begin{cases} \frac{1}{T_N} & \text{if } \lambda_1 > 0\,, \\ \frac{1}{N} & \text{if } \lambda_1 = 0\,. \end{cases}$$

Our proof uses the eigenvalue asymptotics for $\mathrm{t}_r^{(\Lambda)}$ and for the lower bound combinatorial asymptotics for numbers of partitions from the literature:

$$\mathbb{P}\Big(\sum_{r=T_N}^{j} r Y_r = k\Big) \sim \frac{p_1(k/j)}{j}, \qquad N^{2/d} \log^2(N) \leq j \leq k \leq N,$$

where $Y_r \sim \mathrm{Poi}_{1/r}$, and $\sum_{r=1}^m \frac{1}{r} \sim \log m$ as $m \to \infty$. Here $p_1 \colon (0, \infty) \to [0, \infty)$ is the density of the distribution on $(0, \infty)$ with Laplace transform

$$(0, \infty) \ni s \mapsto \exp\left(-\int_0^1 \left(1 - \mathrm{e}^{-sx} \frac{1}{x}\right) \mathrm{d}x\right).$$

The upper bound is technical: it uses clever decompositions and elementary estimates for Poisson probabilities.