

Feynman cycles in the Bose gas

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We study the lengths of the cycles formed by trajectories in the Feynman-Kac representation of the Bose gas. We discuss the occurrence of infinite cycles and their relation to Bose-Einstein condensation. © 2006 American Institute of Physics. [DOI: [10.1063/1.2383008](https://doi.org/10.1063/1.2383008)]

I. INTRODUCTION

Bose and Einstein understood 80 years ago that a curious phase transition occurs in a gas of noninteracting bosons; it is now commonly referred to as the Bose-Einstein condensation. Real particles interact, however, and for many years there were doubts that this transition takes place in natural systems. London suggested in 1938 that superfluid helium undergoes a Bose-Einstein condensation, and this idea is largely accepted nowadays. Bogoliubov considered interacting systems; careful approximations allowed him to get back to a noninteracting gas but with a different dispersion relation. See Refs. 16 and 8 for more discussion and partial justifications of the Bogoliubov theory.

In 1953 Feynman studied the system in the Feynman-Kac representation.⁵ The partition function can be expanded as a gas of trajectories living in $(d+1)$ dimensions. The extra dimension is commonly referred to as “the time,” although it is not related to physical time. The situation is illustrated in Fig. 1. A finite system with N particles induces a probability on the group S_N of permutations of N elements. Feynman considered the probability for a given particle to belong to a cycle of length n . In the thermodynamic limit, there may be strictly positive probability for infinite cycles to be present, and Feynman suggested to use this as an order parameter for Bose-Einstein condensation.

A few years later, in 1956, Penrose and Onsager introduced the concept of “off-diagonal long-range order.”⁹ Formally, it is a correlation between positions x and y given by $\sigma(x,y) = \langle c^\dagger(x)c(y) \rangle$. The system displays off-diagonal long-range order when this correlation is strictly positive, uniformly in the size of the system and in $|x-y| \rightarrow \infty$. One can write a Feynman-Kac version of this correlation, and it involves a special cycle starting at x and ending at y ; this cycle may wind many times around the imaginary time direction. In the limit where x and y are infinitely distant there corresponds a notion of infinite open cycle that is reminiscent of Feynman’s approach.

Feynman’s order parameter is simpler; it is often used in numerical simulations or in order to gain heuristic understanding. On the other hand, everybody agrees that the Penrose and Onsager order parameter is the correct one. Surprisingly, the question of their equivalence is usually eluded, and many physicists implicitly assume equivalence to hold. The first mathematical investigation of this question is due to Sütő, who showed that equivalence holds in the ideal gas. Indeed, he proved that infinite cycles occur in the presence of condensation,¹² and that no infinite cycles occur in the absence of condensation;¹³ the latter result uses probabilistic methods from the theory of large deviations. These results have been extended to mean-field systems in Refs. 1 and 3.

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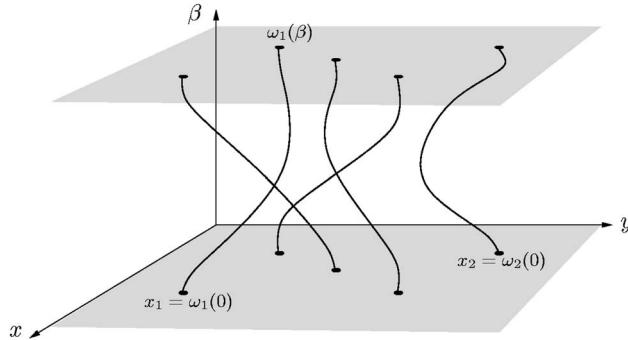


FIG. 1. The Feynman-Kac representation of the partition function for a gas of bosons. The horizontal plane represents the d spatial dimensions, and the vertical axis is the imaginary time dimension. The picture shows a situation with five particles and two cycles, of respective lengths 4 and 1.

In this paper we explore the links between Feynman cycles and off-diagonal long-range order. Let $\sigma(x)$ denote the off-diagonal correlation between the origin and $x \in \mathbb{R}^d$, and $\varrho(n)$ denote the density of particles in cycles of length n . We propose the following formula that relates both concepts:

$$\sigma(x) = \sum_{n \geq 1} c_n(x) \varrho(n) + c_\infty(x) \varrho(\infty). \quad (1.1)$$

Mathematically, the problem is not well posed. Many choices for the coefficients c_n are possible—a trivial choice is $c_n(x) = \sigma(x)/\rho$ for all n , including $n=\infty$. We will see, however, that there is a natural definition for $c_n(x)$ in terms of Wiener trajectories. In any case, we conjecture that Eq. (1.1) holds with coefficients satisfying

$$0 \leq c_n(x) \leq 1, \quad 0 \leq c_\infty(x) \leq 1,$$

for all n, x . In addition, we should have

$$\lim_{n \rightarrow \infty} c_n(x) = c_\infty(x)$$

for any x , and

$$\lim_{|x| \rightarrow \infty} c_n(x) = 0$$

for any finite n , but not uniformly in n ; $c_\infty(x)$ may converge to a strictly positive constant c . If $c=1$, we get from the dominated convergence theorem that $\lim_{|x| \rightarrow \infty} \sigma(x) = \varrho(\infty)$ —in which case the off-diagonal long-range order parameter is equal to the density of cycles of infinite lengths.

We establish this formula and these properties in the case of the ideal gas, where we show that

$$c_n(x) = e^{-x^2/4n\beta}, \quad c_\infty(x) = 1. \quad (1.2)$$

We discuss the validity of formula (1.1) in the interacting gas, proving that these properties hold true in a regime without the Bose-Einstein condensation. The two order parameters should not be always equivalent, however. It is argued in Ref. 15 that they differ when the bosons undergo a regular condensation into a crystalline phase. There is no off-diagonal long-range order, but infinite cycles may be present.

We work in the Feynman-Kac representation of the Bose gas. This representation is standard, see, e.g., Ref. 4 for a clear and concise review and Ref. 6 for a complete introduction. We assume the reader to possess some familiarity with it and in Sec. II we directly define the main

expressions—partition functions, density of cycles, and off-diagonal long-range order—in terms of space-time trajectories. But basic notions and properties are reviewed in Appendix A.

The situation simplifies in the absence of interactions; we consider the ideal gas in Sec. III, where we state and prove the formula that relates the two order parameters. The ideal gas is best discussed in the canonical ensemble. Rigorous proofs of macroscopic occupation of the zero mode have been proposed and they involve the grand-canonical ensemble, with a chemical potential that depends on the volume. Appendix B proposes a simple proof in the canonical ensemble.

Interacting systems constitute a formidable challenge; they are discussed in Sec. IV, where partial results are obtained.

In this paper, we denote finite volume expressions in plain characters, and infinite volume expressions in bold characters. Further, we always consider the canonical and grand-canonical ensembles where the temperature $1/\beta$ is fixed; we alleviate the notation by omitting the β dependence of all quantities.

II. FEYNMAN CYCLES AND OFF-DIAGONAL LONG-RANGE ORDER

A. Partition functions

Our Bose gas occupies a d -dimensional domain D , always a cubic box of size L and volume $V=L^d$. We consider periodic boundary conditions. Let ρ denote the particle density, β the inverse temperature, and μ the chemical potential. The canonical partition function in the Feynman-Kac representation is given by

$$\begin{aligned} Y(N) = & \sum_{k=1}^N \frac{1}{k!} \sum_{\substack{n_1, \dots, n_k \geq 1 \\ n_1 + \dots + n_k = N}} \int_{D^k} dx_1 \cdots dx_k \int dW_{x_1 x_1}^{n_1 \beta}(\omega_1) \cdots dW_{x_k x_k}^{n_k \beta}(\omega_k) \\ & \times \left[\prod_{j=1}^k \frac{1}{n_j} e^{-\beta \mathcal{U}(\omega_j)} \right] \prod_{1 \leq i < j \leq k} e^{-\beta \mathcal{U}(\omega_i, \omega_j)}. \end{aligned} \quad (2.1)$$

This expression is illustrated in Fig. 1. In words, we sum over the number k of closed trajectories and over their respective winding numbers n_1, \dots, n_k . We integrate over the initial positions x_1, \dots, x_k . We integrate over trajectories $\omega_j: [0, n_j \beta] \rightarrow D$ that start and end at x_j ; here, W_{xx}^β denotes the Wiener measure. See Appendix A for more information and, in particular, Eq. (A10) for the normalization condition. Trajectories wind around the time direction according to their winding numbers; because of periodic boundary conditions, they may also wind around space directions.

Given a trajectory ω with winding number n , the function $\mathcal{U}(\omega)$ denotes the interactions between different legs; explicitly,

$$\mathcal{U}(\omega) = \sum_{0 \leq i < j \leq n-1} \frac{1}{\beta} \int_0^\beta U(\omega(i\beta + s) - \omega(j\beta + s)) ds. \quad (2.2)$$

And $\mathcal{U}(\omega, \omega')$ denotes the interactions between closed trajectories ω and ω' , of respective winding numbers n and n' ,

$$\mathcal{U}(\omega, \omega') = \sum_{\substack{0 \leq i \leq n-1 \\ 0 \leq j \leq n'-1}} \frac{1}{\beta} \int_0^\beta U(\omega(i\beta + s) - \omega'(j\beta + s)) ds. \quad (2.3)$$

The function $U(x)$ represents the pair interaction potential between two particles separated by a distance $|x|$. We suppose that $U(x)$ is non-negative and spherically symmetric. We can allow the value $+\infty$; all that is needed is that $e^{-\beta \mathcal{U}(\omega)}$ and $e^{-\beta \mathcal{U}(\omega, \omega')}$ be measurable functions with respect to the Wiener measure—any piecewise continuous function $D \rightarrow [0, \infty]$ can be considered at this point.

The grand-canonical partition function is

$$Z(\mu) = \sum_{N \geq 0} e^{\beta \mu N} Y(N) \quad (2.4)$$

[with the understanding that $Y(0)=1$]. We also need partition functions where a given trajectory ω_0 is present—these will be needed in the expression for cycle densities, see Eqs. (2.8) and (2.9). Namely, we define

$$\begin{aligned} Y(N; \omega_0) = & \sum_{k=1}^N \frac{1}{k!} \sum_{\substack{n_1, \dots, n_k \geq 1 \\ n_1 + \dots + n_k = N}} \int_{D^k} dx_1 \cdots dx_k \int dW_{x_1 x_1}^{n_1 \beta}(\omega_1) \cdots dW_{x_k x_k}^{n_k \beta}(\omega_k) \\ & \times \left[\prod_{j=1}^k \frac{1}{n_j} e^{-\beta \mathcal{U}(\omega_j)} \right] \prod_{0 \leq i < j \leq k} e^{-\beta \mathcal{U}(\omega_i, \omega_j)}. \end{aligned} \quad (2.5)$$

The dependence on ω_0 comes from the last term, where the product includes terms with $i=0$. Notice that

$$Y(N; \omega) \leq Y(N), \quad (2.6)$$

with equality if and only if $U(x) \equiv 0$, i.e., in the absence of interactions. Finally, we introduce

$$Z(\mu, \omega) = \sum_{N \geq 0} e^{\beta \mu N} Y(N, \omega) \quad (2.7)$$

[we set $Y(0, \omega_0)=1$]. We also have $Z(\mu, \omega) \leq Z(\mu)$, with equality if and only if $U(x) \equiv 0$.

B. Cycle lengths

We now introduce the density of particles in cycles of length n , both in the canonical and grand-canonical ensembles. We denote the particle density by $\rho=N/V$. When discussing the canonical ensemble, we always suppose that ρ and V are such that $N=\rho V$ is an integer. The number of particles in cycles of length n is given by the random variable $\sum_{j=1}^k n \delta_{n_j, n}$. Averaging over all configurations of space-time closed trajectories, we get

$$\begin{aligned} \varrho_\rho(n) = & \frac{1}{Y(N)} \sum_{k=1}^N \frac{1}{k!} \sum_{\substack{n_1, \dots, n_k \geq 1 \\ n_1 + \dots + n_k = N}} \left[\frac{1}{V} \sum_{j=1}^k n \delta_{n_j, n} \right] \int_{D^k} dx_1 \cdots dx_k \times \int dW_{x_1 x_1}^{n_1 \beta}(\omega_1) \cdots dW_{x_k x_k}^{n_k \beta}(\omega_k) \\ & \times \left[\prod_{j=1}^k \frac{1}{n_j} e^{-\beta \mathcal{U}(\omega_j)} \right] \prod_{1 \leq i < j \leq k} e^{-\beta \mathcal{U}(\omega_i, \omega_j)} = \int dW_{00}^{n \beta}(\omega) e^{-\beta \mathcal{U}(\omega)} \frac{Y(N-n; \omega)}{Y(N)}. \end{aligned} \quad (2.8)$$

The last line follows from the first line by replacing $\sum_{j=1}^k n \delta_{n_j, n}$ with $nk \delta_{n_1, n}$, isolating the integral over ω_1 , using definition (2.5), using translation invariance, and $\int_D dx_1 = V$. Similarly, we have the grand-canonical expression

$$\varrho_\mu(n) = e^{\beta \mu n} \int dW_{00}^{n \beta}(\omega) e^{-\beta \mathcal{U}(\omega)} \frac{Z(\mu; \omega)}{Z(\mu)}. \quad (2.9)$$

One easily checks that

$$\sum_{n \geq 1} \varrho_\rho(n) = \frac{N}{V} \equiv \rho,$$

$$\sum_{n \geq 1} \varrho_\mu(n) = \left\langle \frac{N}{V} \right\rangle \equiv \rho(\mu).$$

We consider the thermodynamic limits of $\varrho_\rho(n)$ and $\varrho_\mu(n)$. Since $0 \leq \varrho_\rho(n) \leq \rho$ and since n is a discrete index, the Cantor diagonal process yields the existence of a sequence of increasing volumes V_k , with $\rho V_k = N_k$ an integer, such that $\varrho_\rho(n)$ converges to some limit that we denote $\varrho_\rho(n)$. Similarly, we also obtain the infinite volume limit $\varrho_\mu(n)$. Fatou's lemma implies that

$$\sum_{n \geq 1} \varrho_\rho(n) \leq \rho, \quad \sum_{n \geq 1} \varrho_\mu(n) \leq \rho(\mu). \quad (2.10)$$

This suggests to define the density of particles in infinite cycles by

$$\varrho_\rho^{(\infty)} = \rho - \sum_{n \geq 1} \varrho_\rho(n),$$

$$\varrho_\mu^{(\infty)} = \rho(\mu) - \sum_{n \geq 1} \varrho_\mu(n). \quad (2.11)$$

The main question is whether $\varrho^{(\infty)}$ differs from zero at a given temperature and at a given density or chemical potential.

We chose to discuss densities of particles in cycles of given length, but one may consider probabilities as well. Namely, we could introduce the probability for particle 1 to belong to a cycle of length n ; it is given by

$$P_\rho(n) = \int_D dx \int dW_{xx}^{n\beta}(\omega) e^{-\beta U(\omega)} \frac{Y(N-n; \omega)}{NY(N)}. \quad (2.12)$$

Thus $\varrho_\rho(n) = \rho P_\rho(n)$ in the canonical ensemble, and $\varrho_\rho^{(\infty)} = \rho P_\rho^{(\infty)}$. Things are not so simple in the grand-canonical ensemble. The probability $P_\mu(n)$ is

$$P_\mu(n) = \int_D dx \int dW_{xx}^{n\beta}(\omega) \frac{e^{\beta \mu n}}{n} e^{-\beta U(\omega)} \frac{Z'(\mu; \omega)}{Z(\mu)}. \quad (2.13)$$

Here, $Z'(\mu; \omega)$ is like $Z(\mu; \omega)$ given in Eqs. (2.5) and (2.7), but with a factor $1/(k+1)!$ instead of $1/k!$. Heuristically, we should have $\langle V/nk \rangle = 1/\rho(\mu)$ and $\varrho_\mu(n) = \rho(\mu) P_\mu(n)$, but this does not seem easy to establish. The ratio of partition functions in Eq. (2.13) is more difficult to control than the one in Eq. (2.9). We therefore abandon probabilities and discuss densities.

C. Off-diagonal long-range order

Let us turn to the Penrose and Onsager off-diagonal long-range order. Its Feynman-Kac representation involves an open trajectory that starts at x and ends at y , that possibly winds several times around the time direction. Precisely, we introduce

$$\begin{aligned} \sigma_\rho(x) &= \sum_{n=1}^N \int dW_{0x}^{n\beta}(\omega) e^{-\beta U(\omega)} \frac{Y(N-n; \omega)}{Y(N)}, \\ \sigma_\mu(x) &= \sum_{n \geq 1} e^{\beta \mu n} \int dW_{0x}^{n\beta}(\omega) e^{-\beta U(\omega)} \frac{Z(\mu; \omega)}{Z(\mu)}. \end{aligned} \quad (2.14)$$

Thermodynamic limits are denoted $\sigma_\rho(x)$ and $\sigma_\mu(x)$, provided they exist. One may actually restrict $\sigma_\rho(x)$ and $\sigma_\mu(x)$ on rational x and use the Cantor diagonal process to get convergence on a

subsequence of increasing volumes. This is not necessary in this paper, as the limits will be shown to exist in the regimes of parameters under consideration.

Similarities between Eqs. (2.8) and (2.9) on the one hand and Eqs. (2.14) on the other hand are manifested. We can write

$$\begin{aligned}\sigma_\rho(x) &= \sum_{n=1}^N c_{n,\rho}(x) \varrho_\rho(n), \\ \sigma_\mu(x) &= \sum_{n \geq 1} c_{n,\mu}(x) \varrho_\mu(n),\end{aligned}\quad (2.15)$$

where the coefficients $c_{n,\rho}$, $c_{n,\mu}$ are given by

$$\begin{aligned}c_{n,\rho}(x) &= \left[\int dW_{00}^{n\rho}(\omega) e^{-\beta\mathcal{U}(\omega)} \frac{Y(N-n;\omega)}{Y(N)} \right]^{-1} \int dW_{0x}^{n\rho}(\omega) e^{-\beta\mathcal{U}(\omega)} \frac{Y(N-n;\omega)}{Y(N)}, \\ c_{n,\mu}(x) &= \left[\int dW_{00}^{n\mu}(\omega) e^{-\beta\mathcal{U}(\omega)} \frac{Z(\mu;\omega)}{Z(\mu)} \right]^{-1} \int dW_{0x}^{n\mu}(\omega) e^{-\beta\mathcal{U}(\omega)} \frac{Z(\mu;\omega)}{Z(\mu)}.\end{aligned}\quad (2.16)$$

As above, we denote the thermodynamic limits by $c_{n,\rho}(x)$ and $c_{n,\mu}(x)$, provided they exist. One should be careful when sending the volume to infinity in Eqs. (2.15), because a “leak to infinity” may yield a term involving $\varrho^{(\infty)}$ —this actually occurs in the ideal gas, as will be shown in the next section.

III. THE IDEAL GAS

The ideal gas of quantum bosons is fascinating. Particles do not interact, yet they manage to display a phase transition. Historically, the Bose-Einstein condensation is the first theoretical description of a phase transition. The ideal gas has been the object of many studies over the years; let us mention Refs. 17, 7, and 10. A simple proof of macroscopic occupation of the zero Fourier mode is presented in Appendix B.

In this section we elucidate the relation between cycle lengths and off-diagonal long-range order, thus clarifying results that were previously obtained by Sütő.^{12,13} We work in the canonical ensemble and establish formula (1.1) explicitly, for any dimension $d \geq 1$.

Theorem 1: *For any $0 < \beta, \rho < \infty$, there exists a sequence of increasing cubes for which the thermodynamic limits of $\sigma_\rho(x)$, $c_{n,\rho}(x)$, and $\varrho_\rho(n)$ exist for all $x \in \mathbb{R}^d$ and $n \in \mathbb{N}$. Further, we have*

$$\sigma_\rho(x) = \sum_{n \geq 1} e^{-x^2/4n\beta} \varrho_\rho(n) + \varrho_\rho^{(\infty)}.$$

The rest of this section is devoted to the proof of Theorem 1. The coefficient $c_{n,\rho}(x)$, defined in Eq. (2.16), has a simpler expression in the absence of interactions. Indeed, we have $\mathcal{U}(\omega)=0$ and $Y(N;\omega)=Y(N)$. It follows from properties of the Wiener measure in periodic boxes, see Eq. (A10), that

$$c_{n,\rho}(x) = \sum_{z \in \mathbb{Z}^d} e^{-(L^2/4n\beta)((x/L)-z)^2} \left/ \sum_{z \in \mathbb{Z}^d} e^{-(L^2/4n\beta)z^2} \right.. \quad (3.1)$$

Notice that $\lim_{L \rightarrow \infty} c_{n,\rho}(x) = e^{-x^2/4n\beta}$, but the limit is not uniform in n . If the sum over n is restricted to $n \leq cL^2$, with c any finite constant, we can use the dominated convergence theorem and we get

$$\lim_{L \rightarrow \infty} \sum_{n=1}^{cL^2} c_{n,\rho}(x) \varrho_\rho(n) = \sum_{n \geq 1} e^{-x^2/4n\beta} \varrho_\rho(n). \quad (3.2)$$

[The limit is taken along the subsequence of increasing volumes for which $\varrho_\rho(n)$ is known to converge for any n .]

We now consider the terms with $cL^2 < n \leq N$. We estimate the sums in Eq. (3.1) using integrals; we have

$$\int_{-\infty}^{\infty} e^{-a(s-b)^2} ds - 1 \leq \sum_{k \in \mathbb{Z}} e^{-a(k-b)^2} \leq \int_{-\infty}^{\infty} e^{-a(s-b)^2} ds + 1. \quad (3.3)$$

The Gaussian integral is equal to $\sqrt{\pi/a}$. Consequently,

$$\left[\frac{\sqrt{4\pi n\beta} - L}{\sqrt{4\pi n\beta} + L} \right]^d \leq c_{n,\rho}(x) \leq \left[\frac{\sqrt{4\pi n\beta} + L}{\sqrt{4\pi n\beta} - L} \right]^d. \quad (3.4)$$

These bounds hold provided $\sqrt{4\pi n\beta} > L$. Since $n/L^2 > c$, we have

$$\left[\frac{\sqrt{4\pi c\beta} - 1}{\sqrt{4\pi c\beta} + 1} \right]^d \sum_{n=cL^2}^N \varrho_\rho(n) \leq \sum_{n=cL^2}^N c_{n,\rho}(x) \varrho_\rho(n) \leq \left[\frac{\sqrt{4\pi c\beta} + 1}{\sqrt{4\pi c\beta} - 1} \right]^d \sum_{n=cL^2}^N \varrho_\rho(n). \quad (3.5)$$

We obtain

$$\sum_{n=cL^2}^N c_{n,\rho}(x) \varrho_\rho(n) \leq \left[\frac{\sqrt{4\pi c\beta} + 1}{\sqrt{4\pi c\beta} - 1} \right]^d \left(\rho - \sum_{n=1}^{cL^2} \varrho_\rho(n) \right). \quad (3.6)$$

Using Eq. (3.2) with $x=0$ and definition (2.11) of the density of infinite cycles, we see that the last term converges to $\varrho_\rho(\infty)$ as $L \rightarrow \infty$. It then follows from Eqs. (3.2) and (3.6) that

$$\limsup_{L \rightarrow \infty} \sigma_\rho(x) \leq \sum_{n \geq 1} e^{-x^2/4n\beta} \varrho_\rho(n) + \left[\frac{\sqrt{4\pi c\beta} + 1}{\sqrt{4\pi c\beta} - 1} \right]^d \varrho_\rho(\infty). \quad (3.7)$$

This inequality holds for any c , and the fraction is arbitrarily close to 1 by taking c large. A lower bound can be derived in a similar fashion, and we obtain the formula stated in Theorem 1.

IV. THE INTERACTING GAS

The interacting gas is much more difficult to study. We prove in this section the absence of infinite cycles when the chemical potential is negative (Theorem 2). We then study the coefficients $c_{n,\mu}(x)$ at low density and high temperature, using cluster expansion techniques. Their thermodynamic limit can be established, and we show that $c_{n,\mu}(x) \rightarrow 0$ as $|x| \rightarrow \infty$ (Theorem 3).

Theorem 2: Let $0 < \beta < \infty$ and $\mu < 0$; then

$$\varrho_\mu(\infty) = 0,$$

and

$$\lim_{|x| \rightarrow \infty} \limsup_{L \rightarrow \infty} \sigma_\mu(x) = 0.$$

Proof: Since $\mathcal{U}(\omega) \geq 0$ and $Z(\mu; \omega) \leq Z(\mu)$, the finite volume density $\varrho_\mu(n)$, Eq. (2.9), is less than

$$\varrho_\mu(n) \leq e^{\beta\mu n} \int dW_{00}^{n\beta}(\omega) = \frac{e^{\beta\mu n}}{(4\pi n\beta)^{d/2}} \sum_{z \in \mathbb{Z}^d} e^{-L^2 z^2 / 4n\beta}. \quad (4.1)$$

The right side is smaller than $e^{\beta\mu n}$ for all L large enough. We can therefore apply the dominated convergence theorem and we obtain

$$\rho = \lim_{L \rightarrow \infty} \sum_{n \geq 1} \varrho_\mu(n) = \sum_{n \geq 1} \varrho_\mu(n). \quad (4.2)$$

It follows that $\varrho_\rho(\infty) = 0$. The statement about the absence of off-diagonal long-range order can be treated similarly. We have the upper bound

$$\sigma_\mu(x) \leq \sum_{n \geq 1} \frac{e^{\beta\mu n}}{(4\pi n\beta)^{d/2}} \sum_{z \in \mathbb{Z}^d} e^{-(x - Lz)^2 / 4n\beta}. \quad (4.3)$$

By dominated convergence,

$$\limsup_{L \rightarrow \infty} \sigma_\mu(x) \leq \sum_{n \geq 1} \frac{e^{\beta\mu n}}{(4\pi n\beta)^{d/2}} e^{-x^2 / 4n\beta}. \quad (4.4)$$

We can again use the dominated convergence theorem for the limit $|x| \rightarrow \infty$, and we get the claim. \square

We continue the study of the interacting gas in the regime where cluster expansion converges. We assume that the chemical potential is negative, that the interaction potential $U(x)$ is integrable, and that the temperature is high enough. The condition in Theorem 3 is stronger than necessary, but it is very explicit. We will invoke a weaker condition in the proof of the theorem that is based on the “Kotecký-Preiss criterion” for the convergence of cluster expansion. Notice that Ginibre’s survey⁶ uses Kirkwood-Salzburg equations; it applies to a broader range of potentials, but things are terribly intricate.

Theorem 3: Assume that β , μ , and U satisfy

$$\frac{1}{(4\pi\beta)^{d/2}} \int_{\mathbb{R}^d} U(x) dx \sum_{n \geq 1} n^{-d/2} \leq -\mu.$$

The thermodynamic limits of $c_{n,\mu}(x)$ and $\varrho_\mu(n)$ exist, and we have

$$\lim_{|x| \rightarrow \infty} c_{n,\mu}(x) = 0$$

for any n .

Proof: We need some notation in order to cast the grand-canonical partition function in a form suitable for the cluster expansion. Let us introduce a measure for trajectories that wind arbitrarily many times around the time direction. Namely, let \mathcal{X}_n denote the measure space of continuous trajectories $\omega: [0, n\beta] \rightarrow D$, and let $\mathcal{X} = \bigcup_{n \geq 1} \mathcal{X}_n$ be the set of trajectories in D with arbitrary winding numbers. We introduce the measure ν on \mathcal{X} whose integral means the following:

$$\int F(\omega) d\nu(\omega) = \sum_{n \geq 1} \frac{e^{\beta\mu n}}{n} \int_D dx \int dW_{xx}^{n\beta}(\omega) e^{-\beta\ell(\omega)} F(\omega). \quad (4.5)$$

It is clear that ν is a genuine measure on a reasonable measure space. But we describe the measure ν with more details for readers who are interested in analytic technicalities. The σ algebra on \mathcal{X}_n is the smallest σ algebra that contains the sets $\{\omega \in \mathcal{X}_n : \omega(t) \in B\}$, for any $0 \leq t \leq n\beta$, and any Borel set $B \subset D$. Trajectories of \mathcal{X}_1 can be dilated in the time direction so as to yield trajec-

tories with arbitrary winding numbers. One can then consider the product space $\mathcal{X}_1 \times \mathbb{N}$ with the product σ algebra (the σ algebra on \mathbb{N} being the power set). The measure of a set of the kind $A \times \{n\}$, with A a measurable subset of \mathcal{X}_1 , is defined as

$$\nu(A \times \{n\}) = \frac{e^{\beta \mu n}}{n} \int dx \int_{A'} dW_{xx}^{n\beta}(\omega') e^{-\beta \mathcal{U}(\omega')}. \quad (4.6)$$

Here, we introduced

$$A' = \{\omega' \in \mathcal{X}_n : \omega'(t) = \omega(nt) \text{ for some } \omega \in A\}. \quad (4.7)$$

There is a unique extension to a measure on $\mathcal{X}_1 \times \mathbb{N}$. There is a natural correspondence between \mathcal{X} and $\mathcal{X}_1 \times \mathbb{N}$, and we consider ν to be a measure on \mathcal{X} .

With this notation, the grand-canonical partition function (2.4) is given by

$$Z(\mu) = \sum_{k \geq 0} \frac{1}{k!} \int_{\mathcal{X}^k} d\nu(\omega_1) \cdots d\nu(\omega_k) \prod_{1 \leq i < j \leq k} [e^{-\beta \mathcal{U}(\omega_i, \omega_j)} - 1]. \quad (4.8)$$

The term $k=0$ is equal to 1 by definition. Then $Z(\mu)$ has exactly the form assumed, e.g., in Ref. 14. The Kotecký-Preiss criterion for the convergence of the cluster expansion requires the existence of a function $a: \mathcal{X} \rightarrow \mathbb{R}_+$ such that the following inequality holds for any $\omega \in \mathcal{X}$:

$$\int_{\mathcal{X}} [1 - e^{-\beta \mathcal{U}(\omega, \omega')}] e^{a(\omega')} d\nu(\omega') \leq a(\omega). \quad (4.9)$$

Choosing $a(\omega) = -\beta \mu n$ (with n the winding number of the trajectory ω), it was shown in Ref. 14 that Eq. (4.9) is a consequence of the condition in Theorem 3.

The main result of the cluster expansion is that the partition function (4.8) is given by the exponential of a convergent series. Namely,

$$Z(\mu) = \exp \left\{ \sum_{k \geq 1} \int_{\mathcal{X}^k} d\nu(\omega_1) \cdots d\nu(\omega_k) \varphi(\omega_1, \dots, \omega_k) \right\}. \quad (4.10)$$

The combinatorial function $\varphi(\omega_1, \dots, \omega_k)$ is equal to 1 if $k=1$, and is otherwise equal to

$$\varphi(\omega_1, \dots, \omega_k) = \frac{1}{k!} \sum_G \prod_{(i,j) \in G} [e^{-\beta \mathcal{U}(\omega_i, \omega_j)} - 1]. \quad (4.11)$$

The sum is over *connected* graphs with k vertices, and the product is over edges of G . A proof for relation (4.10) that directly applies here can be found in Ref. 14.

Observe now that the partition function $Z(\mu; \omega)$ is given by an expression similar to Eq. (4.8), where each $\nu(\omega_j)$ is replaced by $e^{-\beta \mathcal{U}(\omega, \omega_j)} \nu(\omega_j)$. Since $\mathcal{U}(\omega, \omega_j)$ is positive, the criterion (4.9) is satisfied with this new measure. It follows that $Z(\mu; \omega)$ has an expansion similar to Eq. (4.10), and we obtain the following expression for the ratio of partition functions:

$$\frac{Z(\mu; \omega)}{Z(\mu)} = \exp \left\{ - \sum_{k \geq 1} \int_{\mathcal{X}^k} d\nu(\omega_1) \cdots d\nu(\omega_k) \left[1 - \prod_{j=1}^k e^{-\beta \mathcal{U}(\omega, \omega_j)} \right] \varphi(\omega_1, \dots, \omega_k) \right\}. \quad (4.12)$$

It is not hard to check that

$$1 - \prod_{j=1}^k e^{-\beta \mathcal{U}(\omega, \omega_j)} = \sum_{j=1}^k (1 - e^{-\beta \mathcal{U}(\omega, \omega_j)}) \prod_{i=1}^{j-1} e^{-\beta \mathcal{U}(\omega, \omega_i)} \leq \sum_{j=1}^k (1 - e^{-\beta \mathcal{U}(\omega, \omega_j)}). \quad (4.13)$$

Then Eq. (5) in Ref. 14 gives the necessary estimate for the exponent in Eq. (4.12), namely,

$$\sum_{k \geq 1} \int_{\mathcal{X}^k} d\nu(\omega_1) \cdots d\nu(\omega_k) \left[\sum_{j=1}^k (1 - e^{-\beta \mathcal{U}(\omega, \omega_j)}) \right] |\varphi(\omega_1, \dots, \omega_k)| \leq -\beta \mu n. \quad (4.14)$$

This bound is uniform in the size of the domain, which is important. It follows that, as $L \rightarrow \infty$, the ratio $Z(\mu; \omega)/Z(\mu)$ converges pointwise in μ and ω . The thermodynamic limits of $c_{n,\mu}(x)$ and $\varrho_\mu(n)$ then clearly exist. Further, $c_{n,\mu}(x)$ is bounded by

$$c_{n,\mu}(x) \leq \left[\int dW_{00}^{n\beta}(\omega) e^{-\beta \mathcal{U}(\omega)} \right]^{-1} e^{-2\beta \mu n} \int dW_{0x}^{n\beta}(\omega). \quad (4.15)$$

It is not hard to show that the bracket is bounded away from zero uniformly in L (but not uniformly in β and n). From Eq. (A10), we have

$$\lim_{|x| \rightarrow \infty} \lim_{L \rightarrow \infty} \int dW_{0x}^{n\beta}(\omega) = 0.$$

This implies that $c_{n,\mu}(x)$ vanishes in the limit of infinite $|x|$.

V. CONCLUSION

We introduced formula (1.1) that relates the off-diagonal correlation function and the densities of cycles of given length. This formula involves coefficients c_n that have a natural definition in terms of integrals of Wiener trajectories. We conjectured several properties for the coefficients—these properties can actually be proven in the ideal gas for all temperatures and in the interacting gas for high temperatures. These results seem to indicate that the order parameters of Feynman and Penrose and Onsager agree. However, heuristic considerations based on the present framework¹⁵ suggest that, if the gas is in a crystalline phase, the coefficients satisfy $c_n(x) \leq e^{-a|x|}$ for some $a > 0$ and for all n (including $n = \infty$). Besides, one expects that $\varrho(\infty) > 0$ if the temperature is sufficiently low. The order parameters are not equivalent in this case.

An open problem is to establish the equivalence of the order parameters in weakly interacting gases in the presence of the Bose-Einstein condensation. Another question is whether $c_\infty(x)$ converges, as $|x| \rightarrow \infty$, to a number that is strictly between 0 and 1. The corresponding phase would display a Bose condensate whose density is less than the density of particles in infinite cycles.

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APPENDIX A: FEYNMAN-KAC REPRESENTATION OF THE BOSE GAS

In this appendix we recall some properties of the Wiener measure, and we review the derivation of the Feynman-Kac representation of the partition functions and of the off-diagonal long-range order parameter. A complete account can be found in the excellent notes of Ginibre;⁶ Faris wrote a useful survey.⁴

Let D be the d -dimensional cubic box of size L and volume $V=L^d$. We work with periodic boundary conditions, meaning that D is the d -dimensional torus \mathbb{T}_L^d . The state space is the Hilbert space $\mathcal{H}_{D,N}$ of square-summable complex functions on D^N that are symmetric with respect to their arguments. Let S denote the symmetric projector on $L^2(D^N)$, i.e.,

$$S\psi(x_1, \dots, x_N) = \frac{1}{N!} \sum_{\pi \in S_N} \psi(x_{\pi(1)}, \dots, x_{\pi(N)}), \quad (A1)$$

where $x_1, \dots, x_N \in D$ and the sum is over all permutations of N elements. The state space for N bosons in D is therefore $\mathcal{H}_{D,N}=SL^2(D^N)$, the projection of $L^2(D^N)$ onto symmetric functions.

The Hamiltonian of the system is the sum $H=T+V$ of kinetic and interaction energies. The kinetic energy is $T=-\sum_{j=1}^N \Delta_j$, where Δ_j is the Laplacian for the j th particle. Interactions are given by the multiplication operator $V=\sum_{1 \leq i < j \leq N} U(x_i-x_j)$.

Recall that β and μ denote the inverse temperature and the chemical potential, respectively. The canonical and grand-canonical partition functions are

$$Y(\beta, V, N) = \text{Tr}_{\mathcal{H}_{D,N}} e^{-\beta H}, \quad (\text{A2})$$

$$Z(\beta, V, \mu) = \sum_{N \geq 0} e^{\beta \mu n} Y(\beta, V, N). \quad (\text{A3})$$

Under the assumption that $U(x)$ is a stable potential and that it decays faster than $|x|^{-d}$ as $|x| \rightarrow \infty$, one can establish the existence of the thermodynamic potentials (see Ref. 11)

$$f(\beta, \rho) = \lim_{V \rightarrow \infty} -\frac{1}{\beta V} \log Y(N), \quad (\text{A4})$$

$$p(\beta, \mu) = \lim_{V \rightarrow \infty} \frac{1}{V} \log Z(\mu). \quad (\text{A5})$$

Further, f and p are related by a Legendre transform,

$$f(\beta, \rho) = \sup_{\mu} \left[\rho \mu - \frac{1}{\beta} p(\beta, \mu) \right]. \quad (\text{A6})$$

This equation is useful to find f from p in the case of the ideal gas, where p can be computed explicitly.

The Feynman-Kac representation allows to express $e^{-\beta H}$ in terms of Wiener trajectories (Brownian motion). We briefly review the main properties of the Wiener measure. Let \mathcal{X}_1 be the set of continuous paths $\omega: [0, \beta] \rightarrow D$. Consider a function $F: \mathcal{X}_1 \rightarrow \mathbb{R}$ of the kind

$$F(\omega) = f(\omega(t_1), \dots, \omega(t_n)), \quad (\text{A7})$$

where f is a bounded measurable function on D^n , and $0 < t_1 < \dots < t_n < \beta$; we extend f on \mathbb{R}^d by periodicity. The integral of F with respect to the Wiener measure W_{xy}^β is given by

$$\begin{aligned} \int_{\mathcal{X}} F(\omega) dW_{xy}^\beta(\omega) &= \sum_{z \in \mathbb{Z}^d} \int_{\mathbb{R}^{dn}} g_{t_1}(x_1 - x) g_{t_2 - t_1}(x_2 - x_1) \cdots g_{\beta - t_n}(y + Lz - x_n) \\ &\quad \times f(x_1, \dots, x_n) dx_1 \cdots dx_n, \end{aligned} \quad (\text{A8})$$

where g_t is the normalized Gaussian function with mean zero and variance $2t$,

$$g_t(x) = \frac{1}{(4\pi t)^{d/2}} e^{-x^2/4t}. \quad (\text{A9})$$

The sum over z accounts for periodic boundary conditions. A special case of Eq. (A8) is when the function F is the constant function $F(\omega) \equiv 1$; we get

$$\int dW_{xy}^\beta(\omega) = (4\pi\beta)^{-d/2} \sum_{z \in \mathbb{Z}^d} -e^{-(x-y+Lz)^2/4\beta}. \quad (\text{A10})$$

Only the term $z=0$ remains in the limit $L \rightarrow \infty$. It can be proven that such a measure exists and is unique.⁶ The Wiener measure W_{xy}^β is concentrated on Hölder continuous trajectories (with any

Hölder constant less than $\frac{1}{2}$) that start at x and end at y . Integration with respect to W_{xy}^β and W_{00}^β are related as follows. Define $\omega'(t) = \omega(t) - t[(y-x)/\beta]$; then

$$\int F(\omega) dW_{xy}^\beta(\omega) = e^{-(y-x)^2/4\beta} \int F(\omega') dW_{00}^\beta(\omega). \quad (\text{A11})$$

The Feynman-Kac formula states that $e^{-\beta H}$ is given by an integral operator.^{2,4,6} We are actually dealing with bosonic particles, and it is more convenient to consider the operator $e^{-\beta H} S$ that also projects onto symmetric functions. We have

$$e^{-\beta H} S \psi(x_1, \dots, x_N) = \int_{D^N} K(x_1, \dots, x_N; y_1, \dots, y_N) \psi(y_1, \dots, y_N) dy_1 \cdots dy_N, \quad (\text{A12})$$

where the kernel K is given by

$$K(x_1, \dots, x_N; y_1, \dots, y_N) = \frac{1}{N!} \sum_{\pi \in S_N} \int dW_{x_1 y_{\pi(1)}}^\beta(\omega_1) \cdots dW_{x_N y_{\pi(N)}}^\beta(\omega_N) \\ \times \exp \left\{ - \sum_{i < j} \int_0^\beta U(\omega_i(s) - \omega_j(s)) ds \right\}. \quad (\text{A13})$$

The canonical partition function is then given by

$$Y(N) = \sum_{\pi \in S_N} \frac{1}{N!} \int_{D^N} dx_1 \cdots dx_N \int dW_{x_1 x_{\pi(1)}}^\beta(\omega_1) \cdots dW_{x_N x_{\pi(N)}}^\beta(\omega_N) \\ \times \exp \left\{ - \sum_{i < j} \int_0^\beta U(\omega_i(s) - \omega_j(s)) ds \right\}. \quad (\text{A14})$$

We now group the cycles into closed trajectories, that may wind several times around the time direction. The number of permutations of N elements with k cycles of lengths n_1, \dots, n_k (with $\sum_j n_j = N$) is

$$\frac{N!}{k! \prod_j n_j}.$$

Further, we have

$$\int_{D^{n-1}} dx_2 \cdots dx_n \int dW_{x_1 x_2}^\beta(\omega_1) \cdots dW_{x_n y}^\beta(\omega_n) F(\omega) = \int dW_{xy}^{n\beta}(\omega) F(\omega). \quad (\text{A15})$$

The trajectory $\omega: [0, n\beta] \rightarrow D$ in the right side is the concatenation of $\omega_1, \dots, \omega_n$. The partition function (A14) can then be rewritten in the form of Eq. (2.1).

Let us turn to the Penrose and Onsager off-diagonal long-range order.⁹ Given a single particle function $\varphi \in L^2(D)$, we define the operator N_φ that represents the number of particles in the state φ . The action of this operator is given by

$$(N_\varphi \psi)(x_1, \dots, x_N) = \sum_{j=1}^N \int_D \overline{\varphi(x)} \psi(x_1, \dots, \underbrace{x}_{j\text{th place}}, \dots, x_N) \varphi(x_j) dx. \quad (\text{A16})$$

It is clear that $0 \leq N_\varphi \leq N$ and that $[N_\varphi, S] = 0$. Let $\varphi_0(x) \equiv 1/\sqrt{V}$ denote the single particle ground state in the absence of interactions. It is also the Fourier function with mode $k=0$. The average occupation of the zero mode is given by

$$\varrho_{\rho}^{(0)} = \lim_{V \rightarrow \infty} \frac{1}{Y(N)} \text{Tr}_{\mathcal{H}_{D,N}} \left[\frac{N_{\varphi_0}}{V} e^{-\beta H} \right]. \quad (\text{A17})$$

We set $N=\rho V$, and the limit exists at least along a subsequence of increasing volumes. A criterion for the Bose-Einstein condensation is that $\varrho_{\rho}^{(0)}$ differs from zero. We can derive a Feynman-Kac expression for this order parameter. From Eqs. (A12), (A13), and (A16), we have

$$\begin{aligned} \text{Tr}_{\mathcal{H}_{D,N}} N_{\varphi} e^{-\beta H} &= \frac{1}{(N-1)!} \int_D dx \overline{\varphi(x)} \int_D dy \varphi(y) \int_{D^{N-1}} dx_2 \cdots dx_N \sum_{\pi \in S_N} \\ &\times \int dW_{x_1 \hat{x}_{\pi(1)}}^{\beta}(\omega_1) \cdots dW_{x_N \hat{x}_{\pi(N)}}^{\beta}(\omega_N) \exp \left\{ - \sum_{i < j} \int_0^{\beta} U(\omega_i(s) - \omega_j(s)) \right\}. \end{aligned} \quad (\text{A18})$$

Here, we set $x_1=x$, $\hat{x}_1=y$, and $\hat{x}_j=x_j$ for $2 \leq j \leq N$. Then $\varrho_{\rho}^{(0)}$ can be written as

$$\varrho_{\rho}^{(0)} = \lim_{V \rightarrow \infty} \frac{1}{V^2} \int_{D^2} \sigma_{\rho}(x-y) dx dy, \quad (\text{A19})$$

where

$$\begin{aligned} \sigma_{\rho}(x-y) &= \frac{1}{Y(\beta, V, N)} \frac{1}{(N-1)!} \int_{D^{N-1}} dx_2 \cdots dx_N \sum_{\pi \in S_N} \times \int dW_{x_1 \hat{x}_{\pi(1)}}^{\beta}(\omega_1) \cdots dW_{x_N \hat{x}_{\pi(N)}}^{\beta}(\omega_N) \\ &\times \exp \left\{ - \sum_{i < j} \int_0^{\beta} U(\omega_i(s) - \omega_j(s)) \right\}. \end{aligned} \quad (\text{A20})$$

This expression involves an open cycle from x to y , winding n times around the time direction, with $n=1, \dots, N$. Using the concatenation property (A15) and thanks to the combinatorial factor $(N-1)!/(N-n)!$, we obtain expression (2.14) for $\sigma_{\rho}(x-y)$. The system displays off-diagonal long-range order if $\sigma_{\rho}(x)$ is strictly positive, uniformly in V, x .

APPENDIX B: A SIMPLE PROOF OF MACROSCOPIC OCCUPATION IN THE IDEAL GAS

In this section, we give a proof of the macroscopic occupation of the zero mode at low temperature. This is usually established in the grand-canonical ensemble, using a chemical potential that varies with the volume and tends to zero in the thermodynamic limit. This approach is rather un-natural and requires large deviation techniques to control the fluctuations of the number of particles. The present proof is simpler and stays within the canonical ensemble.

The computation of the pressure and of the density in the grand-canonical ensemble can be found in any textbook dealing with quantum statistical mechanics. The chemical potential must be strictly negative. The infinite volume pressure is

$$p(\beta, \mu) = - \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \log(1 - e^{-\beta(k^2 - \mu)}) dk, \quad (\text{B1})$$

and the density is

$$\rho(\beta, \mu) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{dk}{e^{\beta(k^2 - \mu)} - 1} = \frac{1}{(4\pi\beta)^{d/2}} \sum_{n \geq 1} e^{\beta\mu n} n^{-d/2}. \quad (\text{B2})$$

The limit of $\rho(\beta, \mu)$ as $\mu \nearrow 0$ is finite for $d \geq 3$ and gives the *critical density* of the ideal Bose gas, ρ_c . The graph of $p(\beta, \mu)$ in three dimensions is plotted in Fig. 2(a). Its Legendre transform, Eq. (A6), gives $f(\beta, \rho)$, see Fig. 2(b); it is nonanalytic at ρ_c . The value of $a(\beta)$ is given by

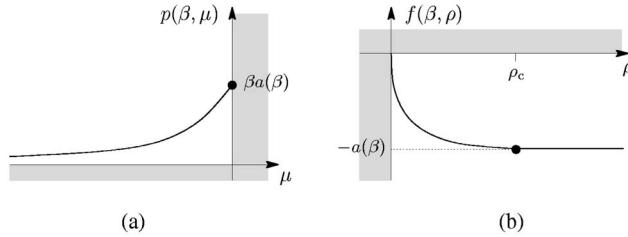


FIG. 2. The pressure and the free energy of the ideal gas in three dimensions.

$$a(\beta) = \lim_{\mu \nearrow 0} \frac{1}{\beta} p(\beta, \mu) = \lim_{\rho \rightarrow \infty} -f(\beta, \rho). \quad (\text{B3})$$

The very nature of the Bose-Einstein condensation is that the occupation number for $k=0$ becomes macroscopic. The average occupation of the zero mode $\varrho_\rho^{(0)}$, see Eq. (A17), can be rewritten as

$$\varrho_\rho^{(0)} = \lim_{V \rightarrow \infty} \frac{1}{Y(N)} \sum_{(n_k):N} \frac{n_0}{V} e^{-\beta \sum_k n_k k^2}. \quad (\text{B4})$$

Here, $N=V\rho$, and the sum is over all occupation numbers $n_k \geq 0$, with indices $k \in ((2\pi/L)\mathbb{Z})^d$, such that $\sum_k n_k = N$. The heart of the Bose-Einstein condensation is the following result.

Theorem 4: For $d \geq 3$, the single particle ground state is macroscopically occupied if $\rho > \rho_c$. More precisely,

$$\varrho_\rho^{(0)} = \max(0, \rho - \rho_c).$$

Proof: It is clear that $\varrho_\rho^{(0)} \geq 0$. We now establish that $\varrho_\rho^{(0)} \geq \rho - \rho_c$. Let us introduce the average occupation of the mode k ,

$$\langle n_k \rangle = \frac{1}{Y(N)} \sum_{(n_k):N} n_k e^{-\beta \sum_k' n_k' k'^2}.$$

Thanks to the sum rule $N = \sum_k \langle n_k \rangle$, we have

$$\varrho_\rho^{(0)} = \rho - \lim_{V \rightarrow \infty} \sum_{k \neq 0} \frac{\langle n_k \rangle}{V}. \quad (\text{B5})$$

We can view n_k as a random variable taking positive integer values; its expectation is therefore given by

$$\langle n_k \rangle = \sum_{i \geq 1} \text{Prob}(n_k \geq i), \quad (\text{B6})$$

where we defined

$$\text{Prob}(n_k \geq i) = \frac{1}{Y(N)} \sum_{(n_k'):N,i} -e^{-\beta \sum_k' n_k' k'^2}. \quad (\text{B7})$$

The sum is restricted to (n_k') such that $\sum n_k' = N$ and $n_k \geq i$. The change of variable $n_k \rightarrow n_k - i$ leads to

$$\text{Prob}(n_k \geq i) = e^{-\beta k^2} \frac{Y(N-i)}{Y(N)}. \quad (\text{B8})$$

The ratio of partition functions is also equal to the probability $\text{Prob}(n_0 \geq i)$, which is smaller than 1. Equations (B6) and (B8) give a bound for the occupation numbers of all modes $k \neq 0$, namely,

$$\langle n_k \rangle \leq \frac{1}{e^{\beta k^2} - 1}. \quad (\text{B9})$$

Notice that $\langle n_k \rangle \leq 1/\beta k^2 \leq L^2/4\pi^2\beta$ for $k \neq 0$. This shows that only the zero mode can be macroscopically occupied (for $d \geq 3$). Inserting this bound into Eq. (B5), we obtain

$$\varrho_\rho^{(0)} \geq \rho - \frac{1}{(2\pi)^d} \lim_{V \rightarrow \infty} \sum_{k \neq 0} \left(\frac{2\pi}{L}\right)^d \frac{1}{e^{\beta k^2} - 1}. \quad (\text{B10})$$

The limit converges to expression (B2) with $\mu=0$, which is equal to ρ_c .

There remains to show that $\varrho_\rho^{(0)} \leq \max(0, \rho - \rho_c)$. From Eq. (B8) with $k=0$, and using the equivalence of ensembles, we have for any fixed a ,

$$\lim_{V \rightarrow \infty} \frac{1}{\beta V} \log \text{Prob}(n_0 \geq Va) = f(\beta, \rho) - f(\beta, \rho - a). \quad (\text{B11})$$

The right side of Eq. (B11) is strictly negative when $a > \max(0, \rho - \rho_c)$. There exists $\delta > 0$ such that for large enough volumes,

$$\text{Prob}(n_0 \geq Va) \leq e^{-V\delta}. \quad (\text{B12})$$

Let us assume that $\rho - \rho_c > 0$; the case $\rho - \rho_c \leq 0$ can be treated similarly. Using Eq. (B6) with $k=0$, together with Eq. (B12), we get

$$\frac{\langle n_0 \rangle}{V} = \frac{1}{V} \sum_{1 \leq i \leq aV} \text{Prob}(n_0 \geq i) + \frac{1}{V} \sum_{aV < i \leq N} \text{Prob}(n_0 \geq i) \leq a + \rho e^{-V\delta}. \quad (\text{B13})$$

It follows that $\varrho_\rho^{(0)}$ is less than any number $a > \rho - \rho_c$, hence $\varrho_\rho^{(0)} \leq \rho - \rho_c$.

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