Canonical ensemble ground state and correlation entropy of Bose–Einstein condensate

Anatoly Svidzinsky¹,³, Moochan Kim¹, Girish Agarwal¹ and Marlan O Scully¹,²

¹ Texas A&M University, College Station TX 77843, United States
² Baylor University, Waco, TX 76706, United States
³ Author to whom any correspondence should be addressed

E-mail: asvid@physics.tamu.edu

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Abstract

Constraint of a fixed total number of particles yields a correlation between the fluctuation of particles in different states in the canonical ensemble. Here we show that, below the temperature of Bose–Einstein condensation (BEC), the correlation part of the entropy of an ideal Bose gas is cancelled by the ground-state contribution. Thus, in the BEC region, the thermodynamic properties of the gas in the canonical ensemble can be described accurately in a simplified model which excludes the ground state and assumes no correlation between excited levels.

Realization of Bose–Einstein condensation (BEC) of weakly interacting gases has given rise to renewed interest in the canonical ensemble statistics. The trapped atomic clouds are small enough so that finite particle effects are potentially observable. Experimentally, the trapped atoms are isolated so that there is no exchange of particles. Magnetic or optical confinement suggests that the system is also thermally isolated and, hence, microcanonical description is needed. In this microcanonical ensemble the total particle number and the total energy are both exactly conserved. On the other hand, in experiments with two (or many) component BECs, Bose–Fermi mixtures, and additional gas components, e.g., for sympathetic cooling, there is an energy exchange between the components. As a result, each of the components can be described by the canonical ensemble that applies to systems with a conserved particle number while exchanging energy with a heat bath of a given temperature. Such a description is also appropriate for dilute $^4$He in a porous medium [1] or for hadronic matter which under certain conditions resembles an ideal Bose gas with its associated Bose condensation [2].

Theoretical treatment of BEC of trapped atoms in the canonical ensemble is challenging since evaluation of the canonical partition function is impeded by the constraint that the total particle number $N$ is fixed. Thermodynamics [3, 4] and statistics of such systems [5, 6] is an interesting and rich area for scientific analysis. Thermodynamics of BEC clouds was studied experimentally using phase-contrast imaging [7].

Among others, the issue of the fluctuations in the number of condensed atoms is of central importance. It has been shown that the difference between using grand canonical and canonical ensembles is substantial for the condensate statistics. For Bose gas, the fluctuations of the condensate fraction were calculated in a series of papers [5, 8–17] by a variety of approximate methods for various trapping potentials and in a different number of dimensions. Fairly accurate analytical expression for the condensate statistics in the canonical ensemble was obtained using a non-equilibrium master equation approach based on the quantum theory of laser [18, 19]. The number statistics was measured for a degenerate Bose gas confined in an optical trap [20], for a mesoscopic ensemble of cold atoms in a dipole trap [21] and in optical lattices [22, 23].

Because of the constraint on the total particle number, exact analytical results in the canonical ensemble are available only for the simplest systems. For an ensemble of bosons trapped in a one-dimensional harmonic potential, an analytical formula for the canonical partition function was found in [24–26]. However, there is no known simple analytic expression for the canonical partition function for higher dimensional traps.

Here we study an ideal Bose gas with a fixed number of particles and temperature in a harmonic trap and show that below the temperature of BEC transition the canonical ensemble correlations can be very accurately
taken into account analytically in a simple effective model. We consider a system of \( N \) particles with energies of the single-particle states \( \varepsilon_n, \nu = 0, 1, 2, \ldots \). The ground state corresponds to \( \nu = 0 \). In the canonical ensemble the total number of particles \( N \) is fixed and the probability to find the system in a microstate \( \{ n \} = \{ n_0, n_1, \ldots \} \), here \( n_\nu \) is the number of particles in the state \( \nu \), is given by the Boltzmann distribution

\[
P_{\{n\}} = \frac{1}{Z_N} \exp \left( -\frac{E_{\{n\}}}{k_B T} \right) \delta_{n_0 + n_1 + \ldots, N},
\]

where \( E_{\{n\}} \) is the energy of the microstate

\[
E_{\{n\}} = \sum_{\nu=0}^{\infty} \varepsilon_\nu n_\nu,
\]

and \( Z_N \) is the canonical partition function

\[
Z_N = \sum_{\{n\}} \exp \left( -\frac{E_{\{n\}}}{k_B T} \right) \delta_{n_0 + n_1 + \ldots, N}.
\]

The average energy of the system is given by

\[
\langle E \rangle = \sum_{\{n\}} E_{\{n\}} P_{\{n\}} = k_B T^2 \frac{\partial \ln Z_N}{\partial T},
\]

while the Gibbs entropy of the system is

\[
S = -k_B \sum_{\{n\}} P_{\{n\}} \ln P_{\{n\}} = k_B \frac{\partial (T \ln Z_N)}{\partial T}.
\]

Equations (3) and (4) yield

\[
\frac{\partial S}{\partial T} = \frac{1}{T} \frac{\partial \langle E \rangle}{\partial T}.
\]

For the canonical ensemble, the contributions to the entropy from each state are not independent because of the constraint on the total number of particles. One can write the total entropy as

\[
S = S_{\text{ind}} + S_{\text{corr}},
\]

where \( S_{\text{ind}} \) is the entropy of the system obtained if state contributions are treated as independent and \( S_{\text{corr}} \) is the remaining part called the correlation entropy. \( S_{\text{ind}} \) is given by the formula

\[
S_{\text{ind}} = \sum_{\nu=0}^{\infty} S_\nu,
\]

where

\[
S_\nu = -k_B \sum_{n=0}^{N} n_p_{n,\nu} \ln n_p_{n,\nu}
\]

and \( n_p_{n,\nu} \) is the distribution function for state \( \nu \) (probability of finding \( n \) particles occupying the single-particle state \( \nu \)).

Here we consider an ideal Bose gas of \( N \) particles confined in an isotropic harmonic trapping potential. Energies of a particle in the trap are

\[
\varepsilon_{n lm} = \hbar \omega (n + l + m),
\]

where \( n, l \) and \( m \) are non-negative integers. We assume that the ground-state energy is equal to zero. The thermodynamic limit formula for the critical temperature of BEC transition is

\[
T_c = \frac{\hbar \omega}{k_b} \left( \frac{N}{\zeta(3)} \right)^{1/3},
\]

where \( \zeta (x) \) is the Riemann zeta function.

For the canonical ensemble, one can calculate the partition function \( Z_N (T) \) using the following recursion relation [12]

\[
Z_N = \frac{1}{N} \sum_{k=1}^{N} Z_k (k) \cdot Z_{N-k},
\]
where \( Z_0 = 1 \) and

\[
Z_t(k) = \sum_{n,l,m=0}^{\infty} \exp \left( -\frac{k_{\text{adm}}}{k_B T} \right) = \frac{1}{1 - \exp \left( -\frac{k_{\text{adm}}}{k_B T} \right)}.
\]

If we know \( Z_N(T) \), then entropy \( S \) can be obtained using equation (4). On the other hand, in the canonical ensemble the distribution function for the state \( \nu \) is given by

\[
p_{\nu} = e^{-\frac{m_{\nu}^2}{2k_B T}} \frac{Z_{N-n}^n}{Z_N} - e^{-\frac{(n+1)m_{\nu}^2}{2k_B T}} \frac{Z_{N-n-1}^{n+1}}{Z_N}.
\]

Using this formula and equation (6), one can find \( S_{\text{ind}} \) and then calculate \( S_{\text{corr}} = S - S_{\text{ind}} \).

In figure 1 we plot \( S_{\text{corr}}/S \) as a function of temperature obtained numerically for \( N = 200 \) particles in the harmonic trap. The figure shows that \( S_{\text{corr}} \) is negative and its absolute value becomes comparable with the total entropy \( S \) at low \( T \). Thus, correlation between particles gives substantial contribution to the thermodynamic quantities at low temperatures and must be taken into account in the proper description of the system.

Here we show, however, that canonical ensemble correlations can be accurately accounted for by replacing the system of correlated particles with an effective model which has no correlations. One can decompose \( S_{\text{ind}} \) into the ground and excited state contributions

\[
S_{\text{ind}} = S_{\text{ground}} + S_{\text{exc}},
\]

where \( S_{\text{ground}} = S_0 \) and

\[
S_{\text{exc}} = \sum_{\nu=1}^{\infty} S_{\nu}.
\]

In figures 2 and 3 we plot the correlation entropy \( S_{\text{corr}} \) and the ground-state entropy \( S_{\text{ground}} \) as a function of temperature for \( N = 200 \) (figure 2) and \( N = 1000 \) (figure 3) particles in the harmonic trap. Plots show that below the temperature of BEC transition

\[
S_{\text{corr}} = -S_{\text{ground}}
\]

with incredible accuracy. To demonstrate this, in figure 4 we plot the relative difference between the two quantities for \( N = 200 \) and 1000. The figure shows that \( |S_{\text{corr}} + S_{\text{ground}}|/S_{\text{corr}} < 10^{-20} \) when \( T < 0.77 T_c \) (for \( N = 1000 \)). Thus, in the BEC state \( S_{\text{ground}} \approx 0 \) and the total entropy of the correlated system reduces to a simple expression \( S = S_{\text{exc}} \), where \( S_{\text{exc}} \) is the entropy of the excited states treated disregarding correlations.

Hence, the system of correlated particles in the canonical ensemble can be replaced by an effective model which omits correlations but excludes the ground-state contribution. In this model, the constrained canonical partition function (2) is replaced with the unconstrained partition function

\[
Z = \sum_{\{\hat{n}\}} \exp \left( -\frac{E_{\{\hat{n}\}}}{k_B T} \right),
\]

where summation is taken over microstates \( \{\hat{n}\} = \{n_1, n_2, \ldots\} \) that do not contain the ground state.

Equation (10), however, is simply the partition function in the grand canonical ensemble with zero chemical
potential \( \mu \). Recall that in the grand canonical ensemble the grand canonical partition function is given by

\[
Z_{\mu} = \sum_{\{n\}} \exp \left( \frac{\mu N_{\{n\}} - E_{\{n\}}}{k_B T} \right),
\]

where \( N_{\{n\}} \) is the number of particles in the microstate \( \{ n \} \) that has energy \( E_{\{n\}} \). For an ideal Bose gas, \( Z_{\mu} \) reduces to

\[
Z_{\mu} = \prod_{i=0}^{\infty} \frac{1}{1 - \exp \left( \frac{\mu - \mu_i}{k_B T} \right)},
\]

In terms of \( Z_{\mu} \), the entropy is given by

\[
S = k_B \frac{\partial [T \ln(Z_{\mu})]}{\partial T} \Bigg|_{V,\mu}.
\]

Our findings indicate that below \( T_c \), the entropy in the canonical ensemble can be very accurately calculated using the grand canonical formula with zero chemical potential in which contribution from the ground state is excluded. Namely, the canonical partition function is approximated as
which yields the following expression for the entropy

\[ S = \ln(1 \text{ exp} \left( \frac{\varepsilon}{k_B T} \right)). \]

It is interesting to compare equation (13) with the exact canonical partition function for \( N \) particles in one-dimensional harmonic trap [26]

\[ Z_N = \prod_{\nu=1}^{N} \frac{1}{1 - \exp\left( -\frac{\varepsilon_{\nu}}{k_B T} \right)}. \]

To illustrate the accuracy of equation (14), we calculate entropy for \( N = 1000 \) particles in the harmonic trap numerically using equations (4), (7) for the canonical ensemble and equation (14). Figure 5 shows entropy \( S \) as a function of temperature \( T \) obtained in the two approaches. The two curves are essentially identical below \( T_c \). In figure 6 we plot the relative difference between the two curves for \( N = 200 \) and 1000. The figure shows that for \( N = 1000 \) the relative difference is smaller than \( 10^{-20} \) when \( T < 0.77 T_c \).

Since other thermodynamic quantities can be expressed in terms of the entropy, they also can be very accurately calculated using the simplified effective model. For example, the mean energy of the system can be...
obtained from equation (5), which then can be used to calculate Helmholtz free energy $F = E - TS$ and heat capacity.

The result obtained above by numerical calculations can be also proved analytically. Indeed, canonical partition function (2) involves summation over particle configurations \( \{ n \} = \{ n_0, n_1, \ldots \} \). Separating the sum over \( n_0 \) and introducing summation index \( \delta n_0 \) we obtain

\[
Z_N = \sum_{n_0 = 0}^{N} \sum_{\{ \delta \}} \exp \left( - \frac{E(\delta)}{k_b T} \right) \delta n_0 + n_1 + \ldots
\]

\[
= Z = \sum_{n = N+1}^{\infty} \sum_{\{ \delta \}} \exp \left( - \frac{E(\delta)}{k_b T} \right) \delta n_0 + n_1 + \ldots,
\]

where \( Z \) is the grand canonical partition function with \( \mu = 0 \) and no ground-state contribution given by equation (10). Dividing both sides by \( Z \) yields

\[
\frac{Z - Z_N}{Z} = P_{n > N},
\]

where \( P_{n > N} \) is the probability that in the grand canonical ensemble with \( \mu = 0 \) the number of particles in excited states \( n \) is greater than \( N \). Below \( T_c \) this probability is exponentially small. One can estimate \( P_{n > N} \) by approximating the distribution function for the particle number in the excited states \( P_n \) as Gaussian

\[
P_n = \frac{1}{\sqrt{2\pi}\sigma^2} \exp \left( - \frac{(n - \bar{n})^2}{2\sigma^2} \right)
\]

with average

\[
\bar{n} = \sum_{\nu = 1}^{\infty} \bar{n}_\nu
\]

and variance

\[
\sigma^2 = \sum_{\nu = 1}^{\infty} \sigma^2_\nu = \sum_{\nu = 1}^{\infty} (\bar{n}_\nu^2 + \bar{n}_\nu),
\]

where \( \bar{n}_\nu = 1/(e^{\bar{E}_\nu/k_b T} - 1) \). For the isotropic harmonic trap in the thermodynamic limit we have [19]

\[
\bar{n} = N \left( \frac{T}{T_c} \right)^3, \quad \sigma^2 = \frac{\zeta(2)}{\zeta(3)} \bar{n}
\]

and \( P_{n > N} \) is given by

\[
P_{n > N} = \frac{1}{2} - \frac{1}{2} \text{erf} \left( \frac{N - \bar{n}}{\sqrt{2} \sigma} \right)
\]

where \( \text{erf}(x) \) is the error function. For \( N - \bar{n} \gg \sqrt{\bar{n}} \) using the asymptotic of the error function \( \text{erf}(x) \approx 1 - \exp(-x^2)/\sqrt{\pi} x \) we obtain that \( P_{n > N} \) is exponentially small, namely

![Figure 6. Relative difference between exact entropy in the canonical ensemble $S_{\text{can}}$ and approximate expression $S_{\text{GC}}$ given by formula (15) for $N = 200$ and $1000$ particles in isotropic harmonic trap.](image-url)
\[
P_{n>N} = 0.47 \frac{\sqrt{\bar{n}}}{\bar{n}_0} \exp \left( -0.37 \frac{\bar{n}_0^2}{\bar{n}} \right).
\]

Here \( \bar{n}_0 = N - \bar{n} \) is the average number of particles in the ground state. For \( T \ll T_c \), \( P_{n>N} \) is proportional to the exponentially small factor \( \exp (-0.37NT_c^2/T^3) \). Thus, below \( T_c \), the canonical partition function \( Z_N \) is equal to \( Z \) with exponential accuracy.

Plugging \( Z_N \approx Z \) in equation (8) yields that statistics of particles in the excited levels is accurately described by the equation

\[
P_{0,n} = (1 - e^{-\epsilon_n/k_B T}) e^{-\epsilon_n/k_B T}
\]

which coincides with the photon distribution in a thermal field. Equation (15) is not applicable for the ground state: \( P_{0,0} \) can be obtained as a mirror image of statistics of the number of particles in the excited states: \( P_{0,0} = P_{N-n} \).

Our findings can be understood from the following arguments. Below \( T_c \), the noncondensate particles can be treated as being in contact with a big reservoir of condensate particles. As a consequence, description of the noncondensate particles in the grand canonical picture is accurate below \( T_c \). In this picture there is no correlation between excited levels and fluctuations of particles at the excited states occur mainly via their exchange with the large condensate reservoir. However, such exchange yields correlations between the ground and excited states. Since fluctuations of particles in the ground state is the mirror image of the noncondensate particle fluctuations (which are already included in the grand canonical picture) the addition of the ground state to the system should not change the total entropy. Thus, the ground-state contribution must be cancelled by the term describing correlation between ground and excited states.

In summary, we show that in canonical ensemble below the temperature of BEC transition the correlation part of the entropy of an ideal Bose gas is equal to the ground-state contribution with the opposite sign. Thus, in the BEC region, the thermodynamic properties of the gas in the canonical ensemble can be accurately described in a simplified model which excludes the ground state and assumes no correlation between excited levels. Mathematically, the model corresponds to the grand canonical description with zero chemical potential and no ground state. Our findings provide new insight on the canonical ensemble correlations and yield substantial simplification of calculation of various thermodynamic quantities in the canonical ensemble.

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