

Fluctuation statistics of mesoscopic Bose-Einstein condensates: Reconciling the master equation with the partition function to reexamine the Uhlenbeck-Einstein dilemma

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The atom fluctuation statistics of an ideal, mesoscopic, Bose-Einstein condensate are investigated from several different perspectives. By generalizing the grand canonical analysis (applied to the canonical ensemble problem), we obtain a self-consistent equation for the mean condensate particle number that coincides with the microscopic result calculated from the laser master equation approach. For the case of a harmonic trap, we obtain an analytic expression for the condensate particle number that is very accurate at all temperatures, when compared with numerical canonical ensemble results. Applying a similar generalized grand canonical treatment to the variance, we obtain an accurate result only below the critical temperature. Analytic results are found for all higher moments of the fluctuation distribution by employing the stochastic path integral formalism, with excellent accuracy. We further discuss a hybrid treatment, which combines the master equation and stochastic path integral analysis with results obtained based on the canonical ensemble quasiparticle formalism [Kocharovskiy *et al.*, Phys. Rev. A **61**, 053606 (2000)], producing essentially perfect agreement with numerical simulation at all temperatures.

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I. INTRODUCTION

The problem of fluctuation statistics in a mesoscopic Bose-Einstein condensate (BEC) is a rich one—even, somewhat surprisingly, for the noninteracting Bose gas, as well as for the interacting Bose gas [1]. Take, for example, a trapped gas of N bosons, and lower the temperature below the critical temperature T_c to form a condensate. Count the number of atoms that are in the condensate. Do this many times at the same temperature and total boson number N to get the statistics. What is the distribution of the condensed atoms, and how does it change when moving the temperature through T_c ? The noninteracting, mesoscopic Bose gas is a problem whose fluctuation characteristics are still not completely understood. Contrary to standard lore, we stress that the fluctuations are not Gaussian, even in the thermodynamic limit. The discussion goes back to the Uhlenbeck-Einstein dilemma [2,3]: Uhlenbeck's criticism that Einstein's expression for the average boson number $\langle n_0 \rangle$ had an abrupt cusp at T_c . The manner in which this cusp is smoothed by fluctuations is of great interest for mesoscopic systems, which is one focus of the present paper. Even more subtle is the question of the higher-order moments of the condensate fluctuations, especially in the vicinity of T_c .

Despite the conceptual simplicity of the above question, the fluctuation statistics are not known analytically, because while the canonical ensemble partition function can be formally written, it can be accurately calculated only numerically. We note that the work by Holthaus and Kalinowski obtains accurate approximations for the first few moments, employing a refined saddle-point approximation of the canonical partition function [4]. However, the equation for the saddle point still has to be solved numerically.

The time-dependent master equation is an excellent alternative approach to attack this question, developed in the pioneering papers of Scully [5] (hereafter referred to as CNB1) and Kocharovskiy, Scully, Zhu, and Zubairy [6] (hereafter referred to as CNB2). This approach is capable of investigating dynamical phenomena, as well as being a viable option when we include interactions, or when the system is out of equilibrium. The master equation approach, within the canonical framework, has successfully calculated moments of the fluctuation distribution to good accuracy. Other advantages of this method are that it provides a simple physical picture of the condensation process with a gas of cold atoms via a detailed balance of the elementary processes of heating and cooling, and that the theory shows a vivid analogy between atomic BEC and the photon laser by demonstrating that the BEC and laser master equations are identical. This analogy can explain the atom-laser linewidth [7], and might also be able to explain the transient dynamics of the phase transition to the BEC. In the master equation approach, the cooling of the BEC is accomplished by the noncondensate interaction with a thermal environment. In typical BEC experiments, the cooling is accomplished with evaporative techniques. However, in the experiments by Reppy and co-workers [8], the BEC was cooled by a thermal reservoir associated with the Vycor glass host—exactly the situation we presently consider. The master equation takes a given bath model for the calculation, so one natural question is if a different bath model alters the physics of the BEC statistics. While different models will certainly alter the dynamics of the condensation, we expect the statistics to be robust, just as the analogous partition function is.

How does all of this relate to traditional statistical physics, in particular the microcanonical, canonical, and grand

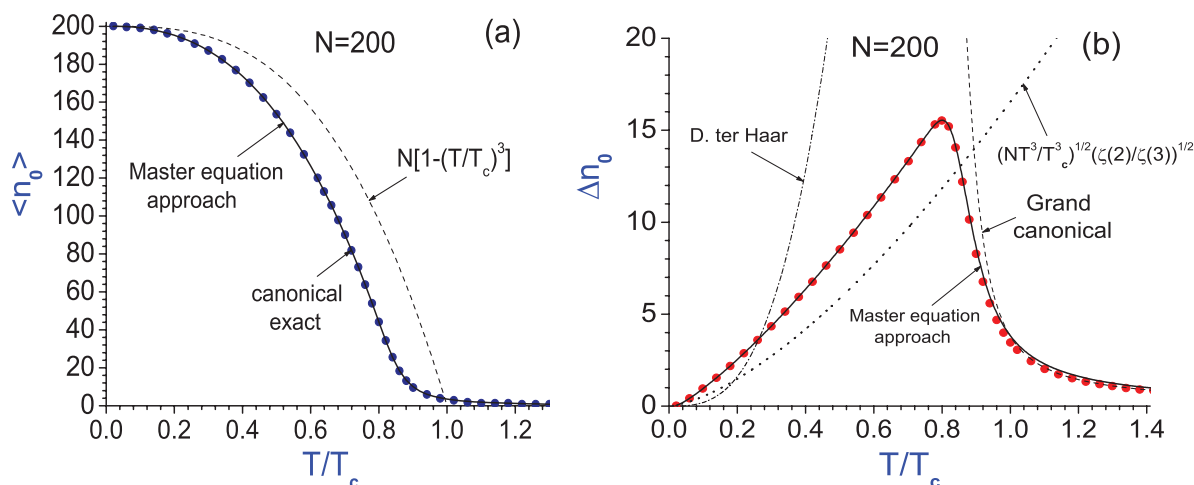


FIG. 1. (Color online) (Left) The average boson number in the condensate is plotted versus temperature. The master equation approach (solid line) is compared with numerical simulation of canonical results (dots), as well as the thermodynamic limit (dashed line). (Right) The variance of the distribution is plotted versus temperature. The grand canonical result (dashed line) deviates near and below the critical temperature, leading to the grand canonical catastrophe. The results of ter Haar [10] (dash dotted line) and Politzer [11] (small dots) (derived in the thermodynamic limit) are also shown. The results are shown for $N=200$ particles in a harmonic trap.

canonical formalism? Recall that Einstein predicted BEC by analyzing the grand canonical formula [9]. Both grand canonical ensemble and canonical ensemble approaches describe the occurrence of BEC equally well in the dramatic rise of the mean condensate number $\langle n_0 \rangle$ in the ground state. However, near the critical temperature and below, the grand canonical approach gives grossly different results for the variance and higher moments, the so-called “grand canonical catastrophe” illustrated in Fig. 1(b).

The question of fluctuations in Bose-Einstein condensation has attracted renewed interest. Grossmann and Holthaus [12,13] previously obtained an analytical expression for the mean condensate particle number in a harmonic trap for finite N using the grand canonical approach. However, their analytical expression does not show a smooth crossover near T_c . Grossmann and Holthaus [12] and Ketterle and Druten [14] found the crossover behavior only by numerical solution of the equation for the condensate particle number. Politzer also obtains an approximate expression for the variance in the thermodynamic limit [11].

The purpose of the present paper is to report advances on several fronts. One goal is to connect the master equation formalism with the partition function analysis in thermal equilibrium. To this end, we review the master equation formalism, and derive an approximate result for the mean condensate particle number, which can be expressed in terms of elementary functions. This result is then connected with standard statistical mechanics by extending the grand canonical approach (applied to the canonical ensemble problem) to obtain an approximate result for the mean condensate particle number that is quite accurate through the critical temperature. This is done by deriving a self-consistent equation for the condensate particle number by eliminating the chemical potential. The equation may be approximately solved, and the solution exactly coincides with the approximate master equation result.

Next, we investigate fluctuations, a more subtle problem. The analogous treatment for the variance via the generalized

grand canonical analysis works quite well for low temperatures, but fails for temperatures near or greater than the critical temperature. In order to obtain a more accurate analytic result from the master equation approach, we first reformulated the master equation as a stochastic path integral. The stochastic path integral formalism [15,16] allows for an accurate approximation of all cumulants of the fluctuation statistics in terms of elementary functions, by applying the saddle-point approximation, whose large parameter is the number of condensed atoms. It is straightforward to generalize the results, and present the fluctuation statistics of a general boson master equation, with arbitrary heating and cooling coefficients.

Finally, by combining the master equation and stochastic path integral predictions with the previous results of Kocharovskiy *et al.* based on the canonical ensemble quasiparticle formalism [17] (hereafter referred to as CNB3), which is very accurate at low temperature, we are able to formulate a hybrid theory, whose results are in near-perfect agreement with exact numerical simulation. The idea is to use the low- T results of CNB3 to fix the values of three master equation parameters via the first three moments. Then the master equation predictions for several higher moments and cumulants are compared with the numerical results at all temperatures. They are in near-perfect agreement.

The paper is organized as follows. In Sec. II we review the master equation approach, and derive an approximate solution for the mean atom number in the condensate. This solution is connected with standard partition function methods in Sec. III by extending the grand canonical analysis, and deriving a self-consistent equation for the mean atom number, which coincides with the result of Sec. II. In Sec. IV, we consider a harmonic trap, and give improved analytic results for the heating coefficient. We go on to apply the extended grand canonical analysis to the variance of the distribution. In Sec. V, we give the stochastic path integral treatment of the problem, which yields approximate expression for all cumulants in terms of the master equation parameters. In Sec.

VI, we introduce a hybrid theory, combining the predictions of the master equation and stochastic path integral with those of CNB3 to obtain excellent agreement with numerical simulation. We conclude in Sec. VII. Appendixes A and B contain the details of the calculations for the grand canonical approach, and Appendix C contains the details of the stochastic path integral calculations.

II. MASTER EQUATION APPROACH

Let us review the results of the master equation approach. Consider a trapped Bose gas, whose single-particle energy levels are ϵ_k . The master equation formalism begins with the elementary transitions of atoms between the condensate and noncondensate. We are primarily interested in the condensate statistics, and therefore focus on the probability p_{n_0} of having n_0 atoms in the condensate, given that there are N total atoms. The master equation describing the heating and cooling processes of a Bose-Einstein condensate is given by [5]

$$\dot{p}_{n_0} = -\kappa[K_{n_0}(n_0+1)p_{n_0} - K_{n_0-1}n_0p_{n_0-1} + H_{n_0}n_0p_{n_0} - H_{n_0+1}(n_0+1)p_{n_0+1}], \quad (1)$$

where in the low-temperature limit

$$K_{n_0} = N - n_0, \quad H_{n_0} = \mathcal{H}, \quad (2)$$

$$\mathcal{H} = \sum_{k>0} \frac{1}{e^{\beta\epsilon_k} - 1}, \quad (3)$$

and κ is a rate constant. The steady-state solution for the distribution is [5]

$$p_{n_0} = \frac{N!}{(N-n_0)!} \frac{\mathcal{H}^{N-n_0}}{e^{\mathcal{H}} \Gamma(N+1, \mathcal{H})}, \quad (4)$$

where

$$\Gamma(N+1, x) = \int_x^\infty t^N e^{-t} dt \quad (5)$$

is an incomplete Gamma function. Higher-order moments may be found via $\langle n_0^s \rangle = \sum_{n_0} n_0^s p_{n_0}$. We introduce the notation $\mu_s \equiv \langle (n_0 - \bar{n}_0)^s \rangle$ for the central moments of the distribution. The equation for the probability distribution can also be converted to an equation for the mean atom number $\langle n_0 \rangle$ to find

$$\langle \dot{n}_0 \rangle = -\kappa[(-N+1+\mathcal{H})\langle n_0 \rangle - N + \langle n_0^2 \rangle]. \quad (6)$$

Approximating $\langle n_0^2 \rangle \approx \langle n_0 \rangle^2$, and considering the stationary case, the solution for $\langle n_0 \rangle$ is

$$\langle n_0 \rangle \approx \frac{1}{2} [N - \mathcal{H} - 1 + \sqrt{(N - \mathcal{H} - 1)^2 + 4N}]. \quad (7)$$

In contrast to CNB1, this approximate answer can be simply expressed in terms of \mathcal{H} and N , yet still catches the smooth transition in the vicinity of T_c (where $N - \mathcal{H} \sim \sqrt{N}$) (see Fig. 2 below). We will show in the next section that this same (approximate) result can be derived within the context of the

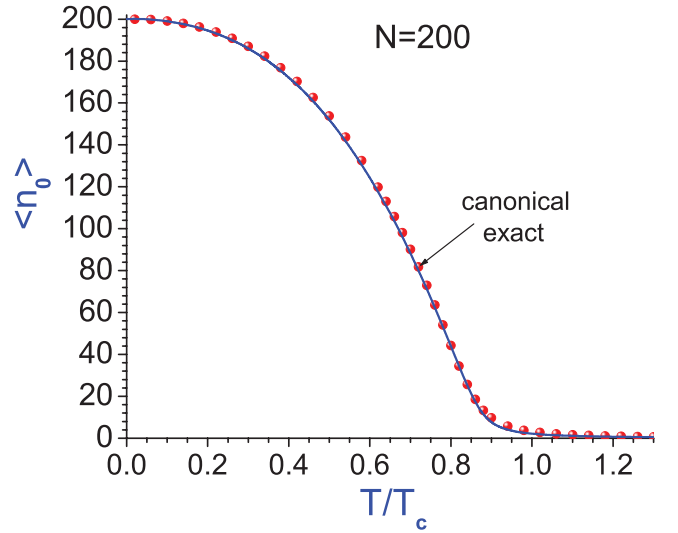


FIG. 2. (Color online) The average condensate particle number is plotted versus temperature for $N=200$ particles in an isotropic harmonic trap. The approximate analytic result given by Eqs. (7) [or (13)] and (14) (solid line) is compared with the “exact canonical dots” computed numerically, with good agreement.

grand canonical formalism, and later in Sec. V, how to derive similar results for all higher moments from the stochastic path integral formalism.

III. GRAND CANONICAL TREATMENT

In order to see how the same result for the average condensate particle number emerges from a modified grand canonical treatment, we recall that the grand canonical formula for the average of the total particle number N is [18]

$$N = \sum_{k=0}^{\infty} \frac{1}{e^{\beta(\epsilon_k - \mu)} - 1} = \sum_{k=0}^{\infty} \langle n_k \rangle, \quad (8)$$

where the sum runs over all states of energy ϵ_k , $\beta^{-1} = k_B T$, and the chemical potential μ is related to the mean condensate particle number $\langle n_0 \rangle$ as (we assume $\epsilon_0 = 0$)

$$\mu = -\beta^{-1} \ln \left(\frac{1}{\langle n_0 \rangle} + 1 \right). \quad (9)$$

Various thermodynamic quantities of the gas such as the chemical potential μ , the internal energy $U = \int \mu dN$, and the specific heat $C = dU/dT$ can be obtained analytically if we have an analytic expression for $\langle n_0 \rangle$. Equation (9) shows that μ is nonzero for finite N , in contrast to the thermodynamic limit $N \rightarrow \infty$ where μ vanishes.

By using Eq. (9), $\langle n_0 \rangle$ can be singled out from Eq. (8) as

$$N - \langle n_0 \rangle = \sum_{k>0} \frac{1}{(1/\langle n_0 \rangle + 1)e^{\beta\epsilon_k} - 1}, \quad (10)$$

which may be rewritten as

$$N - \langle n_0 \rangle = \frac{1}{(1/\langle n_0 \rangle + 1)} \sum_{k>0} \frac{1}{e^{\beta\epsilon_k} - \langle n_0 \rangle / (\langle n_0 \rangle + 1)}. \quad (11)$$

This gives a self-consistent equation for the mean particle number $\langle n_0 \rangle$. In the limit $\langle n_0 \rangle \gg 1$, the term $\langle n_0 \rangle / (\langle n_0 \rangle + 1)$ inside the summation may be approximated by 1. As in the previous section, we denote the summation over k as

$$\mathcal{H} = \sum_{k>0} \frac{1}{e^{\beta\epsilon_k} - 1}, \quad (12)$$

yielding a quadratic equation for the mean number of particles in the ground state

$$N - \langle n_0 \rangle = \frac{\mathcal{H}}{1/\langle n_0 \rangle + 1},$$

whose solution is

$$\langle n_0 \rangle = \frac{1}{2} [N - \mathcal{H} - 1 + \sqrt{(N - \mathcal{H} - 1)^2 + 4N}], \quad (13)$$

which exactly coincides with (7), linking the two approaches. It is natural to ask about the physical significance of this coincidence. The master equation result is derived from a particle-number-conserving formalism, which already has the canonical ensemble property built in. However, the master equation is solved approximately in Eq. (7) under the condition of large condensate particle number. On the other hand, the result of the grand canonical analysis, Eq. (13), is derived by trading the chemical potential for the average particle number, which corresponds to imposing the total particle number constraint on average. The resulting equation is further solved self-consistently, also under the large-condensate-number assumption. The coincidence of results in this approximation, and the excellent agreement with the numerical canonical ensemble simulation, indicates that a strict accounting of the canonical ensemble constraint is unnecessary for the calculation of $\langle n_0 \rangle$.

One should mention that the trick used in Eq. (11) is nontrivial. A straightforward expansion in $1/\langle n_0 \rangle$ yields very poor accuracy. We discuss this in Appendix A.

IV. ANALYTIC EXPRESSIONS FOR MEAN CONDENSATE PARTICLE NUMBER AND VARIANCE WITHIN THE GENERALIZED GRAND CANONICAL APPROACH

It is of interest to have an accurate analytic expression for the mean number of particles in a mesoscopic condensate that is valid for all temperatures. Let us specialize to the case of an isotropic harmonic trap. Single-particle energy levels are then $\epsilon_k = \hbar\Omega(l+m+n)$, where Ω is the trap frequency and $k = \{l, m, n\}$ denotes the quantum numbers. In this case, the coefficient \mathcal{H} can be evaluated approximately by the method shown in Appendix B. The idea of this method is to first convert the triple sum into a single sum, and then to approximate the single sum as an integral. We obtain

$$\mathcal{H} \approx \frac{\zeta(3)}{a^3} + \left(\frac{\pi}{2a}\right)^2 + \frac{1}{a}(\ln 2 - \ln a), \quad (14)$$

where $a = \beta\hbar\Omega$. The first term has been previously obtained in Ref. [12], and here we find subdominant corrections in a . Thus, we have an analytical expression for $\langle n_0 \rangle$ given by Eq. (13), where the term $N - \mathcal{H} - 1$ can be expressed as

$$N - \mathcal{H} - 1 \approx N \left[1 - \left(\frac{T}{T_c}\right)^3 \right] - \frac{\pi^2}{4} \left(\frac{N}{\zeta(3)}\right)^{2/3} \left(\frac{T}{T_c}\right)^2 - 1 + \left(\frac{N}{\zeta(3)}\right)^{1/3} \frac{T}{T_c} \left\{ \ln \left[\left(\frac{\zeta(3)}{N}\right)^{1/3} \frac{T_c}{T} \right] - \ln 2 \right\}, \quad (15)$$

and the critical temperature $T_c = [N/\zeta(3)]^{1/3} \hbar\Omega/k_B$ has been introduced. For large N , the second line of (15) may be neglected, and if we also take $(N - \mathcal{H} - 1)^2 \gg 4N$, then Eq. (13) reduces to Eq. (8) of Ref. [12]:

$$\langle n_0 \rangle \approx N \left[1 - \left(\frac{T}{T_c}\right)^3 \right] - \left(\frac{N}{\zeta(3)}\right)^{2/3} \left(\frac{\pi T}{2T_c}\right)^2, \quad (16)$$

which further reduces to $\langle n_0 \rangle \approx N[1 - (T/T_c)^3]$ in the thermodynamic limit.

We now consider fluctuations of the number of particles in the condensate, starting with the variance. The variance of the *condensate* particles can be expressed in terms of the *noncondensate* variance using the identity $n_0 = N - \sum_{k>0} n_k$. In the grand canonical approach, $\langle n_k^s \rangle$ can be evaluated from

$$\langle n_k^s \rangle = \frac{1}{Z_k} \sum_{n_k} n_k^s e^{-\beta(E_k - \mu)n_k} = \frac{1}{Z_k} \beta^{-s} \partial_\mu^s Z_k, \quad (17)$$

where $Z_k = (1 - e^{-\beta(E_k - \mu)})^{-1}$. It follows from Eq. (17) that

$$\langle n_k^2 \rangle = 2\langle n_k \rangle^2 + \langle n_k \rangle. \quad (18)$$

We then obtain

$$\begin{aligned} \mu_2 &= \langle (n_0 - \langle n_0 \rangle)^2 \rangle \approx \sum_{k>0} [\langle n_k^2 \rangle - \langle n_k \rangle^2] \approx \sum_{k>0} [\langle n_k \rangle^2 + \langle n_k \rangle] \\ &\approx \sum_{k>0} \left(\frac{1}{(Ae^{\beta\epsilon_k} - 1)^2} + \frac{1}{Ae^{\beta\epsilon_k} - 1} \right), \end{aligned} \quad (19)$$

where $A = 1 + 1/\langle n_0 \rangle$. We have assumed that fluctuations of n_k ($k \neq 0$) are uncorrelated ($\langle n_k n_m \rangle = \langle n_k \rangle \langle n_m \rangle$, $k \neq m$). This is the case provided $\langle n_0 \rangle$ is much larger than its variance, so that particle exchange with the condensate reservoir is the main channel of fluctuations of n_k . Near and above T_c , the correlations become substantial, which yields the failure of Eq. (19). Taking the chemical potential μ as given in (9) and using the method described in Appendix B, we find the following analytic expression for the variance in the generalized grand canonical analysis:

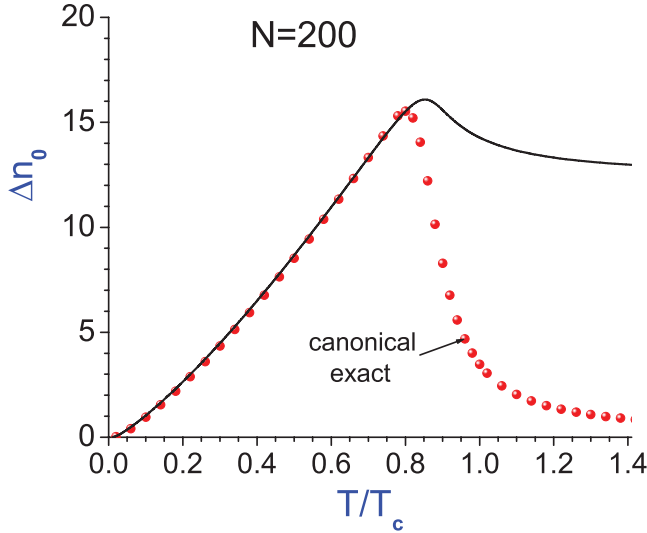


FIG. 3. (Color online) The variance of the condensate distribution is plotted versus temperature for $N=200$. The approximate analytic result within the generalized grand canonical approach (solid line) is compared with the exact dots computed numerically in the canonical ensemble. The analytic result is in good agreement for low temperature, but fails at temperatures comparable to the critical temperature and above. The reason for the high-temperature discrepancy is that the modified grand canonical theory neglects correlations between excited levels.

$$\begin{aligned} \mu_2 \approx & \frac{7Ae^{a/2} + 8}{8a(Ae^{a/2} - 1)} + \frac{3}{2a^2} \ln\left(\frac{A}{Ae^{a/2} - 1}\right) \\ & + \frac{1}{a^3} \left[\frac{\pi^2}{6} + \ln\left(\frac{Ae^{a/2} - 1}{\sqrt{A}}\right) \ln A + \text{dilog}(Ae^{a/2}) \right], \end{aligned} \quad (20)$$

where $a = \beta \hbar \Omega$ and $\text{dilog}(x) = \int_1^x dt \ln(t)/(1-t)$. In the limit $k_B T \gg \hbar \Omega$ and $\langle n_0 \rangle \gg 1$, Eq. (20) yields $\mu_2 \approx \pi^2/6a^3 = \pi^2 T^3 N/6T_c^3 \zeta(3)$ which agrees with Eq. (11) of Ref. [11].

The analytic results are compared with numerical simulation in Figs. 2 and 3. Figure 2 shows an excellent agreement between $\langle n_0 \rangle$ computed analytically from Eqs. (13) and (14) and the exact numerical simulation obtained in the canonical ensemble [19]. In Fig. 3 we plot the variance Δn_0 as a function of temperature obtained from Eq. (20) (solid line), as well as the exact canonical dots obtained from numerical computation [19]. While the analytic result is good at low temperature, at temperatures comparable to T_c and above, there is substantial deviation from the canonical ensemble

result because correlations between excited levels are neglected.

V. ANALYTIC EXPRESSION FOR ALL CUMULANTS VIA THE STOCHASTIC PATH INTEGRAL FORMALISM

While the master equation is a powerful approach, it is often the case that a simple analytic solution cannot be found. It is therefore of great interest to pursue alternative treatments that give an approximate analytic solution of the master equation that is asymptotically valid in the physically relevant limit of many particles in the condensate, $\langle n_0 \rangle \gg 1$. Just such an approach was developed in Refs. [15,16], by solving the fluctuation statistics problem with a stochastic path integral. The stochastic path integral formalism is complementary to the master equation approach as will be shown below. However, we stress that it can also be applied in cases where it is impossible to even write down a differential master equation, as demonstrated in Ref. [16].

The calculational details are given in Appendix C, but the basic idea is to translate the master equation into the stochastic path integral, whose action functional contains all rate information, and also imposes local particle conservation. The fluctuation statistics can then be calculated in saddle-point approximation by finding the “zero energy lines” of the dynamics—the statistical trajectory in phase space that is most likely, similar to the instanton trajectory of Ref. [20]. From this trajectory, the generating function may be found as an area in phase space.

Rather than solving the original master equation (1), we skip to the generalization of CNB2 [6], where

$$K_{n_0} = (N - n_0)(1 + \eta), \quad H_{n_0} = \mathcal{H} + (N - n_0)\eta, \quad (21)$$

which applies also to higher temperatures, and η is defined as

$$\eta = \mathcal{H}^{-1} \sum_{k>0} \frac{1}{(e^{\beta \epsilon_k} - 1)^2}. \quad (22)$$

We introduce the notation κ_n for the cumulants of the distribution [21], and define the nonstandard cumulant generating function $Q(\lambda)$ as

$$\kappa_s = \partial_\lambda^{s-1} Q(\lambda)|_{\lambda=0}. \quad (23)$$

According to the calculations in Appendix C, this function is given by the solution of the equation

$$(Q + 1)K_Q(e^\lambda - 1) + QH_Q(e^{-\lambda} - 1) = 0, \quad (24)$$

for any K, H . For the special case of (21), the result is

$$Q(\lambda) = \frac{-\mathcal{H} + (1 + \eta)(N - 1)e^\lambda - N\eta + \sqrt{4e^\lambda(1 + \eta)[- \eta + e^\lambda(1 + \eta)]N + [\mathcal{H} - e^\lambda(1 + \eta)(N - 1) + \eta N]^2}}{-2\eta + 2e^\lambda(1 + \eta)}. \quad (25)$$

Applying Eq. (23), the average value ($\kappa_1 = \langle n_0 \rangle$) is given by

$$\langle n_0 \rangle = (1/2)[(N - \mathcal{H} - 1 - \eta) + \sqrt{(N - \mathcal{H} - \eta - 1)^2 + 4N(1 + \eta)}], \quad (26)$$

which coincides with (7) in the $\eta=0$ limit. The second central moment ($\kappa_2 = \mu_2$) is given by

$$\mu_2 = \frac{(1 + \eta)(\eta + \mathcal{H})\sqrt{(N - \mathcal{H} - \eta - 1)^2 + 4N(1 + \eta)} - (1 + \eta)[\eta^2 + \mathcal{H}(1 + \mathcal{H} - N) + \eta(1 + 2\mathcal{H} + N)]}{2\sqrt{(N - \mathcal{H} - \eta - 1)^2 + 4N(1 + \eta)}}, \quad (27)$$

in terms of elementary functions.

All higher cumulants and central moments may be easily computed from (25). Figures comparing these approximate results with the exact master equation solution (shown in Fig. 1) are not shown, simply because for $N=200$, they are indistinguishable.

VI. HYBRID THEORY: COMBINING CNB3 WITH THE MASTER EQUATION ANALYSIS

We now demonstrate how to combine ideas from the canonical ensemble quasiparticle formalism of CNB3 [17] (which works well at low temperature when $\sqrt{\mu_2} \ll \bar{n}_0$) with the physics of the master equation approach, in order to obtain essentially perfect quantitative agreement with the exact numerical solution of the canonical partition function at all temperatures for the fluctuation statistics of the Bose gas.

Defining the function F_{n_0} as the ratio between the probabilities to find n_0+1 and n_0 particles in the ground state,

$$F_{n_0} = \frac{P_{n_0+1}}{P_{n_0}}, \quad (28)$$

we note that the canonical ensemble constraint is imposed by $F_N=0$ because if all the particles are in the condensate, it is impossible to cool further, or, in other words, the probability to find $N+1$ particles in the condensate is equal to zero. It is then useful to consider an expansion of this function in $N - n_0$. Rather than Taylor expand, a better approach is to approximate this function by a ratio of two power series and then determine both the numerator and denominator coefficients, a procedure known as a Padé approximation. Padé approximations are usually superior to Taylor expansions when functions contain poles, because the use of rational functions allows them to be well represented. We approximate

$$F_{n_0} = \frac{K_{n_0}}{H_{n_0+1}}, \quad (29)$$

where the functions H, K are both polynomials in $N - n_0$,

$$\begin{aligned} H_{n_0} &= \mathcal{H} + \eta(N - n_0) + \alpha(N - n_0)^2, \\ K_{n_0} &= (1 + \eta)(N - n_0) + \alpha(N - n_0)^2, \end{aligned} \quad (30)$$

and truncate the expansion at second order. Knowledge of the function F_{n_0} allows the construction of the entire distribution,

$$p_{n_0} = Z_N^{-1} \prod_{m=n_0}^{N-1} F_m^{-1}, \quad Z_N = \sum_{n_0=0}^N \prod_{m=n_0}^{N-1} F_m^{-1}, \quad (31)$$

or

$$p_{n_0} = C \frac{(N - n_0 - 1 + x_1)! (N - n_0 - 1 + x_2)!}{(N - n_0)! [N - n_0 + (1 + \eta)/\alpha]}, \quad (32)$$

where $x_{1,2} = (\eta \pm \sqrt{\eta^2 - 4\alpha\mathcal{H}})/2\alpha$ and C is the normalization constant determined by $\sum_{n_0=0}^N p_{n_0} = 1$. The functions H, K take the same form as in the master equation, but now the coefficients $\mathcal{H}, \eta, \alpha$ are treated as free parameters to be fixed by comparison with CNB3 [17] at low temperatures.

The further analytic input for the theory is the first three moments of the distribution described by the heating and cooling coefficients (30) in the low-temperature limit. These moments are used to fix the free parameters $\mathcal{H}, \eta, \alpha$. The calculation is done in Appendix C for the complete generating function using the stochastic path integral formalism, but here we only reproduce the needed first three:

$$\langle n_0 \rangle = N - \mathcal{H}, \quad (33)$$

$$\mu_2 = \mathcal{H}(1 + \eta + \alpha\mathcal{H}), \quad (34)$$

$$\mu_3 = -\mathcal{H}(1 + \eta + \alpha\mathcal{H})(1 + 2\eta + 4\alpha\mathcal{H}). \quad (35)$$

Comparison with the CNB3 result [17] at low temperature allows us to obtain the parameters $\mathcal{H}, \eta, \alpha$:

$$\begin{aligned} \mathcal{H} &= \sum_{k \neq 0} \bar{n}_k, \\ \eta &= \frac{1}{2} \left(- \frac{\sum_{k \neq 0} (2\bar{n}_k^3 + 3\bar{n}_k^2 + \bar{n}_k)}{\sum_{k \neq 0} (\bar{n}_k^2 + \bar{n}_k)} - 3 + \frac{4 \sum_{k \neq 0} (\bar{n}_k^2 + \bar{n}_k)}{\sum_{k \neq 0} \bar{n}_k} \right), \\ \alpha &= \frac{1}{\sum_{k \neq 0} \bar{n}_k} \left(\frac{1}{2} - \frac{\sum_{k \neq 0} (\bar{n}_k^2 + \bar{n}_k)}{\sum_{k \neq 0} \bar{n}_k} + \frac{\sum_{k \neq 0} (2\bar{n}_k^3 + 3\bar{n}_k^2 + \bar{n}_k)}{2 \sum_{k \neq 0} (\bar{n}_k^2 + \bar{n}_k)} \right), \end{aligned} \quad (36)$$

where $\bar{n}_k = (e^{\beta\epsilon_k} - 1)^{-1}$. Knowing these parameters allows the complete specification of the entire distribution in this approximation. To sum up, the theory uses (i) the master equation and stochastic path integral formalism to determine the first three moments at low temperature, and (ii) the results of

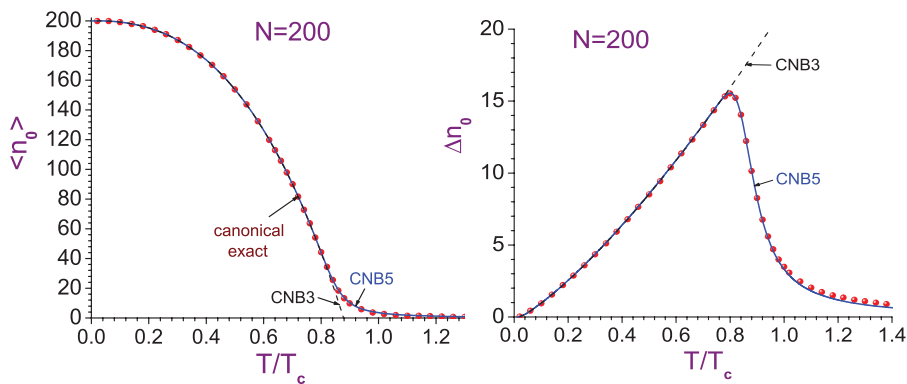


FIG. 4. (Color online) The present hybrid theory, which we call CNB5 (solid line), is compared with the exact numerical results obtained in the canonical ensemble (dots). (left) The average condensate particle number $\langle n_0 \rangle$ and (right) the variance Δn_0 are plotted for $N=200$ versus temperature. The predictions of CNB3 [17] (dashed line) are also shown.

CNB3 (which works well in the low-temperature limit) to fix the three undefined parameters. The distribution function (32) together with Eqs. (36) then gives predictions for all central moments and cumulants [21] at all temperatures.

The theory is put to the test in Figs. 4 and 5 for the first few central moments and cumulants of a thermal Bose gas in a harmonic trap, for the mesoscopic case $N=200$. The hybrid treatment yields perfect agreement with the exact numerical dots obtained in the canonical ensemble.

VII. CONCLUSIONS

We have discussed the fluctuation statistics of an ideal mesoscopic Bose-Einstein condensate from several different perspectives. First, we have reviewed the master equation approach, and derive an approximate analytic solution for the mean condensate particle number. By generalizing the grand canonical analysis, the same result from the approximate solution of a self-consistent equation has been recovered for the mean condensate particle number. Improved analytic results are obtained for the mean condensate particle number in

the case of a three-dimensional (3D) harmonic trap, which are quite accurate when compared with numerical calculation of the canonical partition function result. Analogous treatment of the variance of the distribution in the generalized grand canonical picture have given results that are very accurate below the critical temperature, but substantially deviate at or above the critical temperature. The reason for this discrepancy is because correlations of excited energy levels were neglected in the calculation.

Next, we have presented an (approximate) analytic solution for the generating function of the fluctuation statistics from the master equation perspective. This is done by employing the stochastic path integral formalism, with the saddle-point approximation, giving results that are asymptotically valid in the physically relevant limit of many particles in the condensate. The general solution is discussed for arbitrary heating and cooling coefficients, and specific results are given in terms of elementary functions for the Bose-Einstein condensate heating and cooling coefficients of CNB2. These results are in excellent agreement with exact master equation solution when compared numerically.

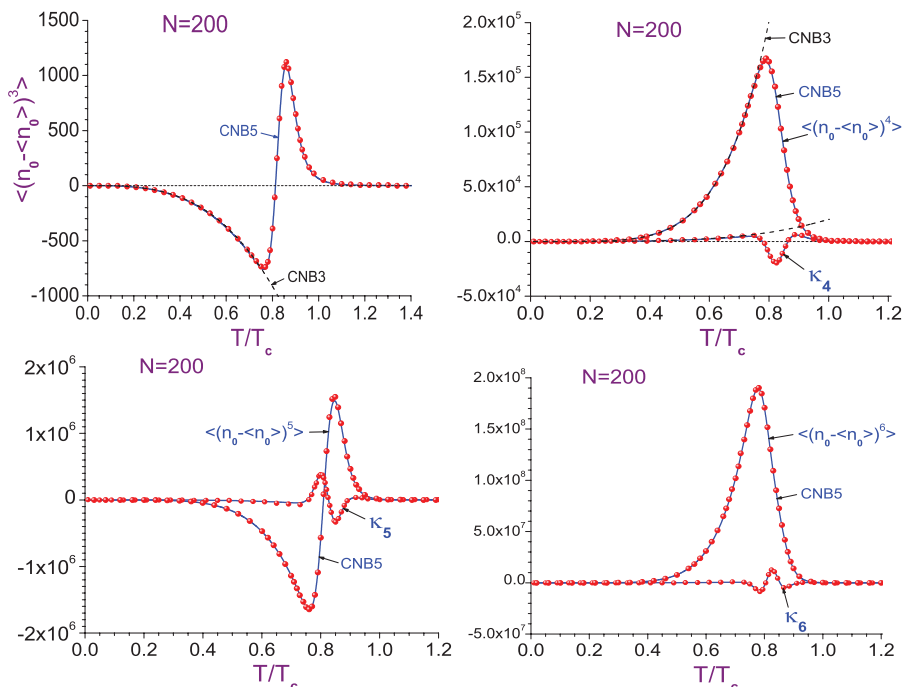


FIG. 5. (Color online) As in Fig. 4, for the third, fourth, fifth, and sixth centered moments, denoted by $\langle (n_0 - \langle n_0 \rangle)^n \rangle$, as well as cumulants κ_n [21].

A hybrid theory has been put forth that combines the master equation and stochastic path integral with the approach of CNB3. The theory applies the results of CNB3 in the low-temperature limit, together with the predictions of the master equation and stochastic path integral. This is accomplished by preserving the physical structure of the master equation, while using the first three moments of CNB3 to fix the numerical values of the heating and cooling parameters. These predictions are then examined for several higher moments (or cumulants), at all temperatures. The predictions of this theory are essentially in perfect agreement with numerical simulation of the exact canonical partition function.

Finally, we briefly discuss how our methods and results extend in the presence of weak interactions. As will be shown in Ref. [22], it is easy to generalize the hybrid approach to the interacting case and take the first three central moments (in the low-temperature limit) from CNB3. From the microscopic master equation point of view, interactions generally lead to “off-diagonal” transitions in the density matrix, demanding a fully coherent treatment of the problem. However, it will be demonstrated elsewhere that good agreement with CNB3 (in the applicable low-temperature limit) may be obtained with only diagonal transitions, where the heating and cooling coefficients are determined from Bogoliubov theory.

ACKNOWLEDGMENTS

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APPENDIX A: GRAND CANONICAL FORMALISM: SIMPLE EXPANSION WITH TRIPLE SUMMATION

Before calculating the analytic expressions for the average and variance of the condensate fluctuations, it is instructive to first take another path, different from the one presented in Sec. III. Rather than make the step (11), we make the simple expansion

$$N - \langle n_0 \rangle = \sum_{r=1}^{\infty} \sum_{k>0} \frac{1}{(e^{\beta\epsilon_k} - 1)^r} \left(-\frac{e^{\beta\epsilon_k}}{\langle n_0 \rangle} \right)^{r-1} \simeq A(T) - \frac{1}{\langle n_0 \rangle} B(T), \quad (\text{A1})$$

where

$$A(T) = \sum_{k>0} \frac{1}{e^{\beta\epsilon_k} - 1}, \quad B(T) = \sum_{k>0} \frac{e^{\beta\epsilon_k}}{(e^{\beta\epsilon_k} - 1)^2}. \quad (\text{A2})$$

The above expansion is in the small parameter $e^{\beta\epsilon_k}/[(e^{\beta\epsilon_k} - 1)\langle n_0 \rangle]$. Equation (A1) has the solution

$$\langle n_0 \rangle = \frac{1}{2} [N - A + \sqrt{(N - A)^2 + 4B}]. \quad (\text{A3})$$

For an isotropic harmonic trap, $\epsilon_k = \hbar\Omega(l+m+n)$, and since $e^{-a(l+m+n)} < 1$ (here $a = \beta\hbar\Omega$) we make the series expansion

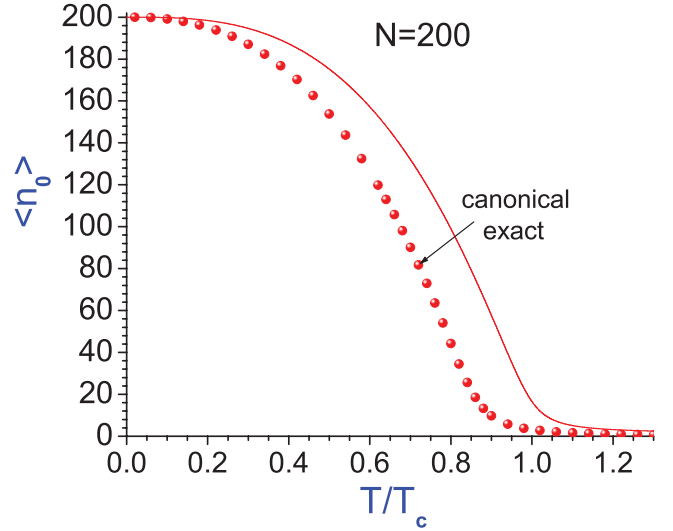


FIG. 6. (Color online) The average condensate particle number is plotted versus temperature for $N=200$. The approximate analytic result (A6) within the grand canonical approach (solid line) is compared with the exact canonical dots. The triple sum together with the simple expansion gives a poor fit.

$$\begin{aligned} A(T) &= \sum_{l,m,n=1}^{\infty} \frac{e^{-a(l+m+n)}}{1 - e^{-a(l+m+n)}} = \sum_{l,m,n=1}^{\infty} \sum_{s=0}^{\infty} e^{-(s+1)a(l+m+n)} \\ &= \sum_{s=0}^{\infty} \left(\sum_{n=1}^{\infty} e^{-(s+1)an} \right)^3 = \sum_{s=1}^{\infty} \left(\sum_{n=1}^{\infty} e^{-san} \right)^3 \\ &\simeq \sum_{s=1}^{\infty} \left(\frac{1}{a} \int_0^{\infty} e^{-sz} dz \right)^3 \rightarrow \frac{1}{a^3} \zeta(3), \end{aligned} \quad (\text{A4})$$

where $\zeta(n) = \sum_{s=1}^{\infty} 1/s^n$ is the Riemann zeta function and the conversion to integration is based on the assumption $a < 1$. Similarly we find

$$\begin{aligned} B(T) &= \sum_{l,m,n=1}^{\infty} \frac{e^{a(l+m+n)}}{(e^{a(l+m+n)} - 1)^2} = \sum_{l,m,n=1}^{\infty} \sum_{s=0}^{\infty} (s+1) e^{-(s+1)a(l+m+n)} \\ &= \sum_{s=0}^{\infty} (s+1) \left(\sum_{n=1}^{\infty} e^{-(s+1)an} \right)^3 = \sum_{s=1}^{\infty} s \left(\frac{1}{a} \int_a^{\infty} e^{-sz} dz \right)^3 \\ &= \frac{1}{a^3} \zeta(2). \end{aligned} \quad (\text{A5})$$

Finally, by noting that $A(T) = N(T/T_c)^3$, $B = N(T/T_c)^3 \zeta(2)/\zeta(3)$, where $T_c = [N/\zeta(3)]^{1/3} \hbar\Omega/k_B$ is the critical temperature in the thermodynamic limit, we obtain

$$\langle n_0 \rangle = \frac{N}{2} \left[1 - \left(\frac{T}{T_c} \right)^3 \right] + \frac{N}{2} \sqrt{\left[1 - \left(\frac{T}{T_c} \right)^3 \right]^2 + \frac{\zeta(2)}{\zeta(3)} \frac{4}{N} \left(\frac{T}{T_c} \right)^3}. \quad (\text{A6})$$

For large N , Eq. (A6) reproduces the thermodynamic limit. However, the triple-sum formula is inaccurate for small N especially near T_c . The result (A6) is plotted in Fig. 6. The fit is poor because $N=200$ is not sufficiently large. We note that

this expansion may be systematically improved by keeping more terms in the $1/\langle n_0 \rangle$ expansion, and evaluating the coefficients in a similar manner. In the next appendix, this analysis is improved.

APPENDIX B: GRAND CANONICAL FORMALISM: IMPROVED EXPANSION WITH SINGLE SUMMATION

The goal of this appendix is to obtain an improved analytical expression for both the average and variance of the condensate distribution for an isotropic harmonic trap. Equation (A1) is obtained from Eq. (10) by neglecting the terms with $1/\langle n_0 \rangle^2$ and higher under the condition $\langle n_0 \rangle \gg e^{\beta\epsilon_k}/(e^{\beta\epsilon_k}-1)$. For the enhanced expansion (11), it is not difficult to see that the validity condition is $\langle n_0 \rangle + 1 \gg (e^{\beta\epsilon_k}-1)^{-1}$, allowing for a better approximation.

After this point, there are two more key steps: (1) convert the triple summation into a single summation and (2) make an integral approximation to the single summation. We first recall that

$$\mathcal{H} = \sum_{k>0} \frac{1}{(e^{\beta\epsilon_k} - 1)}, \quad (\text{B1})$$

where for a harmonic trap $\beta\epsilon_k = a(l+m+n)$ and we have introduced $a = \hbar\Omega\beta$. The triple summation can be reduced to a single summation over s , where $s = l+m+n$, and weighting this sum with the number of ways W to put s quanta into three boxes, $W = (s+2)!/(s!2!) = (s+2)(s+1)/2$,

$$\mathcal{H} = \sum_{s=1}^{\infty} \frac{(s+2)(s+1)}{2(e^{as} - 1)}. \quad (\text{B2})$$

In order to find an analytical expression for \mathcal{H} , we interpret the summation as a Riemann summation, and convert it (approximately) to an integral using the midpoint rule, $\sum_{s=1}^{\infty} f_s \approx \int_0^{\infty} ds f(s+1/2)$. The midpoint rule gives the better approximation because it compromises between the lower and upper summations. Reparametrizing the integral yields

$$\begin{aligned} \mathcal{H} &\approx \frac{1}{2} \int_{a/2}^{\infty} \left(\frac{x^2}{a^2} + \frac{3x}{a} + 2 \right) \frac{1}{e^x - 1} \frac{dx}{a} \\ &= \frac{\zeta(3)}{a^3} - \frac{2 \ln \frac{4}{a+4}}{a^3} - \frac{1}{2a^2} \\ &\quad + \frac{\pi^2}{4a^2} + \frac{3}{2a^2} \text{dilog}(e^{a/2}) + \frac{3}{16} \\ &\quad + \frac{1}{2} - \frac{1}{a} \ln(e^{a/2} - 1) \end{aligned} \quad (\text{B3})$$

$$\approx \frac{\zeta(3)}{a^3} + \left(\frac{\pi}{2a} \right)^2 + \frac{1}{a} (\ln 2 - \ln a), \quad (\text{B4})$$

where $\text{dilog}(x) = \int_1^x dt \ln(t)/(1-t)$. This derivation gives Eq. (14), one of our main results.

Turning to the variance, we proceed in the same manner to obtain an analytical expression for μ_2 . The conversion from the triple sum to the single sum yields

$$\mu_2 = \sum_{s=1}^{\infty} \frac{(s+2)(s+1)}{2} \left(\frac{1}{(Ae^{as} - 1)^2} + \frac{1}{Ae^{as} - 1} \right), \quad (\text{B5})$$

where $A = 1 + 1/\langle n_0 \rangle$. Next, we convert the sum into an integral as before to yield

$$\mu_2 \approx \int_{a/2}^{\infty} \frac{Ae^x}{(Ae^x - 1)^2} \frac{1}{2} \left(\frac{x^2}{a^2} + 3\frac{x}{a} + 2 \right) \frac{dx}{a}. \quad (\text{B6})$$

Then we integrate by parts to find

$$\mu_2 \approx \frac{15}{8a(Ae^{a/2} - 1)} + \frac{1}{2a^2} \int_{a/2}^{\infty} \frac{2x/a + 3}{Ae^x - 1} dx. \quad (\text{B7})$$

The integral in Eq. (B7) can be calculated analytically to find

$$\begin{aligned} \mu_2 &\approx \frac{7Ae^{a/2} + 8}{8a(Ae^{a/2} - 1)} + \frac{3}{2a^2} \ln \left(\frac{A}{Ae^{a/2} - 1} \right) \\ &\quad + \frac{1}{a^3} \left[\frac{\pi^2}{6} + \ln \left(\frac{Ae^{a/2} - 1}{\sqrt{A}} \right) \ln A + \text{dilog}(Ae^{a/2}) \right]. \end{aligned} \quad (\text{B8})$$

This derivation gives Eq. (20), another main result.

APPENDIX C: STOCHASTIC PATH INTEGRAL SOLUTION OF THE MASTER EQUATION

The purpose of this appendix is to provide approximate expressions for all cumulants of the stationary condensate fluctuations using elementary functions, starting from the master equation approach. In order to accomplish this, we employ the stochastic path integral formalism [15,16].

Consider a general differential master equation of the form

$$\dot{P}_n(t) = \sum_m [W_{nm}P_m(t) - W_{mn}P_n(t)], \quad (\text{C1})$$

where W_{nm} is a transition rate from m to n , and P_n is the probability of occupying state n . Applying this equation to our BEC problem, the microscopic rates to different states are taken from CNB2 [6]:

$$W_{n_0, n_0-1} = \kappa(1 + \eta)(N + 1 - n_0)n_0,$$

$$W_{n_0, n_0+1} = \kappa[\mathcal{H} + \eta(N - n_0 - 1)](n_0 + 1), \quad (\text{C2})$$

where n_0 is the number of particles in the condensate, κ is a rate constant, \mathcal{H} is given in (12), and η is given in (22). We now express this master equation as a stochastic path integral, by going to a continuous representation where the discrete number of particles in the ground state n_0 is replaced by an effectively continuous variable Q ,

$$U(Q_f, Q_i, t) = \int \mathcal{D}Q \mathcal{D}\lambda \exp[S(Q, \lambda)], \quad (\text{C3})$$

$$S(Q, \lambda) = \int_0^t dt' [-\lambda \dot{Q} + H(Q, \lambda)]. \quad (\text{C4})$$

The object U is the evolution operator going from one particle configuration Q_i to another particle configuration Q_f in time t . It is expressed as a path integral over Q and λ . The auxiliary variable λ is a canonically conjugate variable and imposes local particle number conservation. In the continuous limit, (and suppressing the overall rate constant κ) the CNB2 [6] rates may be expressed as

$$\begin{aligned} W(Q', Q) = & (1 + \eta)(N + 1 - Q')Q' \delta(Q' - Q - 1) \\ & + [\mathcal{H} + \eta(N - Q' - 1)](Q' + 1) \delta(Q' - Q + 1). \end{aligned} \quad (\text{C5})$$

According to the prescription of Ref. [16], the Hamiltonian $H(Q, \lambda)$ of the stochastic path integral is found from the equation

$$H(Q, \lambda) = \int dQ' (e^{Q' - Q\lambda} - 1) W(Q', Q). \quad (\text{C6})$$

For the rates (C5), we find

$$\begin{aligned} H(Q, \lambda) = & (1 + \eta)(N - Q)(Q + 1)(e^\lambda - 1) \\ & + [\mathcal{H} + \eta(N - Q)]Q(e^{-\lambda} - 1), \end{aligned} \quad (\text{C7})$$

or for the general master equation (1) with arbitrary coefficients H, K , we find

$$H(Q, \lambda) = K_Q(Q + 1)(e^\lambda - 1) + H_Q Q(e^{-\lambda} - 1). \quad (\text{C8})$$

This result has a simple physical interpretation: On a short time scale, the elementary transitions into and out of the

condensate are Poissonian, witnessed by the generators \mathcal{G} of Poissonian statistics, $\mathcal{G} = \Gamma[\exp(\pm\lambda) - 1]$ [counting an incoming (+) or outgoing (-) boson]. These boson transitions are described with a rate into the condensate $\Gamma_{\text{in}} = K_Q(Q + 1)$, and a rate out of the condensate $\Gamma_{\text{out}} = H_Q Q$.

The stochastic path integral (C3) may be evaluated in saddle-point approximation, where the large parameter of the expansion is $\langle n_0 \rangle \gg 1$, the number of particles in the condensate. Applying this approximation gives the analog of Hamilton's equations of motion,

$$\dot{Q} = \partial_\lambda H, \quad \dot{\lambda} = -\partial_Q H. \quad (\text{C9})$$

To solve the problem of instantaneous particle number statistics in this approximation, we generalize the method of Ref. [16], following the method of Ref. [20], by first finding the “zero-energy lines,” implicitly defined by the equation $H(Q, \lambda) = 0$. For time scales longer than the relaxation time κ^{-1} , any Q -distributed initial state will be projected onto the zero-energy lines. The trivial zero-energy line is given by $\lambda_0 = 0$ and must exist for the probability distribution to be normalized. The instantaneous fluctuation statistics (to leading order) can be found by calculating the statistical action (C4) along the nontrivial zero-energy line. This action $S(\chi)$ is also the generating function of the cumulants of the fluctuation statistics. On the zero-energy line, the Hamiltonian vanishes, leaving only the dynamical part of the action,

$$S(\chi) = - \int_0^t dt' \lambda(t') \dot{Q}(t') = \int_0^\chi Q(\lambda) d\lambda, \quad (\text{C10})$$

and we have changed variables from time to phase space coordinates. In the case of Bose-Einstein condensation (C7), the nontrivial zero-energy line $Q(\lambda)$ is given by

$$Q(\lambda) = \frac{-\mathcal{H} + (1 + \eta)(N - 1)e^\lambda - N\eta + \sqrt{4e^\lambda(1 + \eta)[- \eta + e^\lambda(1 + \eta)]N + [\mathcal{H} - e^\lambda(1 + \eta)(N - 1) + \eta N]^2}}{-2\eta + 2e^\lambda(1 + \eta)}, \quad (\text{C11})$$

In order to have a generating function, it is unnecessary to perform the integral (C10) because $dS/d\chi = Q(\chi)$. Therefore, all cumulants of the distribution can be found from

$$\kappa_s = \partial_\lambda^{s-1} Q(\lambda)|_{\lambda=0}. \quad (\text{C12})$$

This result generalizes the discussion of Ref. [16] for any two Poissonian processes in series (equilibrium or not), and is easily generalized to arbitrary elementary processes. Equations (C11) and (C12) recover Eqs. (23) and (25) and are main results.

In Sec. VI, this same method is used to calculate the cumulants where the heating and cooling coefficients are given by

$$K_{n_0} = (1 + \eta)(N - n_0) + \alpha(N - n_0)^2,$$

$$H_{n_0} = \mathcal{H} + \eta(N - n_0) + \alpha(N - n_0)^2. \quad (\text{C13})$$

As before, we define $Q(\lambda)$ as the solution of the approximate zero-energy equation, $e^\lambda = H_Q/K_Q$, where the low-temperature limit allows the approximation $Q + 1 \rightarrow Q$. The solution is

$$Q(\lambda) = N - \frac{\eta - e^\lambda(1 + \eta) + \sqrt{4\alpha\mathcal{H}(e^\lambda - 1) + [\eta - (1 + \eta)e^\lambda]^2}}{2\alpha(e^\lambda - 1)}. \quad (\text{C14})$$

The first three cumulants are given in Eqs. (33)–(35), which coincide with the first three central moments.

We also briefly note that time-averaged fluctuation statistics may be easily calculated within the stochastic path integral formalism. Consider a detector that has finite time reso-

lution. The physical quantity that is of interest is then the condensate particle number, averaged over some time window τ ,

$$Q_\tau = (1/\tau) \int_0^\tau dt' n_0(t'), \quad (\text{C15})$$

where we take τ longer than any dynamical time scale, for simplicity. Following the method of Ref. [16], we find that

the distribution $P(Q_\tau)$ is approximately given by the expression

$$\log P(Q_\tau) = -\pi(\sqrt{\Gamma_{\text{in}}} - \sqrt{\Gamma_{\text{out}}})^2, \quad (\text{C16})$$

where $\Gamma_{\text{in}} = K_{Q_\tau}(Q_\tau + 1)$, $\Gamma_{\text{out}} = H_{Q_\tau} Q_\tau$. Interestingly, this result is of the same form as the time-averaged electron fluctuations on a mesoscopic cavity, out of equilibrium [16]. This similarity of statistics for radically different physical systems originates from the fact that both systems can be described as two Poissonian processes in series.

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