Correlations of occupation numbers in the canonical ensemble and application to a Bose-Einstein condensate in a one-dimensional harmonic trap

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We study statistical properties of N noninteracting identical bosons or fermions in the canonical ensemble. We derive several general representations for the p-point correlation function of occupation numbers $\overline{n_1 \cdots n_p}$. We demonstrate that it can be expressed as a ratio of two $p \times p$ determinants involving the (canonical) mean occupations $\overline{n_1}$, ..., $\overline{n_p}$, which can themselves be conveniently expressed in terms of the k-body partition functions (with $k \leqslant N$). We draw some connection with the theory of symmetric functions and obtain an expression of the correlation function in terms of Schur functions. Our findings are illustrated by revisiting the problem of Bose-Einstein condensation in a one-dimensional harmonic trap, for which we get analytical results. We get the moments of the occupation numbers and the correlation between ground-state and excited-state occupancies. In the temperature regime dominated by quantum correlations, the distribution of the ground-state occupancy is shown to be a truncated Gumbel law. The Gumbel law, describing extreme-value statistics, is obtained when the temperature is much smaller than the Bose-Einstein temperature.

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I. INTRODUCTION

The theory of noninteracting identical quantum particles is a fundamental block of the basic education in statistical physics [1–3]. In the standard approach, calculations are performed in the grand canonical ensemble because it provides the clearest and most efficient tools to relate single-particle and thermodynamic properties. One can then use the equivalence between statistical physics ensembles in the thermodynamic limit to get the thermodynamic observables as a function of the relevant parameters (energy or temperature, number of particles or chemical potential, etc). One should, however, keep in mind that the correspondence between ensembles in the thermodynamic limit only holds for *averages* of observables, and not for their fluctuations [2,3].

Recently, remarkable progress in atomic physics of ultracold atoms has raised many questions concerning many-body effects in those systems [4]. Simpler questions related to quantum correlations in noninteracting gases have also been put forward, as experiments deal with extremely diluted gases, for which the noninteracting limit is often a good starting point. Depending on whether we deal with bosons or fermions, the situation can be rather different. This difference manifests itself, for example, in the presence of a harmonic confinement, as is realized in experiments with optical traps. For bosonic gases, although the low-temperature properties are dominated by interactions, many basic properties such as the energy or density profile can then be obtained within a mean-field approximation [5]. In fermionic gases, the Pauli principle strongly suppresses the effect of interactions at low temperature, which makes the noninteracting description a good starting point, from which interaction can be treated perturbatively [6]. Due to cooling techniques by evaporation, a trapped ultracold atomic gas only contains a moderately large number of atoms (a few thousand to a few million), which has led, before considering interaction effects, to reexamine the differences between the various statistical physics ensembles for noninteracting particles [7–16], as the microcanonical or canonical ensembles are more relevant in this case (see review in Ref. [5]).

A. Occupation numbers

Not only thermodynamic properties and global observables are of interest, but, motivated by the remarkable achievement of the "atomic microscope" [17–19], also local observables have been studied recently (for a review see Ref. [20]). A basic ingredient of such studies is the knowledge of the number of particles n_λ in each individual eigenstate $|\lambda\rangle$. The *grand canonical* mean occupation is given by the Bose-Einstein or Fermi-Dirac distribution

$$\overline{n_\lambda}^{\mathrm{g}} = \frac{1}{1/(x_\lambda \varphi) \mp 1}, \quad x_\lambda = e^{-\beta\varepsilon_\lambda}, \tag{1}$$

where φ is the fugacity, $\{\varepsilon_\lambda\}$ are the individual energy levels, and $\beta = 1/(k_B T)$ is the inverse temperature. $\overline{\cdots}^{\mathrm{g}}$ is the grand canonical average. In this formula, the upper ($-$) and lower ($+$) signs stand for bosons and fermions, respectively. For a fixed number N of particles, the *canonical* mean occupation numbers can be expressed in terms of the k-body canonical partition functions with $k = 1, \ldots, N$. The canonical partition function $Z_N(\beta)$ for N bosons or fermions can be obtained by recursion from the formula [21–25]

$$Z_N(\beta) = \frac{1}{N}\sum_{k=1}^{N} (\pm 1)^{k-1} Z_1(k\beta) Z_{N-k}(\beta), \tag{2}$$

where $Z_1(\beta) = \sum_\lambda e^{-\beta\varepsilon_\lambda}$ is the canonical partition function for one particle, and the upper ($+$) and lower ($-$) signs stand for bosons and fermions, respectively. The canonical mean occupation number is then given by

$$\overline{n_\lambda} = \sum_{k=1}^{N} (\pm 1)^{k-1} \frac{Z_{N-k}}{Z_N} x_\lambda^k, \tag{3}$$

with $Z_0 = 1$ [10,15,26]. The canonical average is simply denoted $\overline{\cdots}$. This expression is expected to coincide with Eq. (1) in the thermodynamic limit, provided that the fugacity φ in Eq. (1) is chosen in such a way that the condition $\sum_\lambda \overline{n_\lambda}^{\mathrm{g}} = N$ is fulfilled. The power of the grand canonical ensemble lies in the *independence* of individual energy-level properties (which leads to many useful additivity properties for the thermodynamic observables), i.e., the absence of correlations between occupation numbers,

$$\overline{n_{\lambda_1} \cdots n_{\lambda_p}}^{\mathrm{g}} = \overline{n_{\lambda_1}}^{\mathrm{g}} \times \cdots \times \overline{n_{\lambda_p}}^{\mathrm{g}}. \tag{4}$$

However, in the canonical ensemble, the constraint on the total number of particles $\sum_\lambda n_\lambda = N$ implies nontrivial correlations between occupation numbers, $\overline{n_1 n_2} \neq \overline{n_1} \times \overline{n_2}$. In the present paper, we focus on the canonical ensemble and study these correlations.

B. Main results

Our main results are complementary expressions for the correlation function. To lighten notations, we consider the correlations of the first p levels; this does not imply any restriction on the generality of the discussion, because levels all play an equivalent role. The first expression we obtained is in terms of the canonical partition functions and of $x_\lambda = e^{-\beta\varepsilon_\lambda}$ and reads

$$\overline{n_1 \cdots n_p} = \frac{(\pm 1)^p}{Z_N} \times \sum_{\substack{k_1,\dots,k_p=1 \\ k_1+\cdots+k_p \leqslant N}}^{N} (\pm x_1)^{k_1} \cdots (\pm x_p)^{k_p} Z_{N-k_1-\cdots-k_p}. \tag{5}$$

This generalizes Eq. (3). The second expression is a representation in terms of two $p \times p$ determinants,

$$\overline{n_1 n_2 \cdots n_p} = (\mp 1)^{p-1} \frac{\begin{vmatrix} \overline{n_1} & x_1 & \cdots & x_1^{p-1} \\ \overline{n_2} & x_2 & \cdots & x_2^{p-1} \\ \vdots & \vdots & \ddots & \vdots \\ \overline{n_p} & x_p & \cdots & x_p^{p-1} \end{vmatrix}}{\begin{vmatrix} 1 & x_1 & \cdots & x_1^{p-1} \\ 1 & x_2 & \cdots & x_2^{p-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_p & \cdots & x_p^{p-1} \end{vmatrix}}, \tag{6}$$

where the denominator is a Vandermonde determinant. A remarkable observation is that the p-point correlation function can be expressed only in terms of the mean values $\overline{n_1},\dots,\overline{n_p}$. It can also be expressed in terms of q-point functions with $q < p$; see Eq. (38) below. Equation (6) turns out to be valid also in the grand canonical ensemble. A particular instance of this general relation for $p = 2$,

$$\overline{n_1 n_2} = \mp \frac{e^{\beta\varepsilon_1}\overline{n_1} - e^{\beta\varepsilon_2}\overline{n_2}}{e^{\beta\varepsilon_1} - e^{\beta\varepsilon_2}}, \tag{7}$$

was recently used for the study of fluctuations of certain observables for trapped noninteracting one-dimensional fermions [27]. Equations (5) and (7) were obtained very recently in Ref. [28] in the fermionic case.

In the case of bosons, we could express the general correlation function for arbitrary integer powers $r_1,\dots,r_p$ as

$$\overline{n_1^{r_1} \cdots n_p^{r_p}} = \frac{1}{Z_N} \sum_{\substack{k_1,\dots,k_p=1 \\ k_1+\cdots+k_p \leqslant N}}^{N} a_{k_1}(r_1) x_1^{k_1} \cdots a_{k_p}(r_p) x_p^{k_p} Z_{N-k_1-\cdots-k_p}, \tag{8}$$

where

$$a_k(r) = k^r - (k-1)^r. \tag{9}$$

Equation (8) generalizes Eq. (5).

We illustrate these formulas by considering the study of Bose-Einstein condensation in a one-dimensional harmonic trap. We obtain several simple analytical results for the occupation numbers of single-particle levels. In particular, we have obtained the distribution $\mathscr{P}_{k,N}$ of the occupation number n_k, with $k \in \mathbb{N}$, for N bosons in the canonical ensemble. In the quantum regime $\omega \ll T \ll N\omega$, where ω is the trap frequency, we have obtained the scaling form

$$\mathscr{P}_{k,N}(n) \simeq \frac{\omega}{T} Q_{k,z}\left(\frac{\omega n}{T}\right), \tag{10}$$

where

$$Q_{k,z}(\xi) = \theta_{\mathrm{H}}(\xi) e^z (k + z e^\xi) \exp\{-k\xi - z e^\xi\}, \tag{11}$$

with $z = (T/\omega)\exp[-N\omega/T]$ and θ_{H} being the Heaviside step function. This expression can be compared with the similar distribution obtained in the grand canonical ensemble $\mathscr{P}_k^{\mathrm{g}}(n) \propto \varphi^n e^{-n\beta\varepsilon_k}$, which would give, after the same rescaling as above, $Q_k^{\mathrm{g}}(\xi) \propto \varphi^{T\xi/\omega} e^{-k\xi}$. The case of the ground state is of special interest: Eqs. (10) and (11) simplify as

$$\mathrm{Proba}\left\{ n_0 = N - \frac{T \ln(T/\omega)}{\omega} + \frac{T}{\omega}\zeta \right\} \propto \theta_{\mathrm{H}}(\zeta - \ln z) \exp\{\zeta - e^\zeta\}, \tag{12}$$

which corresponds to a truncated Gumbel law.

C. Outline

The outline of the article is as follows: in Sec. II, we recall the connection between our problem and the theory of symmetric functions, which will allow us to introduce some useful tools. Our main results expressing correlations between occupation numbers, Eqs. (5) and (6), are derived in Sec. III. Finally, in Sec. IV, we illustrate our results on the problem of Bose-Einstein condensation in a one-dimensional harmonic trap.

II. SYMMETRIC FUNCTIONS

The connection between the problem of identical particles and the theory of symmetric functions has been discussed in Refs. [22,29]. In Ref. [24], Schmidt and Schnack have pointed out that the relation (2) for fermions, which is attributed to Landsberg [21] in many articles, is nothing else but the well-known Newton identity. In this section, we introduce some useful notation. As a simple illustration, we recover the relations (2). For a recent reference on the mathematical theory of symmetric functions, see the monograph [30].

A. Families of symmetric polynomials

A function ϕ in M variables $x_1,x_2,\dots,x_M$ is said to be symmetric if $\phi(x_{\sigma(1)},\dots,x_{\sigma(M)})=\phi(x_1,\dots,x_M)$ for any permutation σ of the M indices. We now introduce three useful families of symmetric polynomials.

The *elementary symmetric polynomials* are defined as

$$e_N(x_1,\dots,x_M)=\sum_{\lambda_1<\lambda_2<\cdots<\lambda_N} x_{\lambda_1}x_{\lambda_2}\cdots x_{\lambda_N}, \tag{13}$$

with $e_0=1$ and $e_k=0$ for $k>M$. For example, $e_1(x_1,\dots,x_M)=x_1+x_2+\cdots+x_M$ and $e_2(x_1,\dots,x_M)=x_1x_2+x_1x_3+\cdots$. Their generating function is given by

$$\Xi^{\mathrm{F}}(\varphi)=\sum_{N=0}^{M} e_N\varphi^N=\prod_{\lambda=1}^{M}(1+\varphi x_\lambda). \tag{14}$$

The *complete homogeneous symmetric polynomials* are defined as

$$h_N(x_1,\dots,x_M)=\sum_{\lambda_1\leqslant\lambda_2\leqslant\cdots\leqslant\lambda_N} x_{\lambda_1}x_{\lambda_2}\cdots x_{\lambda_N}, \tag{15}$$

with $h_0=1$. For example, $h_3(x_1,x_2,x_3)=(x_1^3+x_2^3+x_3^3)+(x_1^2x_2+x_1^2x_3+\cdots)+(x_1x_2x_3)$. Their generating function is given by

$$\Xi^{\mathrm{B}}(\varphi)=\sum_{N=0}^{\infty} h_N\varphi^N=\prod_{\lambda=1}^{M}(1-\varphi x_\lambda)^{-1}. \tag{16}$$

Note that, contrary to the sum in the definition of $\Xi^{\mathrm{F}}(\varphi)$, the sum here extends to infinity, as $h_N\neq 0$ for $N>M$.

The *power sum polynomials* are defined as

$$p_k(x_1,\dots,x_M)=\sum_{\lambda=1}^{M} x_\lambda^k \text{ for } k\geqslant 1. \tag{17}$$

Their generating function is given by

$$P(\varphi)=\sum_{k=1}^{\infty} p_k\varphi^{k-1}=\sum_{\lambda=1}^{M}\frac{x_\lambda}{1-\varphi x_\lambda} \tag{18}$$

(for convenience the definition is slightly different from those of the previous generating functions because we did not introduce a p_0).

Correspondence with the problem of identical particles. Let us consider N particles in M energy levels (possibly infinite). Setting $x_\lambda=e^{-\beta\varepsilon_\lambda}$ as in Eq. (1), one readily sees that the canonical partition function for bosons $Z_N^{\mathrm{B}}(\beta)$ coincides with h_N, while the canonical partition function for fermions $Z_N^{\mathrm{F}}(\beta)$ coincides with e_N. Moreover, one obviously has $p_1=h_1=e_1$, and $p_k(x_1,\dots,x_M)=e_1(x_1^k,\dots,x_M^k)=h_1(x_1^k,\dots,x_M^k)$, so that the single-particle canonical partition function at inverse temperature $k\beta$, which is $Z_1^{\mathrm{B}}(k\beta)$ or $Z_1^{\mathrm{F}}(k\beta)$, coincides with p_k. One can thus establish the following dictionary between the mathematician's and the physicist's notations :

$$\begin{aligned}
x_\lambda &\longrightarrow e^{-\beta\varepsilon_\lambda},\\
e_N &\longrightarrow Z_N^{\mathrm{F}}(\beta),\\
h_N &\longrightarrow Z_N^{\mathrm{B}}(\beta),\\
p_k &\longrightarrow Z_1^{\mathrm{B}}(k\beta)=Z_1^{\mathrm{F}}(k\beta).
\end{aligned}$$

The generating functions $\Xi^{\mathrm{B}}(\varphi)$ and $\Xi^{\mathrm{F}}(\varphi)$ coincide with the grand canonical partition functions for bosons and fermions, respectively.

B. Newton identity

There exist various identities relating the generating functions $\Xi^{\mathrm{B}}(\varphi)$, $\Xi^{\mathrm{F}}(\varphi)$, and $P(\varphi)$. Expanding these identities in powers of φ provides some relations between the three families of symmetric polynomials defined above. For instance, the duality relation

$$\Xi^{\mathrm{B}}(\varphi)\Xi^{\mathrm{F}}(-\varphi)=1, \tag{19}$$

readily obtained from Eqs. (14) and (16), allows us to express the e_k in terms of the h_k, or conversely.

Another identity that can be easily obtained from the expressions of the previous section is

$$P(\varphi)=\frac{d}{d\varphi}\ln\Xi^{\mathrm{B}}(\varphi)=-\frac{d}{d\varphi}\ln\Xi^{\mathrm{F}}(-\varphi); \tag{20}$$

that is,

$$-\frac{d}{d\varphi}\Xi^{\mathrm{F}}(-\varphi)=P(\varphi)\Xi^{\mathrm{F}}(-\varphi) \tag{21}$$

and

$$\frac{d}{d\varphi}\Xi^{\mathrm{B}}(\varphi)=P(\varphi)\Xi^{\mathrm{B}}(\varphi). \tag{22}$$

Expanding explicitly Eq. (21) in powers of φ yields

$$\sum_{N=1}^{M} N(-\varphi)^{N-1}e_N=\sum_{k=1}^{\infty}p_k\varphi^{k-1}\sum_{j=0}^{M}(-\varphi)^j e_j. \tag{23}$$

Identification of terms in φ^{N-1} in the right-hand side (r.h.s.) gives the relation

$$e_N=\frac{1}{N}\sum_{k=1}^{N}(-1)^{k-1}p_k e_{N-k}. \tag{24}$$

This is precisely Eq. (2) for fermions, according to the above dictionary. The relation (24) was derived by Isaac Newton in his book, published in 1666 (see Ref. [31], p. 519). It is known as the Newton identity [30]. Several instances of the relation, for $N=1,2,3,$ and 4, were obtained earlier by Albert Girard in 1629 (see Ref. [32] page F2, i.e., page ∼50 of the manuscript, where the elementary polynomial e_k is called "kth meslé").

Similarly, expanding Eq. (22) in powers of φ gives

$$\sum_{N=1}^{\infty} N\varphi^{N-1}h_N = \sum_{k=1}^{\infty} p_k\varphi^{k-1}\sum_{j=0}^{\infty}\varphi^j h_j, \tag{25}$$

leading to the relation

$$h_N = \frac{1}{N}\sum_{k=1}^{N} p_k h_{N-k}. \tag{26}$$

This corresponds to Eq. (2) for bosons.

The theory of symmetric functions also provides a determinantal representation of elementary symmetric polynomials in terms of power sum polynomials (p. 28 of Ref. [30]) as

$$e_N = \frac{1}{N!}\begin{vmatrix} p_1 & 1 & 0 & \cdots & 0 \\ p_2 & p_1 & 2 & & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ p_{N-1} & p_{N-2} & & & N-1 \\ p_N & p_{N-1} & p_{N-2} & \cdots & p_1 \end{vmatrix}. \tag{27}$$

This provides an explicit expression of the N-body partition function $Z_N^{\mathrm{F}}(\beta)$ in terms of the one-particle partition function $Z_1(k\beta)$. The homogeneous polynomials h_N can also be expressed by the r.h.s. of Eq. (27), but with the determinant replaced by a permanent [22]. Alternatively, they can be expressed in terms of a determinant [30] as

$$h_N = \frac{1}{N!}\begin{vmatrix} p_1 & -1 & 0 & \cdots & 0 \\ p_2 & p_1 & -2 & & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ p_{N-1} & p_{N-2} & & & -N+1 \\ p_N & p_{N-1} & p_{N-2} & \cdots & p_1 \end{vmatrix}, \tag{28}$$

which provides an expression of $Z_N^{\mathrm{B}}(\beta)$ in terms of $Z_1(k\beta)$.

III. CORRELATION FUNCTIONS

The tools developed in the previous section allow us to easily derive Eqs. (5) and (6), as we now show.

A. Canonical and grand canonical ensembles

We consider N identical particles in M (possibly infinite) energy levels. The occupation number of the individual eigenstate $|\lambda\rangle$ of energy ε_λ is denoted by n_λ. Thus we have $n_\lambda \in \{0,1\}$ for fermions and $n_\lambda \in \mathbb{N}$ for bosons. A basis of Fock space is given by the many-body states $|\{n_\lambda\}\rangle$, which are fully specified by the knowledge of all occupation numbers. We can express the canonical (Gibbs) distribution at inverse temperature β as

$$\mathscr{P}_N^{\mathrm{c}}(\{n_\lambda\}) = \frac{\prod_\lambda x_\lambda^{n_\lambda}}{Z_N}\delta_{N,\sum_\lambda n_\lambda}, \quad x_\lambda = e^{-\beta\varepsilon_\lambda}, \tag{29}$$

which gives the probability of occupying the quantum state $|\{n_\lambda\}\rangle$. Here Z_N is the N-body canonical partition function, and the Kronecker symbol constrains the number of particles to be N. On the other hand, the grand canonical distribution is controlled by the fugacity φ and reads

$$\mathscr{P}^{\mathrm{g}}(\{n_\lambda\};\varphi) = \frac{\prod_\lambda (x_\lambda\varphi)^{n_\lambda}}{\Xi(\varphi)}, \tag{30}$$

with $\Xi(\varphi) = \prod_\lambda (1 \mp \varphi x_\lambda)^{\mp 1}$ the grand canonical partition function given by Eq. (14) or (16). For bosons, the convergence of the series is ensured by the condition $\varphi x_0 < 1$, where ε_0 is the individual ground state ($x_0 = e^{-\beta\varepsilon_0}$).

Using these distributions, one can relate the grand canonical average $\overline{\cdots}^{\mathrm{g}}$ and the canonical average $\overline{\cdots}^{(N)}$ for N particles (the superscript will only be introduced if needed). Indeed, if $\mathcal{A}(\cdot)$ is any function of the occupation numbers, then, from Eqs. (29) and (30) one has

$$\Xi(\varphi)\overline{\mathcal{A}(\{n_\lambda\})}^{\mathrm{g}} = \sum_{N=0}^{\infty} Z_N \overline{\mathcal{A}(\{n_\lambda\})}^{(N)}\varphi^N. \tag{31}$$

B. p-point correlation functions

1. Proof of equations (5) and (6)

We now apply Eq. (31) to $\mathcal{A}(\{n_\lambda\}) = n_1\cdots n_p$. In the grand canonical ensemble, the occupation numbers are independent [see Eq. (4)], and they are given by Eq. (1). We thus get from Eq. (31),

$$\sum_{N=p}^{\infty} Z_N\overline{n_1\cdots n_p}^{(N)}\varphi^N = \frac{\Xi(\varphi)}{[1/(x_1\varphi)\mp 1]\cdots[1/(x_p\varphi)\mp 1]}. \tag{32}$$

The expansion of Eq. (32) and the identification of each power of φ directly gives Eq. (5). Consider for example $p=1$. We have explicitly

$$\sum_{N=1}^{\infty} Z_N\overline{n_1}^{(N)}\varphi^N = x_1\varphi\sum_{k=0}^{\infty}(\pm x_1\varphi)^k\sum_{m=0}^{\infty} Z_m\varphi^m. \tag{33}$$

Identification of the φ^N terms on both sides gives $Z_N\overline{n_1}^{(N)} = \sum_{q=1}^{N}(\pm 1)^{q-1}x_1^q Z_{N-q}$, which is Eq. (3).

We now introduce the $p\times p$ determinant

$$\sum_{N=1}^{\infty} Z_N\begin{vmatrix} \overline{n_1}^{(N)} & x_1 & x_1^2 & \cdots & x_1^{p-1} \\ \overline{n_2}^{(N)} & x_2 & x_2^2 & \cdots & x_2^{p-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \overline{n_p}^{(N)} & x_p & x_p^2 & \cdots & x_p^{p-1} \end{vmatrix}\varphi^N = \begin{vmatrix} \sum_N Z_N\overline{n_1}^{(N)}\varphi^N & x_1 & x_1^2 & \cdots & x_1^{p-1} \\ \sum_N Z_N\overline{n_2}^{(N)}\varphi^N & x_2 & x_2^2 & \cdots & x_2^{p-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sum_N Z_N\overline{n_p}^{(N)}\varphi^N & x_p & x_p^2 & \cdots & x_p^{p-1} \end{vmatrix}. \tag{34}$$

Inserting Eq. (33) in the right-hand side of this expression, we get

$$\begin{vmatrix} \frac{x_1\varphi\,\Xi(\varphi)}{1\mp x_1\varphi} & x_1 & x_1^2 & \cdots & x_1^{p-1} \\ \frac{x_2\varphi\,\Xi(\varphi)}{1\mp x_2\varphi} & x_2 & x_2^2 & \cdots & x_2^{p-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{x_p\varphi\,\Xi(\varphi)}{1\mp x_p\varphi} & x_p & x_p^2 & \cdots & x_p^{p-1} \end{vmatrix} = \frac{x_1\cdots x_p\varphi\,\Xi(\varphi)}{(1\mp x_1\varphi)\cdots(1\mp x_p\varphi)}$$

$$\times\begin{vmatrix}1 & (1\mp x_1\varphi) & x_1(1\mp x_1\varphi) & \cdots & x_1^{p-1}(1\mp x_1\varphi)\\ 1 & (1\mp x_2\varphi) & x_2(1\mp x_2\varphi) & \cdots & x_2^{p-1}(1\mp x_2\varphi)\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 1 & (1\mp x_p\varphi) & x_p(1\mp x_p\varphi) & \cdots & x_p^{p-1}(1\mp x_p\varphi)\end{vmatrix}. \tag{35}$$

From linear combinations of columns in the determinant we then obtain

$$\frac{x_1\cdots x_p\varphi\Xi(\varphi)}{(1\mp x_1\varphi)\cdots(1\mp x_p\varphi)}(\mp\varphi)^{p-1}$$
$$\times\begin{vmatrix}1 & x_1 & x_1^2 & \cdots & x_1^{p-1}\\ 1 & x_2 & x_2^2 & \cdots & x_2^{p-1}\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 1 & x_p & x_p^2 & \cdots & x_p^{p-1}\end{vmatrix}$$
$$=(\mp 1)^{p-1}\begin{vmatrix}1 & x_1 & x_1^2 & \cdots & x_1^{p-1}\\ 1 & x_2 & x_2^2 & \cdots & x_2^{p-1}\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 1 & x_p & x_p^2 & \cdots & x_p^{p-1}\end{vmatrix}$$
$$\times\sum_{N=p}^{\infty} Z_N\overline{n_1\cdots n_p}^{(N)}\varphi^N, \tag{36}$$

where we have used Eq. (32) for the last equality. Identifying terms in φ^N in the left-hand side of Eq. (34) and in the right-hand side of Eq. (36) demonstrates Eq. (6). To prove Eq. (6) in the grand canonical case, it suffices to replace $\Xi(\varphi)$ by 1 in the left-hand sides of Eqs. (35) and (36) and use the absence of correlation between occupation numbers Eq. (4).

2. Generalization

The same technique allows us to generalize Eq. (6) straightforwardly: the p-point correlation function can be expressed in terms of q-point correlation functions for any $q<p$. For instance, for $q=2$ we have

$$\overline{n_1n_2\cdots n_p}=\mp\frac{\begin{vmatrix}\overline{n_1n_3\ldots n_p} & x_1\\ \overline{n_2n_3\ldots n_p} & x_2\end{vmatrix}}{\begin{vmatrix}1 & x_1\\ 1 & x_2\end{vmatrix}}, \tag{37}$$

and other such relations obtained by picking different indices among the $p(p-1)/2$ pairs of indices (such an expression was obtained for fermions in Ref. [28]). More generally, as a function of q-point correlation functions we have

$$\overline{n_1n_2\cdots n_p}=(\mp)^{q-1}\frac{\begin{vmatrix}\overline{n_1n_{q+1}\ldots n_p} & x_1 & \cdots & x_1^{q-1}\\ \overline{n_2n_{q+1}\ldots n_p} & x_2 & \cdots & x_2^{q-1}\\ \vdots & \vdots & \ddots & \vdots\\ \overline{n_qn_{q+1}\ldots n_p} & x_q & \cdots & x_q^{q-1}\end{vmatrix}}{\begin{vmatrix}1 & x_1 & \cdots & x_1^{q-1}\\ 1 & x_2 & \cdots & x_2^{q-1}\\ \vdots & \vdots & \ddots & \vdots\\ 1 & x_q & \cdots & x_q^{q-1}\end{vmatrix}}, \tag{38}$$

and other such relations obtained by picking any q indices among the $\binom{p}{q}$ possibilities. The steps are exactly the same as in Eqs. (34)–(36), replacing the correlators in the determinant by their expression (32). For $q=p$ we obviously recover Eq. (6). Again, substituting $\Xi(\varphi)$ by 1 in the proof shows that Eq. (38) is valid also for the grand canonical ensemble.

3. Relation with Schur polynomials

The ratio of determinants in Eq. (6) allows us to identify another interesting connection with the theory of symmetric functions; namely, with a fourth family of symmetric functions, the so-called Schur polynomials [30]. The definition of these polynomials is given in Appendix A; they are expressed as a ratio of two determinants.

The Schur polynomials naturally appear if one replaces the $\overline{n_i}$ in the numerator of Eq. (6) by their expression (3). By linear expansion of the determinant with respect to its first column we directly obtain

$$\overline{n_1\cdots n_p}=\frac{x_1\cdots x_p}{Z_N}\sum_{k=p}^{N}(\pm 1)^{p+k}Z_{N-k}s_{\varpi_k}(x_1,\ldots,x_p), \tag{39}$$

where s_{ϖ_k} are the Schur polynomials for the partition $\varpi_k=(k-p,0^{p-1})$; cf. Appendix A. We recall that Z_{N-k} is identified with either the elementary symmetric polynomial $e_{N-k}(x_1,\ldots,x_M)$, or the homogeneous symmetric polynomial $h_{N-k}(x_1,\ldots,x_M)$, where M is the dimension of the one-particle Hilbert space. Introducing the Schur functions has allowed us to reduce the p-fold sum in Eq. (5) to a single sum in Eq. (39).

C. Correlation functions with higher powers (bosons): Proof of equation (8)

In the case of bosons, we can also consider higher moments of the occupation numbers (for fermions we have of course $n_\lambda^r=n_\lambda$). This question has attracted a lot of attention for the characterization of the number of condensed bosons in a BEC [9,11,12,14,33]. In the grand canonical ensemble, the integer moments of each occupation number can be obtained simply from the individual grand partition function $\xi_\lambda=(1-\varphi x_\lambda)^{-1}$ for individual eigenstate $|\lambda\rangle$ as

$$\overline{n_\lambda^r}^{\mathrm{g}}=\frac{1}{\xi_\lambda}\left(\varphi\frac{d}{d\varphi}\right)^r\xi_\lambda=\sum_{k=1}^{\infty}a_k(r)(x_\lambda\varphi)^k, \tag{40}$$

with $a_k(r)=k^r-(k-1)^r$ and $r\in\mathbb{N}$. Applying Eq. (31) to $\mathcal{A}(\{n_\lambda\})=n_1^{r_1}\cdots n_p^{r_p}$, and making use of the independence of the occupation numbers in the grand canonical ensemble as in Eq. (4), we readily obtain Eq. (8). For instance, for the second moment we have

$$\overline{n_\lambda^2}=\sum_{k=1}^{N}(2k-1)\frac{Z_{N-k}}{Z_N}x_\lambda^k. \tag{41}$$

This representation will be of practical use in the following section.

IV. CONDENSATION OF BOSONS IN A ONE-DIMENSIONAL HARMONIC TRAP

As a simple illustration of our results, we consider N bosons in a one-dimensional harmonic trap with frequency ω. The problem has been studied within the grand canonical [7,34–37], the canonical [7,10,11,26], and the microcanonical [9,10,12,38] ensembles [39]. In particular, some limiting behavior of the ground-state occupancy for $T \to 0$, recalled below, was obtained in several of these references. The probability distribution of the occupation number of the kth level was obtained in Ref. [11] :

$$\mathscr{P}_{k,N}(n) = \overline{\delta_{n_k,n}}^{(N)} = x^{kn}[1 - x^k + x^{N-n+k}]\frac{Z_{N-n}}{Z_N}, \quad (42)$$

where $x = e^{-\beta\omega}$. It is, however, not straightforward to extract simple information, like moments or cumulants, or to analyze the large-N asymptotics of this distribution. Here we show that the canonical formulas obtained in the previous sections lead to simple analytical results appropriate to discuss the large-N limit.

A. Thermodynamic properties

Up to a shift in energy, the one-body spectrum is $\varepsilon_n = n\omega$ for $n \in \mathbb{N}$ (we set $\hbar = k_B = 1$). The N-body partition function [3,40]

$$Z_N = \prod_{n=1}^{N}(1 - e^{-n\beta\omega})^{-1} \quad (43)$$

corresponds to N independent bosonic modes with frequencies $\Omega_n = n\omega$ for $n = 1,\dots,N$.

The problem involves three characteristic temperature scales. (i) The lowest scale, $T_Q = \omega$, separates the regime where the spectrum should be considered discrete ($T \ll T_Q$) from the one where it can be described as a continuous spectrum ($T \gg T_Q$). (ii) The scale $T_* = N\omega$ separates the quantum regime $T \ll T_*$, where the upper modes are frozen in their ground state [see Eq. (43)], from the classical regime $T \gg T_*$ where all the modes can be described as classical oscillators, in which case we recover the Maxwell-Boltzmann partition function $Z_N \simeq (1/N!)(\beta\omega)^{-N}$ corresponding to neglecting the effect of quantum correlations. (iii) The third temperature scale is the Bose-Einstein temperature

$$T_{\rm B} = \frac{N\omega}{\ln N}, \quad (44)$$

below which a macroscopic fraction of bosons accumulates in the individual ground state. It can be obtained from the analysis of the canonical chemical potential $\mu^{\rm c} = F_N - F_{N-1}$ or the fugacity $\varphi^{\rm c} = e^{\beta\mu^{\rm c}} = Z_{N-1}/Z_N = 1 - e^{-N\beta\omega}$. Introducing (incorrectly) this expression in the grand canonical expression of the ground-state occupancy, $\overline{n_0}^{\rm g} = [1/\varphi - 1]^{-1}$, Eq. (1), shows that $\overline{n_0}^{\rm g} \sim N$ for $\varphi \sim 1 - 1/N$, i.e., $T \sim T_{\rm B} = N\omega/\ln N$.

In the following, we will not describe the effect of the discrete nature of the spectrum and will always consider the limit $T \gg \omega$ (the condition will be implicit in the rest of the paper). In particular, we can treat the sum over the spectrum in $\ln Z_N$ as an integral, so that Eq. (43) yields $\ln Z_N \simeq -\int_0^N dn \ln(1 - e^{-n\beta\omega})$. The latter expression can be reformulated in terms of the polylogarithm function $\mathrm{Li}_2(x) = \sum_{n=1}^{\infty} x^n/n^2 = -\int_{-\ln x}^{+\infty} dy \ln(1 - e^{-y})$ (see §25 of Ref. [41]). The free energy is then given by

$$F_N = -\frac{1}{\beta}\ln Z_N \simeq \frac{\mathrm{Li}_2(e^{-N\beta\omega}) - \mathrm{Li}_2(1)}{\beta^2\omega}. \quad (45)$$

B. Mean occupation numbers

1. Classical regime: $T \gg T_*$

In the classical regime $T \gg T_*$, i.e., $N\beta\omega \ll 1$, one can use the asymptotic behavior $\mathrm{Li}_2(1-\epsilon) \simeq \pi^2/6 + \epsilon(\ln\epsilon - 1)$ for $\epsilon \ll 1$. From Eq. (45) we recover the classical (Maxwell-Boltzmann) result $Z_N \sim e^N(N\beta\omega)^{-N}$, which coincides with the expression given above since $N! \sim N^N e^{-N}$. The mean occupation number, given by Eq. (3), is dominated by the first term, so that for the kth level ε_k it is given by $\overline{n_k} \simeq N\beta\omega e^{-\beta\varepsilon_k}$. Since the canonical fugacity behaves as $\varphi^{\rm c} \simeq N\beta\omega$, we get $\overline{n_k} \simeq \varphi^{\rm c} e^{-\beta\varepsilon_k}$, which coincides with the well-known grand canonical behavior.

2. Quantum regime: $T \ll T_*$

We now turn to the more interesting regime where $T \ll T_*$ (and $T \gg T_Q$). The sum in Eq. (3) can be replaced by an integral. Using Eq. (45) for the expression of Z_N, the mean occupation number can be reexpressed as

$$\overline{n_k} \simeq N\int_0^1 dy \times \exp\left\{-N\beta\varepsilon_k y + \frac{\mathrm{Li}_2\left(e^{-N\beta\omega}\right) - \mathrm{Li}_2\left(e^{-N\beta\omega(1-y)}\right)}{\beta\omega}\right\}, \quad (46)$$

where $\varepsilon_k = k\omega$. While the exact form (3) is only tractable for small N in practice, the integral representation (46) has the advantage that it allows us to study the occupation without restriction on N. One must, however, keep in mind that Eq. (46) only holds in the intermediate regime $\omega \ll T \ll N\omega$.

The integral expression (46) can be further simplified by using the behavior of the polylogarithm function in the vicinity of 0, $\mathrm{Li}_2(x) \simeq x$ for $x \to 0$. Indeed, in the regime where $N\beta\omega \gg 1$, one can replace $\mathrm{Li}_2(e^{-N\beta\omega})$ by $e^{-N\beta\omega}$. Moreover, when $\beta\omega \ll 1$ one can also replace $\mathrm{Li}_2(e^{-N\beta\omega(1-y)})$ by $e^{-N\beta\omega(1-y)}$, since in the vicinity of $y = 1$, where this approximation breaks down, the integrand becomes proportional to $e^{-1/(\beta\omega)} \ll 1$. For the same reason one can extend the integral to infinity. Equation (46) thus reduces to

$$\overline{n_k} \simeq N\int_0^\infty dy \exp\left\{-N\beta\varepsilon_k y + \frac{e^{-N\beta\omega} - e^{-N\beta\omega(1-y)}}{\beta\omega}\right\}. \quad (47)$$

Introducing the parameter

$$z = \frac{e^{-N\beta\omega}}{\beta\omega} = \frac{T}{\omega}N^{-T_{\rm B}/T} \quad (48)$$

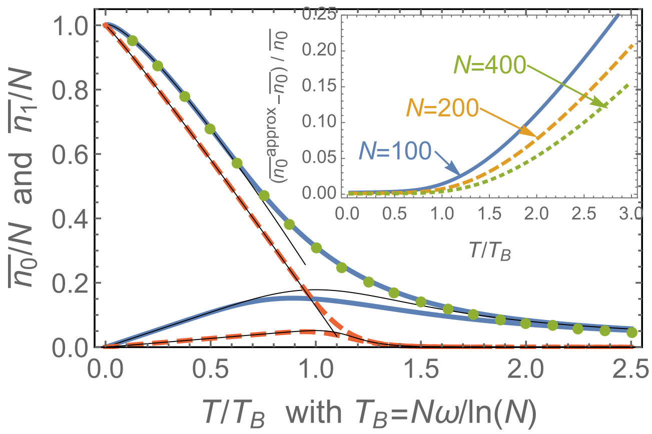

FIG. 1. Occupations of the ground state and the first-excited state, Eq. (49), for $N = 100$ (blue solid line) and $N = 10^8$ (red dashed). The green dots correspond to the exact result (3) for the ground state with $N = 100$. Thin black lines are (50) and (51). Inset shows the relative difference between the approximate form (49) and the exact form (3).

and making the change of variables $u = ze^{N\beta\omega y}$, Eq. (47) yields a representation in terms of the incomplete Gamma function,

$$\overline{n_k} \simeq \frac{1}{\beta\omega} z^k e^z \Gamma(-k,z). \tag{49}$$

In the inset of Fig. 1 we compare Eq. (49) with the exact expression (3): the difference is below 1% on the interval $[0,T_{\rm B}]$ for relatively small N and we can see that the temperature range over which the difference remains small grows as N increases.

3. *Ground state*

Setting $k = 0$ in Eq. (49), the incomplete Gamma function reduces to the exponential integral $\Gamma(0,z) = E_1(z)$. The $T \ll T_{\rm B}$ regime corresponds to the limiting behavior $E_1(z) = \ln[e^{-\gamma}/z] + O(z)$ for $z \to 0$, where $\gamma \simeq 0.577$ is the Euler-Mascheroni constant. Hence

$$\frac{\overline{n_0}}{N} \simeq 1 - \frac{T\ln(e^{\gamma}T/\omega)}{N\omega} \quad \text{for } T \ll T_{\rm B}. \tag{50}$$

This behavior was already obtained in Ref. [14] by a different approach (see also Appendix B, where we recall how the limiting behavior can be obtained within a grand canonical treatment [37]). In Fig. 1 we compare the approximate expression (50) with the exact sum (3). For large-enough N the behavior (50) is indistinguishable from the exact result up to $T \sim T_{\rm B}$.

4. *Excited states*

For the excited states, because of the factor $e^{-N\beta\varepsilon_k y}$, the integral (46) is dominated by the neighborhood of the lower boundary. In this case we can use $e^{-N\beta\omega} - e^{-N\beta\omega(1-y)} \simeq -N\beta\omega y e^{-N\beta\omega}$ for $y \to 0$. This is equivalent to replacing Eq. (49) by the approximation $z^k e^z \Gamma(-k,z) \simeq 1/(k+z)$, which corresponds to the interpolation between the two limiting behaviors $\simeq 1/k$ for $z \to 0$ and $\simeq 1/z$ for $z \to \infty$ [the agreement with $1/(k+z)$ becomes excellent at large k].

As a result we get the approximate form

$$\overline{n_k} \simeq \frac{T}{\varepsilon_k + Te^{-N\omega/T}} \tag{51}$$

for $k \geqslant 1$. For $T \ll T_{\rm B}$ we get the linear behavior $\overline{n_k} \simeq T/\varepsilon_k$. However, unlike Eq. (50), Eq. (51) also describes the crossover from this linear behavior to the decaying behavior above $T_{\rm B}$, as illustrated in Fig. 1. Equation (51) shows that the mean occupation reaches its maximum for $T = N\omega/\ln(N/k) \simeq T_{\rm B}$, with

$$\overline{n_k}\Big|_{\max} \simeq \frac{N/k}{\ln(N/k)}. \tag{52}$$

The presence of the logarithm in the denominator shows that only the ground state has a macroscopic occupation below $T_{\rm B}$, as expected when BEC occurs.

For the highest excited states, such that $\varepsilon_k \gg T$, the continuous approximation of the sum (3), leading to the integral (46), fails, and the occupation decays exponentially as $\overline{n_k} \simeq e^{-\beta\varepsilon_k}$. This is the expected classical behavior (for $\varphi^{\rm c} \simeq 1$), as weakly occupied levels can be considered in the classical regime.

C. Variance of the ground-state occupation

We now study the fluctuations around the mean occupation number. We restrict ourselves to the ground state, which has attracted some attention in higher dimension [14,33]. The exact expression for $\overline{n_0^2}$ is given by Eq. (41). In the most interesting regime, $T_Q = \omega \ll T \ll T_* = N\omega$, we get an integral representation similar to Eq. (46): the coefficient $a_k(2) = 2k - 1$ in the sum (41) translates into a factor $2Ny - 1 \simeq 2Ny$ in the integral (46), so that

$$\overline{n_0^2} \simeq 2N^2 \int_0^1 dy\, y\, e^{[\mathrm{Li}_2(e^{-N\beta\omega}) - \mathrm{Li}_2(e^{-N\beta\omega(1-y)})]/(\beta\omega)}. \tag{53}$$

Performing the same approximations as above and using the asymptotics $\int_x^\infty du\, \ln(u)e^{-u}/u \simeq (1/2)[-\ln^2 x + \gamma^2 +$

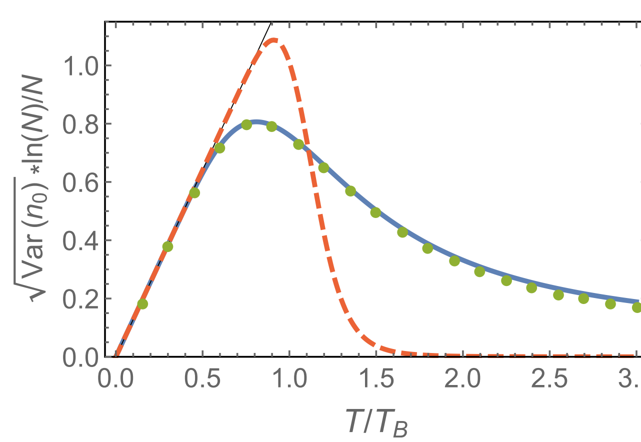

FIG. 2. Fluctuations of the ground-state occupancy as a function of the rescaled temperature, for $N = 100$ (blue solid line) and 10^8 (red dashed), from Eq. (61). Thin black line corresponds to (54). Green dots show exact expression from Eqs. (3)–(41).

$\pi^2/6]$ as $x \to 0$, we obtain

$$\mathrm{Var}(n_0) \simeq \frac{1}{6}\left(\frac{\pi T}{\omega}\right)^2 \text{ for } T \ll T_{\mathrm{B}}. \tag{54}$$

This behavior was obtained in Refs. [11,14] by a different canonical calculation [42]. It was also obtained within the microcanonical ensemble in Refs. [9,12]. The variance deduced from Eq. (53), which is plotted in Fig. 2, presents a peak close to $T \sim T_{\mathrm{B}}$, with a scaling $\mathrm{Var}(n_0)|_{T=T_{\mathrm{B}}} \sim N^2/\ln^2 N$. A careful analysis of the expression (61) derived below, with the help of the software MATHEMATICA, shows that the peak in the variance scales as

$$\mathrm{Var}(n_0)\big|_{\max} \simeq \frac{\pi^2 N^2}{6\ln^2 N}\left[1 - \frac{(\ln\ln N)^2}{\ln N} + O\left(\frac{\ln\ln N}{\ln N}\right)\right], \tag{55}$$

thus the relative fluctuations are $\delta n_0/\overline{n_0} \sim 1/\ln N$. Due to this slow decay, n_0 cannot be considered self-averaging in practice.

D. Distribution of occupation numbers

1. Characteristic function

To demonstrate the efficiency of our formalism, we now derive the full distribution of the ground-state occupancy. We start from the general expression of the moments, Eq. (8). As for the first two moments, we replace the sum by an integral, which is valid for $T_Q = \omega \ll T \ll T_* = N\omega$. For $r \geqslant 1$, we have

$$\begin{aligned}\overline{n_k^r} \simeq & N^{r+1}\int_0^1 dy\left[y^r - \left(y - \frac{1}{N}\right)^r\right]e^{-N\beta\varepsilon_k y}\\ &\times \exp\left\{\frac{\mathrm{Li}_2(e^{-N\beta\omega}) - \mathrm{Li}_2(e^{-N\beta\omega(1-y)})}{\beta\omega}\right\},\end{aligned} \tag{56}$$

where $\varepsilon_k = k\omega$. Weighting this expression by $(\alpha\beta\omega)^r/r!$ and summing over r, we get the characteristic function

$$\begin{aligned}\overline{\exp\{\alpha\beta\omega n_k\}} \simeq & 1 + \frac{1 - e^{-\alpha\beta\omega}}{\beta\omega}z^{k-\alpha}\int_z^{1/(\beta\omega)} du\, u^{\alpha-k-1}\\ &\times \exp\left\{\frac{\mathrm{Li}_2(\beta\omega z) - \mathrm{Li}_2(\beta\omega u)}{\beta\omega}\right\},\end{aligned} \tag{57}$$

where z is given by Eq. (48) and we made the change of variables $u = ze^{N\beta\omega y}$. In the limit where $\beta\omega \to 0$ (continuous approximation), keeping z finite (i.e., probing $T \sim T_{\mathrm{B}}$), one can again use $\mathrm{Li}_2(x) \simeq x$ for $x \to 0$. We recognize the integral representation of the incomplete Gamma function $\Gamma(\alpha - k, z)$. We finally get

$$\overline{e^{\alpha\beta\omega n_k}} \simeq 1 + \alpha e^z z^{k-\alpha}\Gamma(\alpha - k, z) \equiv G_{k,z}(\alpha), \tag{58}$$

where we introduced the moment-generating function $G_{k,z}(\alpha)$. We define a rescaled variable ξ by $G_{k,z}(\alpha) = \overline{e^{\alpha\xi}}$. It is such that $\xi \simeq \beta\omega n_k$. In this regime, the generating function of the occupation number for the kth excited state only depends on the nontrivial combination of parameters given by z defined in Eq. (48).

We can get the moments by expanding the generating function as

$$G_{k,z}(\alpha) = \sum_{r=0}^{\infty}\frac{\mu_r(z,k)}{r!}\alpha^r \quad \text{with } \overline{n_k^r} \simeq \frac{\mu_r(z,k)}{(\beta\omega)^r}. \tag{59}$$

We get

$$\mu_1(z,k) = z^k e^z \Gamma(-k,z), \tag{60}$$

which coincides with Eq. (49), as it should. The higher moments are expressed in terms of Meijer G functions:

$$\mu_r(z,k) = r!\,e^z G_{r,r+1}^{r+1,0}\left(z\,\middle|\,\begin{matrix}1+k,\ldots,1+k\\ 0,k,\ldots,k\end{matrix}\right). \tag{61}$$

These expressions are valid in the full range of temperature $T \sim T_{\mathrm{B}}$ where quantum correlations dominate. The cumulants of the occupations can be deduced from the expansion

$$\ln G_{k,z}(\alpha) = \sum_{r=1}^{\infty}\frac{c_r(z,k)}{r!}\alpha^r \text{ with } \overline{n_k^r}^{\mathrm{cum}} \simeq \frac{c_r(z,k)}{(\beta\omega)^r}. \tag{62}$$

However, we have not found any expression for the cumulants that would be simpler than that obtained from the moments.

2. Distribution

Using the integral representation $\Gamma(a,z) = z^a\int_0^\infty d\xi \exp\{a\xi - ze^\xi\}$, we rewrite the generating function (58) as

$$G_{k,z}(\alpha) = \overline{e^{\alpha\xi}} = 1 + e^z\int_0^\infty d\xi\,\alpha e^{\alpha\xi}e^{-k\xi - ze^\xi}. \tag{63}$$

An integration by parts makes it clear that the rescaled occupation number $\xi \simeq \beta\omega n_k$ is distributed according to the law

$$Q_{k,z}(\xi) = \theta_{\mathrm{H}}(\xi)e^z(k + ze^\xi)\exp\{-k\xi - ze^\xi\}, \tag{64}$$

where $\theta_{\mathrm{H}}(\xi)$ is the Heaviside function. Although the connection is not obvious, this distribution is the large-N limit of Eq. (42).

We can compare our result (64) with the simple result given by the grand canonical ensemble. In this case, occupations are independent and the distribution of the occupation is exponential, $\mathscr{P}_k^{\mathrm{g}}(n) \propto \varphi^n e^{-n\beta\varepsilon_k}$, where φ is the fugacity; cf. Eq. (30). The rescaled variable $\xi \simeq \beta\omega n_k$ is then distributed according to the law $Q_k^{\mathrm{g}}(\xi) \propto \varphi^{T\xi/\omega}e^{-k\xi}$. The two distributions thus significantly differ, and in particular the large deviations, as shown in the inset of Fig. 3.

As stressed by Schönhammer [28], the deviation from the purely exponential distribution in the canonical ensemble can be interpreted as a deviation from the Wick theorem induced by the constraint on the number of particle number.

3. Ground state

In the case of the ground state, it is more convenient to shift the rescaled variable as $\zeta = \xi + \ln z \simeq \beta\omega n_0 + \ln z$. The new variable is thus distributed according to

$$F_z(\zeta) \equiv Q_{0,z}(\xi) = \theta_{\mathrm{H}}(\zeta - \ln z)\exp\{z + \zeta - e^\zeta\}, \tag{65}$$

which is the *truncated* Gumbel distribution. In the limit $z \to 0$, we get the Gumbel law $F_0(\zeta) = \exp\{\zeta - e^\zeta\}$, defined on $\mathbb{R}$, describing extreme-value statistics of independent random

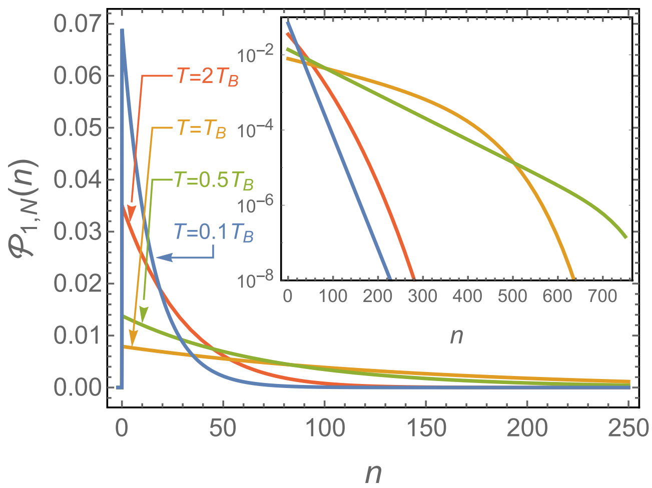

FIG. 3. Distribution $\mathscr{P}_{1,N}(n)$ of the number of bosons in the first-excited state for $N = 1000$. Temperature is $T/T_{\rm B} = 2$ (red), 1 (orange), 0.5 (green), and 0.1 (blue), obtained from Eq. (64). The plot in log-linear scale in the inset shows that the distribution is far from exponential when $T \gtrsim T_{\rm B}$.

variables [43,44]. The probability distribution for the ground-state occupancy n_0 can then be written as

$$\mathscr{P}_{0,N}(n) \simeq \frac{\omega}{T} F_z\left(\frac{\omega}{T}\left(n - N + \frac{T}{\omega}\ln(T/\omega)\right)\right). \tag{66}$$

This distribution is plotted in Fig. 4 for different temperatures. The curves correspond at first sight with the plot of Eq. (42) in Ref. [11], although the connection with the Gumbel distribution was not made in that paper.

The distribution simplifies in the regime $T \ll T_{\rm B}$, as well as the moments: when $z \to 0$, Eq. (58) yields $\ln G_{0,z}(\alpha) \simeq -\alpha \ln z + \ln \Gamma(1+\alpha)$, leading to

$$\ln G_{0,z}(\alpha) \simeq -\alpha \ln z + \sum_{r=1}^{\infty} \frac{\psi^{(r-1)}(1)}{r!}\alpha^r \text{ as } z \to 0, \tag{67}$$

where $\psi(x)$ is the digamma function. This leads in particular to $\mu_1(z,0) = c_1(z,0) = -\ln z + \psi(1) + O(z) \simeq -\ln z - \gamma$, in accordance with Eq. (50), and $c_2(z,0) = \psi'(1) + O(z\ln z) \simeq \pi^2/6$, in accordance with Eq. (54). In general, we have for $r \geqslant 2$ the expression $c_r(z,0) = \psi^{(r-1)}(1) + O(z \ln^{r-1} z)$ as $z \to 0$, thus

$$\overline{n_0^r}^{\rm cum} \simeq \psi^{(r-1)}(1)\left(\frac{T}{\omega}\right)^r \text{ for } r \geqslant 2, \tag{68}$$

which coincide with the cumulants of the Gumbel law, as it should. Again, recall that this behavior holds in the regime $T_Q \ll T \ll T_{\rm B}$.

4. *Excited states*

The study of the fluctuations of the occupation numbers for the excited states follows the same lines as for the ground state. For instance, the second moment $\overline{n_k^2}$ is given by inserting a factor $2Ny$ in the integral (46). Similar approximations as for the calculation of the mean value lead to $\overline{n_k^2} \simeq 2(\overline{n_k})^2$,

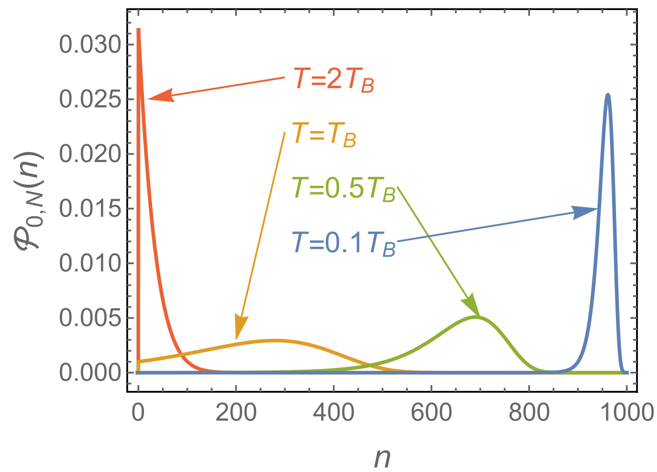

FIG. 4. Distribution $\mathscr{P}_{0,N}(n)$ of the number of condensed bosons for $N = 1000$. Temperature is (from left to right) $T/T_{\rm B} = 2$ (red), 1 (orange), 0.5 (green), and 0.1 (blue), obtained from Eq. (66).

thus

$$\mathrm{Var}(n_k) \simeq (\overline{n_k})^2 \text{ for } T \ll T_{\rm B}. \tag{69}$$

As is turns out, this approximation reproduces quite well the variance in the whole regime $T \ll T_*$. As for the ground state, we get a quadratic behavior at low temperature, $\mathrm{Var}(n_k) \sim (T/\varepsilon_k)^2$ for $\omega \ll T \ll T_{\rm B}$. The fluctuations are maximum for $T \simeq T_{\rm B}$ with $\mathrm{Var}(n_k)|_{\max} \simeq (N/k)^2/\ln^2(N/k)$. Hence, the maximal fluctuations in the excited states are of the same order as the fluctuations in the ground state

$$\delta n_k \sim \frac{1}{k}\delta n_0 \text{ for } T \sim T_{\rm B}; \tag{70}$$

however, the relative fluctuations are larger in the excited states, $\delta n_k/\overline{n_k} \sim 1$, than in the ground state, $\delta n_0/\overline{n_0} \sim 1/\ln N$.

The distribution of the occupation number is given by Eq. (64). We remark that the distribution simplifies in the low-temperature limit as $Q_{k,0}(\xi) = \theta_{\rm H}(\xi) k e^{-k\xi}$, i.e., $\mathscr{P}_{k,N}(n) \simeq \beta\varepsilon_k e^{-n\beta\varepsilon_k}$ for $T \ll T_{\rm B}$. Interestingly, in this limit, this distribution coincides with the similar distribution obtained in the grand canonical ensemble (see Sec. IV D 2) $\mathscr{P}_k^{\rm g}(n) \propto e^{-n\beta\varepsilon_k}$ with $\varphi = 1$. This supports the fact that the condensed bosons in the ground state play the role of a reservoir for the excited bosons in this regime [33] (cf. Appendix B).

For $T \gtrsim T_{\rm B}$, the distribution presents a decay faster than exponential (see Fig. 4).

5. *Correlations*

We can also study the correlations between occupation numbers. For example, by using Eq. (7) we can easily get $\overline{n_k n_0}$. Let us study the $T \to 0$ limit of the correlator, when $\overline{n_0} \simeq N$ and $\overline{n_k} \simeq 1/(\beta\varepsilon_k)$. In the continuum limit ($\beta\omega \ll 1$) and for small-enough k, we can expand the exponential $e^{\beta\varepsilon_k} \simeq 1 + \beta\varepsilon_k$. As a result we obtain $\mathrm{Cov}(n_0,n_k) = \overline{n_k n_0} - \overline{n_k} \times \overline{n_0} \simeq -(\overline{n_k})^2$. Denoting by $N_{\rm ex} = \sum_{k>0} n_k$ the number of excited bosons, this result implies that $\mathrm{Cov}(n_0, N_{\rm ex}) \simeq -\sum_{k>0}(\overline{n_k})^2 \simeq$

$-(T/\omega)^2 \sum_{k>0} 1/k^2 = -(1/6)(\pi T/\omega)^2 \simeq -\mathrm{Var}(n_0)$, as it should since $\mathrm{Cov}(n_0,N_{\mathrm{ex}}) = -\mathrm{Var}(n_0) = -\mathrm{Var}(N_{\mathrm{ex}})$ follows from the constraint that $n_0 + N_{\mathrm{ex}} = N$ is fixed. Furthermore, we see that the anticorrelations

$$\frac{\overline{n_k n_0} - \overline{n_k} \times \overline{n_0}}{\sqrt{\mathrm{Var}(n_k)\mathrm{Var}(n_0)}} \simeq -\sqrt{\frac{\mathrm{Var}(n_k)}{\mathrm{Var}(n_0)}} \simeq -\frac{\sqrt{6}}{\pi k} \text{for } T \ll T_{\mathrm{B}}, \tag{71}$$

decay as higher excited states are considered.

V. CONCLUSION

We obtain several general results for the occupation numbers in the *canonical* ensemble for bosons and for fermions: mean occupations, fluctuations, and correlation functions. We show that the p-point correlation function for N particles is expressed in terms of the k-body canonical partition functions, with $k = 1,\dots,N$, where these partition functions can be obtained by using a well-known recursion formula. We have also obtained a representation of the p-point correlation function in terms of the ratio of two determinants, involving the mean occupations, which can therefore be viewed as the only fundamental quantities controlling any correlation function. An open question would be to extend our determinantal representation to correlation functions involving arbitrary powers (in the bosonic case) and clarify the connection with the theory of symmetric functions in this case.

The two-point correlation function and the relation (7) have recently found an application in Ref. [27], where the variance of a specific observable for a gas of noninteracting fermions in a one-dimensional harmonic trap was analyzed in detail. We demonstrate the efficiency of our results by deriving some analytical expressions for the problem of Bose-Einstein condensation in a one-dimensional gas harmonically trapped. We obtain significant deviations with the results given by the traditional grand canonical treatment where the constraint on the number of bosons is introduced *a posteriori* (cf. Appendix B). This detailed analysis relies on the knowledge of the exact canonical partition function. A study of higher dimensions or other situations would be interesting.

We demonstrate that, in the regime where quantum correlations dominate ($T_Q = \omega \ll T \ll T_* = N\omega$), the distribution of the individual ground-state occupancy has the form of a truncated Gumbel law. Moreover, in the regime $T \ll T_{\mathrm{B}}$, we get the Gumbel distribution. Interestingly, this is not the first time that a connection is established between thermodynamical properties of a Bose gas and extreme-value statistics: in Ref. [45], the spectral density of a Bose gas (not necessarily harmonically confined) was shown to be related to the different extreme-value distributions for identical and independently distributed random variables. Depending on the exponent controlling the single-particle density of states $\rho(\varepsilon) \propto \varepsilon^{\alpha-1}$, the different universality classes (Gumbel, Fréchet, or Weibull) can be obtained. For the one-dimensional harmonically trapped Bose gased studied here, the connection between the ground-state occupancy distribution and extreme-value statistics still remains to be explained.

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APPENDIX A: SCHUR FUNCTIONS

Consider the integer partition $\lambda = (\lambda_1,\lambda_2,\dots,\lambda_n)$ with $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$. If an integer is repeated, we may use the notation $(2,1,1,1) \equiv (2,1^3)$, here for the partition of 5. We introduce the specific partition $\delta = (n-1,n-2,\dots,1,0)$. Addition of partitions is simply obtained by adding integers term by term $\lambda + \delta = (\lambda_1 + n - 1,\lambda_2 + n - 2,\dots,\lambda_{n-1} + 1,\lambda_n)$. We introduce the determinant

$$a_\lambda(x_1,\dots,x_n) = \begin{vmatrix} x_1^{\lambda_1} & x_1^{\lambda_2} & \cdots & x_1^{\lambda_n} \\ \vdots & \vdots & \ddots & \vdots \\ x_n^{\lambda_1} & x_n^{\lambda_2} & \cdots & x_n^{\lambda_n} \end{vmatrix}. \tag{A1}$$

The Vandermonde determinant is then $a_\delta(x_1,\dots,x_n)$, up to a sign. The Schur function is defined by [30]

$$s_\lambda(x_1,\dots,x_n) = \frac{a_{\lambda+\delta}(x_1,\dots,x_n)}{a_\delta(x_1,\dots,x_n)}. \tag{A2}$$

APPENDIX B: GRAND CANONICAL TREATMENT OF BOSONS IN A ONE-DIMENSIONAL HARMONIC TRAP

In this appendix, we recall the grand canonical treatment for bosons in a harmonic trap. A first rough description can be found in Refs. [35,36], which corresponds to slightly adapting the usual treatment valid for $d > 1$ [2,3]: while for $d > 1$ the fugacity reaches $\varphi = 1$ at the Bose-Einstein temperature, one needs to introduce a cutoff in one dimension and set $\varphi = 1 - 1/N$. This leads to the linear behavior [46]. $\overline{n_0}/N \simeq 1 - T/T_{\mathrm{B}}$ for $T < T_{\mathrm{B}}$. In practice, the linear behavior is only reached for huge numbers of bosons because the fluctuation region is rather large in one-dimension [37]. A refined treatment was proposed in Ref. [34] (see also Ref. [37]): assuming that the occupations are given by the usual Bose-Einstein factor (1), one splits the sum $N = \sum_\lambda \overline{n_\lambda}^{\mathrm{g}}$ between strongly occupied low energy levels and weakly occupied high

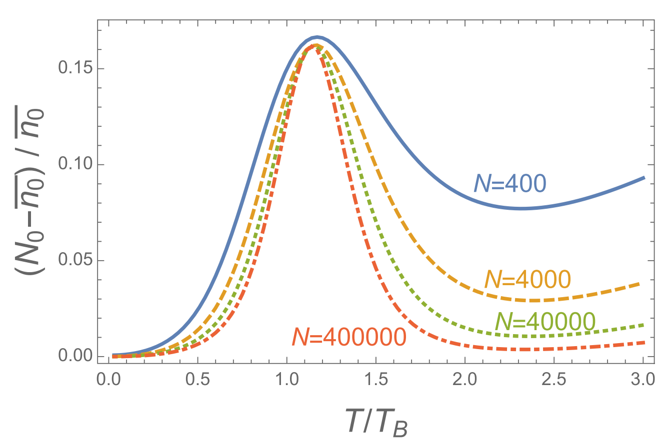

FIG. 5. Comparison between the form (46), obtained within the canonical treatment, and the result of the grand canonical treatment, solution of Eq. (B1).

energy levels. This leads to the equation for the condensate fraction [34,37]

$$N - \frac{T}{\omega}\ln(T/\omega) = N_0 - \frac{T}{\omega}\psi\left(1 + \frac{T}{N_0\omega}\right), \tag{B1}$$

where $\psi(z)$ is the digamma function [we use a different notation for the (exact) canonical condensate fraction $\overline{n_0}$ and its counterpart N_0 in the (approximate) grand canonical approach]. From this equation, it is possible to recover the limiting behavior (50). However, a precise comparison with Eq. (46) shows a relative difference of $\sim$16% when $T \sim T_{\mathrm{B}}$, irrespectively how large N is, as shown in Fig. 5 [note that this discrepancy cannot be attributed to the continuous approximation leading to Eq. (46); cf. inset of Fig. 1].

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