1.1 Phase Transitions of Condensation Type in Interacting Particle Systems

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One of the greatest unsolved problems in contemporary mathematical physics is a mathematical understanding of the famous *Bose–Einstein condensation (BEC)* phase transition. In 1924, the young and then unknown Indian mathematical physicist Sateyendra Nath Bose kindly asked the already famous Albert Einstein to help publishing his achievement, a new calculation method for the free energy of a simple model (i.e., without particle interactions) for a large particle system at very low temperatures. Einstein helped him, but also noticed that this new method even had detected a previously unknown and very weird phase transition, in particular, a new kind of condensation phase of an ensemble of undistinguishable particles. In this state of matter, a positive fraction would remain in the same quantum mechanical state, a kind of "super atom" having strange properties. He predicted that this effect would arise also at positive, but very low temperature and under realistic conditions, i.e., with some interaction between the particles.

For a long time, this prediction did not lead to much research activity, since the anticipated phase transition was seen mostly as a kind of curiosity, a mathematical foundation seemed to represent a major undertaking, and an experimental verification was far out of reach. Nevertheless, a few theoretical physicists started developing some preliminary modeling in the 1940s and triggered the interest of the physics community. By the 1990s, the opinion emerged that an experimental realization would be a hot candidate for a Nobel Prize. In 1992, a team of experimental physicists created a temperature of 10^{-6} Kelvin for some ten thousands of particles, which did not suffice for obtaining the condensation, but lead to the Physics Nobel Prize being awarded for the year 1997. In 1995, finally, two teams reached a temperature of 10^{-9} Kelvin and did obtain the condensation phase experimentally. As expected, three members of the two teams were awarded jointly the Physics Nobel Prize for the year 2001 for this success. This development triggered substantial activity by mathematical physicists and later probabilists searching for a rigorous mathematical understanding of BEC. Since then, for many simplified models, this phase transition has been successfully analyzed mathematically, but not in the situation that is considered the most realistic and important one, namely the thermodynamic limit of the canonical model at positive temperature with some pair interaction between the particles, the *interacting quantum Bose gas*.

The interacting quantum Bose gas

There is a generally acknowledged model for the description of the predicted condensation effect. It is given via an ensemble of many interacting Brownian bridges (Brownian motions conditioned on terminating at their initial site) of various lengths of their time intervals, where the number of particles carried by a bridge is proportional to this length. The condensation effect is seen in the emergence of a positive fraction of the particles that sit in cycles of lengths that tend to infinity as the total particle number diverges. This positive fraction is—in this model—equal to the Bose–Einstein condensate. The famous conjecture is that it exists in dimensions larger or equal to three at sufficiently low temperatures (or equivalently at sufficiently large particle densities), but not in dimensions less than or equal to two. More precisely, this phase transition is expected to be a *saturation effect*, i.e., up to a certain critical particle density, all particles should be organized in microscopic structures (i.e., in cycles of finite lengths), and if this threshold is exceeded, then the condensate emerges, and the microscopic structures remain essentially unchanged if the particle density is further increased. Each of the long cycles corresponds to an above said “super atom”, the novel aggregate state of matter that fascinated Einstein and Bose.

Let us give a more precise description of the model. We consider a canonic interacting bosonic many-body system in a large box in $\mathbb{R}^d$ at positive temperature $1/\beta \in (0,\infty)$ with fixed particle density $\rho \in (0,\infty)$ and kinetic energy in the thermodynamic limit, i.e., N particles in a large box Λ_N of volume N/ρ. We denote by

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

the N-particle *Hamilton operator* with kinetic energy given by the Laplace operator and mutual energy given by a pair-interaction function $v\colon [0,\infty) \to \mathbb{R}$. There is no particular canonical choice of v in view of the Bose gas, but a typical requirement is a short-distance repulsion (i.e., $v(r) \to \infty$ as $r \downarrow 0$) and a strong decay at infinity. Otherwise, one requires v often to be nonnegative or of *Lennard-Jones-type*, i.e., with some attraction at moderate distance (i.e., a strict negative minimum at some positive point). We are interested in *bosons* and introduce a symmetrization, i.e., we project $\mathcal{H}_N$ on the set of symmetric, i.e., permutation-invariant, wave functions. For this, we consider the trace of the operator $\mathrm{e}^{-\beta\mathcal{H}_N}$ in Λ_N with symmetrization,

$$Z_N(\beta,\Lambda_N) = \mathrm{Tr}_{\Lambda_N,+}(\mathrm{e}^{-\beta\mathcal{H}_N}), \tag{1}$$

where the index $+$ indicates the symmetrization. This trace is the *partition function* of the model, the integral over all realizations of the system of N indistinguishable particles in Λ_N, equipped with the two energies. The kinetic energy is expressed in terms of an expectation with respect to N Brownian bridges (cycles) on the time interval $[0,\beta]$, and the symmetrization appends each bridge at the end of another, according to some uniformly-at-random-picked permutation of the N bridges. Since every permutation decomposes into cycles, these bridges are glued together to bridges of various time lengths, by the virtue of the Markov property. This is summarized in terms of a well-known variant of the *Feynman–Kac formula*, which we formulate now.

For $k \in \mathbb{N}$, we put $q_k = \frac{1}{k}(4\pi\beta k)^{-d/2}$ and pick the starting sites of all the bridges of length k (i.e., with time interval $[0,\beta k]$) as the points of a *Poisson point process* with intensity q_k; hence they are uniformly distributed over Λ_N, and their number is Poisson distributed with expectation $q_k|\Lambda_N|$. Each bridge B of length k has exactly k particles $B_0, B_\beta, B_{2\beta}, \dots, B_{(k-1)\beta}$ and has k legs $(B_t)_{t\in[(j-1)\beta, j\beta]}$ with $j = 1,\dots,k$. All these families of cycles are independently superposed over $k \in \mathbb{N}$, and the total number of all the motions is put equal to N. The interaction of the ensemble is equal to a sum over all pairs of any two legs of any of the bridges and given by the functional

$$(f, g) \mapsto \int_0^\beta v(f(t) - g(t))\,\mathrm{d}t. \qquad (2)$$

Let us denote the ensemble by $\mathfrak{B} = (B^{(k,i)})_{k,i}$ with corresponding expectation $\mathbb{E}$ and the total interaction by $\mathfrak{V}$, then the announced trace formula reads

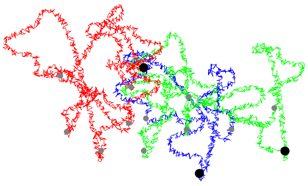

Fig. 1: Illustration of three Brownian cycles (red, blue, green) attached to Poisson points (black) and carrying particles (gray)

$$Z_N(\Lambda_N) = \mathbb{E}\Big[\mathrm{e}^{-\mathfrak{V}}\mathbb{1}\{L(\mathfrak{B}) = N\}\Big], \qquad (3)$$

where $L(\mathfrak{B})$ denotes the total number of particles in the system, i.e., the sum of all the lengths of the cycles. We have arrived at a probabilistic description of the trace in terms of an interacting ensemble of many random cycles (in this case, Brownian bridges) of various, unbounded lengths, with a pair interaction for each pair of legs and a total number of N legs. In particular, this is a spatial distribution of N indistinguishable particles in terms of a marked Poisson point process in the box Λ_N, see Figure 1.

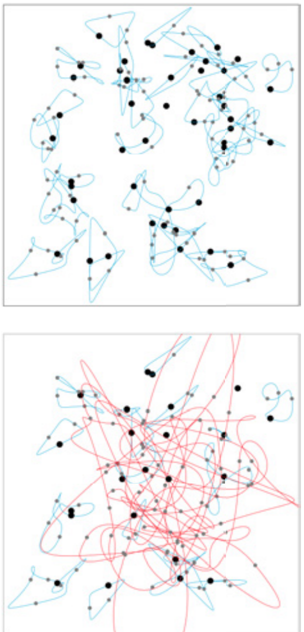

Fig. 2: Up: Illustration of a cycle ensemble without emergence of a condensate. Down: Illustration of a cycle ensemble with a very long cycle (red), interpreted as condensate

The main goal is to prove that, in the limit as $N \to \infty$, in dimension $d \geq 3$ (but not in $d \leq 2$) and for all sufficiently large particle densities ρ, the main contribution to this expected value comes from those configurations that have a *positive fraction of particles* (i.e., of legs) in *"very long"* cycles, i.e., cycles of lengths that depend on N and diverge as $N \to \infty$, see Figure 2. The totality of all these long cycles is then interpreted as the *condensate*. The occurrence of such a macroscopic structure at sufficiently large particle density is supposed to be a *condensation phase transition*, i.e., there should be a critical threshold $\rho_c \in (0, \infty)$ such that long cycles occur for $\rho > \rho_c$, but not for $\rho < \rho_c$. The idea is that, if ρ grows, i.e., when addding more and more particles to the container Λ_N, then first the particles are organized in finite-length cycles until *saturation* is reached, and if the threshold ρ_c is exceeded, then all additional particles condensate, and the density of the finite-cycle particles does not change anymore.

Large deviations ansatz

One familiar ansatz for deriving large-N asymptotics for the partition function is based on the idea to derive a *characteristic variational formula* for its large-N exponential rate, i.e., for the *free energy* per unit volume, given by

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

This formula should be able to express the contributions of the decisive quantities like energy, entropy, and particle density in terms of an infimum over all the three random ingredients (cycle lengths, locations of Poisson points, cycle trajectories), to distribute all the random cycles. A decisive step towards this aim was made in [1], where, for all sufficiently small ρ, it was proved that

$$f(\rho) = \inf\big\{I(P) + \Phi(P) \colon P \in \mathcal{M}_1^{(\mathrm{s})}, \mathcal{N}(P) = \rho\big\}, \qquad (4)$$

where $\mathcal{M}_1^{(\mathrm{s})}$ is the set of (distributions P of) translation-invariant marked point processes in $\mathbb{R}^d$ (the marks being the random cycles starting and ending at the points); furthermore, $I(P)$ is the *relative entropy density* of P with respect to the above reference Poisson point process, $\Phi(P)$ the *energy* of P, and $\mathcal{N}(P)$ the *effective particle density* of P, i.e., the number of particles that P puts on an average into a unit volume. It should be noted that P is able to express only microscopic structures, not the condensate.

The methods employed in [1] failed to extend this statement to all particle densities ρ, nor to say anything about the existence nor non-existence of minimizers P in that formula. The latter question is conjectured to be decisive for the question about occurrence of BEC. Indeed, if the formula admits a minimizer, then this should be interpreted as the non-existence of a condensate, while a lack of a minimizer should indicate that there is something in the system that cannot be expressed in terms of such processes P – this should be the condensate. It is conjectured by the WIAS team that there is a critical value ρ_c (which is finite in dimensions $d \geq 3$) such that a minimizer P exists for $\rho < \rho_c$, but not for $\rho > \rho_c$. Mathematically, much of the problem stems from the fact that the map $P \mapsto \mathcal{N}(P)$ is lower semicontinuous, but not continuous.

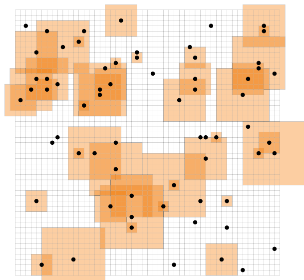

Fig. 3: *Illustration of a realization of the simplified quantum Bose gas in a finite box. Poisson points on $\mathbb{Z}^d$ carry marks given by finite grids of varying size*

In order to solve a problem of this kind, a WIAS team worked in 2020 on a slightly simplified model, where $\mathbb{R}^d$ is replaced by the lattice $\mathbb{Z}^d$ and the (random) Brownian cycles are replaced by (deterministic) grids, see Figure 3 for an illustration. The team is about to finish the derivation of a characteristic variational formula that features a serious extension of (4): an extended probability space that is able to encode also the macroscopic structure:

$$f(\rho) = \inf_{\rho_1 \in [0,\rho]} \inf_{\psi \in \mathcal{M}_1(\mathbb{N}_0):\ \sum_{a\in\mathbb{N}_0} a\psi(a) = \rho-\rho_1} \inf\left\{ I(P_\psi) + \Phi(P_\psi) \colon P_\psi \in \mathcal{M}_1^{(s)}, \mathcal{N}(P_\psi) = \rho_1 \right\}.$$

Here, $\psi(a)$ is the percentage of the area in which precisely a macroscopic grids overlap (this defines something like an environment of condensates), and P_ψ is the distribution of the microscopic grids given the spatial distribution of the condensate and $\Phi(P_\psi)$ its total expected energy (within and between all microscopic and macroscopic particles), and $\mathcal{N}(P_\psi)$ is the number of microscopic particles that P_ψ puts on an average at one site. Then ρ_1 is the particle density in microscopic grids, and $\rho - \rho_1$ is the density of particles in the condensate.

This formula admits a minimizer for any value of ρ and a clear distinction between the mass of microscopic particles and the condensate. Standard variational techniques give criteria for existence of minimizers with a non-trivial value of $\rho - \rho_1$. The WIAS team is working on a proof that, as long as $\sum_k kq_k$ is finite (recall that q_k is the spatial *a priori* density of cycles of length k), this criterion is satisfied for any sufficiently large ρ, i.e., a proof of the occurrence of BEC in this model. We are confident of addressing the original interacting quantum Bose gas with an extension and adaptation of this methodology in the future.

Reflection positivity ansatz

A second approach, which is currently explored by another WIAS team, consists of an application of reflections to the family of random cycles and the deduction of useful correlation inequalities. This technique has previously produced good results in models of random cycles (often called *random loops* in this connection) in the spatially and temporally discrete setting, and offers good perspectives for extensions to the interacting quantum Bose gas in the future. Currently, there is a high interest in the study of models of interacting random loops in large boxes of various types, written in terms of random geometric permutations in the spirit of the formulation of the trace in (1) above; see [2].

The model to which this technique was applied in 2020 at WIAS is the following. We work in a large box in $\mathbb{Z}^d$ with nearest-neighbor edges (and periodic boundary conditions). On each edge in the box, there is a random number of links connecting the two vertices, satisfying the constraint that the number of links connecting any vertex is even. Each link connecting a vertex is paired to precisely one other link connecting that vertex. As a result, we obtain a random collection of closed loops as in Figure 4. We denote by m_e the number of links on the edge e and by n_x the number of pairings at the vertex x. A given configuration obtains a weight proportional to

$$\Big(\prod_{\text{edges } e} \frac{\gamma^{m_e}}{m_e!}\Big)\Big(\prod_{\text{vertices } x,y} \mathrm{e}^{-v(|x-y|)n_x n_y}\Big) K^{\#\text{ loops}}, \tag{5}$$

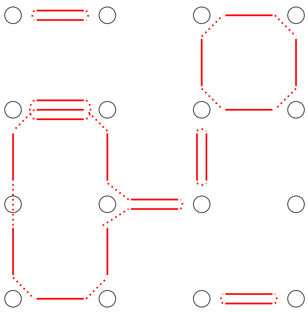

Fig. 4: *Representation of a link and pairing configuration with six closed loops. The circles represent the vertices of the graph. Paired links are connected by a dotted line*

where $v\colon [0,\infty) \to \mathbb{R}$ is an interaction function like in (2), and $\gamma, K \in (0,\infty)$ are two parameters. The parameter γ controls the number of links and, hence, also the number of particles, i.e., it plays the role of the particle density (called ρ above). Large values of the parameter K favor a large number of loops, i.e., suppress their lengths. This random loop model is defined in the spirit of the interacting quantum Bose gas; however, the precise relation between the two models is not clear yet.

For this model the team is in progress to prove the existence of a regime of occurrence of macroscopic loops for all sufficiently large values of γ. The central technique uses a special property of the random loop measure, which is a correlation inequality called *reflection positivity*. For an arbitrary plane through edges that is orthogonal to one of the Cartesian axes, we consider a bilinear form defined on the set of functions that depend only on the configuration on one half of the box. It is given by the expected value of the product of two such functions, where one of them is reflected at the plane. Reflection positivity means that this bilinear form is symmetric and positive semidefinite, giving us a Cauchy–Schwarz-type inequality. The first step is to prove that the random loop measure (5) indeed enjoys this property, which is due to the particular form of its weights and to the periodic boundary conditions.

The by far more serious part is to use this correlation inequality to derive, for sufficiently large γ, a positive lower bound on the expected length of the loops, uniformly in the volume of the box. (This part is too involved to be explained here.)

The technique of reflection positivity was developed in the late 1970s by Fröhlich, Simon and Spencer who employed it for establishing the occurrence of a phase transition in lattice spin models. In [3], this property was used to prove a phase transition in a modified version of the above model, in which the "loop" containing the origin is open, i.e., it starts at the origin and ends at an arbitrary vertex of the box that differs from the origin.

For $K = 2$, the team is convinced that they will obtain a connection with the spatially discrete and temporally continuous version (i.e., with continuous-time random walks in $\mathbb{Z}^d$) of the interacting quantum Bose gas, at least in the grand canonical ensemble (where the particle number is not fixed, but a Poisson random number).

References

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