Condensation of $N$ bosons IV: A simplified Bogoliubov master equation analysis of fluctuations in an interacting Bose gas

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(Dated: June 28, 2018)

A nonequilibrium master equation analysis for $N$ interacting bosons, with Bogoliubov quasiparticles as the reservoir is presented. The analysis is based on a simplified Hamiltonian. The steady state solution yields the equilibrium density matrix. The results are in good agreement with and extend our previous rigorous canonical ensemble equilibrium statistical treatment leading to a quantum theory of the atom laser.

I. INTRODUCTION

We here analyze the condensate fluctuations of $N$ interacting bosons via a master equation analysis based on a simple truncated Hamiltonian. The strategy is to regard excited states of the Bose gas, as well as collective excitations, as reservoir variables which we ultimately trace over, in order to obtain a master equation for the condensate. We find that the steady state solution of the resulting kinetic equations provides a good description of Bose-Einstein condensate (BEC) \[1\]. Fig. 1 shows the condensate fraction as a function of temperature and is one of our main results. This is in accord with the wit and wisdom of Wigner:

With classical thermodynamics, one can calculate almost everything crudely; with kinetic theory, one can calculate fewer things, but more accurately; and with statistical mechanics, one can calculate almost nothing exactly.

In particular, we discuss several subtle issues concerning the statistics of condensate atoms in the region of $T \approx T_c$. This is analogous to studying the photon statistics of the laser in the passage from below to above threshold. In fact, BEC is often referred to as an atom laser, and the question of the atom statistics of the mesoscopic BEC (containing a few $10^3$ or $10^4$ atoms), is the subject of this paper. The answer is given by the diagonal elements of the BEC density matrix, $\rho_{n_0,n_0}$, where $n_0$ is the number of atoms in the BEC ground state. In the present case of a gas of $N$ weakly interacting bosons, in one limit we find

$$\rho_{n_0,n_0} = \frac{\mathcal{H}_I^{N-n_0}}{(N-n_0)!} Z_N^{-1}, \quad Z_N = e^{\mathcal{H}_I} \Gamma(N+1,\mathcal{H}_I)/N!$$

(1)

where $Z_N$ is a normalization (partition function) factor expressed in terms of the incomplete gamma function $\Gamma(N+1,\mathcal{H}_I)$; and $\mathcal{H}_I$ is a simple heating coefficient governing the rate of removal of atoms from the ground state due to scattering by Bogoliubov quasiparticles, which is given by

$$\mathcal{H}_I = \sum_{k \neq 0} \left( \frac{u_k^2 + v_k^2}{e^{\beta \omega_k} - 1} + v_k^2 \right).$$

(2)

FIG. 1: Solid lines are the present work results showing the mean number of condensate particles as a function of temperature for $N = 200$ particles in a box calculated via the solution of the condensate master equation for an interacting (Bogoliubov) gas with $an^{1/3} = 0.1$ and an ideal (Bose) gas $an^{1/3} = 0$. Dots are the exact numerical results obtained in the canonical ensemble for the ideal Bose gas \[2\]. Squares are the results of CNB3 (please note that repulsive interaction increases $T_c$). Dashed line is a plot of $N[1 - (T/T_c)^{3/2}]$ which is valid for the ideal gas in the thermodynamic limit. The temperature is normalized by the ideal gas thermodynamic critical temperature in the box $T_c = 2\pi\hbar^2 n^{2/3}/k_B M \zeta(3/2)^{1/3}$, where $M$ is the particle mass.
In the above the usual Bogoliubov amplitudes are

\[ u_k = \frac{1}{\sqrt{1-A_k}} \quad v_k = \frac{A_k}{\sqrt{1-A_k}} \]
\[ A_k = \frac{V}{\bar{n}_0 U_k} \left( \epsilon_k - \frac{\hbar^2 k^2}{2 M} - \bar{n}_0 U_k \right) \]

where \( M \) is the atomic mass, \( V \) is the condensate volume and \( U_k \) is the atom-atom scattering energy; the quasiparticle energy \( \epsilon_k \) is given by

\[ \epsilon_k = \sqrt{\left( \frac{\hbar^2 k^2}{2 M} + \bar{n}_0 U_k \right)^2 - \left( \frac{\bar{n}_0 U_k}{V} \right)^2} \]

The simple expression, Eq. (4), is valid in the limit in which, for the case of an ideal gas in a box, \( H_I = N \left( T/T_c \right)^{3/2} \) where \( T \) is the temperature of the gas and \( T_c \) is the usual critical temperature. This was the main result of the first paper on the Condensation of \( N \) Bosons (CNB1) in this series [2], in which we focused on the statistics of \( N \) noninteracting (ideal) bosons. In the second paper [2] (CNB2) the approximations were improved, as discussed in section III below. In CNB1,2 we solved for the condensate statistics of an ideal Bose gas and found, surprisingly, that the fluctuations are not Gaussian even in the thermodynamic limit. The treatment of CNB1,2 is patterned after the quantum theory of the laser, i.e., based on a master equation for the condensate density matrix. As such, it has the useful (and intriguing) feature of working equally well at all temperatures from \( T = 0 \) to \( T_c \) and above. Atom-atom interactions are, however, ignored in those papers.

Paper CNB3 [2] includes interactions. The analysis of CNB3 is based on the Girardeau-Arnoldi approximation of Bogoliubov’s approach to BEC. In CNB3, we give a “rigorous” statistical mechanical treatment of the fluctuations, valid provided the average number of condensate particles is much larger than its variance; that is valid for temperatures not too near \( T_c \). This condition implies that the excited atom numbers \( n_k \) fluctuate independently, \(< n_k n_m > = \bar{n}_n \bar{n}_m \), \( k \neq m \), by exchanging particles with the condensate reservoir. For \( N = 200 \) CNB3 is valid from \( T = 0 \) to \( T \approx 0.7T_c \). However, near and above \( T_c \) the correlations become substantial which yields failure of such a treatment. In a broad temperature range, interactions increase the condensate number \( \langle n_0 \rangle \), and the fluctuations are found to be one half those of the ideal Bose gas. This remarkable fact is due to the \( \left( \bar{k} - \bar{k} \right) \) pairing of atoms.

In the present paper, we utilize a master equation analysis for the interacting Bose gas based on the simple truncated Hamiltonian given by Eq. (13). In particular we derive the average number of particles in the lowest energy level, \( \langle n_0 \rangle \) and the fluctuation about the average \( \Delta n_0^2 = \langle (n_0 - \langle n_0 \rangle)^2 \rangle \). These are plotted in Figs. 1 and 2 and constitute our main results.

We note that the present analysis yields an expression for \( \langle n_0 \rangle \), in good agreement with the rigorous results of CNB3, in the temperature region where that analysis is valid; and extends those results to higher temperature up to \( T_c \) and beyond, as per Fig. 1.

We emphasize that the problem of the interacting Bose gas near \( T_c \) is a difficult one. It is therefore worthwhile to investigate simple models designed to capture the essential physics. To that end, the next section is based on a simple “toy” model which works surprisingly well. Encouraged by the results of that analysis we then present a physically motivated model yielding a similar Hamiltonian. The analysis based on a more general treatment will be published elsewhere.

In the next section we derive the relevant master equation which we solve in section III to obtain the condensate statistics. In section IV we discuss the results and make contact with previous work.

II. MASTER EQUATION FOR WEAKLY INTERACTING BOSE GAS

Having set the stage, we proceed to sketch a simple approach extending our master equation analysis to the case of the interacting Bose gas. The present treatment is based on simple extension of CNB1,2 via a “toy” model and then a more realistic (but still heuristic) formulation.
However the results are in good agreement with "rigorous" results of CNB3 for temperatures where that theory is valid and provide answers in the vicinity of $T_c$ where it does breakdown.

In CNB1,2 the basic model interaction Hamiltonian describing the statistical dynamics of the condensate was taken to be

$$V = \sum_k g_k \hat{a}_k \hat{b}_k + \text{adj.}$$

where $\hat{a}_k$ and $\hat{b}_k$ are atom and phonon annihilation operators, likewise $\hat{a}_0$ is the condensate annihilation operator and $g_k$ is the corresponding coupling strength for the collision of a ground state atom and an atom having momentum $k$ scattering into the BEC. This models the dilute gas BEC experiments of Reppy and coworkers 1. Moreover the results for the condensate particle number, obtained by the master equation approach of CNB2 and exact numerical simulation for the ideal gas in the canonical ensemble 2, are in excellent agreement as indicated in Fig. 1.

A. Toy Model for an Interacting Bose Gas

As a first step toward obtaining $\bar{n}_0$ and $\Delta n_0$ for an interacting Bose gas, we derive a master equation for $\rho_{n_0,n_0}$ by simply replacing the phonon operators $\hat{b}_k$ and $\hat{b}_k^\dagger$ in Eq. 2 by operators $\hat{b}_k$ and $\hat{b}_k^\dagger$ related to $\hat{a}_k$ and $\hat{a}_k^\dagger$ by the usual Bogoliubov transformation

$$\hat{b}_k = u_k \hat{a}_k + v_k \hat{a}_k^\dagger$$
$$\hat{b}_k^\dagger = u_k \hat{a}_k^\dagger + v_k \hat{a}_k$$

where $u_k$ and $v_k$ are given in Eq. 3. $\beta_0 = \sqrt{1/(e^{\beta \epsilon_k} - 1)}$, $\epsilon_k$ is the Bogoliubov quasiparticle energy given by the Eq. 4.

The present master equation for the condensate is now obtained via the phenomenological analysis of this subsection on a more physically motivated footing.

B. A Physical Argument Based on Bogoliubov-Girardeau-Arnowitt Formalism

We work with the particle number conserving creation and annihilation operators of Girardeau and Arnowitt 2 passing the operators $\hat{b}_k$ and $\hat{b}_k^\dagger$ in Eq. 4 by the quasiparticle operators $\hat{a}_k$ and $\hat{a}_k^\dagger$ of Eq. 5, and find the new heating coefficient

$$\mathcal{H} = \sum_{k\neq 0} \frac{1}{e^{\beta \epsilon_k} - 1}$$

where $\beta = 1/k_B T$.

In the present toy model all we do is replace the phonon operators $\hat{b}_k$ and $\hat{b}_k^\dagger$ in Eq. 3 by the quasiparticle operators $\hat{a}_k$ and $\hat{a}_k^\dagger$ of Eq. 5, and find the new heating coefficient

$$\mathcal{H} = \sum_{k\neq 0} \left[ \frac{u_k^2 + v_k^2}{e^{\beta \epsilon_k} - 1} \right] \equiv \mathcal{H}_f.$$ (10)

The results of this simple analysis are summarized in Figs. 1 and 2. Encouraged by these results we next present a simple argument which puts the phenomenological analysis of this subsection on a more physically motivated footing.
C. The Master Equation

The present master equation for the condensate is now derived by focusing on the truncated scattering Hamiltonian Eq. (14), which adds (removes) atoms from the condensate with the annihilation (creation) of an excited atom and the emission (absorption) of a quasiparticle. As in CNB1 and CNB2 we treat the phonon like quasiparticle states as reservoir states for the condensate.

The dynamical evolution of the condensate thus involves three components: the ground state (condensate) atoms, excited (noncondensate) and the phonon like canonical ensemble excitations, $\hat{\beta}_k$ and $\hat{\beta}_k^\dagger$. We proceed to treat the $\hat{\beta}_k$ quasiparticles as a thermal reservoir which we trace over to obtain the density matrix equation for the ground state, as in CNB1,2. Some details of the master equation analysis are given in Appendix A. As will be discussed further elsewhere, the equation of motion for the probability to find $n_0$ particles in the condensate $\rho_{n_0,n_0} = P_{n_0}$ is now given by

$$\frac{1}{\kappa} \dot{P}_{n_0} = -K_{n_0}(n_0 + 1)P_{n_0} + K_{n_0-1}n_0 P_{n_0-1}$$

$$H_{n_0,n_0}P_{n_0} + H_{n_0+1}(n_0 + 1)P_{n_0+1}.$$  

(15)

As in CNB1,2, we have divided the physical process into two kinds of terms: the $K_{n_0}$ and $K_{n_0-1}$ terms describing the cooling of the gas which increases the condensate number and heating terms $H_{n_0}$ and $H_{n_0+1}$ which decrease it. The constant $\kappa$ is an uninteresting overall rate factor. The cooling and heating coefficients are given by

$$K_{n_0} = \sum_{k \neq 0} \langle n_k \rangle_{n_0} \left( 1 + \langle \hat{\beta}_k^\dagger \hat{\beta}_k \rangle \right),$$

$$H_{n_0} = \sum_{k \neq 0} \langle \hat{\beta}_k^\dagger \hat{\beta}_k \rangle \left( 1 + \langle n_k \rangle_{n_0} \right).$$

(16)

(17)

Equation (14) was obtained previously in a similar form for the ideal gas; the essential difference being that the average $\langle \hat{\beta}_k^\dagger \hat{\beta}_k \rangle$ is replaced by an average number of thermal phonons in our earlier work. The physics behind $\omega_k$ is best understood by going to a "low temperature limit" such that $\langle \hat{\beta}_k^\dagger \hat{\beta}_k \rangle \ll 1$ and we may write Eq. (16) as

$$K_{n_0} = \sum_{k \neq 0} \langle n_k \rangle_{n_0} = N - n_0,$$

(18a)

and $\langle n_k \rangle_{n_0} \ll 1$ so that we may write Eq. (17) as

$$H_{n_0} = \sum_{k \neq 0} \langle \hat{\beta}_k^\dagger \hat{\beta}_k \rangle \equiv \mathcal{H}_I.$$  

(18b)

We proceed by writing the $\hat{\beta}_k$ and $\hat{\beta}_k^\dagger$ operators in terms of the Bogoliubov quasiparticle operators

$$\hat{\beta}_k = u_k \hat{b}_k + v_k \hat{b}_k^\dagger$$

$$\hat{\beta}_k^\dagger = u_k \hat{b}_k^\dagger + v_k \hat{b}_k$$

where, as usual, $[\hat{b}_k, \hat{b}_k^\dagger] = \delta_{k,k'}$, hence

$$\langle \hat{\beta}_k^\dagger \hat{\beta}_k \rangle = u_k^2 + v_k^2 \left( \hat{b}_k \hat{b}_k - 1 \right) = \frac{u_k^2 + v_k^2}{e^{\beta \epsilon_k} - 1} + v_k^2 \equiv \mathcal{H}_{k}.$$  

(19)

$$\langle \hat{\beta}_k^\dagger \hat{\beta}_k \rangle = \frac{1}{e^{\beta \epsilon_k} - 1}. $$

(22)

Finally, we note that in the useful notation of CNB3 the $\mathcal{H}_I$ coefficient found from Eqs. (18b) and (22) reads

$$\mathcal{H}_I = \frac{1}{2} \sum_{k \neq 0} \left( \frac{1}{z(A_k) - 1} + \frac{1}{z(-A_k) - 1} \right),$$

(23)

where

$$z(A_k) = \frac{A_k - e^{\beta \epsilon_k}/T}{A_k e^{\beta \epsilon_k}/T - 1}.$$  

(24)

and $A_k$ is given by Eq. (9).

In the low temperature limit the cooling and heating coefficients are given by Eqs. (18a) and (18b). However, as was shown in CNB2, the cross coefficient

$$\sum_{k \neq 0} \langle n_k \rangle_{n_0} \langle \hat{\beta}_k^\dagger \hat{\beta}_k \rangle$$

(25)

as it appears in Eqs. (16) and (17) is necessary in order to obtain an accurate description of the condensate. As was shown in CNB2 and as sketched in the appendix B, for the ideal gas we have

$$\sum_{k \neq 0} \langle n_k \rangle_{n_0} \langle \hat{b}_k^\dagger \hat{b}_k \rangle = (N - n_0) \eta$$

(26)
where the phonon average number \( \langle \hat{b}_k^\dagger \hat{b}_k \rangle = (e^{\beta E_k} - 1)^{-1} \equiv \eta_k \) and the CNB2 cross coupling coefficient \( \eta \) is defined by

\[
\eta = \sum_{k \neq 0} \frac{\eta_k^2}{\mathcal{H}} 
\]

where

\[
\mathcal{H} = \sum_{k \neq 0} \eta_k. 
\]

For the interacting gas the heating coefficient \( \mathcal{H}_I \) and the cross coupling coefficient can now be written as

\[
\mathcal{H}_I = \sum_{k \neq 0} \left( \frac{u_k^2 + v_k^2}{e^{\beta E_k} - 1} + v_k^2 \right) = \sum_{k \neq 0} \eta_k^I. 
\]

and

\[
\sum_{k \neq 0} \langle n_k \rangle_{n_0} \langle \hat{b}_k^\dagger \hat{b}_k \rangle = \sum_{k \neq 0} \langle n_k \rangle_{n_0} \eta_k = (N - n_0) \eta_I, 
\]

where

\[
\eta_I = \sum_{k \neq 0} \frac{\eta_k^2}{\mathcal{H}_I}. 
\]

Written in terms of \( \mathcal{H}_I \) and \( \eta_I \) the master equation for the interacting Bose gas is finally

\[
\frac{1}{\kappa} \dot{P}_{n_0} = -(N - n_0)(1 + \eta_I)(n_0 + 1)P_{n_0} + 
\]

\[
[N - (n_0 - 1)](1 + \eta_I)n_0 P_{n_0 - 1} - [\mathcal{H}_I + (N - n_0) \eta_I]n_0 P_{n_0} + 
\]

\[
[\mathcal{H}_I + (N - (n_0 + 1)) \eta_I](n_0 + 1)P_{n_0 + 1}. 
\]

III. CONDENSATE STATISTICS VIA STEADY STATE SOLUTION TO MASTER EQUATION

The BEC atom statistical distribution is now obtained by solving the master equation (22). The resulting distribution is given by essentially the same expression as was obtained for the ideal Bose gas in CNB2, namely

\[
P_{n_0} = \frac{1}{\mathcal{Z}_N} \frac{(N - n_0 + \mathcal{H}_I/\eta_I - 1)!}{(\eta_I/1 + \eta_I)^{N - n_0}}, 
\]

\[
\mathcal{Z}_N = \sum_{n_0=0}^N \left( \frac{N - n_0 + \mathcal{H}_I/\eta_I - 1}{N - n_0} \right) \left( \frac{\eta_I}{1 + \eta_I} \right)^{N - n_0}, 
\]

where \( \mathcal{H}_I \) and \( \eta_I \) for the interacting gas are given in Table 1.

In the low temperature limit we set \( \eta_I \) to zero and obtain the distribution given by Eq. (11). The average condensate particle number from Eq. (11) is

\[
\langle n_0 \rangle = N - \mathcal{H}_I + \mathcal{H}_I^{-1}N! 
\]

This is in good agreement with the average value obtained in CNB3 namely \( \langle n_0 \rangle = N - \mathcal{H}_I \) valid for \( T \) not in the vicinity of \( T_c \). The extra term \( \mathcal{H}_I^{-1}N! \) as given in Eq. (25) removes the unphysical cusp at \( T = T_c \) and extends the treatment of CNB3 through the critical temperature. Equation (11) and the associated \( \langle n_0 \rangle \) is essentially the extension of the results of CNB1 to include atom-atom interaction.

In general the \( \eta_I \) parameter is important and the quasithermal \( \langle n_0 \rangle \) obtained from Eq. (28) is

\[
\langle n_0 \rangle = N - \mathcal{H}_I + P_0(\eta_I N + \mathcal{H}_I), 
\]

it is plotted in Fig. 1.

The squared variance

\[
\Delta n_0^2 = \langle n_0^2 \rangle - \langle n_0 \rangle^2 
\]

can be calculated analytically from Eq. (33) to find

\[
\Delta n_0^2 = (1 + \eta_I)\mathcal{H}_I - P_0(\eta_I N + \mathcal{H}_I)(N - \mathcal{H}_I + 1 + \eta_I) - 
\]

\[
P_0^2(\eta_I N + \mathcal{H}_I)^2, 
\]

where

\[
P_0 = \frac{1}{\mathcal{Z}_N} \frac{(N + \mathcal{H}_I/\eta_I - 1)!}{(\eta_I/1 + \eta_I)^N} \left( \frac{\eta_I}{1 + \eta_I} \right)^N, 
\]

is the probability that there are no atoms in the condensate.

If the temperature is not too close to the critical temperature, only the first term in Eq. (37) remains, resulting in

\[
\Delta n_0^2 \simeq (1 + \eta_I)\mathcal{H}_I = \sum_k (\eta_k^2 + \eta_k^I) . 
\]

We plot the variance in Fig. 2 for the case of 200 atoms in a box and the values of gas parameter \( an^{1/3} = 0, 0.1 \). Here \( a = MU/\pi \hbar^2 \) is the s-wave scattering length, \( M \) is the atom mass, \( U \simeq U_{kl} \) is the scattering matrix element in Eq. (13) and \( n \) is the particle density in the box. Squares show the result obtained from CNB3, that is

\[
\langle (n_0 - \bar{n}_0)^2 \rangle = \frac{1}{2} \sum_{k \neq 0} \left[ \frac{1}{z(A_k) - 1} \right]^2 + \frac{1}{z(-A_k) - 1} + 
\]

\[
\frac{1}{z(A_k) - 1} + \frac{1}{z(-A_k) - 1}, 
\]

which is in agreement with Ref. [8].
Table 1 shows $\mathcal{H}_I$ and $\eta_I$ in different approximations. The interacting Bose gas values of $\mathcal{H}_I$ and $\eta_I$ are given in column one in the CNB1 low temperature limit in which $\eta_I = 0$. The second column gives the heating $\mathcal{H}_I$ and cross coupling $\eta_I$ coefficients according to the Eqs. (29) and (31). However, we have specific information from CNB3 such that we know $\Delta n_0$ etc. exactly at, say, $T = 0$. We use that information to improve the present treatment of $\Delta n_0$ by shifting $\mathcal{H}_I$ by a constant value $\Delta \bar{n}$ so that we match $\Delta n_0$ of CNB3 at $T = 0$.

Figure 4 compares the variance $\Delta n_0$ of the condensate particle number as a function of temperature for $N = 200$ particles in a box calculated via the solution of the condensate master equation for $\bar{n}^{1/3} = 0.1$ in different approximations. Dash-dot line is obtained in the low temperature limit. Dashed line is the quasithermal approximation. Squares show the result of Ref. [8] and CNB3. Solid line is calculated in the quasithermal approximation by a shift of $\mathcal{H}_I$ to match the CNB3 value at $T = 0$.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|}
\hline
 & low temperature & quasithermal approximation & quasithermal approximation improved by CNB3 \\
\hline
$\mathcal{H}_I$ & $\sum_{k \neq 0} N_k$ & $\sum_{k \neq 0} N_k$ & $\Delta + \sum_{k \neq 0} N_k$ \\
$\eta_I$ & 0 & $\sum_{k \neq 0} \beta \epsilon_k$ & $\sum_{k \neq 0} \beta \epsilon_k$ \\
\hline
\end{tabular}
\caption{Expressions for $\mathcal{H}_I$ and $\eta_I$ in three limits of operation corresponding to the three previous treatments extended to the present model. The average particle number in the excited level is given by $N_k = \frac{\eta_k^2}{\epsilon_k - \epsilon_{k-1}} + v_k^2$.}
\end{table}

IV. DISCUSSION AND SUMMARY

A. Mean number of particles in the condensate

The calculation of $\langle n_0 \rangle$ for the interacting “Bose-Bogoliubov” gas is in good agreement with and extends the results of CNB3. For example, the Uhlenbeck cusp dilemma [8] is resolved for the interacting gas just as it was for the ideal gas. The master equation approach gives an excellent treatment of the temperature dependence average number of atoms in the condensate. The agreement with the rigorous results of CNB3 is gratifying. Note in particular the ground state depletion at $T = 0$, due to atom-atom interactions, is handled very well by the present approach. Likewise the increase in the number of atoms in the ground state, for temperature $0.3 \lesssim T/T_c \lesssim 1.0$, is modelled very well by the master equation approach. For temperatures well above $T_c$ ($T/T_c \lesssim 1.4$) the ideal gas treatment is valid and agrees with our result. Furthermore, and most significantly from the vantage point of this paper, the master equation approach works well for the temperature region near $T_c$ where the other treatments fail.

As one can see from Fig. 1 repulsive interaction between Bose particles stimulates BEC and yields an increase in $\bar{n}_0$ at intermediate temperature as compared to the ideal gas [11]. The reason is energetic: bosons in different but mutually overlapping states interact stronger than when they are in the same state. For example, when two particles are in the same state is the lowest energy configuration. This favors multiple occupation of a single one-particle state. Such an effect is sometimes called an attraction in momentum space [11]. One can see from Fig. 1 that repulsive interaction also increases $T_c$. 
B. Fluctuations $\Delta n_0$

As Einstein taught us long ago, fluctuation phenomena contains much more physics than mean values do. He used the difference between the fluctuation properties of waves and particles to show the particle side of the photon [12] and the wave side of matter [13]. Note that the latter was well in advance of the Schrödinger equation, and provided support for the wave nature of matter.

The extension of the ideal gas work of CNB2, as per column 2 of Table 1 to the present problem yields the dashed curve which is better but not good for $T = 0$. However, CNB3 provides a good description of the central moments $\langle (n_0 - \bar{n}_0)^m \rangle$ for low temperatures. Thus we can improve our description of the fluctuations by using the known low temperature behavior from CNB3 to improve the heating coefficients as in column 3 of Table 1. The utilization of the low temperature results of CNB3 to improve on $K_{n_0}$ and $H_{n_0}$ yields an excellent description of the central moments, as will be shown elsewhere.

C. Connection with previous studies and future work

The experiments in dilute Bose gases of rubidium, lithium and sodium have reopened the old BEC questions, e.g., the Uhlenbeck cusp dilemma [9] and the question of condensate fluctuations. See for example the recent review [16] and references therein. Likewise the condensate time development [17] is an exciting frontier.

In earlier work [3, 4] we found that there is a useful connection between BEC of an ideal Bose gas [18], and the quantum theory of the laser [19, 20]. We recall that the saturation nonlinearity in the radiation matter interaction is essential for laser coherence [21]. Indeed, the coherence generating nonlinearity in the case of the ideal Bose gas is the particle number constraint which provides the essential nonlinearity in BEC. However, in the case of the interacting gas, the problem of fluctuation is rather subtle and requires a more refined approach. Although useful papers have been published dealing with various limiting cases [8, 22], so far there has been no treatment of this problem valid at all temperatures. Apart from general theoretical interest, condensate fluctuations can be measured, in principle, by means of a scattering of series of short pulses [23], see also [24].

The problem of $N$ ideal bosons in a 3D harmonic potential coupled to a thermal reservoir turns out to be surprisingly rich. The $N$ particle constraint is included naturally in the present formulation and introduces an essential nonlinearity yielding accurate results as shown in Fig. 4 and 2.

Given the utility of the quantum theory of the laser-master equation approach in the ideal Bose gas problem it is natural to look at the interacting gas from a quantum optical perspective, and that was the vantage of Ref. [3]. Other fascinating studies in this regard include the paper by Lewenstein and You on quantum phase diffusion [25], Graham [26] who applied quantum noise analysis to the BEC linewidth question and Wiseman and Thomson on reducing the linewidth of an atom laser by feedback [27].

The time dependent master equation analysis of Gardiner and Zoller is presented in a heroic series of strong papers [28]. The paper of Parkins and Walls [29] on the BEC is another important work in this field. Reference to many

![Graph of $\Delta n_0$ vs $T/T_c$](image)

FIG. 5: Variance $\Delta n_0 = \sqrt{\langle n_0^2 \rangle - \langle n_0 \rangle^2}$ of the condensate particle number as a function of temperature for an ideal Bose gas of $N = 200$ atoms in an isotropic harmonic trap. Solid line is a solution of the condensate master equation. Dots are the exact numerical results obtained in the canonical ensemble for the ideal Bose gas [2]. Squares are result of CNB3. Dashed line is a plot of $\Delta n_0 = \sqrt{\langle n_0^2 \rangle - \langle n_0 \rangle^2}$ which is obtained in the thermodynamic limit [14]. Dash-dot line is a plot of $\Delta n_0 = N - \langle n_0 \rangle = N \left( \frac{T}{T_c} \right)^3$, which is proposed by D. ter Haar [15] in the low temperature regime (adapted to a harmonic trap). This had the correct zero limit as $T \to 0$, but is not right for higher temperatures.

Likewise fluctuations are central to our investigation. We find that even in the ideal Bose gas the fluctuation physics is quite rich, see Fig. 5. The atomic statistical distribution, and its first two central moments, as plotted in Fig. 1 (for $\bar{n}_0$) and Fig. 2 (for $\Delta n_0$) make our point. The low temperature approximation used to get Eq. 1 works quantitatively well for $\bar{n}_0$. However, the treatment of fluctuations in this approximation is only qualitative (see Fig. 4). To get a good description of fluctuations we must extend the improved approach of CNB2, with appropriate modifications, to the case of the interacting gas.
obtain a useful equation of motion for the density matrix of motion for \( \dot{\rho} \). Integrating for representation was given by the "gas+reservoir" system density matrix in the interaction and the Robert A. Welch Foundation (Grant No. A-1261).

APPENDIX A: THE MASTER EQUATION

In CNB1,2 the equation of motion for the total "gas+reservoir" system density matrix in the interaction representation was given by

\[
\dot{\rho}_{\text{total}}(t) = -i[V(t), \rho_{\text{total}}(t)]/\hbar. \tag{A1}
\]

Integrating for \( \rho_{\text{total}} \), inserting it back into the equation of motion for \( \dot{\rho}(t) \), and tracing over the reservoir, we obtain a useful equation of motion for the density matrix of the Bose-gas subsystem

\[
\dot{\rho}(t) = -\frac{1}{\hbar^2} \int_0^t dt' \text{Tr}_{\text{res}}[V(t'), [V(t'), \rho_{\text{total}}(t')]], \tag{A2}
\]

where \( \text{Tr}_{\text{res}} \) denotes the trace over the \( \hat{\beta}_k \) degrees of freedom.

We proceed by assuming that the phonon reservoir (in the spirit of the experiments of Reppy and coworkers) remains unchanged during the interaction with the Bose gas. As discussed in detail in CNB1,2, the density operator for the total system "gas+reservoir" can then be factored, i.e., \( \rho_{\text{total}}(t') \approx \rho(t') \otimes \rho_{\text{res}}, \) where \( \rho_{\text{res}} \) is the equilibrium density matrix of the reservoir. If the spectrum is smooth, we are justified in making the Markov approximation, viz. \( \rho(t') \rightarrow \rho(t) \).

In the present analysis we do not invoke an external (phonon) reservoir. Instead we regard the excited states of our weakly interacting gas to be reservoir-like. In this regard the excited states are nearly analogous to the atoms in the quantum theory of the laser. There we calculate the change in the laser radiation density matrix due to one atom and multiply by the rate of such atomic interaction to obtain a coarse-grained equation of motion for the laser density matrix.

Following the laser approach explicitly (in CNB1,2 it was only implicitly) we first calculate \( \delta \rho(\hat{a}_0, \hat{a}_0^\dagger, t) \) due to a collision between two atoms, which adds (or removes) atoms to the ground state and then multiply by the rate of such collisions to find our master equation for \( \rho(\hat{a}_0, \hat{a}_0^\dagger, t) \). The small change \( \delta \rho \) is given by

\[
\delta \rho(\hat{a}_0, \hat{a}_0^\dagger, t) = -\frac{1}{\hbar^2} \int dt' \int dt'' \text{Tr}_{\text{exc}}[V(t'), [V(t''), \rho(t')]], \tag{A3}
\]

where the collision time \( \tau_c \) is of the order of the scattering length divided by the thermal velocity and is some nanoseconds in duration. The excited states, \( \{n_k\} \), are not much influenced by a single collision and the density matrix \( \rho(t) \) is taken to be \( \rho(t) = \rho_{\text{res}}(t) \otimes \rho(\hat{a}_0, \hat{a}_0^\dagger, t) \). It is important to note that the trap frequencies are of order a few hundred Hertz and the integrals over \( t' \) and \( t'' \) can be simply replaced by \( \tau_c^2/2 \). The rate of collisions \( r \) is governed by the particle mean free path, the thermal velocity and the number of (density of) excited states. The rate \( r \) will contribute only to the constant \( \kappa \) of e.g. Eq. \( \text{(A3)} \) and is of interest here.

Using Eq. \( \text{(A3)} \) and the interaction Hamiltonian Eq. \( \text{(A4)} \) we obtain the following coarse grained equation of motion for the reduced density operator of the interacting Bose gas

\[
\dot{\rho}(\hat{a}_0, \hat{a}_0^\dagger, t) = r \delta \rho = -\frac{\kappa}{2} \sum_{k \neq 0} \text{Tr}[\hat{\beta}_k \hat{\beta}_k^\dagger \rho_{\text{res}}] \{\hat{a}_k \hat{a}_k^\dagger \hat{a}_0 \hat{a}_0^\dagger \rho(t) - \hat{a}_k \hat{a}_0^\dagger \rho(t) \hat{a}_0 \hat{a}_k^\dagger + \text{adj.}\} - \frac{\kappa}{2} \sum_{k \neq 0} \text{Tr}[\hat{\beta}_k \hat{\beta}_k^\dagger \rho_{\text{res}}] \{\hat{a}_k^\dagger \hat{a}_k \hat{a}_0 \hat{a}_0^\dagger \rho(t) - \hat{a}_k^\dagger \hat{a}_0 \hat{a}_0^\dagger \rho(t) \hat{a}_k \hat{a}_k^\dagger + \text{adj.}\}. \tag{A4}
\]

The constant \( \kappa \) is an overall rate which plays no role in the present problem.

In this paper, we are most interested in the atomic statistics of the condensate and hence define the joint probability for having \( n_k \) atoms in the condensate and \( n_1, n_2, \ldots, n_k, \ldots = \{n_k\} \) atoms in the various excited states as:

\[
P(\{n_k\}, n_0) = \langle \{n_k\}, n_0 | \rho | \{n_k\}, n_0 \rangle \tag{A5}
\]

In view of the definition \( \text{(A5)} \), Eq. \( \text{(A4)} \) implies

\[
\dot{P}(\{n_k\}; n_0) = -\frac{\kappa}{2} \sum_{k \neq 0} (\langle \hat{\beta}_k^\dagger \hat{\beta}_k \rangle + 1) [n_k(n_k + 1)P(\{n_k\}; n_0) - P(\{n_k\}; n_0)].
\]
\[ n_k n_0 P(\{n_k\}; n_0 - 1) + \text{adj.} - \]
\[
\frac{K}{2} \sum_{k \neq 0} (\hat{\beta}_k^\dagger \hat{\beta}_k)[(n_k + 1)n_0 P(\{n_k\}; n_0) - \\
(n_k + 1)(n_0 + 1)P(\{n_k\}; n_0 + 1) + \text{adj.}] \quad (A6)
\]

The condensate statistical distribution \(P(n_0)\) is then related to the joint probability distribution \(P(\{n_k\}; n_0)\) and the conditional probability \(P(\{n_k\}|n_0)\) via Bayes rule
\[
P(\{n_k\}; n_0) = P(\{n_k\}|n_0)P(n_0). \quad (A7)
\]

We obtain \(P(n_0)\) from \(P(\{n_k\}; n_0)\) directly by summing over all excited states \(\{n_k\}\)
\[
P(n_0) = \sum_{\{n_k\}} P(\{n_k\}; n_0), \quad (A8)
\]
so that we have
\[
\dot{P}_{n_0} = -\kappa \sum_{k \neq 0} ((\hat{\beta}_k^\dagger \hat{\beta}_k) + 1)[(n_k)n_0(n_0 + 1)P_{n_0} - \\
\langle n_k \rangle_{n_0-1} n_0 P_{n_0-1}] - \kappa \sum_{k \neq 0} (\hat{\beta}_k^\dagger \hat{\beta}_k)[(n_k)n_0+1)n_0 P_{n_0} - \\
\langle n_k \rangle_{n_0+1} n_0 P_{n_0+1} + 1)(n_0+1)P_{n_0+1}] \quad (A9)
\]
where we have introduced the convenient conditional average notation
\[
\langle n_k \rangle_{n_0} = \sum_{n_k} n_k P(\{n_k\}|n_0). \quad (A10)
\]

The master equation obtained here is diagonal. More general master equation can be off-diagonal, as we discuss in Appendix C.

**APPENDIX B: THE CROSS COUPLING COEFFICIENTS**

In this appendix, we present a brief reminder of how the heating and cooling coefficients \(H_{n_0}\) and \(K_{n_0}\) were handled in CBN2 for an ideal gas. There, we encountered the heating and cooling coefficients
\[
K_{n_0} = \sum_{k \neq 0} \langle n_k \rangle_{n_0} (1 + \langle \hat{b}_k^\dagger \hat{b}_k \rangle), \quad (B1)
\]
and
\[
H_{n_0} = \sum_{k \neq 0} \langle \hat{b}_k^\dagger \hat{b}_k \rangle (1 + \langle n_k \rangle_{n_0}). \quad (B2)
\]
Defining
\[
\eta_k = \langle \hat{b}_k^\dagger \hat{b}_k \rangle = \frac{1}{e^{\beta \nu_k} - 1}, \quad (B3)
\]
where \(\beta = 1/k_{\beta}T\). Eqs. \((B1)\) and \((B2)\) now read
\[
K_{n_0} = \sum_{k \neq 0} \langle n_k \rangle_{n_0} (1 + \eta_k), \quad (B4)
\]
and
\[
H_{n_0} = \sum_{k \neq 0} \eta_k (1 + \langle n_k \rangle_{n_0}). \quad (B5)
\]

We then approximate the conditional thermal average as
\[
\langle n_k \rangle_{n_0} = (N - n_0) \sum_{k \neq 0} \frac{\tilde{n}_k}{\eta_k}, \quad (B6)
\]
where the usual atomic thermal average is given by
\[
\tilde{n}_k = \frac{1}{e^{\beta \nu_k} - 1}. \quad (B7)
\]
Now an ensemble of atoms and phonons in an ordinary gas obeys the simple rate equation
\[
\frac{d}{dt} \tilde{n}_k = \gamma (\tilde{n}_k + 1) \eta_k - \gamma \tilde{n}_k (\eta_k + 1), \quad (B8)
\]
where \(\gamma\) is an uninteresting rate factor. At steady state Eq. \((B8)\) yields
\[
(\tilde{n}_k + 1) \eta_k = \tilde{n}_k (\eta_k + 1), \quad (B9)
\]
which implies that \(\eta_k = \tilde{n}_k\) and we may write Eq. \((B8)\) as
\[
\langle n_k \rangle_{n_0} = (N - n_0) \sum_{k \neq 0} \frac{\eta_k}{\sum_{k \neq 0} \eta_k}. \quad (B10)
\]
Hence we have
\[
\sum_{k \neq 0} \langle n_k \rangle_{n_0} \eta_k = \frac{(N - n_0)}{\mathcal{H}} \sum_{k \neq 0} \eta_k^2 = (N - n_0) \eta \quad (B11)
\]
where we have introduced the notations
\[
\mathcal{H} = \sum_{k \neq 0} \eta_k \quad \text{and} \quad \eta = \frac{\sum_{k \neq 0} \eta_k^2}{\mathcal{H}}. \quad (B12)
\]
In this way we arrive at the \(K_{n_0}\) and \(H_{n_0}\) coefficients of CBN2 given by
\[
K_{n_0} = (N - n_0)(1 + \eta), \quad (B13)
\]
and
\[
H_{n_0} = \mathcal{H} + (N - n_0) \eta. \quad (B14)\]
APPENDIX C: MASTER EQUATION GENERALIZATIONS

Our interaction Hamiltonian can yield an off-diagonal master equation. That is, the main working master equation in operator form is

\[
\frac{1}{\kappa} \frac{d \rho(t)}{dt} = - \sum_{k \neq 0} < \hat{\beta}^\dagger_k \hat{a}_k \hat{a}^\dagger_k >_{n_0} (\hat{a}^\dagger_k \hat{a}_k \rho(t) - \hat{a}_k \hat{a}^\dagger_k \rho(t) \hat{a}_k) + \text{adj.} - J \left[ \sqrt{n_0(n_0 - 1)} \rho_{n_0 - 2, n_0} + \sqrt{(n_0 + 2)(n_0 + 1)} \rho_{n_0, n_0 + 2} - 2 \sqrt{n_0(n_0 + 1)} \rho_{n_0 - 1, n_0 + 1} \right] - \frac{1}{2 \kappa} \rho_{n_0, n_0} = -(N - n_0)(1 + \eta_1)(n_0 + 1) \rho_{n_0, n_0} + (N - n_0 + 1)(1 + \eta_1) n_0 \rho_{n_0 - 1, n_0 - 1} - [H_I + (N - n_0) \eta_1] n_0 \rho_{n_0, n_0} + [H_I + (N - n_0 - 1) \eta_1] (n_0 + 1) \rho_{n_0 + 1, n_0 + 1} - 2 \sqrt{n_0(n_0 + 1)} \rho_{n_0 + 1, n_0 + 1} \right] \]

New contribution of the form \( \hat{a}^\dagger_k \hat{a}_k \rho(t) - \hat{a}_k \hat{a}^\dagger_k \rho(t) \hat{a}_k \) and \( \hat{a}_k \hat{a}^\dagger_k \rho(t) - \hat{a}_k \hat{a}^\dagger_k \rho(t) \hat{a}_k \) yields off-diagonal terms in the density matrix equation. Taking into account that

\[
< \hat{\beta}^\dagger_k \hat{\beta}^\dagger_{-k} > = \hat{a}_k \hat{a}^\dagger_k = \frac{2}{e^\beta - 1} + 1 \]

we obtain a master equation which couples the diagonal and off-diagonal terms in the density matrix

\[
\frac{1}{2 \kappa} \rho_{n_0, n_0} = -(N - n_0)(1 + \eta_1)(n_0 + 1) \rho_{n_0, n_0} + (N - n_0 + 1)(1 + \eta_1) n_0 \rho_{n_0 - 1, n_0 - 1} - [H_I + (N - n_0) \eta_1] n_0 \rho_{n_0, n_0} + [H_I + (N - n_0 - 1) \eta_1] (n_0 + 1) \rho_{n_0 + 1, n_0 + 1}
\]

where \( H_I \) and \( \eta_I \) are given by previous formulas \[20\] and \[31\], and

\[
J = \sum_{k \neq 0} u_k^2 v_k^2 \left[ \frac{2}{e^\beta - 1} + 1 \right]^2 \]

The more general analysis of fluctuations with off-diagonal terms will be presented elsewhere. We have also studied a two atom master equation in which two atoms at a time are added or removed from the condensate. This is analogous to the two photon laser. The results of such an analysis are in basic agreement with the present findings and will be published elsewhere.

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