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

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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 $T \simeq T_c$. 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's or 100's of atoms), is the subject of this paper. The answer is given by the diagonal elements of the BEC density matrix, ρ_{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

$$\rho_{n_0,n_0} = \frac{\mathcal{H}_I^{N-n_0}}{(N-n_0)!} \mathcal{Z}_N^{-1}, \qquad \mathcal{Z}_N = e^{\mathcal{H}_I}\Gamma(N+1,\mathcal{H}_I)/N! \tag{1}$$

where $\mathcal{Z}_N$ 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
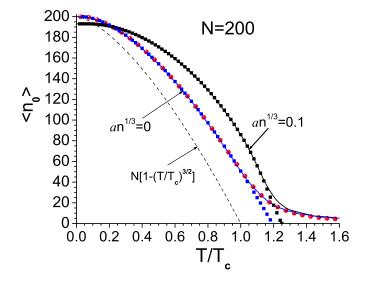

FIG. 1: Solid lines are the present work results showing the mean number of condensate particles as a function of temperature for N = 200 particles in a box calculated via the solution of the condensate master equation for an interacting (Bogoliubov) gas with $an^{1/3} = 0.1$ and an ideal (Bose) gas $an^{1/3} = 0$. 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 $T_c = 2\pi\hbar^2 n^{2/3}/k_B M \zeta(3/2)^{2/3}$, where M is the particle mass.

given by

$$\mathcal{H}_I = \sum_{\mathbf{k}\neq\mathbf{0}} \left(\frac{u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2}{e^{\beta\varepsilon_{\mathbf{k}}} - 1} + v_{\mathbf{k}}^2 \right). \tag{2}$$

In the above the usual Bogoliubov amplitudes are

$$u_{\mathbf{k}} = \frac{1}{\sqrt{1 - A_{\mathbf{k}}^2}}, \ v_{\mathbf{k}} = \frac{A_{\mathbf{k}}}{\sqrt{1 - A_{\mathbf{k}}^2}},$$
$$A_{\mathbf{k}} = \frac{V}{\bar{n}_0 U_{\mathbf{k}}} \left(\epsilon_{\mathbf{k}} - \frac{\hbar^2 k^2}{2M} - \frac{\bar{n}_0 U_{\mathbf{k}}}{V} \right), \qquad (3)$$

where M is the atomic mass, V is the condensate volume and $U_{\mathbf{k}}$ is the atom-atom scattering energy; the quasiparticle energy $\epsilon_{\mathbf{k}}$ is given by

$$\epsilon_{\mathbf{k}} = \sqrt{\left(\frac{\hbar^2 k^2}{2M} + \frac{\bar{n}_0 U_{\mathbf{k}}}{V} \right)^2 - \left(\frac{\bar{n}_0 U_{\mathbf{k}}}{V} \right)^2}. \qquad (4)$$

The simple expression, Eq. (1), is valid in the limit in which, for the case of an ideal gas in a box, $\mathcal{H}_I = N (T/T_c)^{3/2}$ 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 [3], in which we focused on the statistics of N noninteracting (ideal) bosons. In the second paper [4] (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., is 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 [5] includes interactions. The analysis of CNB3 is based on the Girardeau-Arnowitt adaptation 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, $< n_k n_m > = \bar{n}_k \bar{n}_m$, $k \neq m$, by exchanging particles with the condensate reservoir. For $N = 200$ CNB3 is valid from $T = 0$ to $T \approx 0.7 T_c$. 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 $\left(\vec{k} - \vec{k} \right)$ 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. (14). 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
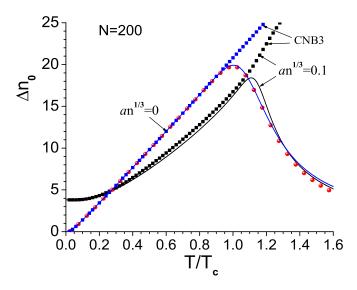

FIG. 2: Variance Δn_0 of the condensate particle number as a function of temperature for N = 200 particles in a box calculated via the solution of the condensate master equation for $an^{1/3} = 0$ and 0.1 (solid lines). Dots are obtained by exact numerical calculations for the ideal Bose gas in the canonical ensemble [2]. Squares are the result of CNB3. For $an^{1/3} = 0.1$ the solid line is obtained from the master equation by a shift of $\mathcal{H}_I$ to match the CNB3 value at T = 0 (see Table 1 column three).

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

$$V = \sum_{\mathbf{k}} g_{\mathbf{k}} \, \hat{a}_0^\dagger \, \hat{b}_{\mathbf{k}}^\dagger \, \hat{a}_{\mathbf{k}} + \text{adj.} \tag{5}$$

where $\hat{a}_{\mathbf{k}}$ and $\hat{b}_{\mathbf{k}}$ are atom and phonon annihilation operators, likewise $\hat{a}_0$ is the condensate annihilation operator and $g_{\mathbf{k}}$ is the corresponding coupling strength for the collision of a ground state atom and an atom having momentum $\mathbf{k}$ scattering into the BEC. This models the dilute gas BEC experiments of Reppy and coworkers [6]. 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 Δn_0 for an interacting Bose gas, we derive a master equation for ρ_{n_0,n_0} by simply replacing the phonon operators $b_{\mathbf{k}}$ and $b_{\mathbf{k}}^\dagger$ in Eq. (5) by operators $\hat{\text{ß}}_{\mathbf{k}}$ and $\hat{\text{ß}}_{\mathbf{k}}^\dagger$ related to $\hat{b}_{\mathbf{k}}$ and $\hat{b}_{\mathbf{k}}^\dagger$ by the usual Bogoliubov transformation

$$\begin{aligned}
\hat{\text{ß}}_{\mathbf{k}} &= u_{\mathbf{k}} \hat{b}_{\mathbf{k}} + v_{\mathbf{k}} \hat{b}_{-\mathbf{k}}^\dagger \\
\hat{\text{ß}}_{\mathbf{k}}^\dagger &= u_{\mathbf{k}} \hat{b}_{\mathbf{k}}^\dagger + v_{\mathbf{k}} \hat{b}_{-\mathbf{k}},
\end{aligned} \tag{6}$$

where $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are given in Eq. (3), $< \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} > = 1/(e^{\beta \epsilon_{\mathbf{k}}} - 1)$, $\epsilon_{\mathbf{k}}$ is the Bogoliubov quasiparticle energy given by Eq. (4).

The present master equation for the condensate is now obtained via the phenomenological interaction Hamiltonian

$$V = \sum_{\mathbf{k}} \tilde{g}_{\mathbf{k}} \, \hat{a}_{\mathbf{k}} \, \hat{\text{ß}}_{\mathbf{k}}^\dagger \, \hat{a}_0^\dagger + \text{adj.} \tag{7}$$

which adds (removes) atoms from the condensate with the annihilation (creation) of an excited atom and the emission (absorption) of a quasiparticle.

We recall that the simple ideal gas master equation for the probability P_{n_0} of finding n_0 atoms in the N atom gas ground state was found to be [3]

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

$$\mathcal{H} n_0 P_{n_0} + \mathcal{H}(n_0 + 1) P_{n_0 + 1}, \tag{8}$$

where κ is an uninteresting overall rate factor and the phonon heating coefficient was given by

$$\mathcal{H} = \sum_{\mathbf{k} \neq \mathbf{0}} \frac{1}{e^{\beta \epsilon_{\mathbf{k}}} - 1}, \tag{9}$$

where $\beta = 1/k_B T$.

In the present toy model all we do is replace the phonon operators $\hat{b}_{\mathbf{k}}$ and $\hat{b}_{\mathbf{k}}^\dagger$ in Eq. (5) by the quasiparticle operators $\hat{\text{ß}}_{\mathbf{k}}$ and $\hat{\text{ß}}_{\mathbf{k}}^\dagger$ of Eq. (6), and find the new heating coefficient

$$\mathcal{H} \Rightarrow \sum_{\mathbf{k} \neq \mathbf{0}} \left[\frac{u_k^2 + v_k^2}{e^{\beta \epsilon_{\mathbf{k}}} - 1} + v_k^2 \right] \equiv \mathcal{H}_I. \tag{10}$$

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.

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 [7]

$$\hat{\beta}_{\mathbf{k}}^\dagger = \hat{a}_{\mathbf{k}}^\dagger \hat{\beta}_0, \qquad \hat{\beta}_{\mathbf{k}} = \hat{\beta}_0^\dagger \hat{a}_{\mathbf{k}}, \qquad \hat{\beta}_0 = (1 + \hat{n}_0)^{-1/2} \hat{a}_0. \tag{11}$$

These operators describe canonical-ensemble quasiparticles which obey the Bose canonical commutation relations

$$[\hat{\beta}_{\mathbf{k}}, \hat{\beta}_{\mathbf{k}}^\dagger] = \delta_{\mathbf{k}, \mathbf{k}'}, \tag{12}$$

see CNB3. The canonical-ensemble quasiparticles $\hat{\beta}_{\mathbf{k}} = \hat{\beta}_0^\dagger \hat{a}_{\mathbf{k}}$ describe transitions between ground ($\mathbf{k} = \mathbf{0}$) and excited ($\mathbf{k} \neq \mathbf{0}$) states.

Consider next the conventional atom-atom interaction Hamiltonian as sketched in Fig. 3. Thus we may write

$$V_1 = \sum_{\mathbf{k}, \mathbf{l}} U_{\mathbf{k}\mathbf{l}} \hat{a}_{\mathbf{l} - \mathbf{k}}^\dagger \hat{a}_{\mathbf{k}}^\dagger \hat{a}_0 \hat{a}_{\mathbf{l}} = \sum_{\mathbf{k}, \mathbf{l}} \tilde{U}_{\mathbf{k}\mathbf{l}} \hat{a}_{\mathbf{l} - \mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{l}} \tag{13}$$

where we have introduced the canonical-ensemble quasiparticles $\hat{a}_{\mathbf{k}}^\dagger \hat{a}_0 \approx \sqrt{\bar{n}_0} \hat{a}_{\mathbf{k}}^\dagger (1 + \hat{n}_0)^{-1/2} \hat{a}_0 = \sqrt{\bar{n}_0} \hat{\beta}_{\mathbf{k}}^\dagger$, and the notation $\tilde{U}_{\mathbf{k}\mathbf{l}} = \sqrt{n_0} U_{\mathbf{k}\mathbf{l}}$ with $U_{\mathbf{k}\mathbf{l}}$ being the scattering matrix element. Finally we take $\mathbf{l} = \mathbf{k}$ (leading term) and thus write the interaction Hamiltonian

$$V = \sum_{\mathbf{k}} \tilde{U} \hat{a}_0^\dagger \hat{\beta}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \text{adj.} \tag{14}$$

It is important to note that this Hamiltonian involves two different kinds of operators. The operators $\hat{a}_0^\dagger$ and $\hat{a}_{\mathbf{k}}$ are single particle operators which create and annihilate particles. The $\hat{\beta}_{\mathbf{k}}^\dagger$ operator, by construction conserves particle number as befits a phonon like quasiparticle.
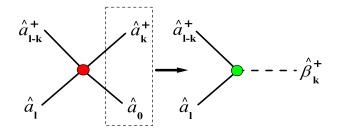
FIG. 3: Two particle scattering process involving the condensate, and the same process in terms of canonical ensemble quasiparticles.

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, $\hat{\beta}_{\mathbf{k}}$ and $\hat{\beta}_{\mathbf{k}}^{\dagger}$. We proceed to treat the $\hat{\beta}_{\mathbf{k}}$ 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

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

$$H_{n_0}n_0 P_{n_0} + H_{n_0+1}(n_0+1)P_{n_0+1}. \qquad (15)$$

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 κ is an uninteresting overall rate factor. The cooling and heating coefficients are given by

$$K_{n_0} = \sum_{\mathbf{k}\neq\mathbf{0}} \langle n_{\mathbf{k}}\rangle_{n_0}\left(1 + \left\langle\hat{\beta}_{\mathbf{k}}^{\dagger}\hat{\beta}_{\mathbf{k}}\right\rangle\right), \qquad (16)$$

$$H_{n_0} = \sum_{\mathbf{k}\neq\mathbf{0}} \left\langle\hat{\beta}_{\mathbf{k}}^{\dagger}\hat{\beta}_{\mathbf{k}}\right\rangle\left(1 + \langle n_{\mathbf{k}}\rangle_{n_0}\right). \qquad (17)$$

Equation (15) was obtained previously in a similar form for the ideal gas; the essential difference being that the average $\left\langle\hat{\beta}_{\mathbf{k}}^{\dagger}\hat{\beta}_{\mathbf{k}}\right\rangle$ is replaced by an average number of thermal phonons in our earlier work. The physics behind (15) is best understood by going to a "low temperature limit" such that $\left\langle\hat{\beta}_{\mathbf{k}}^{\dagger}\hat{\beta}_{\mathbf{k}}\right\rangle \ll 1$ and we may write Eq. (16) as

$$K_{n_0} = \sum_{\mathbf{k}\neq\mathbf{0}} \langle n_{\mathbf{k}}\rangle_{n_0} = N - n_0, \qquad (18a)$$

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

$$H_{n_0} = \sum_{\mathbf{k}\neq\mathbf{0}} \left\langle\hat{\beta}_{\mathbf{k}}^{\dagger}\hat{\beta}_{\mathbf{k}}\right\rangle \equiv \mathcal{H}_I. \qquad (18b)$$

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

$$\hat{\beta}_{\mathbf{k}} = u_{\mathbf{k}}\hat{\mathfrak{b}}_{\mathbf{k}} + v_{\mathbf{k}}\hat{\mathfrak{b}}_{-\mathbf{k}}^{\dagger} \qquad (19)$$

$$\hat{\beta}_{-\mathbf{k}}^{\dagger} = u_{\mathbf{k}}\hat{\mathfrak{b}}_{-\mathbf{k}}^{\dagger} + v_{\mathbf{k}}\hat{\mathfrak{b}}_{\mathbf{k}} \qquad (20)$$

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

$$\left\langle\hat{\beta}_{\mathbf{k}}^{\dagger}\hat{\beta}_{\mathbf{k}}\right\rangle = u_{\mathbf{k}}^2\left\langle\hat{\mathfrak{b}}_{\mathbf{k}}^{\dagger}\hat{\mathfrak{b}}_{\mathbf{k}}\right\rangle + v_{\mathbf{k}}^2\left\langle\hat{\mathfrak{b}}_{-\mathbf{k}}\hat{\mathfrak{b}}_{-\mathbf{k}}^{\dagger}\right\rangle$$

$$= \frac{u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2}{e^{\beta\epsilon_{\mathbf{k}}} - 1} + v_{\mathbf{k}}^2 \equiv \mathfrak{N}_{\mathbf{k}}. \qquad (21)$$

In the preceding we have taken the quasi-particle to be in thermal equilibrium such that

$$\left\langle\hat{\mathfrak{b}}_{\mathbf{k}}^{\dagger}\hat{\mathfrak{b}}_{\mathbf{k}}\right\rangle = \left\langle\hat{\mathfrak{b}}_{-\mathbf{k}}^{\dagger}\hat{\mathfrak{b}}_{-\mathbf{k}}\right\rangle = \frac{1}{e^{\beta\epsilon_{\mathbf{k}}} - 1}. \qquad (22)$$

Finally, we note that in the useful notation of CNB3 the $\mathcal{H}_I$ coefficient found from Eqs. (18b) and (21) reads

$$\mathcal{H}_I = \frac{1}{2}\sum_{\mathbf{k}\neq\mathbf{0}}\left(\frac{1}{z(A_{\mathbf{k}}) - 1} + \frac{1}{z(-A_{\mathbf{k}}) - 1}\right), \qquad (23)$$

where

$$z(A_{\mathbf{k}}) = \frac{A_{\mathbf{k}} - e^{\varepsilon_{\mathbf{k}}/T}}{A_{\mathbf{k}}e^{\varepsilon_{\mathbf{k}}/T} - 1} \qquad (24)$$

and $A_{\mathbf{k}}$ is given by Eq. (3).

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

$$\sum_{\mathbf{k}\neq\mathbf{0}} \langle n_k\rangle_{n_0}\left\langle\hat{\beta}_{\mathbf{k}}^{\dagger}\hat{\beta}_{\mathbf{k}}\right\rangle \qquad (25)$$

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

$$\sum_{\mathbf{k}\neq\mathbf{0}} \langle n_k\rangle_{n_0}\left\langle\hat{b}_{\mathbf{k}}^{\dagger}\hat{b}_{\mathbf{k}}\right\rangle = (N - n_0)\eta \qquad (26)$$

where the phonon average number $\left\langle \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}} \right\rangle = (e^{\beta \epsilon_{\mathbf{k}}} - 1)^{-1} \equiv \eta_{\mathbf{k}}$ and the CNB2 cross coupling coefficient η is defined by

$$\eta = \sum_{\mathbf{k} \neq \mathbf{0}} \eta_{\mathbf{k}}^2 / \mathcal{H} \qquad (27)$$

where

$$\mathcal{H} = \sum_{\mathbf{k} \neq \mathbf{0}} \eta_{\mathbf{k}}. \qquad (28)$$

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

$$\mathcal{H}_I = \sum_{\mathbf{k} \neq \mathbf{0}} \left(\frac{u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2}{e^{\beta \varepsilon_{\mathbf{k}}} - 1} + v_{\mathbf{k}}^2 \right) \equiv \sum_{\mathbf{k} \neq \mathbf{0}} \mathfrak{N}_{\mathbf{k}} \qquad (29)$$

and

$$\sum_{\mathbf{k} \neq \mathbf{0}} \langle n_k \rangle_{n_0} \left\langle \hat{\beta}_{\mathbf{k}}^{\dagger} \hat{\beta}_{\mathbf{k}} \right\rangle = \sum_{\mathbf{k} \neq \mathbf{0}} \langle n_k \rangle_{n_0} \mathfrak{N}_k = (N - n_0) \eta_I, \quad (30)$$

where

$$\eta_I = \sum_{\mathbf{k} \neq \mathbf{0}} \mathfrak{N}_{\mathbf{k}}^2 / \mathcal{H}_I. \qquad (31)$$

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

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

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

$$[\mathcal{H}_I + (N - (n_0 + 1)) \eta_I](n_0 + 1) P_{n_0 + 1}. \qquad (32)$$

III. CONDENSATE STATISTICS VIA STEADY STATE SOLUTION TO MASTER EQUATION

The BEC atom statistical distribution is now obtained by solving the master equation (32). The resulting distribution is given by essentially the same expression as was obtained for the ideal Bose gas in CNB2, namely

$$P_{n_0} = \frac{1}{\mathcal{Z}_N} \frac{(N - n_0 + \mathcal{H}_I / \eta_I - 1)!}{(\mathcal{H}_I / \eta_I - 1)!(N - n_0)!} \left(\frac{\eta_I}{1 + \eta_I} \right)^{N - n_0}, \qquad (33)$$

$$\mathcal{Z}_N = \sum_{n_0 = 0}^{N} \binom{N - n_0 + \mathcal{H}_I / \eta_I - 1}{N - n_0} \left(\frac{\eta_I}{1 + \eta_I} \right)^{N - n_0}, \qquad (34)$$

where $\mathcal{H}_I$ and η_I for the interacting gas are given in Table 1.

In the low temperature limit we set η_I to zero and obtain the distribution given by Eq. (1). The average condensate particle number from Eq. (1) is

$$\langle n_0 \rangle = N - \mathcal{H}_I + \mathcal{H}_I^{N+1} / \mathcal{Z}_N N! \qquad (35)$$

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 $\mathcal{H}_I^{N+1} / \mathcal{Z}_N N!$ as given in Eq. (35) removes the unphysical cusp at $T = T_c$ and extends the treatment of CNB3 through the critical temperature. Equation (1) and the associated $\langle n_0 \rangle$ is essentially the extension of the results of CNB1 to include atom-atom interaction.

In general the η_I parameter is important and the quasithermal $\langle n_0 \rangle$ obtained from Eq. (33) 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

$$\Delta n_0^2 = \langle n_0^2 \rangle - \langle n_0 \rangle^2 \qquad (36)$$

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

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

$$P_0^2 (\eta_I N + \mathcal{H}_I)^2, \qquad (37)$$

where

$$P_0 = \frac{1}{\mathcal{Z}_N} \frac{(N + \mathcal{H}_I / \eta_I - 1)!}{N!(\mathcal{H}_I / \eta_I - 1)!} \left(\frac{\eta_I}{1 + \eta_I} \right)^N \qquad (38)$$

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

$$\Delta n_0^2 \simeq (1 + \eta_I) \mathcal{H}_I \equiv \sum_{\mathbf{k}} (\mathfrak{N}_{\mathbf{k}}^2 + \mathfrak{N}_{\mathbf{k}}). \qquad (39)$$

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 $a = MU / 4\pi \hbar^2$ is the s-wave scattering length, M is the atom mass, $U \simeq U_{\mathbf{kl}}$ 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

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

$$\left. \frac{1}{z(A_{\mathbf{k}}) - 1} + \frac{1}{z(-A_{\mathbf{k}}) - 1} \right], \qquad (40)$$

which is in agreement with Ref. [8].

	low temperature approximation	quasithermal approximation	quasithermal approximation improved by CNB3
$\mathcal{H}_I$	$\sum_{k \neq 0} \mathfrak{N}_k$	$\sum_{k \neq 0} \mathfrak{N}_k$	$\Delta + \sum_{k \neq 0} \mathfrak{N}_k$
η_I	0	$\frac{\sum_{k \neq 0} \mathfrak{N}^2_k}{\sum_{k' \neq 0} \mathfrak{N}_k}$	$\frac{\sum_{k \neq 0} \mathfrak{N}^2_k}{\sum_{k' \neq 0} \mathfrak{N}_k}$

TABLE I: Expressions for $\mathcal{H}_I$ and η_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 $\mathfrak{N_k} = \frac{u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2}{e^{\beta \varepsilon_{\mathbf{k}}} - 1} + v_{\mathbf{k}}^2$.

Table 1 shows $\mathcal{H}_I$ and η_I in different approximations. The interacting Bose gas values of $\mathcal{H}_I$ and η_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 η_I coefficients according to the Eqs. (29) and (31). However, we have specific information from CNB3 such that we know Δn_0 etc. exactly at, say, $T = 0$. We use that information to improve the present treatment of Δn_0 by shifting $\mathcal{H}_I$ by a constant value Δ so that we match Δn_0 of CNB3 at $T = 0$.

Figure 4 compares the variance Δn_0 of the condensate particle number calculated for $an^{1/3} = 0.1$ in three different approximations. The dash-dot line is obtained in the low temperature limit (Table 1 column one). The dashed line is the quasithermal approximation (Table 1 column two). The solid curve was obtained from $\mathcal{H}_I$ and η_I of Table 1 column three.

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 [9] 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 ($T/T_c \gtrsim 1.4$) 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 in-
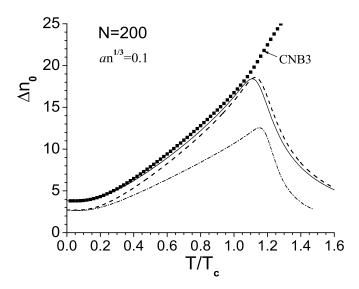

FIG. 4: Variance $\Delta n_0 = \sqrt{\langle n_0^2 \rangle - \langle n_0 \rangle^2}$ of the condensate particle number as a function of temperature for $N = 200$ particles in a box calculated via the solution of the condensate master equation for $an^{1/3} = 0.1$ in different approximations. Dash-dot 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 $T = 0$.

crease in $\bar{n}_0$ at intermediate temperature as compared to the ideal gas [10]. 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 $\Psi(\mathbf{r}_1, \mathbf{r}_2) = \chi(\mathbf{r}_1)\chi(\mathbf{r}_2)$ and interact via a potential $V = g\delta(\mathbf{r}_1 - \mathbf{r}_2)$, the interaction energy is

$$E_{\text{int}} = \int d\mathbf{r}_1 \int d\mathbf{r}_2 \Psi^*(\mathbf{r}_1, \mathbf{r}_2) V \Psi(\mathbf{r}_1, \mathbf{r}_2) =$$

$$g \int d\mathbf{r}_1 |\chi(\mathbf{r}_1)|^4.$$

However when two particles are in different states such that $\Psi(\mathbf{r}_1, \mathbf{r}_2) = [\varphi(\mathbf{r}_1)\chi(\mathbf{r}_2) + \varphi(\mathbf{r}_2)\chi(\mathbf{r}_1)]/\sqrt{2}$, the interaction energy is

$$E_{\text{int}} = 2g \int d\mathbf{r}_1 |\varphi(\mathbf{r}_1)|^2 |\chi(\mathbf{r}_1)|^2.$$

Then since $|\varphi(\mathbf{r}_1)|^2 \simeq |\chi(\mathbf{r}_1)|^2$ we see that two bosons 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 Δn_0

As Einstein taught us long ago, fluctuation phenomena contains much more physics then 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.
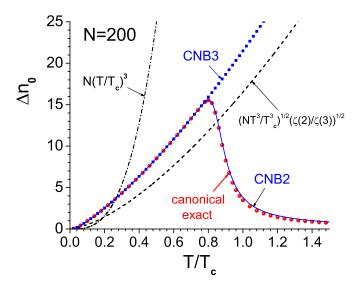

FIG. 5: Variance $\Delta n_0 = \sqrt{\langle n_0^2 \rangle - \langle n_0 \rangle^2}$ of the condensate particle number as a function of temperature for an ideal Bose gas of $N = 200$ atoms in an isotropic harmonic trap. Solid line is a solution of the condensate master equation. Dots are the exact numerical results obtained in the canonical ensemble for the ideal Bose gas [2]. Squares are result of CNB3. Dashed line is a plot of $\Delta n_0 = \sqrt{\frac{\zeta(2)N}{\zeta(3)} \left(\frac{T}{T_c}\right)^3}$ 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 Δn_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.

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. 1 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. [5]. 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

other useful and insightful papers is given in our recent review on fluctuations in the BEC [16].

One basic difference between the classic papers mentioned above is treatment of the BEC of a mesoscopic gas in the critical region near T_c. The present master equation approach is, to our knowledge, unique in that it treats BEC analytically at all temperatures.

In the next paper (CNB5) we shall follow the lead of Section III, see Table I and Fig. 4, wherein we use the statistical mechanical results of CNB3 to find a good (semi-phenomenological) description of all moments at arbitrary temperatures. Then in CNB6 we shall present a detailed analysis including the off-diagonal elements (e.g. $\hat{a}_0^\dagger \hat{a}_0^\dagger \hat{\rho}_0$). Finally we will return to the study of various forms of the dynamics (Hamiltonian) in CNB7, and show that certain formulations do not involve off-diagonal elements and give a good account of the physics via a simple treatment.

V. ACKNOWLEDGMENTS

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

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

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

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

where Tr_{res} denotes the trace over the $\hat{\beta}_{\mathbf{k}}$ degrees of freedom.

We proceeded by assuming that the phonon reservoir (in the spirit of the experiments of Reppy and coworkers [6]) 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 ρ_{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 [19]. 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

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

where the collision time τ_c is of the order of the scattering length divided by the thermal velocity and is some nanoseconds in duration. The excited states, $\{n_{\mathbf{k}}\}$, 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 κ of e.g. Eq. (A4) and is not of interest here.

Using Eq. (A3) and the interaction Hamiltonian Eq. (14) we obtain the following coarse grained equation of motion for the reduced density operator of the interacting Bose gas

$$\dot{\rho}(\hat{a}_0, \hat{a}_0^\dagger, t) = r\delta\rho = -\frac{\kappa}{2} \sum_{\mathbf{k} \neq \mathbf{0}} \text{Tr}\{\hat{\beta}_{\mathbf{k}} \hat{\beta}_{\mathbf{k}}^\dagger \rho_{res}\}[\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \hat{a}_0 \hat{a}_0^\dagger \hat{\rho}(t) -$$

$$\hat{a}_{\mathbf{k}} \hat{a}_0^\dagger \hat{\rho}(t) \hat{a}_0 \hat{a}_{\mathbf{k}}^\dagger + \text{adj.}] -$$

$$\frac{\kappa}{2} \sum_{\mathbf{k} \neq \mathbf{0}} \text{Tr}\{\hat{\beta}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}} \rho_{res}\}[\hat{a}_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{\rho}(t) - \hat{a}_{\mathbf{k}}^\dagger \hat{a}_0 \hat{\rho}(t) \hat{a}_0^\dagger \hat{a}_{\mathbf{k}} + \text{adj.}]. \quad (A4)$$

The constant κ 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_0 atoms in the condensate and $n_1, n_2, .., n_{\mathbf{k}}, .. = \{n_{\mathbf{k}}\}$ atoms in the various excited states as:

$$P(\{n_{\mathbf{k}}\}, n_0) = \langle \{n_{\mathbf{k}}\}, n_0 | \rho | \{n_{\mathbf{k}}\}, n_0 \rangle \quad (A5)$$

In view of the definition (A5), Eq. (A4) implies

$$\dot{P}(\{n_{\mathbf{k}}\}; n_0) = -\frac{\kappa}{2} \sum_{\mathbf{k} \neq \mathbf{0}} (\langle \hat{\beta}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}} \rangle + 1)[n_{\mathbf{k}}(n_0+1)P(\{n_{\mathbf{k}}\}; n_0) -$$

$$n_{\mathbf{k}}n_0 P(\{n_{\mathbf{k}}\}; n_0 - 1) + \text{adj.}] -$$

$$\frac{\kappa}{2} \sum_{\mathbf{k} \neq \mathbf{0}} \langle \hat{\beta}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}} \rangle [(n_{\mathbf{k}} + 1)n_0 P(\{n_{\mathbf{k}}\}; n_0) -$$

$$(n_{\mathbf{k}} + 1)(n_0 + 1)P(\{n_{\mathbf{k}}\}; n_0 + 1) + \text{adj.}] \qquad (A6)$$

The condensate statistical distribution $P(n_0)$ is then related to the joint probability distribution $P(\{n_{\mathbf{k}}\}; n_0)$ and the conditional probability $P(\{n_{\mathbf{k}}\}|n_0)$ via Bayes rule

$$P(\{n_{\mathbf{k}}\}; n_0) = P(\{n_{\mathbf{k}}\}|n_0)P(n_0). \qquad (A7)$$

We obtain $P(n_0)$ from $P(\{n_{\mathbf{k}}\}; n_0)$ directly by summing over all excited states $\{n_{\mathbf{k}}\}$

$$P(n_0) = \sum_{\{n_{\mathbf{k}}\}} P(\{n_{\mathbf{k}}\}; n_0), \qquad (A8)$$

so that we have

$$\dot{P}_{n_0} = -\kappa \sum_{\mathbf{k} \neq \mathbf{0}} (\langle \hat{\beta}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}} \rangle + 1)[\langle n_{\mathbf{k}} \rangle_{n_0}(n_0 + 1)P_{n_0} -$$

$$\langle n_{\mathbf{k}} \rangle_{n_0 - 1} n_0 P_{n_0 - 1}] -$$

$$\kappa \sum_{\mathbf{k} \neq \mathbf{0}} \langle \hat{\beta}_{\mathbf{k}}^\dagger \hat{\beta}_{\mathbf{k}} \rangle [(\langle n_{\mathbf{k}} \rangle_{n_0} + 1)n_0 P_{n_0} - (\langle n_{\mathbf{k}} \rangle_{n_0 + 1} + 1)(n_0 + 1)P_{n_0 + 1}] \qquad (A9)$$

where we have introduced the convenient conditional average notation

$$\langle n_{\mathbf{k}} \rangle_{n_0} = \sum_{n_{\mathbf{k}}} n_{\mathbf{k}} P(\{n_{\mathbf{k}}\}|n_0). \qquad (A10)$$

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 CNB2 for an ideal gas. There, we encountered the heating and cooling coefficients

$$K_{n_0} = \sum_{\mathbf{k} \neq \mathbf{0}} \langle n_{\mathbf{k}} \rangle_{n_0} \left(1 + \left\langle \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} \right\rangle\right), \qquad (B1)$$

and

$$H_{n_0} = \sum_{\mathbf{k} \neq \mathbf{0}} \left\langle \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} \right\rangle \left(1 + \langle n_{\mathbf{k}} \rangle_{n_0}\right). \qquad (B2)$$

Defining

$$\eta_k = \langle \hat{b}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}} \rangle = \frac{1}{e^{\beta \hbar \omega_k} - 1}, \qquad (B3)$$

where $\beta = 1/k_B T$. Eqs. (B1) and (B2) now read

$$K_{n_0} = \sum_{\mathbf{k} \neq \mathbf{0}} \langle n_k \rangle_{n_0}(1 + \eta_k), \qquad (B4)$$

and

$$H_{n_0} = \sum_{\mathbf{k} \neq \mathbf{0}} \eta_k(1 + \langle n_k \rangle_{n_0}). \qquad (B5)$$

We then approximate the conditional thermal average as

$$\langle n_k \rangle_{n_0} = (N - n_0)\frac{\bar{n}_k}{\sum_{\mathbf{k} \neq \mathbf{0}} \bar{n}_k}, \qquad (B6)$$

where the usual atomic thermal average is given by

$$\bar{n}_k = \frac{1}{e^{\beta \epsilon_k} - 1}. \qquad (B7)$$

Now an ensemble of atoms and phonons in an ordinary gas obeys the simple rate equation

$$\frac{d}{dt}\bar{n}_k = \gamma(\bar{n}_k + 1)\eta_k - \gamma\bar{n}_k(\eta_k + 1), \qquad (B8)$$

where γ is an uninteresting rate factor. At steady state Eq. (B8) yields

$$(\bar{n}_k + 1)\eta_k = \bar{n}_k(\eta_k + 1), \qquad (B9)$$

which implies that $\eta_k = \bar{n}_k$ and we may write Eq. (B6) as

$$\langle n_k \rangle_{n_0} = (N - n_0)\frac{\eta_k}{\sum_{\mathbf{k} \neq \mathbf{0}} \eta_k}. \qquad (B10)$$

Hence we have

$$\sum_{\mathbf{k} \neq \mathbf{0}} \langle n_k \rangle_{n_0} \eta_k = \frac{(N - n_0)}{\mathcal{H}} \sum_{\mathbf{k} \neq \mathbf{0}} \eta_k^2 = (N - n_0)\eta \qquad (B11)$$

where we have introduced the notations

$$\mathcal{H} = \sum_{\mathbf{k} \neq \mathbf{0}} \eta_k \text{ and } \eta = \frac{\sum_{\mathbf{k} \neq \mathbf{0}} \eta_k^2}{\mathcal{H}}. \qquad (B12)$$

In this way we arrive at the K_{n_0} and H_{n_0} coefficients of CBN2 given by

$$K_{n_0} = (N - n_0)(1 + \eta), \qquad (B13)$$

and

$$H_{n_0} = \mathcal{H} + (N - n_0)\eta. \qquad (B14)$$

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

$$\frac{1}{\kappa}\frac{d\hat{\rho}(t)}{dt} = -\sum_{\mathbf{k}\neq\mathbf{0}} <\hat{a}_{\mathbf{k}}^{\dagger}\hat{a}_{\mathbf{k}}\hat{\beta}_{\mathbf{k}}\hat{\beta}_{\mathbf{k}}^{\dagger}>_{n_0} (\hat{a}_0\hat{a}_0^{\dagger}\hat{\rho}(t)-\hat{a}_0^{\dagger}\hat{\rho}(t)\hat{a}_0)+\text{adj.}$$

$$-\sum_{\mathbf{k}\neq\mathbf{0}} <\hat{\beta}_{\mathbf{k}}^{\dagger}\hat{\beta}_{\mathbf{k}}\hat{a}_{\mathbf{k}}\hat{a}_{\mathbf{k}}^{\dagger}>_{n_0} (\hat{a}_0^{\dagger}\hat{a}_0\hat{\rho}(t)-\hat{a}_0\hat{\rho}(t)\hat{a}_0^{\dagger})+\text{adj.}-$$

$$-\sum_{\mathbf{k}\neq\mathbf{0}} <\hat{\beta}_{\mathbf{k}}^{\dagger}\hat{\beta}_{-\mathbf{k}}^{\dagger}\hat{a}_{\mathbf{k}}\hat{a}_{-\mathbf{k}}>_{n_0} (\hat{a}_0^{\dagger}\hat{a}_0^{\dagger}\hat{\rho}(t)-\hat{a}_0^{\dagger}\hat{\rho}(t)\hat{a}_0^{\dagger})+\text{adj.}-$$

$$-\sum_{\mathbf{k}\neq\mathbf{0}} <\hat{\beta}_{\mathbf{k}}\hat{\beta}_{-\mathbf{k}}\hat{a}_{\mathbf{k}}^{\dagger}\hat{a}_{-\mathbf{k}}^{\dagger}>_{n_0} (\hat{a}_0\hat{a}_0\hat{\rho}(t)-\hat{a}_0\hat{\rho}(t)\hat{a}_0)+\text{adj.} \tag{C1}$$

New contribution of the form $\hat{a}_0^{\dagger}\hat{a}_0^{\dagger}\hat{\rho}_0(t)-\hat{a}_0^{\dagger}\hat{\rho}(t)\hat{a}_0^{\dagger}$ and $\hat{a}_0\hat{a}_0\hat{\rho}(t)-\hat{a}_0\hat{\rho}(t)\hat{a}_0$ yields off-diagonal terms in the density matrix equation. Taking into account that

$$<\hat{\beta}_{\mathbf{k}}^{\dagger}\hat{\beta}_{-\mathbf{k}}^{\dagger}> = <\hat{a}_{\mathbf{k}}\hat{a}_{-\mathbf{k}}> = u_k v_k \left[\frac{2}{e^{\beta\epsilon_k}-1}+1\right]$$

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

$$\frac{1}{2\kappa}\dot{\rho}_{n_0,n_0} = -(N-n_0)(1+\eta_I)(n_0+1)\rho_{n_0,n_0}+$$

$$+(N-n_0+1)(1+\eta_I)n_0\rho_{n_0-1,n_0-1}-$$

$$-[\mathcal{H}_I+(N-n_0)\eta_I]n_0\rho_{n_0,n_0}+$$

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

$$-J\left[\sqrt{n_0(n_0-1)}\rho_{n_0-2,n_0}+\sqrt{(n_0+2)(n_0+1)}\rho_{n_0,n_0+2}-\right.$$

$$\left.-2\sqrt{n_0(n_0+1)}\rho_{n_0-1,n_0+1}\right]$$

$$-J\left[\sqrt{(n_0+1)(n_0+2)}\rho_{n_0+2,n_0}+\sqrt{n_0(n_0-1)}\rho_{n_0,n_0-2}-\right.$$

$$\left.-2\sqrt{n_0(n_0+1)}\rho_{n_0+1,n_0-1}\right], \tag{C2}$$

where $\mathcal{H}_I$ and η_I are given by previous formulas (29) and (31), and

$$J = \sum_{\mathbf{k}\neq\mathbf{0}} u_k^2 v_k^2 \left[\frac{2}{e^{\beta\epsilon_k}-1}+1\right]^2. \tag{C3}$$

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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[1] For an excellent overview of BEC physics see, e.g., P. Meystre, *Atom Optics*, (Springer-Verlag, New York) (2001).

[2] M. Wilkens and C. Weiss, J. Mod. Opt. **44**, 1801 (1997).

[3] CNB1: M. O. Scully, Phys. Rev. Lett. **82**, 3927 (1999).

[4] CNB2: V. V. Kocharovsky, M. O. Scully, S. Y. Zhu and M. S. Zubairy, Phys. Rev. A **61**, 023609 (2000).

[5] CNB3: V. V. Kocharovsky, Vl. V. Kocharovsky, and M. O. Scully, Phys. Rev. Lett. **84**, 2306 (2000); Phys. Rev. A **61**, 053606 (2000).

[6] B. C. Crooker, B. Hebral, E. N. Smith, Y. Takano, and J. D. Reppy, Phys. Rev. Lett. **51**, 666 (1983); M. H. W. Chan, K. I. Blum, S. Q. Murphy, G. K. S. Wong, and J. D. Reppy, Phys. Rev. Lett. **61**, 1950 (1988); P. A. Crowell, F. W. Van Keuls, and J. D. Reppy, Phys. Rev. Lett. **75**, 1106 (1995). For theory see the pioneering works of M. Fisher and colleagues, e.g. M. Fisher and M. Barber, Phys. Rev. Lett. **29**, 1516 (1972).

[7] M. Girardeau and R. Arnowitt, Phys. Rev. **113**, 755 (1959).

[8] S. Giorgini, L. P. Pitaevskii, and S. Stringari, Phys. Rev. Lett. **80**, 5040 (1998).

[9] Uhlenbeck criticized Einstein that his expression for the average condensate particle number had an abrupt cusp at T_c [G. E. Uhlenbeck, *Over statistische Methoden in de Theorie der Quanta*, Ph.D. thesis, Leiden (1927)]. The manner in which this cusp is smoothed by fluctuations is of great interest for mesoscopic systems and is one focus of the present paper.

[10] A. Leggett, Rev. Mod. Phys. **73**, 307 (2001).

[11] K. Huang, *Statistical mechanics*, 2nd edition (Wiley, New York) (1987).

[12] A. Einstein, Annalen der Physik **17**, 132 (1905).

[13] A. Einstein, *Sitzungsberichte der preussischen Akademie der Wissenschaften*, I. Sitzung der physikalisch-mathematischen Klasse, 8. Januar 1925, p. 3.

[14] H. D. Politzer, Phys. Rev. A **54**, 5048 (1996).

[15] D. ter Haar, *Lectures on selected topics in statistical me-*

chanics (Elsevier, Amsterdam, 1977), Chapter 4; I. Fujiwara, D. ter Haar and H. Wergeland, J. Stat. Phys. 2, 329 (1970).

[16] V.V. Kocharovsky, Vl.V. Kocharovsky, M. Holthaus, C.H.R. Ooi, A.A. Svidzinsky, W. Ketterle and M.O. Scully, Advances in Atomic, Molecular and Optical Physics **53**, 291 (2006).

[17] See especially the time evolution experiments by H.-J. Miesner, D. Stamper-Kurn, M. Andrews, D. Durfee, S. Inouye, and W. Ketterle Science **279**, 1005 (1998); and the theoretical work of D. Jaksch, C. Gardiner, K. Gheri, and P. Zoller, Phys. Rev. A **58**, 1450 (1998); and C. Sackett, H. Stoff, and R. Hulet, Phys. Rev. Lett. **80**, 2031 (1998); M. Andrews, C. Townsend, H.-J. Miesner, D. Durfee, D. Kurn, and W. Ketterle, Science **275**, 637 1997; A. Röhrl, M. Naraschewski, A. Schenzle, and H. Wallis, Phys. Rev. Lett. **78**, 4143 (1997).

[18] The classic works in Bose gas physics by Bogolubov, Huang, Lee, and Yang are well presented in Ref. [11], Chap. 19.

[19] For the quantum theory of the laser as developed by Lamb and Scully using the density matrix treatment, that of Haken and Risken using Fokker-Planck techniques and of Lax and Louisell using a quantum noise approach, see, for example, M. Scully and S. Zubairy, Quantum Optics (Cambridge University, Cambridge, England, 1997).

[20] Insightful "atom-laser" papers include M. Holland, K. Burnett, C. Gardiner, J. Cirac, and P. Zoller, Phys. Rev. A **54**, R1757 (1996); A. Guzman, M. Moore, and P. Meystre, Phys. Rev. A **53**, 977 (1996); H. Wiseman, A. Martins, and D. Walls, Quantum Semiclass. Opt. **8**, 737 (1996); M. Olshanii, Y. Castin, and J. Dalibard, in Proceedings of the 12th International Conference on Laser Spectroscopy, edited by M. Inguscio, M. Allegrini, and A. Lasso (World Scientific, Singapore, 1995).

[21] Pure coherent light is characterized by Poissonian photon statistics. The quantum theory of the laser shows that partially coherent laser light also has a sharp photon distribution (with width several times Poissonian for a typical He-Ne laser). Laser coherence is due to the fact that after emission the atoms become absorbers and this saturation nonlinearity is essential for producing a sharply peaked photon distribution.

[22] J. A. Dunningham, D. F. Walls, and M. J. Collett, Phys. Lett. A **245**, 49 (1998); P. Navez, Mod. Phys. Lett. B **12**, 705 (1998); Z. Idziaszek, M. Gajda, P. Navez, M. Wilkens, and K. Rzazewski, Phys. Rev. Lett. **82**, 4376 (1999); F. Illuminati, P. Navez, and M. Wilkens, J. Phys. B **32**, L461 (1999); F. Meier and W. Zwerger, Phys. Rev. A **60**, 5133 (1999); R. Graham, Phys. Rev. A **62**, 023609 (2000); H. W. Xiong, S. Liu, G. Huang, and Z. Xu, Phys. Rev. A **65**, 033609 (2002); H. Xiong, S. Liu, and G. Huang, Phys. Rev. A **67**, 055601 (2003); S. Liu, H. W. Xiong, G. Huang, and Z. Xu, Phys. Rev. A **68**, 065601 (2003); R. K. Bhaduri, M. V. N. Murthy, and Muoi N. Tran, J. Phys. B **35**, 2817 (2002); A. Y. Cherny, Phys. Rev. A **71**, 043605 (2005); C.-H. Zhang, Phys. Rev. A **73**, 023601 (2006).

[23] Z. Idziaszek, K. Rzazewski, and M. Lewenstein, Phys. Rev. A**61**, 053608 (2000).

[24] The recent experiment of M. Raizen and coworkers on observation of number statistics in a degenerate Bose gas is reported in C.S. Chuu, F. Schreck, T.P. Meyrath, J.L. Hanssen, G.N. Price and M.G. Raizen, Phys. Rev. Lett. **95**, 260403 (2005).

[25] M. Lewenstein and L. You, Phys. Rev. Lett. **77**, 3489 (1996); A. Imamoglu, M. Lewenstein, and L. You, Phys. Rev. Lett. **78**, 2511 (1997).

[26] R. Graham, Phys. Rev. Lett. **81**, 5262 (1998).

[27] H. M. Wiseman and L. K. Thomsen, Phys. Rev. Lett. **86**, 1143 (2001).

[28] C.W. Gardiner and P. Zoller, Phys. Rev. A **55**, 2902 (1997); D. Jaksch, C.W. Gardiner, and P. Zoller, Phys. Rev. A **56**, 575 (1997); C.W. Gardiner and P. Zoller, Phys. Rev. A **58**, 536 (1998); D. Jaksch, C.W. Gardiner, and P. Zoller, Phys. Rev. A **58**, 1450 (1997); C. W. Gardiner and P. Zoller, Phys. Rev. A **61**, 033601 (2000); M. D. Lee and C. W. Gardiner, Phys. Rev. A **62**, 033606 (2000); M. J. Davis, C. W. Gardiner, and R. J. Ballagh, Phys. Rev. A **62**, 063608 (2000).

[29] A. S. Parkins and D. F. Walls, Phys. Rep. **303**, 1 (1998).