Entropy of the Bose-Einstein-condensate ground state: Correlation versus ground-state entropy

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Calculation of the entropy of an ideal Bose-Einstein condensate (BEC) in a three-dimensional trap reveals unusual, previously unrecognized, features of the canonical ensemble. It is found that, for any temperature, the entropy of the Bose gas is equal to the entropy of the excited particles although the entropy of the particles in the ground state is nonzero. We explain this by considering the correlations between the ground-state particles and particles in the excited states. These correlations lead to a correlation entropy which is exactly equal to the contribution from the ground state. The correlations themselves arise from the fact that we have a fixed number of particles obeying quantum statistics. We present results for correlation functions between the ground and excited states in a Bose gas, so as to clarify the role of fluctuations in the system. We also report the sub-Poissonian nature of the ground-state fluctuations.

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I. INTRODUCTION

The properties of a Bose condensate [1,2] are usually studied by using a grand canonical ensemble by making a number of assumptions which can be justified in the thermodynamic limit [3–5]. For a condensate consisting of relatively small number of particles, it is better to use a canonical ensemble. This ensemble is useful in understanding the particle number distribution, as well as the fluctuations in the number of particles in ground states and excited states, has been obtained [6–10]. Such calculations do not require a thermodynamic limit. An important result is the distribution of the number of particles in the ground state. Recent work presents the entropy of the ground state of an ideal N-particle Bose-Einstein condensate (BEC) from the condensate density matrix [11,12]

$$\rho_{n_0 n_0} = \frac{\mathcal{H}^{N-n_0}}{(N-n_0)!} e^{-\mathcal{H}}, \tag{1}$$

where $\mathcal{H} = N(T/T_c)^3$ for a harmonic trap at temperature T and critical temperature T_c and n_0 is the number of atoms in the condensate state.

This distribution has some novel features—it is like the well-known laser distribution for photons in a single mode laser. This distribution can be used to calculate the thermodynamic properties of the ground state; in particular the approximate expression for entropy was obtained. From the von Neumann entropy

$$S = -k_{\rm B} \sum_n \rho_{nn} \ln \rho_{nn}, \tag{2}$$

with Boltzmann constant $k_{\rm B}$, one finds [12]

$$S = k_{\rm B} \ln W + \frac{k_{\rm B}}{2}, \tag{3}$$

where $W = [2\pi(\Delta n_0)^2]^{1/2} = \sqrt{2\pi\mathcal{H}}$. Note that, for $T \to 0$, we need to use the expression (1) or the full canonical ensemble calculation (See Fig. 1).

In this paper we study the Bose gas in a three-dimensional trap. We use the canonical ensemble to obtain *exact* results for the quantum statistical entropy. Our exact results reveal new features of the Bose gas. We consider the density matrix associated with the ground state $\rho_{\rm gnd}$ and for the excited states $\rho_{\rm ex}$ obtained from the full canonical density matrix. The considerations of exact canonical ensemble reveal that the total entropy of the Bose gas at any temperature T is equal to the entropy of the particles in the excited states; although the entropy of the ground-state particles is nonzero. This remarkable result implies the existence of the correlation entropy in a Bose gas and in fact the correlation entropy must cancel the contribution from the ground state. We trace this result to the fact that in the ensemble the number of particles is fixed and thus the total density matrix does not factorize $\rho_{\rm T} \neq \rho_{\rm gnd} \otimes \rho_{\rm ex}$. The nonfactorized nature of the full density matrix is further clarified by calculating the correlation functions between the ground-state and excited-state particles.

In Sec. II, we derive reduced density matrices from the total matrix in number-occupation representation and consider the corresponding entropies. An explicit example is shown in Table I. Furthermore, the equality of the total entropy and entropy of the excited particles is confirmed by comparing the forms of two density matrices. In this procedure, the correlation entropy is also defined. In Sec. III, we derive the explicit relations among the entropies of particles in an ideal BEC, which leads to the joint entropy theorem for the total entropy, as shown in Fig. 2. In Sec. IV, the consideration of correlation functions has provided more clear understanding on the correlation entropy in BEC system. The correlations between the occupations of ground state and that of excited states has shown a similar tendency as the correlation entropy along temperature, as shown in Fig. 3. In Sec. V, we conclude this paper by asserting the equality between two entropies: the total entropy and the entropy of the excited particles of a BEC in the canonical ensemble. Explicit procedures to calculate the partition function and related thermodynamic quantities in a canonical ensemble are shown in Appendixes A and B.

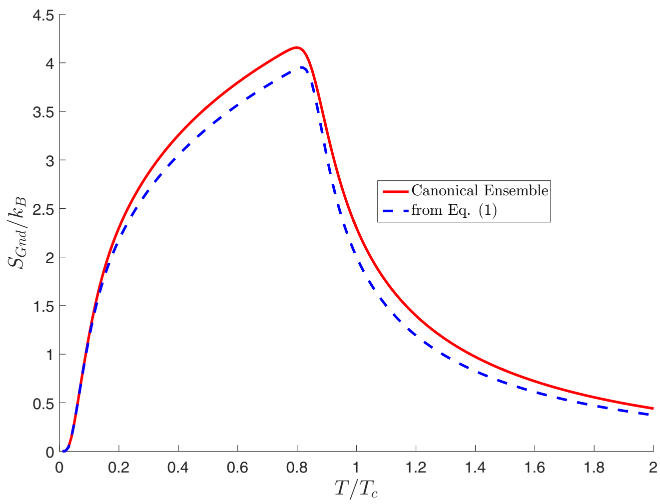


FIG. 1. Entropy of ground state in an ideal Bose gas, which is trapped in a 3D harmonic trap. The total number of particles is $N = 200$. The critical temperature for a 3D harmonic trap is $T_c = \hbar\Omega/k_B[N/\zeta(3)]^{1/3}$, with harmonic trap oscillation frequency Ω, and Riemann's zeta function $\zeta(s)$. This exact result on entropy is calculated by using the canonical ensemble partition function, which is explained in Appendixes A and B and is drawn as a solid red line. From the approximate density matrix, Eq. (1), the corresponding von Neumann's entropy is plotted as a dashed blue line.

II. BOSE-EINSTEIN-CONDENSATE JOINT GROUND-STATE ENTROPY

We first prove that the total entropy of an ideal Bose gas at a temperature T is the same as the entropy of excited states of that system. At equilibrium, the total density matrix for an ideal Bose gas with a *fixed* total number of particles N is given by

$$\rho_T = \sum_{n_0,\{n_i\}} p(n_0,\{n_i\})|n_0,\{n_i\}\rangle\langle n_0,\{n_i\}|\delta_{N-n_0,\sum n_i}, \quad (4)$$

with the occupation distribution $\{n_i\}$ on the excited states constrained by the condition $\sum_i n_i = N - n_0$. The reduced density matrices for the ground state and for the excited states are

$$\rho_{gnd} = \mathrm{Tr}_{\{n_i\}_{n_0}}(\rho_T) \quad (5a)$$

$$= \sum_{n_0} p(n_0)|n_0\rangle\langle n_0|, \quad (5b)$$

and

$$\rho_{ex} = \mathrm{Tr}_{n_0}(\rho_T) \quad (6a)$$

$$= \sum_{\{n_i\}} p\left(n_0 = \sum_i n_i, \{n_i\}\right)|\{n_i\}\rangle\langle\{n_i\}|. \quad (6b)$$

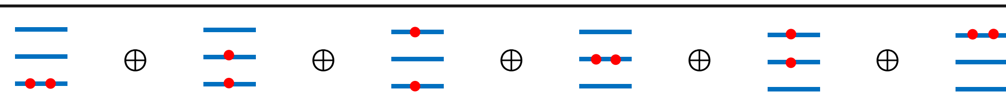
The occupation probability for the ground state is

$$p(n_0) = \sum_{\{n_i\}} p(n_0,\{n_i\}). \quad (7)$$

Note that the probabilities for the states $|\{n_i\}\rangle$ in ρ_{ex} are the same joint probabilities as for the states $|n_0,\{n_i\}\rangle$ in ρ_T. The explicit example for calculating the corresponding probability is explained in Table I.

TABLE I. (a) The system consists of two identical Bose particles (red dots), which are distributed among three different states (blue lines). Due to the Bose statistics, the number of possible configurations is six. (b) The total density matrix ρ_T and the corresponding entropy $S(\rho_T)$ and (c) the reduced density matrix ρ_{ex} for excited states and the corresponding entropy $S(\rho_{ex})$. By comparing insets (b) and (c), we can easily confirm the equality of the two entropies. (d) The density matrix and entropy for the ground state. The relation between the occupation probability for the ground state and the whole joint probability is explicitly shown.

(a)



(b) Total Density Matrix: $\rho_T =$ $p(2_0,0_1,0_2)\|2_00_10_2\rangle\langle 2_00_10_2\| + p(1_0,1_1,0_2)\|1_01_10_2\rangle\langle 1_01_10_2\|$ $+ p(1_0,0_1,1_2)\|1_00_11_2\rangle\langle 1_00_11_2\| + p(0_0,2_1,0_2)\|0_02_10_2\rangle\langle 0_02_10_2\|$ $+ p(0_0,1_1,1_2)\|0_01_11_2\rangle\langle 0_01_11_2\| + p(0_0,0_1,2_2)\|0_00_12_2\rangle\langle 0_00_12_2\|$	Entropy of total system: $S(\rho_T) =$ $p(2_0,0_1,0_2)\ln p(2_0,0_1,0_2) + p(1_0,1_1,0_2)\ln p(1_0,1_1,0_2)$ $+p(1_0,0_1,1_2)\ln p(1_0,0_1,1_2) + p(0_0,2_1,0_2)\ln p(0_0,2_1,0_2)$ $+p(0_0,1_1,1_2)\ln p(0_0,1_1,1_2) + p(0_0,0_1,2_2)\ln p(0_0,0_1,2_2)$
(c) Reduced Density Matrix: $\rho_{ex} =$ $p(2_0,0_1,0_2)\|0_10_2\rangle\langle 0_10_2\| + p(1_0,1_1,0_2)\|1_10_2\rangle\langle 1_10_2\|$ $+ p(1_0,0_1,1_2)\|0_11_2\rangle\langle 0_11_2\| + p(0_0,2_1,0_2)\|2_10_2\rangle\langle 2_10_2\|$ $+ p(0_0,1_1,1_2)\|1_11_2\rangle\langle 1_11_2\| + p(0_0,0_1,2_2)\|0_12_2\rangle\langle 0_12_2\|$	Entropy of excited states: $S(\rho_{ex}) =$ $p(2_0,0_1,0_2)\ln p(2_0,0_1,0_2) + p(1_0,1_1,0_2)\ln p(1_0,1_1,0_2)$ $+p(1_0,0_1,1_2)\ln p(1_0,0_1,1_2) + p(0_0,2_1,0_2)\ln p(0_0,2_1,0_2)$ $+p(0_0,1_1,1_2)\ln p(0_0,1_1,1_2) + p(0_0,0_1,2_2)\ln p(0_0,0_1,2_2)$
(d) Reduced Density Matrix: $\rho_{gnd} =$ $p(2_0)\|2_0\rangle\langle 2_0\| + p(1_0)\|1_0\rangle\langle 1_0\| + p(0_0)\|0_0\rangle\langle 0_0\|$ $= p(2_0,0_1,0_2)\|2_0\rangle\langle 2_0\|$ $+[p(1_0,0_1,1_2) + p(1_0,0_1,1_2)]\|1_0\rangle\langle 1_0\|$ $+[p(0_0,1_1,1_2) + p(0_0,1_1,1_2) + p(0_0,1_1,1_2)]\|0_0\rangle\langle 0_0\|$	Entropy of the ground state: $S(\rho_{gnd}) =$ $p(2_0)\ln p(2_0) + p(1_0)\ln p(1_0) + p(0_0)\ln p(0_0)$

From the von Neumann entropy, Eq. (2), the corresponding entropies are

$$S(\rho_{\rm T}) = -k_{\rm B}{\rm Tr}_{n_0,\{n_i\}}(\rho \ln \rho) \tag{8a}$$
$$= -k_{\rm B}\sum_{n_0,\{n_i\}} p(n_0,\{n_i\}) \ln p(n_0,\{n_i\}), \tag{8b}$$

and

$$S(\rho_{\rm ex}) = -k_{\rm B}{\rm Tr}_{\{n_i\}}(\rho_{\rm ex} \ln \rho_{\rm ex}) \tag{9a}$$
$$= -k_{\rm B}\sum_{n_0,\{n_i\}} p(n_0,\{n_i\}) \ln p(n_0,\{n_i\}), \tag{9b}$$

showing that the entropy of the total system, Eq. (8b), is equal to that for the excited states, Eq. (9b), since the accessible states and corresponding probabilities are the same. Table I shows this property explicitly for a system of two Bose particles in three nondegenerate levels.

Similarly, we can write the entropy of the ground state:

$$S(\rho_{\rm gnd}) = -k_{\rm B}{\rm Tr}_{n_0}(\rho_{\rm gnd} \ln \rho_{\rm gnd}) \tag{10a}$$
$$= -k_{\rm B}\sum_{n_0} p(n_0) \ln p(n_0). \tag{10b}$$

Furthermore, the above result is applicable for any quantum system of identical particles including ideal Fermi atoms in a trap with a *fixed* total number of particles. Hence, we can say that the removal of any single state in the canonical ensemble preserves the entropy, since the total number of particles is fixed by the constraint.

Since the total entropy of the system is same as that of the excited states, what is learned from this result? In a system of N ideal Bose particles, we can divide the system into two parts: one is the ground state and the other is the excited states [Eqs. (5a) and (6a)]. It is also possible to define the entropy of each part [Eqs. (10a) and (9a)]. Since the total density matrix, Eq. (4), does *not* factorize as, $\rho_{\rm T} \neq \rho_{\rm ex} \otimes \rho_{\rm gnd}$, we expect that the entropy of the total system is not the summation of the entropy of each part, $S(\rho_{\rm T}) \neq S(\rho_{\rm gnd}) + S(\rho_{\rm ex})$, and we thus introduce the correlation entropy [13] as

$$S_{\rm cor}(\rho_{\rm gnd},\rho_{\rm ex}) \equiv S(\rho_{\rm gnd}) + S(\rho_{\rm ex}) - S(\rho_{\rm T}). \tag{11}$$

Remarkably, since $S(\rho_{\rm T}) = S(\rho_{\rm ex})$, we see that

$$S_{\rm cor}(\rho_{\rm gnd},\rho_{\rm ex}) = S(\rho_{\rm gnd}). \tag{12}$$

Therefore, the entropy of the ground state can be interpreted as the correlation entropy between the ground state and excited states. According to information theory [14], the correlation entropy $S_{\rm c}(\rho_{\rm gnd},\rho_{\rm ex})$ is called the mutual information. Hence, according to information theory we can say that the status of the excited states can provide total information about the ground state.

III. BOSE-EINSTEIN-CONDENSATE CONDITIONAL GROUND-STATE ENTROPY

In statistics and Shannon's information theory [15], conditional distributions and the conditional entropy are useful concepts. Using the conditional probability, we can identify the amount of contribution of the ground state in entropy to the excited states. The conditional probability for the excited states with a given number of particles in the ground state is

$$p(\{n_i\}|n_0) = \frac{p(n_0,\{n_i\})}{p(n_0)}, \tag{13}$$

where the ground-state occupation probability is given by Eq. (7). The entropy of $\rho_{\rm ex}$ can be further evaluated:

$$S(\rho_{\rm ex}) = -k_{\rm B}\sum_{\{n_i\}}\sum_{n_0}[p(n_0)p(\{n_i\}_{n_0}|n_0)]\ln[p(n_0)]$$
$$-k_{\rm B}\sum_{\{n_i\}}\sum_{n_0}[p(n_0)p(\{n_i\}_{n_0}|n_0)]\ln[p(\{n_i\}_{n_0}|n_0)] \tag{14}$$
$$= -k_{\rm B}\sum_{n_0} p(n_0)\ln p(n_0) - k_{\rm B}\sum_{n_0} p(n_0) \times \sum_{\{n_i\}} p(\{n_i\}_{n_0}|n_0)\ln p(\{n_i\}_{n_0}|n_0) \tag{15}$$
$$= S(\rho_{\rm gnd}) + \sum_{n_0} p(n_0) S(\rho_{\rm ex}^{N-n_0}). \tag{16}$$

where $\rho_{\rm ex}^{N-n_0}$ is the reduced density matrix of excited states with $N-n_0$ particles, and $S(\rho_{\rm ex}^{N-n_0})$ is the corresponding entropy. Hence, the excited states $S(\rho_{\rm ex})$ contain information about the ground state.

Similarly, we can rewrite the above relation for the total entropy as

$$S(\rho_{\rm T}) = S(\rho_{\rm gnd}) + \sum_{n_0} p(n_0) S(\rho_{\rm ex}^{N-n_0}). \tag{17}$$

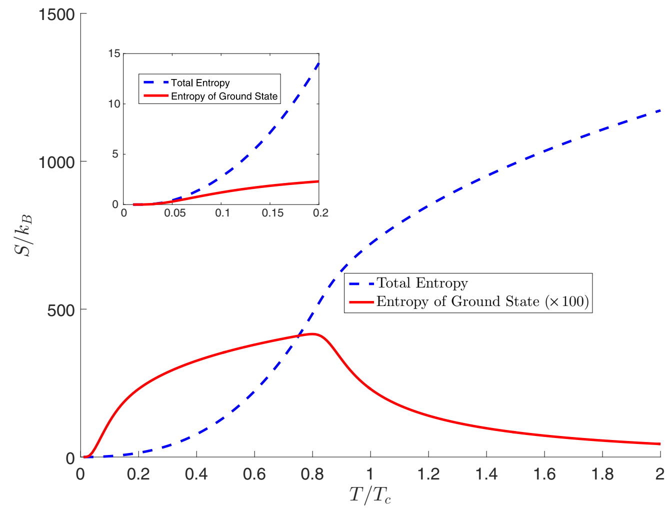


FIG. 2. Entropy for ideal Bose gas which is trapped in a three-dimensional harmonic trap. The detailed parameters are as in Fig. 1. The total entropy is drawn with a dashed blue line, using the procedure in Appendixes A and B, and the entropy of the ground state is in the solid red line. In this picture, the entropy for the ground state is multiplied by 100. From the behavior of the occupation number in the ground state, we can see the entropy contribution of the ground state is important below the critical temperature. In a similar way, in terms of correlation entropy the relevant range of the correlation is also below the critical temperature. The inset shows both entropies below $T/T_c = 0.2$.

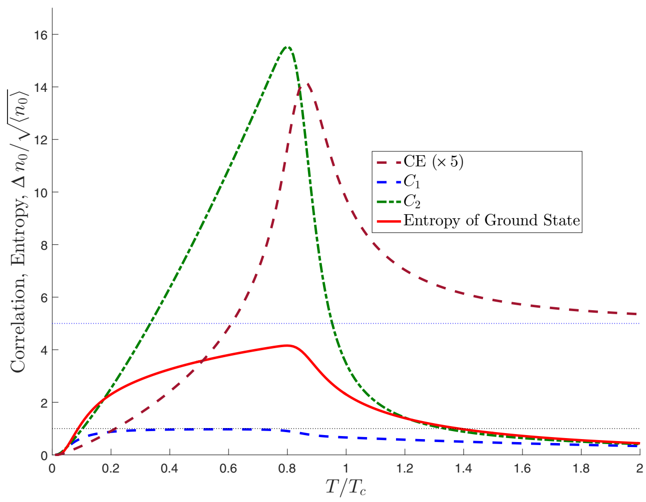


FIG. 3. The system is an ideal Bose gas trapped in a 3D harmonic trap with 200 particles. The parameters are the same as in Fig. 1. The normalized correlation function C_1, Eq. (18), between the ground-state occupation number and that of excited states is plotted as a dashed blue line. C_2, Eq. (20), is plotted as a dotted green line. The correlation entropy, Eq. (12), or the entropy of the ground state, is also drawn as a solid red line. In the figure we also show the sub-Poissonian nature of fluctuations by plotting the parameter $\Delta n_0/\sqrt{\langle n_0\rangle}$ [dashed brown line (×5)]. The strong sub-Poissonian region corresponds to $\Delta n_0/\sqrt{\langle n_0\rangle} \ll 1$.

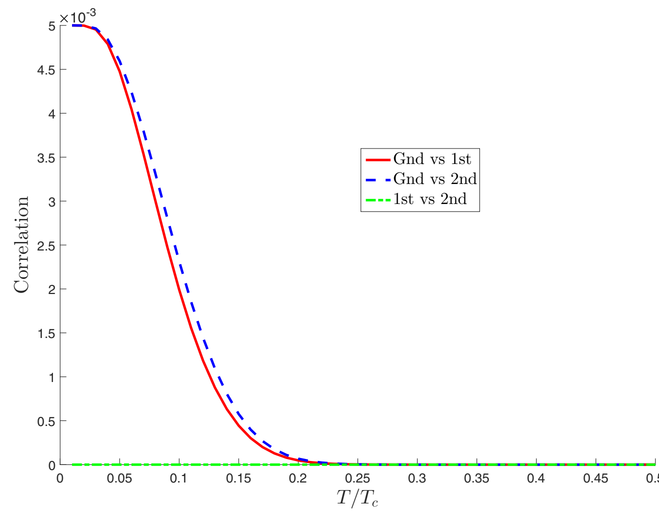


FIG. 4. The correlation function $\tilde{C}_1$, Eq. (21), is drawn among the three lowest states. $\tilde{C}_1(n_0,n_1)$ is drawn as a solid red line, $\tilde{C}_1(n_0,n_2)$ as a blue dashed line, and $\tilde{C}_1(n_1,n_2)$ as a green dashed-dotted line. Since the occupation of the ground state is macroscopic in low temperature, the correlation function is noticeable below $T/T_c \sim 0.2$. The correlation between the first- and the second-excited states is negligible, since the occupation number in each state is small compared with the total number of particles. The system is an ideal Bose gas trapped in a 3D harmonic trap, and the parameters are the same as in Fig. 1.

This relation is known as the joint entropy theorem [14,16,17]. The entropy contribution of the ground state is in the total entropy. We can interpret $S(\rho_{\text{gnd}})$ as the entropy of the ground state and as the correlation entropy.

The explicit procedure to calculate the entropy for $S(\rho_{\text{T}})$ and $S(\rho_{\text{exc}}^{N-n_0})$ is explained in Appendix B. Figure 2 shows the entropy of the ground state, or the correlation entropy, for an ideal Bose gas with 200 particles in a 3D harmonic trap.

IV. CORRELATION FUNCTION

To better appreciate the nature of correlations in the Bose gas at low temperatures, we examine the variety of correlations of occupation numbers between the ground state and the excited states. The entropy is defined by the distribution of occupation numbers; that is, the density matrix, and the correlation function is defined by the corresponding random variables; that is, the occupation numbers. For the ground-state distribution the occupation number n_0 for the ground state is the corresponding variable, and for the excited states the occupation number is $\sum_i n_i = N - n_0$.

As in a statistical description of the correlation between two random variables, we can introduce the correlation between the numbers of particles in the ground state and in excited states as

$$C_1\left(n_0, \sum_i n_i\right) \equiv \frac{\langle n_0 \sum_i n_i\rangle}{\sqrt{\langle n_0{}^2\rangle\left\langle\left(\sum_i n_i\right)^2\right\rangle}} = \frac{\langle n_0(N-n_0)\rangle}{\sqrt{\langle (n_0)^2\rangle\langle (N-n_0)^2\rangle}}. \tag{18}$$

Note that the Schwarz inequality implies that $C_1 \leqslant 1$. We note that over the temperature range $T/T_c \sim [0.2-0.8]$, $C_1 \simeq 1$ implying a very high degree of correlation. Beyond this temperature the correlation starts falling. Next we introduce the correlation defined as the fluctuation around the mean:

$$C_2\left(n_0, \sum_i n_i\right) \equiv \left[\langle n_0\rangle\left\langle \sum_i n_i\right\rangle - \left\langle n_0 \sum_i n_i\right\rangle\right]^{1/2} \tag{19}$$

$$= \sqrt{\langle (n_0)^2\rangle - \langle n_0\rangle^2}. \tag{20}$$

It is interesting that the conservation of total number N of particles makes C_2 identical to the (variance)$^{1/2}$ of the ground-state number. C_2 shows a behavior which has similarities to the behavior of the correlation entropy. However, the correlation entropy shows a much slower dependence on T. This can be understood as the ground-state entropy is the mean value of $p(n_0)$ and is related in principle to all order of moments of n_0. If $p(n_0)$ were to be approximated by a Gaussian, then $\ln p(n_0)$ is directly related to $\ln C_2$ and because of the logarithmic dependence, entropy shows a much slower dependence on T than C_2. In Fig. 3 we also show a very interesting character of the statistics of the fluctuations in the ground state: the fluctuations in the region close to $T/T_c \ll 1$ are predominantly sub-Poissonian as $\Delta n_0/\sqrt{\langle n_0\rangle} < 1$. The result from the approximate expression, Eq. (1), is close to the exact result.

Although the fluctuations of the ground-state populations have not been yet studied experimentally, this is possible in principle from the snapshots of the images of the distribution of particles in the trap. The peak and tail of the snapshots should yield the ground-state and the excited-state distributions. Such images have been used for studying the particle-number fluctuations in a trap when interparticle interactions are important [18].

We next consider the correlation between two specific states defined by

$$\tilde{C}_1(n_i,n_j) \equiv \frac{\langle n_i n_j\rangle}{\sqrt{\langle (n_i)^2\rangle\langle (n_j)^2\rangle}}, \tag{21}$$

where

$$\langle n_i n_j\rangle = \sum_{n_i=1}^{N}\sum_{n_j=1}^{N-n_i} e^{-\beta n_i\epsilon_i-\beta n_j\epsilon_j}\frac{Z_{N-n_i-n_j}(\beta)}{Z_N(\beta)}, \tag{22}$$

which is derived in the supplementary information.

The correlation between the ground state and the first-excited state is shown in Fig. 4. Although the occupation number of the first-excited states is considerable around $T/T_c \sim 1$, the correlation between two states are negligible except at low temperatures $T/T_c \lesssim 0.1$, where it is of order $1/N$.

V. SUMMARY

The most important result of our *exact* calculation based on the canonical ensemble is that the entropy of a Bose gas confined to a three-dimensional harmonic trap is equal to the entropy associated with the atoms in the excited states. This is so even though, at any temperature, the entropy of the particles in the ground state is nonzero. We bring out the reasons for this surprising result by showing that the total entropy associated with the full system consists of three contributions: the entropy of the ground state, the entropy associated with the particles in the excited state, and a contribution which we refer to as the correlation entropy (analog of the mutual information from information theory). We show on a very general ground that the correlation entropy cancels the ground-state contribution. This appears due to the fixed number of particles distributed among the quantum states [19]. The explicit nature of correlations among the particles in the ground state and excited states is brought about by studying different types of correlation functions involving the numbers in the ground state and excited states. Because of number conservation, these correlations become related to the ground-state fluctuations. Since the entropy of the ground state is the mean value of the ln $p(n_0)$, the fluctuations of n_0 determine the value of the entropy of particles in the ground state.

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APPENDIX A: *EXACT* PARTITION FUNCTION AND OCCUPATION PROBABILITY IN CANONICAL ENSEMBLE

The partition function Z_N in a canonical ensemble (CE) can be written in terms of occupation number in each accessible state as

$$Z_N(\beta) = \sum_{n_0=0}^{\infty}\sum_{n_1=0}^{\infty}\cdots\sum_{n_\nu=0}^{\infty}\cdots e^{-\beta n_0\epsilon_0}e^{-\beta n_1\epsilon_1}\cdots \times e^{-\beta n_\nu\epsilon_\nu}\cdots\delta\left(N-\sum_\nu n_\nu\right) \tag{A1}$$

$$= \sum_{n_0,\{n_i\}_{n_0}} e^{-\beta\sum_\nu n_\nu\epsilon_\nu}\delta\left(N-\sum_\nu n_\nu\right), \tag{A2}$$

where $\beta = (k_B T)^{-1}$ is the inverse temperature with the Boltzmann constant $k_{\rm B}$.

Let us consider the probability that state ν has more than n particles. Then, the corresponding summation is restricted to $n_\nu \geqslant n$:

$$P(n_\nu \geqslant n) = \frac{1}{Z_N}\sum_{n_0=0}^{\infty}\sum_{n_1=0}^{\infty}\cdots\sum_{n_\nu=n}^{\infty}\cdots e^{-\beta n_0\epsilon_0}e^{-\beta n_1\epsilon_1}\cdots \times e^{-\beta n_\nu\epsilon_\nu}\cdots\delta\left(N-\sum_\nu n_\nu\right) \tag{A3}$$

$$= e^{-\beta n\epsilon_\nu}\frac{Z_{N-n}(\beta)}{Z_N(\beta)}. \tag{A4}$$

The probability for state ν to have n particles is

$$P(n_\nu = n) = P(n_\nu \geqslant n) - P(n_\nu \geqslant n+1) \tag{A5}$$

$$= \frac{e^{-\beta n\epsilon_\nu}Z_{N-n}(\beta) - e^{-\beta(n+1)\epsilon_\nu}Z_{N-n-1}(\beta)}{Z_N(\beta)}. \tag{A6}$$

The average occupation number in state ν is

$$\langle n_\nu\rangle = \sum_{n_\nu=1}^{N} n_\nu P(n_\nu) = \sum_{n_\nu=1}^{N} e^{-\beta n_\nu\epsilon_\nu}\frac{Z_{N-n_\nu}(\beta)}{Z_N(\beta)}. \tag{A7}$$

The total number of particles is given by sum of the average occupation number of all states,

$$N = \sum_\nu \langle n_\nu\rangle. \tag{A8}$$

By a simple manipulation, we get the following recurrence relation [6,20]:

$$Z_N(\beta) = \frac{1}{N}\sum_{m=1}^{N} Z_1(m\beta)Z_{N-m}(\beta). \tag{A9}$$

Similar to Eq. (A5), we can write the occupation probability for two states:

$$P(n_\nu \geqslant n, n_\mu \geqslant m) = e^{-\beta n\epsilon_\nu-\beta m\epsilon_\mu}\frac{Z_{N-n-m}(\beta)}{Z_N(\beta)}. \tag{A10}$$

So, the probability to find $n_\nu = n$ and $n_\mu = m$ is

$$P(n_\nu = n, n_\mu = m) = P(n_\nu \geqslant n, n_\mu \geqslant m) - P(n_\nu \geqslant n, n_\mu \geqslant m+1) \tag{A11}$$

$$- P(n_\nu \geqslant n+1, n_\mu \geqslant m) + P(n_\nu \geqslant n+1, n_\mu \geqslant m+1). \tag{A12}$$

The correlation function between the two states can be easily obtained. Explicitly, it is

$$\langle n_\nu n_\mu \rangle = \sum_{n=1}^{N} \sum_{m=1}^{N-n} e^{-\beta n \epsilon_\nu - \beta m \epsilon_\mu} \frac{Z_{N-n-m}(\beta)}{Z_N(\beta)}. \tag{A13}$$

APPENDIX B: THERMODYNAMIC QUANTITIES IN CANONICAL ENSEMBLE

The partition function $Z_N(T,V)$ in a canonical ensemble is related to the Helmholtz free energy $A(T,V)$ [3,4]:

$$Z_N(T,V) = e^{-\beta A(T,V)}, \tag{B1}$$

or

$$A(T,V) = -k_B T \ln Z_N(T,V). \tag{B2}$$

Thermodynamic quantities can be calculated from the Helmholtz free energy through the Maxwell relations. For example, the pressure P and entropy S are

$$P = -\left(\frac{\partial A}{\partial V}\right)_T, \tag{B3}$$

$$S = -\left(\frac{\partial A}{\partial T}\right)_V, \tag{B4}$$

$$U = \langle H \rangle = A + TS, \tag{B5}$$

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V, \tag{B6}$$

with isochoric heat capacity C_V.

In terms of the partition function,

$$\frac{A}{k_B} = -T \ln Z_N, \tag{B7}$$

$$\frac{P}{k_B T} = \left(\frac{\partial \ln Z_N}{\partial V}\right)_T, \tag{B8}$$

$$S = k_B \ln Z_N + k_B T\left(\frac{\partial \ln Z_N}{\partial T}\right)_V, \tag{B9}$$

$$U = k_B T^2 \left(\frac{\partial \ln Z_N}{\partial T}\right)_V, \tag{B10}$$

$$C_V = 2k_B T\left(\frac{\partial \ln Z_N}{\partial T}\right)_V + k_B T^2 \left(\frac{\partial^2 \ln Z_N}{\partial T^2}\right)_V. \tag{B11}$$

Derivatives of the partition function $\ln Z_N$ with respect to the temperature T or to the volume V give to the corresponding thermodynamic quantities in canonical ensemble.

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