Percolation transition in the Bose gas

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Abstract

The canonical partition function of a Bose gas gives rise to a probability distribution over the permutations of N particles. We study the probability and mean value of the cycle lengths in the cyclic permutations, their relation to physical quantities like pair correlations, and their thermodynamic limit. We show that in the ground state of most interacting boson gas the mean cycle length diverges in the bulk limit and the particles form macroscopic cycles. In the free Bose gas Bose-Einstein condensation is accompanied by a percolation transition: the appearance of infinite cycles with nonvanishing probability.

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1 Introduction

This paper presents a new approach to phase transitions in bosonic systems. Since this description emerges somewhat accidentally from a study of the ferromagnetism in the Hubbard model, it may be interesting to outline the sequence of ideas connecting these seemingly distant fields.

The magnetization per particle in the Hubbard model (in fact, in any model of spin-1/2 fermions) can be written ([AL], [S1], [S2]) as

$$M(h)=\frac{1}{2}\frac{\sum_{[p]}(\frac{1}{N}\sum_j p_j\tanh\frac{1}{2}p_j\beta h)\epsilon[p]A[p]\prod_j(2\cosh\frac{1}{2}p_j\beta h)}{\sum_{[p]}\epsilon[p]A[p]\prod_j(2\cosh\frac{1}{2}p_j\beta h)}\ . \tag{1.1}$$

Equation (1.1) and the formulas (1.4) and (1.6) below will be derived in full generality in Section 3. At this place let us concentrate on the structure of the above expression. The summations run over the partitions $[p]$ of N, the number of particles:

$$p_1\geq p_2\geq\ldots\geq 1\ \ ,\ \ p_1+p_2+\cdots=N\ . \tag{1.2}$$

$\epsilon[p]=(-1)^{\sum(p_j-1)}$, h is the external field, β is the inverse temperature and $A[p]$ (see Eq.(2.16)) is independent of h. Each partition corresponds to a conjugacy class of the group S_N of permutations of N elements and fixes the cycle lengths of the permutations within the class [LF]. One observes that the magnetization is a rational function of $\tanh\frac{1}{2}\beta h$, which can be expanded to give

$$M(h)=\sum_{n=0}^{\infty}a_n(\tanh\frac{1}{2}\beta h)^{2n+1}\ . \tag{1.3}$$

The zero field magnetic susceptibility χ reads

$$\beta^{-1}\chi=\frac{a_0}{2}=\frac{1}{4}\frac{\sum_{[p]}(\frac{1}{N}\sum_j p_j^2)\epsilon[p]2^{k[p]}A[p]}{\sum_{[p]}\epsilon[p]2^{k[p]}A[p]}=\frac{1}{4}\langle\langle p_j\rangle\rangle\ , \tag{1.4}$$

where $k[p]$ is the number of elements of the partition $[p]$. The above is a sort of mean value of the cycle lengths: The first average is taken with the weights p_j/N, the second is the thermodynamic average. Let $\mathbf{S}(x)$ denote the spin operator at the site x, $S^z(x)$ its z-component and $\mathbf{S}$ the operator of the total spin. Then the fluctuation-dissipation formula

$$\beta^{-1}\chi=\frac{1}{N}\sum_{x,y}\langle S^z(x)S^z(y)\rangle=\frac{1}{3N}\sum_{x,y}\langle\mathbf{S}(x)\mathbf{S}(y)\rangle=\frac{1}{3N}\langle\mathbf{S}^2\rangle \tag{1.5}$$

compared with (1.4) shows that there is a ferromagnetic long-range order if and only if the average cycle length grows like the number of electrons when the thermodynamic limit is taken.

Spin correlations in zero field are connected to the cyclic permutations also locally: For $x\neq y$,

$$\langle\mathbf{S}(x)\mathbf{S}(y)\rangle=\frac{3}{4}\frac{\sum_{g\neq e}\epsilon(g)2^{k(g)}\sum'_{(x_1,\ldots,x_N)}\langle x_{g(1)},\ldots,x_{g(N)}|e^{-\beta H_N}|x_1,\ldots,x_N\rangle}{\sum_g\epsilon(g)2^{k(g)}\sum_{(x_1,\ldots,x_N)}\langle x_{g(1)},\ldots,x_{g(N)}|e^{-\beta H_N}|x_1,\ldots,x_N\rangle} \tag{1.6}$$

(cf. Eq.(3.24)). In this formula H_N is the N-particle Hamiltonian and

$$|x_1, \ldots, x_N\rangle = \otimes |x_i\rangle \ ;$$

g denotes a permutation of $1, 2, ..., N$, $\epsilon(g)$ is the signature and $k(g)$ is the number of disjoint cycles of g, and e is the unit of S_N. The primed sum goes over $(x_1, ..., x_N)$ such that $x_i = x$ and $x_j = y$ for a single pair (i, j), where i and j are in the same cycle of g. The remarkable fact about this formula is that the numerator is a part of the sum constituting the denominator. Were not $\epsilon(g)$ there, we could interprete the ratio as the probability of finding a configuration (x_i) and a permutation g such that x and y are singly occupied and the two particles belong to the same cycle of g. Long-range ferromagnetic order then would mean that spatially extended cycles have nonvanishing probability. This interpretation becomes possible if we drop $\epsilon(g)$. This makes (1.4) turn into a true mean value and (1.6) into a true probability. The system is now a boson gas with a two-valued internal degree of freedom. If we replace the numbers 1/4, 3/4 and 2 respectively by $s(s+1)/3$, $s(s+1)$ and $2s+1$, we obtain the susceptibility and pair correlation of a spin-s boson gas. As a last step, we divide the two equations by s and then set $s = 0$. The right-hand side of the first is still the mean value of the cycle lengths, that of the second is still the probability quoted above. The obvious physical meaning of the left-hand sides has been lost, however they must refer to some thermodynamic properties of the spinless boson gas.

One observes that $\langle\langle p_i \rangle\rangle$ takes on values between 1 and N. At high temperatures and/or low densities $\langle\langle p_i \rangle\rangle$ must be of the order of 1 as N and V increase. This is at least clear for the Bose gas with spin, where in the opposite case we would get non- or slowly decaying magnetic correlations at arbitrarily high temperatures or low densities. The boundedness of $\langle\langle p_i \rangle\rangle$ implies that in the thermodynamic limit all the cycles are finite with full probability. This may not be the case at low temperatures and/or high densities. If a transition occurs it will be a percolation transition in the sense that infinite cycles appear with positive density. This has thermodynamic consequences through the divergence of the response function $\langle\langle p_i \rangle\rangle$.

The aim of this paper is to make the above ideas mathematically more precise. In Section 2 we define a probability distribution $P_{V,N}$ over the symmetric group S_N by using the canonical partition function of a system of N bosons in a volume V. Associated with the cyclic permutations in which any permutation g can be decomposed, we introduce two sets of random variables: $\nu_k(g)$, the number of cycles of length k and $\xi_i(g)$, the length of the cycle containing the number i. The mean value of the first and the probability distribution of the second are related by a simple expression. Section 3, supplemented by an Appendix, contains the derivation of the formulas (1.1),(1.4) and (1.6) in full generality for bosons and fermions. In particular, for the magnetic Bose gas the expectation value $E_{V,N}(\xi_i)$ proves to be the zero field susceptibility while in the nonmagnetic case it is related to some special kind of density-density correlation functions. In Section 4 we sketch the problem of the thermodynamic limit of the probability distribution introduced in Section 2, and give the definition of what we call the cycle percolation. Sections 5 and 6 present examples.

In Section 5 we study $P_{V,N}$ at zero temperature for the interacting Bose gas. We show that if the overall ground state of the Hamiltonian in the spinless Hilbert space (without Bose or Fermi statistics) is unique, the corresponding Bose gas exhibits cycle percolation in the ground state: $E_{V,N}(\xi_i)$ grows proportionally to N and the probability of cycle percolation is 1. This clearly shows the interest in this quantity: being zero at high temperature and 1 in the ground state, it is a good candidate for an order parameter. Notice, in contradistinction, that the non-vanishing of the off-diagonal long-range order (ODLRO, [Ya]) in the ground state of an interacting Bose gas is apparently not easier to establish than to show Bose condensation at positive temperatures. As a rare example, recently Penrose [Pe] proved ODLRO for the hard-core Bose gas on the complete graph, a model solved earlier by Tóth [To1].

The prerequisite to ground state cycle percolation, the uniqueness of the overall ground state in finite volumes holds true rather generally, for example, in two and higher dimensions for pair interactions which are bounded from below everywhere and from above outside the origin or a hard core. (For hard-core interactions the density must be smaller than the closed-packing value.) Strictly speaking, this is proved only for Dirichlet boundary condition on an arbitrary connected domain. Relevant results are due to Rutman ([KR], Theorem 6.3), Glimm and Jaffe ([GJ], § 3.3), Faris [Fa], Faris and Simon [FS] and Simon ([Si], Theorem 21.1). Uniqueness is probably also true for periodic and Neumann boundary condition on rectangular domains where the proof is immediate for noninteracting particles. Natural counterexamples for the uniqueness of the ground state are provided by one-dimensional systems with hard-core or other pair interactions which are repulsive and nonintegrable at the origin. Such interactions cut the phase space into $N!$ disconnected parts ($(N-1)!$ if the boundary condition is periodic) so that there are $N!$ linearly independent ground states. In the corresponding Fermi or Bose gas the exchange is completely prohibited: at any temperature including zero each particle forms a 1-cycle in itself, the fermion and boson partition functions coincide. So there is no cycle percolation and, indeed, no Bose condensation in the case of attractive walls ([BP], [Sm]), although these latter give rise to condensation in the 1D free Bose gas [Ro]. Notice that the uniqueness condition replaces the absence of long-range order which was argued to be necessary for ODLRO in the ground state [PO].

In Section 6 we show that in the free Bose gas Bose-Einstein condensation calls forth the percolation transition. In this case the probabilities $P_{V,N}(\xi_i = k)$ can be obtained explicitly and their asymptotic behaviour for different boundary conditions can be studied. This and other details will be published separately [S3].

Let us finish this introduction with several remarks.

A purely quantum mechanical phase transition in the Bose gas, that is, a phase transition which is entirely due to Bose statistics is driven by the exchange interaction. Exchange acts among particles which are cyclicly permuted. If $E_{V,N}(\xi_i)$ remains finite, the symmetrisation plays a minor role and Boltzmann statistics would give a qualitatively correct description. It is only when $E_{V,N}(\xi_i)$ diverges that Bose statistics becomes relevant. Therefore, the divergence of $E_{V,N}(\xi_i)$ with increasing N and V is probably the most general criterion of such a phase transition: more general than ODLRO and even more general than cycle percolation. (Take, for instance, $P_{V,N}(\xi_i = n) = a_N/n^2$ with normalizing factor a_N, then $E_{V,N}(\xi_i) \approx a_N \ln N$

diverges but

$$\sum_{n=1}^{\infty} \lim_{N\to\infty} P_{V,N}(\xi_i = n) = 6/\pi^2 \sum_{n=1}^{\infty} 1/n^2 = 1$$

and, hence, there is no cycle percolation, see Section 4.) On the other hand, ODLRO implies cycle percolation in the free Bose gas and probably also in interacting systems: The importance of long cycles in the λ-transition in liquid helium was already observed by Feynman [Fe] and Penrose and Onsager [PO]. If the mean cycle length diverges slowly (more slowly than N), there may occur a phase transition analogous to the Kosterlitz-Thouless transition, with or without ODLRO and cycle percolation.

Random walks in connection with path-integral representations of the partition function are realisations of the cyclic permutations in "spacetime". It is in these terms that Feynman [Fe] described the λ-transition in liquid helium. Closely related ideas appear in recent works, mainly in connection with the quantum Heisenberg model [CS], in particular in attempts to describe the ground state of the two-dimensional antiferromagnet [Mi] or the phase transition in the three-dimensional spin-1/2 ferromagnet [To2]. In the set-up of the present paper random walks have no conceptual importance, their introduction can be avoided.

It is interesting to point out the role of the spins in the above description. While spins are not thought to modify the nature of the phase transition, their presence is useful, as they are the most natural markers of the cycles.

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2 Probability distribution over permutations

The canonical partition function of a system of N bosons confined in a volume V can be written as

$$Q_{V,N} = \mathrm{Tr}\, P_+ e^{-\beta H_N} \ . \tag{2.1}$$

With some abuse of notation, V will be used to denote both the domain and the volume (the set of sites and their number in the lattice case). In Eq.(2.1) (and, unless otherwise stated, in all subsequent formulas) the trace is taken in $\mathcal{H}^{\otimes N}$, the N-times tensor product of the one-particle Hilbert space $\mathcal{H}$. The N-particle Hamiltonian is

$$H_N = -\frac{\hbar^2}{2m}\sum_{i=1}^{N} \Delta_i + u_N(x_1, \ldots, x_N) \tag{2.2}$$

where m is the particle mass and Δ_i is the Laplacian acting in the coordinates $x_i = (x_i^1, \ldots, x_i^D)$ of the ith particle. The potential energy u_N is a real symmetric function of its arguments. The only assumption about u_N is that it permits to define the trace of $e^{-\beta H_N}$. In Eq.(2.1),

$$P_+ = N!^{-1} \sum_{g\in S_N} U(g) \ . \tag{2.3}$$

U is the unitary representation of the permutation group S_N in $\mathcal{H}^{\otimes N}$; the action of $U(g)$ is defined by

$$U(g)|\psi_1, \ldots, \psi_N\rangle = |\psi_{g^{-1}(1)}, \ldots, \psi_{g^{-1}(N)}\rangle \ . \tag{2.4}$$

It is easy to verify that P_+ is self-adjoint and $P_+^2 = P_+$, so that P_+ is the orthogonal projection onto the symmetric subspace of $\mathcal{H}^{\otimes N}$. Substituting Eq.(2.3) into Eq.(2.1) we obtain a sum over the permutation group and notice that the summand depends only on the conjugation class to which g belongs. Indeed, let g and h be conjugate to each other, i.e., $h = fgf^{-1}$ for some f in S_N, then

$$\mathrm{Tr}\, U(h)e^{-\beta H_N} = \mathrm{Tr}\, U(f)U(g)U(f)^{-1}e^{-\beta H_N} = \mathrm{Tr}\, U(g)e^{-\beta H_N} \ . \tag{2.5}$$

The first equality holds because U is a representation of S_N, the second because of the cyclicity of the trace and because $U(f)$ commutes with H_N. In virtue of Eq.(2.5), we can rewrite $Q_{V,N}$ as

$$Q_{V,N} = N!^{-1} \sum_{\mathcal{K}} |\mathcal{K}|\, \mathrm{Tr}\, U(g)e^{-\beta H_N} \tag{2.6}$$

where the summation runs over the conjugacy classes of S_N, $|\mathcal{K}|$ is the number of elements in $\mathcal{K}$ and g is any element of $\mathcal{K}$. The class corresponding to the partition $[p]$ (see (1.2)) consists of all the permutations of the form

$$g = g_1 g_2 \ldots = (i_1 \ldots i_{p_1})(i_{p_1+1} \ldots i_{p_1+p_2}) \cdots \tag{2.7}$$

where g_i are cyclic permutations of pairwise disjoint subsets

$$C_1 = \{i_1, \ldots, i_{p_1}\}\ ,\ C_2 = \{i_{p_1+1}, \ldots, i_{p_1+p_2}\}, \ldots \tag{2.8}$$

of $\{1, \ldots, N\}$. If $n_j \geq 0$ denotes the multiplicity of j in $[p]$, the sequence (n_j) satisfies

$$\sum_{j=1}^{N} j n_j = N \ . \tag{2.9}$$

The relation between $[p]$ and (n_j) is one-to-one, therefore the notation

$$q[p] = \prod_{j=1}^{N} \left(\frac{1}{j}\right)^{n_j} \frac{1}{n_j!} \tag{2.10}$$

is unambiguous. Now $N!q[p]$ is the number of elements of the class $[p]$, thus Eq.(2.6) reads

$$Q_{V,N} = \sum_{[p]} q[p]\, \mathrm{Tr}\, U(g)e^{-\beta H_N} \ . \tag{2.11}$$

This formula was the starting point for Matsubara [Ma], Feynman [Fe] and Penrose and Onsager [PO] in the discussion of the λ-transition in liquid helium. Let us remark that the canonical partition function of a system of fermions has the form (2.11) with an extra factor $\epsilon[p]$. This can be obtained by replacing P_+ by

$$P_- = N!^{-1} \sum_{g \in S_N} \epsilon(g)U(g) \tag{2.12}$$

in Eq.(2.1) and by noticing that the signature $\epsilon(g)$ depends only on the class: each j-cycle contributes to it with a factor $(-1)^{j-1}$.

In the simplest situation the one-particle Hilbert space is $L^2(V)$ (or $\ell^2(V)$, lattice case). Another example is when the particles have an internal degree of freedom (spin) which may take on $d = 2s + 1$ values. In this case

$$\mathcal{H} = \mathcal{H}_0 \otimes {}^d \tag{2.13}$$

where $\mathcal{H}_0$ denotes the spinless one-particle Hilbert space. The Hamiltonian acts exclusively in $\mathcal{H}_0$. Therefore the partial trace over $({}^d)^{\otimes N}$ can be performed: Using the notation U_0 and U_1 for the representations of S_N in $\mathcal{H}_0^{\otimes N}$ and $({}^d)^{\otimes N}$, respectively, we obtain

$$\operatorname{Tr} U(g) e^{-\beta H_N} = \operatorname{Tr}_{({}^d)^{\otimes N}} U_1(g) \operatorname{Tr}_{\mathcal{H}_0^{\otimes N}} U_0(g) e^{-\beta H_N} \ . \tag{2.14}$$

The first term on the right-hand side is the character $\chi_N(g)$ of g in the representation U_1. With the decomposition (2.7), this factorises according to the cycles,

$$\chi_N(g) = \prod_{i=1}^{k} \chi_{p_i}(g_i) = d^k \ , \tag{2.15}$$

see also Eq.(A.5). Thus, for $\mathcal{H}$ given by Eq.(2.13),

$$Q_{V,N} = \sum_{[p]} d^{k[p]} q[p] \operatorname{Tr}_{\mathcal{H}_0^{\otimes N}} U_0(g) e^{-\beta H_N} = \sum_{[p]} d^{k[p]} A[p] \ . \tag{2.16}$$

The number of cycles $k[p] = \sum n_j$ includes cycles of length 1. $A[p]$ is defined by Eq.(2.16). It is this quantity which appeared in Eq.(1.1).

In what follows, we will consider S_N as a space of events and assign probabilities to the permutations. The probability of any $g \in S_N$ is defined as

$$P_{V,N}(g) = (N! Q_{V,N})^{-1} \operatorname{Tr} U(g) e^{-\beta H_N} \ . \tag{2.17}$$

To see that this expression is positive write

$$\operatorname{Tr} U(g) e^{-\beta H_N} = \int_V \ldots \int_V dx_1 \ldots dx_N \langle x_1, \ldots, x_N | e^{-\beta H_N} | x_{g(1)}, \ldots, x_{g(N)} \rangle \ . \tag{2.18}$$

The positivity of the integrand can be proved by showing it at first for the free Hamiltonian $-\sum \Delta_i$ and then by passing to H_N with the application of the Trotter formula. For $-\sum \Delta_i$ the proof is done by direct computation if the domain is rectangular and the boundary condition is periodic or Neumann; for Dirichlet boundary condition on arbitrary domain the proof involves path integral arguments ([Gi], [FS]).

To simplify the notation, the labels V and N will be dropped whenever this causes no confusion. Next, we introduce two sets of random variables: $\nu_j(g)$ is the number of j-cycles of g and $\xi_i(g)$ is the length of the cycle containing i $(1 \leq i, j \leq N)$. These are related by

$$\sum \xi_i = \sum j^2 \nu_j \ . \tag{2.19}$$

To see this, observe that both sides depend only on the class $[p]$ and both equal $\sum p_j^2$. All the ξ_i are equally distributed, therefore

$$\xi = N^{-1} \sum \xi_i \tag{2.20}$$

has the same mean value as any of the ξ_i:

$$E_{V,N}(\xi) = E_{V,N}(\xi_i) = N^{-1} \sum j^2 E_{V,N}(\nu_j) \ . \tag{2.21}$$

Again, the labels V and N will often be dropped hereafter. $E(\xi)$ will be referred to as the "mean cycle length", although the true mean cycle length may be smaller:

$$\xi \geq N / \sum \nu_j \ . \tag{2.22}$$

Equation (2.22) is equivalent with the Schwarz inequality

$$N^2 = (\sum j\nu_j)^2 \leq (\sum \nu_j)(\sum j^2 \nu_j) = N\xi \sum \nu_j \ . \tag{2.23}$$

There is a simple relation between the probability distribution of ξ_i and the mean value of the ν_j's. It reads

$$P(\xi_i = n) = \frac{n}{N} E(\nu_n) \ . \tag{2.24}$$

Equation (2.21) could have been obtained from here as well. To get Eq.(2.24) we write

$$P(\xi_i = n) = \sum_j P(\xi_i = n | \nu_n = j) P(\nu_n = j) \tag{2.25}$$

and notice that

$$P(\xi_i = n | \nu_n = j) = \frac{jn}{N} \ . \tag{2.26}$$

A similar simple relation can be derived for the probability that any two different numbers, say i and j, fall in the same cycle of g. Let us denote this event by $i \sim_g j$ or more simply by $i \sim j$.

$$\begin{aligned} P(i \sim j) &= \sum_n P(i \sim j | \xi_i = n) P(\xi_i = n) \\ &= \sum_n \frac{n-1}{N-1} P(\xi_i = n) = \frac{1}{N-1}(E(\xi) - 1) \ . \end{aligned} \tag{2.27}$$

To compute the conditional probabilities in Eqs.(2.26) and (2.27) we used the fact that $P_{V,N}(g)$ is a class function (see Eq.(2.5)), therefore a given number can be found with equal probability in any box of a Young diagram.

If we replace the definition (2.17) by any probability distribution P_N on S_N which is constant on the conjugacy classes, the probability of a class is

$$P_N[p] = N! q[p] P_N(g) \tag{2.28}$$

where g is any element of the class, all ξ_i are equally distributed and the equations (2.21) and (2.24-2.27) remain valid. Equation (2.24) can be generalized as follows.

Let $m_1,\ldots,m_k$ be k different positive integers and $1\le i_1<\cdots<i_k$. If $N\ge\sum m_i$ and $N\ge i_k$,

$$P_N(\xi_{i_1}\!=\!m_1,\ldots,\xi_{i_k}\!=\!m_k)=\frac{m_1m_2\cdots m_k}{N(N\!-\!1)\cdots(N\!-\!k\!+\!1)}E_N(\nu_{m_1}\cdots\nu_{m_k})\ . \tag{2.29}$$

This relation can be verified by direct computation:

$$\begin{aligned}
&P_N(\xi_{i_1}\!=\!m_1,\ldots,\xi_{i_k}\!=\!m_k)\\
&\quad=P_N(\xi_1\!=\!m_1,\xi_{m_1+1}\!=\!m_2,\ldots,\xi_{m_1+\cdots+m_{k-1}+1}\!=\!m_k)\\
&\quad=\frac{(N\!-\!k)!}{(N\!-\!m_1\!-\!\cdots\!-\!m_k)!}\sum_{g\in S(m_1+\cdots+m_k+1,\ldots,N)}P_N(g_1\cdots g_kg)\\
&\quad=(N\!-\!k)!\sum_{[p]_{N-m_1-\cdots-m_k}}q[p]_{N-m_1-\cdots-m_k}P_N(g_1\cdots g_kg)\ .
\end{aligned}\tag{2.30}$$

Above g_i denotes the cyclic permutation $(\sum_1^{i-1}m_j\!+\!1\ldots\sum_1^i m_j)$, $S(L,L\!+\!1,\ldots,N)$ is the group of all the permutations of the numbers $L,L\!+\!1,\ldots,N$ and the notation $[p]_M$ is used to indicate that $[p]$ is a partition of $M\neq N$. In the last line g is any element of the class $[p]_{N-m_1-\cdots-m_k}$. On the other hand, if, as in Eq.(2.10), n_j denotes the multiplicity of j in $[p]$ and the m_i's are all different,

$$n_{m_1}\cdots n_{m_k}q[p]=\frac{1}{m_1\cdots m_k}q[p]_{N-m_1-\cdots-m_k}\ . \tag{2.31}$$

Therefore with Eq.(2.28)

$$\begin{aligned}
E_N(\nu_{m_1}\cdots\nu_{m_k})&=\sum_{[p]:n_{m_1},\ldots,n_{m_k}\ge1}n_{m_1}\cdots n_{m_k}P_N[p]\\
&=\frac{N!}{m_1\cdots m_k}\sum_{[p]_{N-m_1-\cdots-m_k}}q[p]_{N-m_1-\cdots-m_k}P_N(g_1\cdots g_kg)\ .
\end{aligned}\tag{2.32}$$

This and Eq.(2.30) prove Eq.(2.29).

If some of the m_i's coincide, Eq.(2.29) still holds true up to a correction of the order of $1/N$. This is particularly easy to check for $k=2$:

$$\begin{aligned}
P_N(\xi_i\!=\!m,\xi_j\!=\!m)&=P_N(\xi_i\!=\!m)-\sum_{n(\neq m)}P_N(\xi_i\!=\!m,\xi_j\!=\!n)\\
&=\frac{m}{N}E_N(\nu_m)-\frac{m}{N(N\!-\!1)}E_N(\nu_m\sum_{n(\neq m)}n\nu_n)\\
&=\frac{m}{N}E_N(\nu_m)-\frac{m}{N(N\!-\!1)}E_N(\nu_m(N\!-\!m\nu_m))\\
&=\frac{m^2}{N(N\!-\!1)}E_N(\nu_m^2)-\frac{1}{N\!-\!1}P_N(\xi_i\!=\!m)\ .
\end{aligned}\tag{2.33}$$

We used Eqs.(2.24), (2.29) in the second equality and $\sum n\nu_n=N$ in the third one.

It is easy to get an upper bound on the probability (2.29). Since $m_1,\ldots,m_k$ are all different, replacing (m_i) by $(m_{g(i)})$, where $g\in S_k$ is arbitrary, results in a disjoint event of the same probability. Therefore $1/k!$ is an upper bound to (2.29). In general, if $l_1, l_2, \ldots, l_j$ of the numbers m_i are respectively the same ($\sum_{\alpha=1}^{j} l_\alpha = k$), we get

$$P_N(\xi_{i_1} = m_1, \ldots, \xi_{i_k} = m_k) \leq \frac{l_1! \cdots l_j!}{k!} \, . \tag{2.34}$$

These probabilities will reappear in Section 4 where we attempt (without really succeeding) to construct a probability measure in the limit of the infinite system.

3 Cycles and pair correlations

Consider a system of identical particles (bosons or fermions) having a spin of quantum number s: this is the case of Eq.(2.13) with $d = 2s+1$. If the spins are coupled to a homogeneous external magnetic field, the Hamiltonian reads

$$H_N^{(h)} = H_N - h \sum_{i=1}^{N} S_i^z \tag{3.1}$$

where S_i^z is the z-component of the spin of the ith particle. To get the partition function $Q_{V,N}^{(h)}$, one has to replace H_N by $H_N^{(h)}$ in Eq.(2.11). Similarly to Eq.(2.14), the trace over $\mathcal{H}^{\otimes N}$ factorizes according to spatial and spin variables and the partial trace over the spins is easy to performe: If g is a permutation of the form (2.7-2.8),

$$\begin{aligned} \mathrm{Tr}_{({}^d)^{\otimes N}}\, U_1(g) e^{\beta h \sum S_i^z} &= \prod_{j=1}^{k[p]} \mathrm{Tr}_{({}^d)^{\otimes p_j}}\, U_1(g_j) e^{\sum_{i \in C_j} \beta h S_i^z} \\ = \prod_j \sum_{\sigma=-s}^{s} e^{\sigma \beta h p_j} &= \prod_j \frac{\sinh d\beta h p_j/2}{\sinh \beta h p_j/2} \equiv C[p](\beta h/2) \, . \end{aligned} \tag{3.2}$$

With this equality the partition function reads

$$Q_{V,N}^{(h)} = \sum_{[p]} \epsilon[p] A[p] C[p](\beta h/2) \tag{3.3}$$

where $\epsilon[p] = (-1)^{\sum (p_j - 1)}$ for fermions and 1 for bosons. For $h = 0$, Eqs.(3.2) and (3.3) reduce to Eqs.(2.15) and (2.16), respectively.

Let us compute at first the magnetization. We will need

$$\frac{dC[p](\alpha)}{d\alpha} = 2sC[p](\alpha) \sum_{j=1}^{k} p_j B_s(2s\alpha p_j) \tag{3.4}$$

where

$$B_s(x) = \frac{2s+1}{2s} \coth \frac{2s+1}{2s} x - \frac{1}{2s} \coth \frac{1}{2s} x \tag{3.5}$$

is the Brillouin function [AM]. With Eq.(3.4) we find the magnetization

$$\begin{aligned} M(h) &= \frac{1}{2N} \frac{\partial \ln Q_{V,N}^{(h)}}{\partial (\beta h/2)} \\ &= \frac{s}{Q_{V,N}^{(h)}} \sum_{[p]} \left(\frac{1}{N} \sum_j p_j B_s(s\beta h p_j) \right) \epsilon[p] A[p] C[p](\beta h/2) \, . \end{aligned} \tag{3.6}$$

For $s=1/2$ fermions this is just Eq.(1.1).

The zero-field magnetic susceptibility can be obtained easily. $M(h)$ vanishes at $h=0$, therefore

$$\chi = \left.\frac{\partial M}{\partial h}\right|_{h=0} = \frac{1}{\beta N Q_{V,N}} \left.\frac{\partial^2 Q^{(h)}_{V,N}}{\partial h^2}\right|_{h=0} . \tag{3.7}$$

The second derivative of $C[p]$ can be read out from

$$C[p](\beta h/2) = d^{k[p]}\left(1+\frac{1}{6}s(s+1)(\beta h)^2 \sum p_j^2\right) + O(h^4) . \tag{3.8}$$

Combining Eqs.(3.3), (3.7) and (3.8),

$$\chi(s) = \frac{1}{3}s(s+1)\beta \frac{\sum_{[p]}(\frac{1}{N}\sum p_j^2)\epsilon[p]d^{k[p]}A[p]}{\sum_{[p]}\epsilon[p]d^{k[p]}A[p]} \tag{3.9}$$

which, in the bosonic case, still reads

$$\chi(s) = \frac{1}{3}s(s+1)\beta E(\xi) . \tag{3.10}$$

Here $E(\xi)$ is the mean cycle length (2.21). For spin-1/2 fermions we can recognize Eq.(1.4).

Let $\mathbf{S}_i$ denote the spin operator associated with the ith particle. ¿From Eq.(1.5) we get for any $i \neq j$

$$\chi(s) = (\beta/3N)\langle \mathbf{S}^2\rangle = \frac{1}{3}s(s+1)\beta + \frac{1}{3}\beta(N-1)\langle \mathbf{S}_i\mathbf{S}_j\rangle \tag{3.11}$$

because $\langle \mathbf{S}_i\mathbf{S}_j\rangle$ is independent of i,j. Comparison with Eqs.(3.10) and (2.27) shows that for $i\neq j$

$$\langle \mathbf{S}_i\mathbf{S}_j\rangle = s(s+1)P(i\sim j) . \tag{3.12}$$

Thus, the correlations in a gas of spinning bosons are ferromagnetic and ferromagnetic long-range order means that the probability of finding i and j in the same cycle is nonvanishing in the thermodynamic limit.

Equation (3.12) contains no information about the spatial behaviour of the pair correlations. This latter can be inferred from the analogue of Eq.(1.6). For the sake of simplicity, we restrict the discussion to the lattice case. The spin operator at the site x is defined by

$$\mathbf{S}(x) = \sum_{i=1}^{N} \mathbf{S}_i N_i(x) . \tag{3.13}$$

$N_i(x)$ projects the position of particle i to x:

$$N_i(x) = I\otimes\cdots\otimes|x\rangle\langle x|\otimes\cdots\otimes I \tag{3.14}$$

with $|x\rangle\langle x|$ at the ith place and the identity elsewhere. With $x_1,\ldots,x_N$ in V and g in S_N let

$$(x_i) = (x_1,x_2,\ldots,x_N) \ \ , \ \ (x_{g(i)}) = (x_{g(1)},\ldots,x_{g(N)}) . \tag{3.15}$$

The vectors

$$|(x_i)\rangle = |x_1,\ldots,x_N\rangle \tag{3.16}$$

form an orthonormal basis in $\ell^2(V)^{\otimes N}$. For any subset C of $\{1,2,\ldots,N\}$ and x in V let

$$N_C(x) = \sum_{i\in C} N_i(x)\ . \tag{3.17}$$

Any $|(x_i)\rangle$ is an eigenvector of $N_C(x)$ with the eigenvalue

$$n_{C,(x_i)}(x) = \sum_{i\in C}\langle x|x_i\rangle\ . \tag{3.18}$$

For a permutation g let $C_j = C_j(g)$, $j = 1,\ldots,k = k(g)$ stand for the (support of the) cycles of g (see Eq.(2.8)). Now $n_{C_j,(x_i)}(x)$ is a *joint cycle-site occupation number* in the configuration (x_i): it gives the number of particles which are simultaneously at the site x and in the cycle C_j. These numbers can be united in a vector

$$\mathbf{n}_{g,(x_i)}(x) = (n_{C_1,(x_i)}(x),\ldots,n_{C_k,(x_i)}(x))\ . \tag{3.19}$$

The ℓ^1-norm of this vector is independent of g,

$$\|\mathbf{n}_{g,(x_i)}(x)\|_1 = \sum_j n_{C_j,(x_i)}(x) = \sum_{i=1}^N\langle x|x_i\rangle \tag{3.20}$$

and gives the number of particles at x in the configuration (x_i).

Now for $x\neq y$ in V the spin pair correlation reads

$$\begin{aligned}&\langle\mathbf{S}(x)\mathbf{S}(y)\rangle \\ &\quad = s(s{+}1)\frac{\sum_{[p]}\epsilon[p]d^{k[p]}q[p]\sum_{(x_i)}\langle(x_{g(i)})|e^{-\beta H_N}|(x_i)\rangle\mathbf{n}_{g,(x_i)}(x)\mathbf{n}_{g,(x_i)}(y)}{\sum_{[p]}\epsilon[p]d^{k[p]}q[p]\sum_{(x_i)}\langle(x_{g(i)})|e^{-\beta H_N}|(x_i)\rangle}\ .\end{aligned} \tag{3.21}$$

As earlier, g is any element of the class $[p]$; $\sum_{(x_i)}$ is a short-hand for $\sum_{x_1}\ldots\sum_{x_N}$. This formula is derived in the Appendix. One can immediately see that for bosons the pair correlations are strictly positive. Let us introduce an enlarged event space consisting of the couples $(g,(x_i))$ and define the probability of $(g,(x_i))$ as

$$P_{V,N}(g,(x_i)) = \frac{d^{k(g)}}{N!Q_{V,N}}\langle(x_{g(i)})|e^{-\beta H_N}|(x_i)\rangle\ . \tag{3.22}$$

Then for bosons

$$\langle\mathbf{S}(x)\mathbf{S}(y)\rangle = s(s+1)E_{V,N}(\mathbf{n}_{g,(x_i)}(x)\mathbf{n}_{g,(x_i)}(y))\ , \tag{3.23}$$

the expectation value on the right-hand side taken with the probabilities (3.22). Thus, the spin pair correlations are proportional to the density- density correlations restricted to particles belonging to the same cycle. The latter is well-defined also for spinless bosons.

In some cases summing over all terms of the numerator of (3.21) in which $\mathbf{n}_{g,(x_i)}(x)\mathbf{n}_{g,(x_i)}(y) \geq 2$ yields zero. Then Eq.(3.21) can be rewritten more simply as

$$\langle \mathbf{S}(x)\mathbf{S}(y)\rangle = s(s+1)\frac{\sum_{[p]:p_1>1}\epsilon[p]d^{k[p]}q[p]\sum'_{(x_i)}\langle (x_{g(i)})|e^{-\beta H_N}|(x_i)\rangle}{\sum_{[p]}\epsilon[p]d^{k[p]}\sum_{(x_i)}\langle (x_{g(i)})|e^{-\beta H_N}|(x_i)\rangle} \ . \tag{3.24}$$

Here $\sum'$ means that after choosing g in the class $[p]$ the summation is restricted to those configurations in which both x and y are singly occupied and the (labels of the) corresponding two particles belong to the same cycle of g. The restriction $p_1 > 1$ (cf. Eq.(1.2)) excludes the class formed by the unit e of S_N: this is necessary because the inner product in Eq.(3.21) vanishes for $g = e$. Equation (3.24) is valid for bosons and fermions if the interaction contains a hard-core repulsion: Doubly occupied sites being excluded, $\mathbf{n}_{g,(x_i)}(x)\mathbf{n}_{g,(x_i)}(y) = 0$ or 1 for the nonvanishing terms.

Equation (3.24) is also valid for spin-1/2 fermions independently of the form of the interaction. In this case the sum over the classes for fixed (x_i) yields zero if x or y is multiply occupied [S1,S2]. This can be understood by noticing that triple and higher encounters are illicit and a double occupation at, say, x results in a spin singlet on which $\mathbf{S}(x)$ gives 0. The only difference between Eqs.(1.6) and (3.24) is that in the latter we have executed the trivial summation over the permutations within each class.

Let $x \sim y$ denote the event that x and y fall in the same cycle, i.e.,

$$\{x \sim y\} = \{(g,(x_i)) : x_i = x, x_j = y \text{ for some } i \sim_g j\} \ . \tag{3.25}$$

For bosons with a hard-core interaction $\mathbf{n}_{g,(x_i)}(x)\mathbf{n}_{g,(x_i)}(y)$ is the indicator function of $x \sim y$, therefore from (3.23) or (3.24) we get

$$\langle \mathbf{S}(x)\mathbf{S}(y)\rangle = s(s+1)P(x \sim y) \ . \tag{3.26}$$

For the general boson gas, combining Eqs.(1.5), (3.10) and (3.23) we obtain

$$E(\xi) = \frac{1}{N}\sum_{x,y} E(\mathbf{n}_{g,(x_i)}(x)\mathbf{n}_{g,(x_i)}(y)) \tag{3.27}$$

which reduces to

$$E(\xi) = \frac{1}{N}\sum_{x,y} P(x \sim y) \tag{3.28}$$

in the case of a hard-core interaction. These formulas hold true whether or not the bosons have a spin. Equation (3.27) can be obtained also directly by noticing that

$$P(i \sim j) = \sum_{x,y}\sum_{g:i\sim j}\sum_{(x_k):x_i=x,x_j=y} P(g,(x_k)) \tag{3.29}$$

and

$$\sum_{i,j} P(i \sim j) = NE(\xi) \ . \tag{3.30}$$

In contrast to Eq.(3.28), the latter equation is always true and follows from Eq.(2.27) with the definition

$$P(i \sim i) = 1 \ . \tag{3.31}$$

One may observe a resemblance between $E(\mathbf{n}_{g,(x_i)}(x)\mathbf{n}_{g,(x_i)}(y))$ and the one-particle reduced density matrix [PO], although the former is more complicated. However, $E(\xi)$ is much easier to compute, at least in the ground state (see Section 5), than the corresponding sum determining ODLRO (VA_1 in [PO]).

4 Events and probabilities in the infinite system

When speaking about a percolation transition one makes allusion to a phenomenon occurring in an infinite event space. In our case this will be the family of all the bijections from the set of positive integers onto itself, which we denote by S_∞. The permutation group S_N can be embedded into S_∞ by defining $g(i) = i$ for any g in S_N and $i > N$. In this way

$$S_1 \subset S_2 \subset \cdots \subset S_\infty \ . \tag{4.1}$$

Clearly, $S_f \equiv \cup_{N=1}^\infty S_N$ does not exhaust S_∞. S_f is the family of all the finite permutations, i.e., those having a finite number of nontrivial cycles. Let $S_0 = S_\infty - S_f$. S_0 contains bijections all the cycles of which are finite, an example is $g(2i-1) = 2i$, $g(2i) = 2i-1$ for every $i \geq 1$. However, "almost all" elements of S_0 contain at least one infinite cycle because S_0 is an uncountable set, while the family of all the bijections in which every number is in a finite cycle is countable.

The random variables ν_j and ξ_i introduced in Section 2 are naturally defined as functions on S_∞ with values in $[0,\infty]$ and $[1,\infty]$, respectively. The level sets

$$\begin{aligned} B_{in} &= \{\xi_i = n\} \ , \quad n \geq 1 \ , \\ B_{i0} &= \{\xi_i = \infty\} \end{aligned} \tag{4.2}$$

are then subsets of S_∞. For any V and N we redefine $P_{V,N}$ as a probability measure on the σ-algebra $\mathcal{F}(\mathcal{A})$ generated by $\mathcal{A} = \{B_{im}\}_{i\geq 1, m\geq 1}$ by setting

$$P'_{V,N}(\cap_{j=1}^k B_{i_j m_j}) = P_{V,N}(\cap_{j=1}^k B_{i_j m_j} \cap S_N) \tag{4.3}$$

and dropping the prime immediately. Notice that

$$S_N = \cap_{i=N+1}^\infty B_{i1} \ . \tag{4.4}$$

We are interested in the limit of (4.3) when N and V tend to infinity and N/V goes to the density ρ. By the diagonal process [Rud] one can choose a subsequence (V_n, N_n) on which these limits simultaneously exist for every k and $m_1, m_2, \ldots, m_k \geq 1$ finite (thus, for a countable number of events):

$$P_\rho(\cap_{j=1}^k B_{i_j m_j}) = \lim_{n\to\infty} P_{V_n,N_n}(\cap_{j=1}^k B_{i_j m_j}) \ . \tag{4.5}$$

It is obvious that replacing i_j by $g(i_j)$ ($g \in S_\infty$ arbitrary) yields the same limit. Now

$$\sum_{n=1}^\infty P_\rho(B_{in}) \leq 1 \tag{4.6}$$

because the inequality holds for finite sums. Therefore one can define the "probability of cycle percolation" by

$$P_\rho(B_{i0}) = 1 - \sum_{n=1}^{\infty} P_\rho(B_{in}) \ . \tag{4.7}$$

That this is indeed a probability, i.e., that P_ρ extends from (4.5) to a unique probability measure on $\mathcal{F}(\mathcal{A})$, remains to be proved. Let us briefly resume the problem we encounter here. Let $\mathcal{B}$ denote the class of all finite intersections of elements of $\mathcal{A}$. The numerical function P_ρ is defined on $\mathcal{B}$ via Eq.(4.5). Furthermore, let $\mathcal{C}$ be the class of all finite unions of elements of $\mathcal{A}$ and

$$\mathcal{D} = \{B - C | B \in \mathcal{B}, C \in \mathcal{C}\} \ . \tag{4.8}$$

We call the elements of $\mathcal{D}$ "monomials". One can check easily that the class of all finite unions of monomials is just the ring $\mathcal{R}(\mathcal{A})$ generated by $\mathcal{A}$, and the limit P_ρ of P_{V_n,N_n} exists on $\mathcal{R}(\mathcal{A})$ and defines a *content* [Ba]: $0 \leq P_\rho \leq 1$, $P_\rho(\emptyset) = 0$ and $P_\rho(\cup_{i=1}^n A_i) = \sum_{i=1}^n P_\rho(A_i)$ for any finite number of pairwise disjoint sets $A_1, \ldots, A_n \in \mathcal{R}(\mathcal{A})$. If P_ρ is σ-additive on $\mathcal{R}(\mathcal{A})$, it has a unique extension by continuity and complementation as a probability measure on $\mathcal{F}(\mathcal{A})$. Proving σ-additivity is equivalent to show that if (A_i) is an infinite sequence in $\mathcal{R}(\mathcal{A})$, $A_1 \supset A_2 \supset \cdots$ and $\cap_{i=1}^\infty A_i = \emptyset$ then $P_\rho(A_i) \to 0$. If A_i are monomials, this can be seen to be true by using the inequalities (2.34). The general case is much more complicated and Eq.(2.34) may not suffice to get σ-additivity.

Notice that the strict inequality in Eq.(4.6) in itself indicates a phase transition independently of whether or not P_ρ is a probability measure. However, in the absence of this result one has to be careful with the interpretation of the limits of probabilities and expectation values.

One may observe that $\mathcal{F}(\mathcal{A})$ is the smallest σ-algebra on which cycle percolation can be defined. It does not contain the event $i \sim j$, and some interesting random variables like the density of an infinite cycle (see next section) are not $\mathcal{F}$-measurable. The systematic extension of P_ρ could replace in some respects the C^*-algebraic description of infinite Bose systems.

5 Ground state cycle percolation

We consider a system of interacting bosons possibly with a d-valued spin (Eq.(2.13)) and assume that the Hamiltonian (2.2) has a unique overall ground state in the spinless Hilbert space $\mathcal{H}_0^{\otimes N}$. As discussed in the Introduction, this holds true under very general assumptions on the interaction, domain and boundary condition. Uniqueness proofs are based on Perron-Frobenius type theorems ([KR], [GJ]) and show that the ground state wave function can be chosen to be positive. Uniqueness and positivity then implies that it is symmetric under any permutation of the particle positions. As we see below, this suffices to prove ground state cycle percolation. Let $E_0 = E_0(N)$ denote the energy of the ground state. Then

$$\lim_{\beta \to \infty} e^{\beta E_0} Q_{V,N} = N!^{-1} \sum_g d^{k(g)} = \sum_{[p]} d^{k[p]} q[p] \equiv Q_N(d) \ . \tag{5.1}$$

This limit gives the number of linearly independent ground states of the Bose gas. Since the degeneracy comes exclusively from the spins, we have

$$Q_N(d) = \left(\begin{array}{c} d+N-1 \\ N \end{array} \right) , \tag{5.2}$$

the number of ways we can assign d spin values to N undistinguishable particles. The zero temperature limit of the probability distribution for the permutations is

$$P_N(g) = d^{k(g)}/N!Q_N(d) . \tag{5.3}$$

In particular, for $d = 1$ all permutations are equally probable.

We wish to determine $P_N(\xi_i = j)$. This goes via the determination of $E_N(\nu_j)$, see Eq.(2.24), which can be done exactly. However, we start with an approximate method which will be reapplied for the free Bose gas at positive temperatures [S3]. From Eqs.(2.10) and (5.1) for any λ we find

$$P_N((\nu_k)=(n_k)) = e^{-\lambda N} Q_N(d)^{-1} \prod_{k=1}^{N} \left(\frac{de^{\lambda k}}{k}\right)^{n_k} \frac{1}{n_k!} \tag{5.4}$$

if $\sum kn_k = N$ and 0 otherwise. Let us forget about the constraint (2.9) for a moment. Then the ν_j are independent Poisson-distributed random variables with mean value

$$E(\nu_j) = de^{\lambda j}/j . \tag{5.5}$$

Now let us take the constraint into account in average, i.e., choose λ so that

$$\sum_{k=1}^{N} kE(\nu_k) = d\sum_{k=1}^{N} e^{\lambda k} = N . \tag{5.6}$$

One can check that $E(\nu_j)$ determined from (5.5), (5.6) is the most probable value of ν_j obtained as a conditional extremum in a continuous approximation. The Lagrange multiplier λ can be identified with the chemical potential. In particular, for $d = 1$ we get $\lambda = 0$ and

$$E(\nu_j) = 1/j . \tag{5.7}$$

It turns out that this is the exact result. Let us compute $E_N(\nu_j)$ by fully respecting the constraint (2.9). With the notations of Eq.(2.30) the result is

$$\begin{aligned} E_N(\nu_j) &= \sum_m mP_N(\nu_j = m) = \sum_{m\geq 1} m \sum_{[p]:n_j=m} d^{k[p]}q[p]/Q_N(d) \\ &= \frac{d}{j} \sum_{[p]_{N-j}} d^{k[p]_{N-j}} q[p]_{N-j}/Q_N(d) = \frac{d}{j} Q_{N-j}(d)/Q_N(d) \end{aligned} \tag{5.8}$$

which is equal to (5.7) for $d = 1$. For $d > 1$, Eq.(5.5) gives a reasonably good approximation if $j \ll N$. To see this, notice that in this case Eq.(5.8) yields

$$E_N(\nu_j) \approx \frac{d}{j} e^{-\frac{d-1}{N}j} , \tag{5.9}$$

while the solution of Eq.(5.6) for λ is

$$\lambda = -a/N \tag{5.10}$$

with $d-1 < a < d$ [S3]. Let us observe that the ratio of $Q_{N-j}(d)$ and $Q_N(d)$ tends to 1 as N increases, therefore

$$\lim_{N\to\infty} E_N(\nu_j) = d/j \ . \tag{5.11}$$

¿From Eqs.(2.24) and (5.8)

$$P_N(\xi_i = j) = \frac{d}{N} Q_{N-j}(d)/Q_N(d) \ . \tag{5.12}$$

For $d = 1$ all the cycle lengths are equally probable. Moreover,

$$p(n) \equiv P_\rho(B_{in}) = \lim_{N\to\infty} P_N(\xi_i = n) = 0 \tag{5.13}$$

for any $n \geq 1$. Thus the percolation probability $1 - \sum_{n\geq 1} p(n) = 1$. Furthermore, applying Eq.(5.2) and the Pascal triangle identity

$$\sum_{k=0}^{m} \binom{n+k}{n} = \binom{n+m+1}{n+1} \tag{5.14}$$

we obtain

$$E_N(\xi_i) = \frac{N+d}{d+1} \ . \tag{5.15}$$

¿From Eq.(5.12) we can infer the limit distribution of the cycle densities. Let $0 \leq a < b \leq 1$, then using Eq.(5.14) we find

$$\begin{aligned} & P_N(aN < \xi_i \leq bN) \\ & \quad = \frac{d}{N} \binom{N+d-1}{d-1}^{-1} \left\{ \binom{N+d-1-[aN]}{d} - \binom{N+d-1-[bN]}{d} \right\} \\ & \quad \underset{N\to\infty}{\longrightarrow} (1-a)^d - (1-b)^d \equiv \mu((a,b]) \ . \end{aligned} \tag{5.16}$$

Thus, μ is an absolutely continuous probability measure on the interval $[0,1]$, and each ξ_i/N tends to a random variable η_i distributed according to μ. This η_i is the density of the cycle containing i. For $d = 1$, μ is the Lebesgue measure and for general d the probability density corresponding to μ is $d(1-x)^{d-1}$. We can use this density to perform the limit $N \to \infty$ in Eq. (2.27) at $\beta = \infty$:

$$\begin{aligned} \lim_{N\to\infty} P_N(i \sim j) &= \int_0^1 P(i \sim j | \eta_i = x) d\mu(x) = \int_0^1 x d\mu(x) \\ &= E(\eta_i) = d \int_0^1 x(1-x)^{d-1} dx = \frac{1}{d+1} = \frac{1}{2(s+1)} \ . \end{aligned} \tag{5.17}$$

The fact that this is less than 1 and that the percolation probability is 1 implies that the infinite cycle is nonunique. However, we can arrive at a much stronger conclusion: Equation (5.16) shows that as N increases, any particle belongs, with a probability tending to 1, to a macroscopic cycle (the length of which grows proportionally to N). Moreover, macroscopic cycles of different densities coexist, and in the infinite system the number of infinite cycles of positive density is (countable) infinite. This can be seen more clearly if one computes the expected number of cycles with density larger than x: ¿From (5.2) and (5.8) one obtains

$$\lim_{N\to\infty} E_N(\sum_{j\geq xN} \nu_j) \geq d\ln\frac{1}{x} + d(d-1)(1-x) \tag{5.18}$$

(with equality at $d=1$) which diverges as x goes to zero. In this respect, cycle percolation resembles bond percolation on a tree where the number of infinite clusters is infinite when percolation takes place.

A physical consequence of the existence of macroscopic cycles is that the ground state of a system of spinning bosons is ferromagnetic. ¿From Eqs.(3.10) and (5.15) the ground state magnetic susceptibility is

$$\lim_{\beta\to\infty} \beta^{-1}\chi_N = \frac{1}{3}s(s+1)\frac{N+2s+1}{2s+2} = s(N+2s+1)/6\ . \tag{5.19}$$

Comparing with Eq.(1.5) or (3.11), we see that for $s > 1/2$ the magnetic moment cannot saturate: $S_{\max} = Ns$ while

$$\frac{\langle \mathbf{S}^2\rangle}{S_{\max}(S_{\max}+1)} \underset{\beta\to\infty}{\longrightarrow} \frac{1}{2}\frac{N+2s+1}{Ns+1} < 1 \tag{5.20}$$

if $N > 1$. The reason is that there exist ground states with spin quantum number less than Ns, and these are all mixed together when the temperature goes to zero in zero magnetic field.

6 Percolation transition in the free Bose gas

For the free Bose gas

$$H_N = \sum_{i=1}^{N} H_i^0\ \ ,\ \ H_i^0 = -\frac{\hbar^2}{2m}\Delta_i \tag{6.1}$$

and the trace in Eq.(2.16) factorizes according to the cycles: If g has n_k cycles of length k,

$$\mathrm{Tr}_{\mathcal{H}_0^{\otimes N}}\, U_0(g)e^{-\beta H_N} = \prod_{k=1}^{N}\left(\mathrm{tr}\, e^{-\beta k H^0}\right)^{n_k} \tag{6.2}$$

where $\mathrm{tr} = \mathrm{Tr}_{\mathcal{H}_0}$. For the probability of a conjugacy class we find

$$P_{V,N}((\nu_k)\!=\!(n_k)) = \frac{1}{Q_{V,N}}\prod_{k=1}^{N}\left(\frac{d\,\mathrm{tr}\, e^{-\beta k H^0}}{k}\right)^{n_k}\frac{1}{n_k!} \tag{6.3}$$

if $\sum kn_k = N$ and zero otherwise. This yields, similarly to Eqs.(5.8) and (5.12),

$$E_{V,N}(\nu_k) = \frac{d}{k}\,\mathrm{tr}\, e^{-\beta k H^0} Q_{V,N-k}/Q_{V,N} \tag{6.4}$$

and

$$P_{V,N}(\xi_i = k) = \frac{d}{N}\,\mathrm{tr}\, e^{-\beta k H^0} Q_{V,N-k}/Q_{V,N}\ . \tag{6.5}$$

For the sake of simplicity, let V be a D-dimensional hypercube of side L and choose periodic boundary condition. Then due to the zero eigenvalue of H^0

$$Q_{V,N} > Q_{V,N-1}\ . \tag{6.6}$$

On the other hand, by simple computation

$$\mathrm{tr}\, e^{-\beta k H^0} \leq \left[1 + \frac{L}{B\sqrt{k}}\right]^D \tag{6.7}$$

where $B = \hbar(2\pi\beta/m)^{1/2}$. Thus,

$$P_\rho(\xi_i = k) = \lim_{V,N\to\infty} P_{V,N}(\xi_i = k) \leq \frac{d}{\rho B^D} k^{-D/2} \tag{6.8}$$

and therefore

$$\sum_{k=1}^{\infty} P_\rho(\xi_i = k) < 1 \ \text{ if } \ \rho B^D > d \sum_{k=1}^{\infty} k^{-D/2} \tag{6.9}$$

which can be satisfied if $D > 2$. In Eq.(6.8) and below the limit is taken so that N/V goes to ρ. Notice that the second inequality in (6.9) is the well-known condition for the Bose-Einstein condensation (see e.g. [Hu] in the case $d = 1$ and [CL] for $d > 1$). So the probability of cycle percolation is positive when the condition for the condensation is satisfied. To complete the discussion we should prove the converse statement:

$$\sum_{k=1}^{\infty} P_\rho(\xi_i = k) = 1 \ \text{ if } \ \rho B^D < d \sum_{k=1}^{\infty} k^{-D/2}\ , \tag{6.10}$$

in particular, that this holds for any finite density and positive temperature in one and two dimensions. Suppose one can prove: There exists some function $f(k)$ such that $Q_{V,N-k}/Q_{V,N} \leq f(k)$ independently of V and N, and $\sum_{k=1}^{\infty} f(k) < \infty$. Then by the dominated convergence theorem [Rud]

$$\begin{aligned} 1 &= \lim_{V,N\to\infty} \sum_{k=1}^{N} P_{V,N}(\xi_i = k) = \lim_{V,N\to\infty} \sum_{k=1}^{\infty} P_{V,N}(\xi_i = k) \\ &= \sum_{k=1}^{\infty} \lim_{V,N\to\infty} P_{V,N}(\xi_i = k) = \sum_{k=1}^{\infty} P_\rho(\xi_i = k) \end{aligned} \tag{6.11}$$

because $P_{V,N}(\xi_i = k) = 0$ for $k > N$ (cf. Eq.(4.3)) and $\mathrm{tr}\, e^{-\beta k H^0}/N$ can be bounded by a constant. To get such an $f(k)$ observe that, if in (6.10) the inequality holds true, there is no condensation and in the thermodynamic limit the canonical and grand-canonical ensembles are equivalent ([Rue], Thm.3.5.8). For fixed β let $z(\rho) < 1$ be the fugacity corresponding to the density ρ and define

$$z_{V,N} = Q_{V,N-1}/Q_{V,N}\ . \tag{6.12}$$

By adapting the proof of Van der Linden obtained for classical systems [VdL], one can show that $z_{V,N}$ converges to $z(\rho)$ which is continuous, increasing and smaller than 1 for $\rho < \rho_c(\beta)$. This implies that

$$\lim_{V,N\to\infty} Q_{V,N-k}/Q_{V,N} = z(\rho)^k \tag{6.13}$$

for all k. Here we would need the uniformity of the convergence and, in fact, it is plausible to conjecture that for any $\rho_0 < \rho_c(\beta)$ and $\varepsilon > 0$ one can find a $V_0 < \infty$ such that

$$\left|\frac{Q_{V,M-1}}{Q_{V,M}} - z\left(\frac{M}{V}\right)\right| < \varepsilon \tag{6.14}$$

if $V > V_0$ and $0 < M/V < \rho_0$. If such a result holds true, choosing $\varepsilon = (1 - z(\rho))/2$ one finds

$$\frac{Q_{V,N-k}}{Q_{V,N}} = \prod_{i=1}^{k} \frac{Q_{V,N-i}}{Q_{V,N-i+1}} \le [(1 + z(\rho))/2]^k \tag{6.15}$$

for large enough V, and the function on the right can play the role of $f(k)$. However, we cannot prove (6.14) and therefore (6.10) rigorously.

Equations (6.7)-(6.9) remain valid for Dirichlet or Neumann boundary condition. For Dirichlet condition the inequality (6.6) has to be replaced by

$$Q_{V,N} \ge \exp\left(-\frac{\pi D B^2}{4L^2}\right) Q_{V,N-1} \tag{6.16}$$

because the lowest eigenvalue of H^0 is positive, but the percolation transition still takes place above two dimensions. Further details will be given elsewhere [S3].

7 Summary

In this paper we have dealt with phase transitions in the Bose gas which are entirely due to quantum statistics. In a system of bosons there may occur classical phase transitions like ordinary condensation or crystallization in which quantum effects play little and mainly inhibiting role. The particularity of the quantum statistics is that they create a temperature-dependent many-body interaction via particle exchange. This leads to the Bose-Einstein condensation in the free Bose gas and may lead to BE condensation or to some weaker phase transition in an interacting Bose gas.

In order to see better the exchange in action we have not applied the formalism of the second quantization. Projection to the symmetric subspace has been done explicitly by a summation over permutations.

It is reasonable to speak about a system of interacting particles if the canonical partition function cannot be written as a product with each term depending only on the coordinates of a single particle. In this sense the 'free' Bose gas is, indeed, strongly interacting as one can see by combining the formulas (2.16) and (6.2): This, probably the best factorized, form is a sum over products on cycles. Responsible is the exchange which is seen to act among particles which are cyclicly permuted. Additional classical interactions superimpose on and sometimes compete with the creation of cycles by exchange: for example, repulsive interactions prefer the avoiding trajectories and, hence, have a tendency to shorten the cycles.

It seemed to us useful to assign probabilities to the different lengths of the cycle containing a given particle. This was possible because the terms of the sum over the permutations providing the canonical partition function are all positive. The strength of the exchange can then be measured by the mean cycle length (MCL), i.e., the expectation value of the length of the cycle containing, say, particle No.1. If, for given temperature and density, MCL remains bounded as N increases, the exchange is irrelevant. This is typically the case at high temperature or low density. MCL may increase proportionally to N and it does indeed in the ground state of most interacting Bose gas. The divergence of MCL may also be slower than N. If this occurs in a gas of spinning bosons, one encounters a Kosterlitz-Thouless type phase transition (MCL is proportional to the zero field magnetic susceptibility). For spinless bosons we may still apply this appelation by analogy.

A sufficiently rapid divergence of MCL gives rise to cycle percolation. This is detected by *first* taking the $N \to \infty$ limit of the probability of each fixed cycle length and *then* summing these limits over all cycle lenghts. Cycle percolation occurs in the ground state and yields infinitely many infinite cycles of positive density. It also occurs in the free Bose gas as far as the condition for BE condensation is satisfied. The rate of divergence of MCL will be the subject of a forthcoming publication.

The disintegration of long cycles when the temperature is raised is reminiscent of the dissociation of vortex pairs of a Kosterlitz-Thouless phase. One may wonder whether the cycles which appear as purely mathematical objects, the vortices of a Kosterlitz-Thouless phase that we recognize due to the slow divergence of MCL and the vortices of a superfluid phase are not different faces of one and the same reality.

Appendix. Proof of Equation (3.21)

In this formula the denominator is the partition function and the numerator is, for example in the bosonic case,

$$\begin{aligned}
&\mathrm{Tr}\, P_+ e^{-\beta H_N} \mathbf{S}(x)\mathbf{S}(y) \\
&\quad = N!^{-1} \sum_g \mathrm{Tr}_{\ell^2(V)^{\otimes N}} \Big(U_0(g) e^{-\beta H_N}\, \mathrm{Tr}_{(^d)^{\otimes N}}\, U_1(g)\mathbf{S}(x)\mathbf{S}(y) \Big) \qquad \text{(A.1)} \\
&\quad = N!^{-1} \sum_g \sum_{i,j} \mathrm{Tr}_{\ell^2(V)^{\otimes N}} \Big(U_0(g) e^{-\beta H_N} N_i(x) N_j(y) \Big)\, \mathrm{Tr}_{(^d)^{\otimes N}}\, U_1(g)\mathbf{S}_i\mathbf{S}_j \;.
\end{aligned}$$

Let us compute at first the trace over the spin space. Below we use the short-hand Tr_N for this trace. Suppose $g = g_1 g_2 \cdots g_k$ as in Eq.(2.7). Then

$$\begin{aligned}
\mathrm{Tr}_N\, U_1(g)\mathbf{S}_i\mathbf{S}_j &= 3\, \mathrm{Tr}_N\, U_1(g) S^z_i S^z_j = 3\, \mathrm{Tr}_N\, U_1(g_1)\cdots U_1(g_k) S^z_i S^z_j \\
&= 3 \prod_{r=1}^{k} \mathrm{Tr}_{p_r}\, U_1(g_r) W_r = \left\{ \begin{array}{ll} s(s+1)(2s+1)^k, & i \sim_g j \\ 0, & \text{otherwise} \end{array} \right. . \qquad \text{(A.2)}
\end{aligned}$$

Above W_r is one of the four operators $S_i^z, S_j^z, S_i^z S_j^z$ or I according to whether the rth cycle contains only i, only j, both or none, respecively. To prove the last equality, assume at first that i and j are in different cycles and i is in the rth cycle. Without restricting the generality we may also assume that $g_r = (12 \ldots p_r)$. Then

$$\begin{aligned} \mathrm{Tr}_{p_r} U_1(g_r)W_r &= \sum_{\sigma_1,\ldots,\sigma_{p_r}} \langle \sigma_{g(1)},\ldots,\sigma_{g(p_r)} | S_i^z | \sigma_1,\ldots,\sigma_{p_r} \rangle \\ &= \sum_{\sigma_1,\ldots,\sigma_{p_r}} \sigma_i \prod \langle \sigma_{g(l)} | \sigma_l \rangle = \sum_{\sigma=-s}^{s} \sigma = 0 \, . \end{aligned} \tag{A.3}$$

Second, assume that i and j are in the rth cycle. Now

$$\mathrm{Tr}_{p_r} U_1(g_r)W_r = \sum_{\sigma_1,\ldots,\sigma_{p_r}} \sigma_i \sigma_j \prod \langle \sigma_{g(l)} | \sigma_l \rangle = \sum_{\sigma=-s}^{s} \sigma^2 = s(s+1)(2s+1)/3 \, . \tag{A.4}$$

Notice that the last equality holds both for s integer and half-integer. Finally,

$$\mathrm{Tr}_{p_r} U_1(g_r) = \chi_{p_r}(g_r) = \sum_{\sigma_1,\ldots,\sigma_{p_r}} \prod \langle \sigma_{g(l)} | \sigma_l \rangle = \sum_{\sigma=-s}^{s} 1 = 2s+1 = d \, . \tag{A.5}$$

Equations (A.3-A.5) prove Eq.(A.2). We have therefore

$$\begin{aligned} &\mathrm{Tr}_{p_r} P_+ e^{-\beta H_N} \mathbf{S}(x)\mathbf{S}(y) \\ &= \frac{s(s+1)}{N!} \sum_g d^{k(g)} \, \mathrm{Tr}_{\ell^2(V)^{\otimes N}} U_0(g) e^{-\beta H_N} \sum_{i,j: i \sim_g j} N_i(x) N_j(y) \, . \end{aligned} \tag{A.6}$$

Let C_r be the support of g_r (Eq.(2.8)). With the definition (3.17),

$$\sum_{i,j: i \sim_g j} N_i(x) N_j(y) = \sum_{r=1}^{k} N_{C_r}(x) N_{C_r}(y) \, . \tag{A.7}$$

Using (A.7) one can see that the trace in Eq.(A.6) is the same for all permutations within a class: Let $h \in S_N$ be conjugate to g, i.e., $h = fgf^{-1}$ for some $f \in S_N$. If $g_r = (i_1 i_2 \ldots i_{p_r})$ then $h_r \equiv f g_r f^{-1} = (f(i_1) f(i_2) \ldots f(i_{p_r}))$, therefore the support of h_r is

$$C_r(h) = f(C_r(g)) \equiv \{ f(i) | i \in C_r(g) \} \, . \tag{A.8}$$

On the other hand,

$$U_0(f^{-1}) N_{f(C)}(x) N_{f(C)}(y) = N_C(x) N_C(y) U_0(f^{-1}) \tag{A.9}$$

which can be verified on the vectors $|(x_i)\rangle$. With the use of Eqs.(A.7-A.9) the result follows analogously to Eq.(2.5). Partial summation in (A.6) over the class $[p]$ yields a factor $N! q[p]$. The last step is to write the trace in the basis $|(x_i)\rangle$ and apply Eqs.(2.4) and (3.18).

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