Thermodynamic identities and particle number fluctuations in weakly interacting Bose–Einstein condensates

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We derive exact thermodynamic identities relating the average number of condensed atoms and the root–mean–square fluctuations determined in different statistical ensembles for the weakly interacting Bose gas in a box. This is achieved by introducing the concept of auxiliary partition functions for model Hamiltonians that do conserve the total number of particles. Exploiting such thermodynamic identities, we provide the first, completely analytical prediction of the microcanonical particle number fluctuations in the weakly interacting Bose gas. Such fluctuations, as a function of the volume \( V \) of the box are found to behave normally, at variance with the anomalous scaling behavior \( V^{4/3} \) of the fluctuations in the ideal Bose gas.

After the experimental achievement of Bose–Einstein condensation in trapped, cold gases of weakly interacting neutral Bose atoms [1]–[3], a flow of experimental data on the statistical properties of the condensate fraction has become available for theoretical study [4]. Among others, the issue of the fluctuations in the number of condensed atoms is of central importance, and it is foreseeable that it will become experimentally testable in the near future.

Experimentally, the trapped atoms are in a situation of almost complete isolation with respect to the outer environment surrounding the trap: the total number of particles is certainly conserved, while energy exchange with the environment is small, in some cases even negligible. Therefore, the relevant statistical ensemble to consider when attempting to compute the fluctuations should be the canonical or, even more appropriate, the microcanonical one.

For the ideal Bose gas, the fluctuations of the condensate fraction were calculated in a series of papers [5]–[11], both in the microcanonical and the canonical ensembles by a variety of approximate methods: both numerical (based on recurrence formulae and on contour integration) and analytic (asymptotic formulae based on the notion of the Maxwell Demon ensemble), for various trapping potentials and in different number of dimensions.

On the other hand, the issue of fluctuations in the weakly interacting Bose gas is not as well defined, both because there is no unambiguous way of defining the condensate fraction and because the approximate dynamics and energy spectra can be defined in a number of different ways, yielding different model–dependent predictions.

Of the few existing attempts to address the problem, we should mention in particular the calculation of the fluctuations of the interacting Bose gas trapped in a box, that was developed analytically in the canonical ensemble assuming the Bogoliubov number nonconserving description [12]. In this framework, it was predicted an anomalous scaling of the fluctuations with the volume \( V \) of the box, \( < \delta^2 N_0 >, \sim V^{4/3} \) analogous to that of the ideal Bose gas. However, this result can be questioned on the grounds that it has been derived assuming the condensate to act as a particle reservoir, and moreover that in the actual experimental situations the total number of particles \( N \) is a good quantum number.

It is therefore sensible to set up model calculations that avoid these features, and to compare the results thus obtained. As a first step, the fluctuations were calculated analytically in the canonical ensemble and numerically in the microcanonical ensemble, assuming different standard approximate spectra (respectively, the one obtained in Hartree–Fock theory, the two–gas model obtained by reduction of the Bogoliubov approximation, and the spectrum obtained in lowest order perturbation theory). It was shown that the fluctuations are very sensitive to the details of the approximation, resulting in large discrepancies between the different models [13]. On the other hand, they all satisfy the criterion of conservation of the total number of particles, while the lowest order perturbative spectrum includes three– and four–body contributions to the dynamics.

In this letter we address the issue of computing analytically the fluctuations of the condensate fraction in the microcanonical ensemble for a specific number–conserving model interaction. By introducing a so–called auxiliary canonical partition function, defined below, we prove by saddle point evaluation and with the help of standard thermodynamic Legendre transformations that for all model Hamiltonians that do conserve the total number of particles, the microcanonical fluctuations can be expressed in terms of the canonical moments exactly as in the case of the microcanonical fluctuations in the ideal Bose gas [4].

On the other hand, the canonical moments are modified in the presence of the interaction, and so is the final analytic
expression of the microcanonical fluctuations, which we are able to compute. At small but finite coupling (scattering length) the fluctuations scale linearly with the volume $V$ of the box, showing no anomalous behavior. In all actual calculations we assume for the interacting system the energy spectrum obtained in lowest order perturbation theory \cite{14}.

The Bose–Einstein condensation manifests itself in the macroscopic occupation of one of the eigenmodes. In general, the eigenfunctions of the single particle density matrix depend on the total number of atoms $N$, on the trapping potential, on the interatomic interactions and on the statistical ensemble of the system. The exceptionally simple, and hence the best studied, is the case of a system confined in the box with periodic boundary conditions. In this case the single particle density matrix is translationally invariant and periodic, so its spectral decomposition is just the Fourier series, and the index $j$ is the quantized momentum $p = (2\hbar \pi / L)(n_x, n_y, n_z)$, where $L$ is the size of the box.

We are interested in the statistics of a weakly interacting Bose gas for temperatures below the condensation temperature. In this regime, the system may be viewed as being composed of two macroscopic subsystems, a condensate just the Fourier series, and the index $j$ is the quantized momentum $p = (2\hbar \pi / L)(n_x, n_y, n_z)$, where $L$ is the size of the box. In this regime, the system may be viewed as being composed of two macroscopic subsystems, a condensate and the excited subsystem. In this case the single particle density matrix is translationally invariant and periodic, so its spectral decomposition is just the Fourier series, and the index $j$ is the quantized momentum $p = (2\hbar \pi / L)(n_x, n_y, n_z)$, where $L$ is the size of the box.

After splitting the system into its condensed and excited parts we will have to define the approximate dynamics. This needs not to be specified as long as we are concerned with general thermodynamic arguments, but only in the actual calculations.

One commonly made assumption is to neglect the interatomic interaction within the excited subsystem. Thus, the states of the excited atoms are still single particle states in a box, since the condensate is uniform. Accordingly, the energy of the excited subsystem is given by

$$E_{\text{ex}} = \sum_{p \neq 0} \frac{p^2}{2m} \eta_p.$$  \hspace{1cm} (1)

To fully define the problem, we need to specify the relation between the total energy of the system $E$ and $E_{\text{ex}}$, subject to the requirements that the total number of atoms $N$ be a good quantum number, and that higher order contributions beyond the two-body ones be included. We will hence adopt the spectrum obtained in lowest order perturbation theory \cite{14} in its simplified form by neglecting the terms proportional to the product of excited occupation numbers:

$$E(N, N_{\text{ex}}) = \alpha(N^2 + 2N N_{\text{ex}} - N_{\text{ex}}^2) + E_{\text{ex}},$$  \hspace{1cm} (2)

where

$$\alpha = \frac{2\pi \hbar^2}{mV},$$  \hspace{1cm} (3)

and $\alpha$ is the scattering length.

The above, like the other mentioned approximate spectra, depends only on the total number of atoms $N$ and on the total number of excited atoms $N_{\text{ex}}$ (or, equivalently, on $N$ and $N_0$), and not on the detailed distribution among excited states.

To calculate the canonical expressions for mean values and fluctuations and to relate them to the microcanonical ones in an exact thermodynamic setting, we may now proceed as follows: we define an auxiliary canonical partition function for exactly $N$ particles, by introducing the chemical potential $\mu_{\text{ex}}$ pertaining to the subsystem of excited atoms:

$$Z_{\text{aux}}(N, \beta, \mu_{\text{ex}}) = Tr_{N} \left[ \exp \left( - (\beta H - \mu_{\text{ex}} N_{\text{ex}}) \right) \right] = \sum_{N_{\text{ex}}} \exp \left[ - \mu_{\text{ex}} N_{\text{ex}} \right] Z_{\text{ex}}(N, N_{\text{ex}}; \beta).$$  \hspace{1cm} (4)

The crucial observation is now that differentiating the free energy with respect to $\mu_{\text{ex}}$ and evaluating the derivative at $\mu_{\text{ex}} = 0$ yields the canonical average $<N_0>_c$. Furthermore, since $N_{\text{ex}}$ commutes with the total Hamiltonian, second derivative evaluated at $\mu_{\text{ex}} = 0$ yields the canonical fluctuations $<\delta^2 N_0>_c$.

To proceed, one determines first $\ln Z_{\text{ex}}$ by the method of the most probable value. This is done expressing $Z_{\text{ex}}$ in terms of the associated generating function, i.e. the grand–canonical partition function $\Xi_{\text{ex}}$. As explained below, this introduces a further chemical potential $\mu_s$, not to be confused with the chemical potential $\mu_{\text{ex}}$ of the excited atoms introduced in Eq. (1). The saddle point value $\bar{\mu}_s$ of this chemical potential is fixed by the value $\bar{N}_{\text{ex}}$ of $N_{\text{ex}}$ for which $\ln Z_{\text{ex}}$ acquires its maximum. Standard calculations lead to the following expression for the most probable value:
\[ \ln Z_{ex}(N, \bar{N}_{ex}, \beta) = -\beta E(N, \bar{N}_{ex}) + \bar{\mu}_s \bar{N}_{ex} - V \left( \frac{m}{2\pi \beta \hbar^2} \right)^{3/2} g_{5/2}(\exp(-\bar{\mu}_s)), \]  

where \( g_{5/2} \) is the Bose function of order 5/2 and \( \bar{\mu}_s = 2\beta \alpha(N - \bar{N}_{ex}) \) is positive defined. To simplify notations, we have absorbed a factor \( \beta \) in the definition, so that \( \bar{\mu}_s \) is adimensional, in contrast to the chemical potential \( \mu_{ex} \).

Saddle point evaluation of the total free energy at the equilibrium value \( \bar{N}_{ex} \) can now be performed to yield

\[ \ln Z_{aux}(N, \beta, \mu_{ex}) = \ln Z_{ex}(N, \bar{N}_{ex}, \beta) + \beta \mu_{ex} \bar{N}_{ex} + \frac{1}{2} (\beta \mu_{ex})^2 \frac{\partial^2 \ln Z_{ex}(N, \bar{N}_{ex}, \beta)}{\partial \bar{N}_{ex}^2}. \]  

We see by immediate inspection that the first derivative with respect to \( \mu_{ex} \) evaluated at the equilibrium value \( \mu_{ex} = 0 \) yields the canonical mean value \( \langle N_{ex} \rangle_{cn} = \bar{N}_{ex} \), while the second derivative (again evaluated at \( \mu_{ex} = 0 \)) yields the canonical root–mean–square fluctuations \( \langle \delta^2 N_{ex} \rangle_{cn} = \frac{\partial^2 \ln Z_{ex}}{\partial N_{ex}^2} \).

The implicit equation satisfied by the canonical mean number of condensed atoms \( \langle N_0 \rangle_{cn} = \bar{N}_0 \) is \( \bar{N}_{ex} = N - \bar{N}_0 \), where the latter term reads:

\[ N - \bar{N}_0 = V \left( \frac{m}{2\pi \beta \hbar^2} \right)^{3/2} g_{3/2}(\exp(-2\alpha(N - \bar{N}_{ex}))), \]  

where the Bose–Einstein function \( g_n(s) = \sum_{l=1}^{\infty} s^l / l^n \). In the same approximation the canonical fluctuations read

\[ \langle \delta^2 N_0 \rangle_{cn} = \left[ \left( \sum_{p \neq 0} 4 \sinh^2 \left( \frac{\beta}{2} \left( \frac{\beta p^2}{2m} + 2\alpha(N - \bar{N}_{ex}) \right) \right) \right)^{-1} - 2\alpha \beta \right]^{-1}. \]  

These expressions, as it should be, coincide with the ones already obtained by Idziaszek et al. \[13\] in the standard canonical setting. Now, by applying twice the Legendre transformation we can express the microcanonical thermodynamic derivatives (fundamental variables: \( E, N \)) in terms of the canonical ones (fundamental variables: \( \beta, N \)). One has:

\[ \langle \delta^2 N_0 \rangle_{mc} = \frac{\partial^2 \ln Z_{aux}}{\partial \mu_{ex}^2} \bigg|_{\mu_{ex}=0; \beta} + \frac{\partial \beta}{\partial \mu_{ex}} \bigg|_{\mu_{ex}=0; E} \times \frac{\partial^2 \ln Z_{aux}}{\partial \beta \partial \mu_{ex}} \bigg|_{\mu_{ex}=0; \beta}. \]  

The above expression for the microcanonical fluctuations can be recast by simple thermodynamic manipulations in a more transparent form. By noting that

\[ \frac{\partial^2 \beta}{\partial \mu_{ex}^2} \bigg|_{\mu_{ex}=0; E} = - \frac{\partial E}{\partial \mu_{ex}} \bigg|_{\mu_{ex}=0; \beta} \times \frac{\partial \beta}{\partial E} \bigg|_{\mu_{ex}=0}, \]  

we can write

\[ \langle \delta^2 N_0 \rangle_{mc} = \langle \delta^2 N_0 \rangle_{cn} - \frac{\langle \delta N_0 \delta E \rangle_{cn}^2}{\langle \delta^2 E \rangle_{cn}}. \]  

Relation (11) is our first main result. It coincides with the formula derived by Navez et al. \[9\] for the ideal Bose gas. We thus find that the general structure of thermodynamics and thermodynamical fluctuations is not modified by the presence of a model interaction that conserves the total number of particles. In other words, our analysis satisfies the general principle that the thermodynamic relations between different statistical ensembles should be independent of the dynamics (the Hamiltonian), a principle that is violated when resorting to Bogoliubov theory.
Direct analytic evaluation of the microcanonical fluctuations is now possible by computing the derivatives of the approximate free energy (Eq. (6)) appearing in Eq. (9). The final result is:

\[ < \delta^2 N_0 >_{mc} = < \delta^2 N_0 >_{cn} - \frac{[A(\beta)F(\beta, \bar{\mu}_s)]^2}{G(\beta, \bar{\mu}_s)}, \quad (12) \]

where

\[ A(\beta) = V \left( \frac{m}{2\pi \hbar^2} \right)^{3/2}, \]

\[ F(\beta, \bar{\mu}_s) = \frac{3g_{3/2}(\exp(-\bar{\mu}_s)) + 4\alpha \beta \bar{N}_0 g_{1/2}(\exp(-\bar{\mu}_s))}{2\beta[1 - 2A(\beta)\alpha g_{1/2}(\exp(-\bar{\mu}_s))]}, \]

\[ G(\beta, \bar{\mu}_s) = \frac{3}{2}A(\beta) \left[ \frac{\bar{\mu}_s}{\beta^2} - 2\alpha \frac{\partial \bar{N}_0}{\partial \beta} \right] g_{3/2}(\exp(-\bar{\mu}_s)) + \frac{\bar{\mu}_s}{\beta} \frac{\partial \bar{N}_0}{\partial \beta} + \frac{15}{4\beta^2}A(\beta)g_{5/2}(\exp(-\bar{\mu}_s)). \quad (13) \]

The above expression is our second main result. It generalizes the microcanonical fluctuations of the number of condensed atoms in the ideal Bose gas to the interacting case. For small values of the coupling \( \alpha \) (i.e. of the scattering length \( a \)) we can exploit the Robinson–Kac representation of the Bose \( g \) functions [17] up to terms linear in \((-\bar{\mu}_s)^{1/2}\). In this situation, the canonical fluctuations behave normally (scaling linearly with \( V \)) as already shown by Idziaszek et al. [13], while the second term in the right–hand–side of Eq. (12), up to order \( \bar{\mu}_s^{1/2} \) reduces to

\[ -\frac{3A(\beta)}{5g_{5/2}(1)} \left[ g_{3/2}(1) + 2\sqrt{\bar{\mu}_s}^{1/2} \right]^2. \quad (14) \]

It is straightforward to verify that this term too scales linearly with \( V \), also in the thermodynamic limit \( V \rightarrow \infty \), \( N \rightarrow \infty \), \( N/V = const. \) Therefore the total microcanonical fluctuations scale linearly with the volume of the box, and show no anomalous behavior for any finite value of the coupling. Obviously, in our model the thermodynamic limit does not commute with the weak coupling limit, and to recover the anomalous scaling of the fluctuations in the ideal Bose gas one must first perform the thermodynamic limit and then go to the limit \( a \rightarrow 0 \) of vanishing scattering length.

In Fig. 1 the microcanonical root–mean–square fluctuations Eq. (14) are plotted (dotted line) and compared to the canonical results Eq. (14) of Ref. [12] (dot–dashed line), to the canonical fluctuations computed in the framework of Bogoliubov theory, Eq. (8) of Ref. [12] (dashed line) and to the ideal Bose gas behavior (solid line). The fluctuations are plotted as a function of the temperature for \( N = 10^4 \) particles and \( a/L = 5 \times 10^{-4} \). The temperature is measured in units given by the spacing between the two lowest levels in the 3D box: \( \Delta = (2\pi \hbar)^2/(2mL^2) \). The inset displays results for \( N = 10^6 \) and \( a/L = 5 \times 10^{-5} \); the curves correspond to our microcanonical result (dashed), the ideal Bose gas (solid), and the canonical results of Ref. [12] (dashed). The canonical results of Ref. [13] are not shown in the inset because with increasing number of particles they become indistinguishable from the microcanonical prediction, as expected.

We see that our result (14) is in marked disagreement with the predictions obtained in [12]. The emerging picture of ideal versus weakly interacting Bose systems is then the following. In the framework of Bogoliubov approximation: the anomalous scaling behavior of the ideal gas fluctuations is preserved; the general thermodynamic relation between ideal gas fluctuations computed in different ensembles is lost. In the framework of number conserving approximations: the scaling behavior of the ideal Bose gas fluctuations is modified; the ideal Bose gas thermodynamic relations are preserved.

To summarize, we have performed a model calculation of the microcanonical fluctuations of the weakly interacting Bose–Einstein condensate, allowing for analytical solution, to provide a first prediction that may be tested against experiment. We stress this point, since in the real experimental situations the trapped gases are usually in conditions of fantastic isolation, and thus the microcanonical result should be the one to be compared with actual experimental observations (when they will become available).

At variance with the canonical fluctuations predicted in the framework of Bogoliubov theory [12], we find no anomalous scaling of the microcanonical fluctuations for any finite value of the scattering length. On the other hand, exact knowledge of the full energy spectrum is available only for the one–dimensional chain of interacting bosons [16]. In this case, comparison of the exact solution with Bogoliubov theory shows that the Bogoliubov spectrum accounts
only for some subset of the low–lying elementary excitations. The situation for Bogoliubov theory is likely to be even worse in higher dimensions. Furthermore, phonons are collective excitations which do not necessarily change the number of particles in the condensate. It is therefore hardly conceivable that they should play an important role in determining the equilibrium fluctuations in the occupation number, and may therefore be safely ignored in first approximation.

Some of the most subtle aspects of the dynamics and statistical mechanics of many–body interacting Bose systems appear in the above discussion: care is needed in handling the different limits, whose order cannot in general be interchanged, while the non–trivial thermodynamic identities, relating the different statistical ensembles at the level of fluctuations, are found to hold true just as in the case of the ideal Bose gas \[15\].

Looking at the future perspectives, we expect that achieving a deeper understanding of the thermodynamic properties in exactly solvable instances such as the Lieb model in one dimension would be of great help, and studies addressing this problem are currently under way. On the experimental side, we hope that the measurement of the second–order correlation function \(g_2(r_1,r_2)\) will soon become available, allowing for a direct test of the different theoretical predictions.

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FIG. 1. Root–mean–square fluctuations of the ground state occupation number for \(N = 10^4\) and \(a/L = 5 \times 10^{-4}\). Displayed are (i) our microcanonical result Eq. (14) (dotted), (ii) Eq. (14) of Ref. \[13\] (dot–dashed), (iii) the ideal Bose gas (solid line), and (iv) Eq. (8) of Ref. \[12\] (dashed). Inset: root–mean–square fluctuations for \(N = 10^6\) and \(a/L = 5 \times 10^{-5}\). Displayed are (i) our microcanonical result (dotted), (ii) the ideal Bose gas (solid line), and (iii) Eq. (8) of Ref. \[12\] (dashed).

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