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Condensation of N Bosons and the Laser Phase Transition Analogy

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A simple analytic expression for the ground state of a dilute gas of N ideal bosons in a 3D harmonic potential at temperature T is derived from the steady state solutions of nonequilibrium equations of motion. The N particle constraint plays the important role of introducing the essential nonlinearity yielding a Ginzburg-Landau free energy. The present analysis has much in common with the quantum theory of the laser, and with the laser phase transition analogy. [S0031-9007(99)09008-0]

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Bose-Einstein condensation (BEC) in dilute ultracold gases has become a laboratory reality, notably the three pioneering experiments reporting BEC in rubidium [1(a)], lithium [1(b)], and sodium [1(c)] and independent confirmation [2]. Furthermore, BEC experiments on dilute He^4 in porous media [3], excitons in Cu_2O [4], demonstration of interference between condensates [5], and the condensate time development [6] are exciting developments.

It is important, therefore, to understand the connection between BEC [7] and the ideal Bose gas [8], and the quantum theory of the laser [9,10], etc. In the latter context, we recall that the saturation nonlinearity in the radiation matter interaction is essential for laser coherence [11]. Is the corresponding nonlinearity in BEC due solely to atom-atom scattering, or is there a coherence generating nonlinearity even in an ideal Bose gas? We shall see that the latter is the case; the laser phase transition analogy [12] provides insight into such questions.

With the above in mind, and stimulated by a recent article [13], we here extend our previous laser-phase transition analogy to the problem of N ideal bosons in a 3D harmonic potential coupled to a thermal reservoir. This "simple" problem turns out to be surprisingly rich. For example, we obtain, for the first time, a simple analytic expression for the ground state density matrix for N ideal bosons in contact with a thermal reservoir [see Eq. (2)]. The N particle constraint is included naturally in the present formulation and introduces the essential nonlinearity [14].

We emphasize that the present work provides another example [15] in which steady state (detailed balance) solutions to nonequilibrium equations of motion provide a supplementary approach to conventional statistical mechanics (e.g., partition function calculations). This is of interest since, for example, the partition sums in the canonical ensemble are complicated by the restriction to N particles. Stated differently, the present approach lends itself to different approximations, yielding, among other things, a simple (approximate) analytic expression for the ground state density matrix for N trapped bosons [see Eq. (2)].

Thus, we derive a nonequilibrium master equation for the ground state of an ideal Bose gas in a 3D harmonic trap coupled to a thermal reservoir; writing only the diagonal elements (the off-diagonal elements will be presented elsewhere), we find

$$\begin{aligned}\frac{1}{\kappa}\,\dot{\rho}_{n_0,n_0} = &-[(N+1)(n_0+1)-(n_0+1)^2]\rho_{n_0,n_0}\\ &+[(N+1)n_0-n_0^2]\rho_{n_0-1,n_0-1}\\ &-\left(\frac{T}{T_c}\right)^3 N[n_0\rho_{n_0,n_0}-(n_0+1)\rho_{n_0+1,n_0+1}],\end{aligned} \tag{1}$$

where $|n_0\rangle$ is the eigenstate of n_0 bosons, κ is a rate constant, N is the total number of bosons, T is the temperature of the heat bath, and T_c is a transition temperature, the precise meaning of which is discussed later.

The steady state solution for Eq. (1) is

$$\rho_{n_0,n_0} = \frac{1}{Z_N}\left[N\left(\frac{T}{T_C}\right)^3\right]^{N-n_0}\frac{N!}{(N-n_0)!}, \quad (2)$$

where the N boson normalization state function Z_N is an incomplete gamma function which is conveniently expressed as

$$Z_N = \left(\frac{T}{T_c}\right)^{3(N+1)}\int_0^\infty dt\, e^{-t(T/T_c)^3}(t+N)^N. \quad (3)$$

Equation (2) is a main result of this paper; we note that ρ_{n_0,n_0} is not a Poisson distribution as would be expected for a coherent state.

Proceeding further to glean the physics from Eq. (2), we note that it yields the following analytical expressions for the average and the variance [16] of the number of bosons in the ground state (see Fig. 1):

$$\langle n_0\rangle = \left[1-\left(\frac{T}{T_c}\right)^3\right]N + \left(\frac{T}{T_c}\right)^3 N/Z_N', \quad (4)$$

$$\Delta n_0^2 = \langle n_0^2\rangle - \langle n_0\rangle^2 = \left(\frac{T}{T_c}\right)^3 N[1-(\langle n_0\rangle+1)/Z_N'], \quad (5)$$

where $Z_N' = Z_N[N(T/T_c)^3]^{-N}$.

In the limit that $T \to T_c$, we find (by a steepest-descent approximation) $Z_N' \to \sqrt{2/N\pi}$; therefore $\langle n_0(T_c)\rangle \simeq \sqrt{2N/\pi}$, and $\Delta n_0^2(T_c) \simeq N - N(2/\pi + \sqrt{2/N\pi})$.

In developing the laser phase transition analogy the "touch stone" was the Glauber-Sudarshan P distribution. Thus, when we expand the density matrix in terms of coherent (i.e., eigenstates of the annihilation operator)

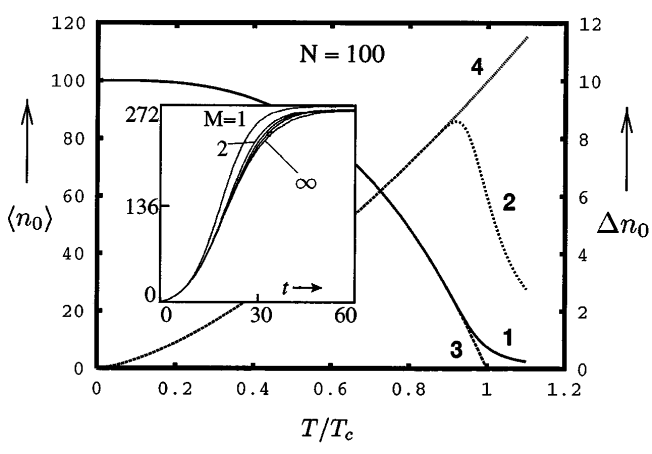

FIG. 1. At sufficiently low temperatures, $\langle n_0\rangle \simeq N[1-(T/T_c)^3]$ (curve 3) and $\Delta n_0 \simeq N^{1/2}(T/T_c)^{3/2}$ (curve 4). Near T_c, corrections are appreciable (of order $\sqrt{N}$); see curves 1 and 2. Inset: time evolution of average number given by integration of Eq. (12) truncated according to Ref. [20] (see text). Parameters are $N = 1600$, $T/T_c = 0.94$, vertical axis $\langle n_0\rangle$, horizontal axis time in units of κ^{-1}.

states $|\Delta\rangle$ using $\rho_{n_0,n_0'} = \int d^2\Delta P(\Delta)\langle n_0|\Delta\rangle\langle\Delta|n_0'\rangle$, we find for $T \simeq T_c$, $P(\Delta) = \exp[-\beta G(\Delta)]/Z$, with the Ginzburg-Landau-type free energy $G(\Delta) = a(T,T_c) \times |\Delta|^2 + b(T,T_c)|\Delta|^4$.

The correspondence between the expression for $P(\Delta)$ and its laser analog is very close, in accord with Ref. [12]. The bosonic ground state is indeed much "like a laser"; and in this context we note that the off-diagonal generalization of Eq. (1) yields a finite "phase diffusion" linewidth for Δ. This will be discussed elsewhere.

Having presented the master equation, Eq. (1), and some of the physics it contains, we sketch its derivation and limitations. Our reservoir consists of an ensemble of simple harmonic oscillators having a large frequency spread so as to ensure Markovian dynamics.

Defining $\rho_{n_0,n_0'} = \sum_{\{n_k\}} \mathrm{Tr}_{\mathrm{Res}}\rho_{n_0,\{n_k\},n_0'\{n_k\}}$, where $\{n_k\} = \{n_1, n_2, \ldots, n_k, \ldots\}$ and $\mathrm{Tr}_{\mathrm{Res}}$ denotes the trace over the reservoir, we seek the equation of motion for $\rho_{n_0,n_0'}$ as it evolves due to interaction with the reservoir [17], which is governed by the interaction Hamiltonian,

$$V(t) = \sum g_{j,k} b_j^\dagger(t) a_k(t) a_0^\dagger(t) + \text{adj.}, \quad (6)$$

where $g_{j,k}$ is the coupling strength between the jth reservoir oscillator and a gas atom being cooled from the kth level of the trap into its ground state. The raising operator for the jth reservoir oscillator is $b_j^\dagger(t) = b_j^\dagger(0)\exp(i\omega_j t)$. The boson annihilation operator is given by $a_k(t) = a_k(0)\exp(-i\nu_k t)$, where $\hbar\nu_k$ is the energy of the kth state of the 3D trap, and $a_0^\dagger(t)$ is the ground state creation operator.

We proceed via the exact dynamical equation

$$\dot\rho_{n_0,n_0} = -\int_{-\infty}^{t} dt' \sum_{\{\eta_j\},\{n_k\}} \langle\{\eta_j\},\{n_k\},n_0| \times [V(t),[V(t'),\rho(t')]]\,|n_0,\{n_k\},\{\eta_j\}\rangle, \quad (7)$$

where $|\{\eta_j\}\rangle = |\eta_1, \eta_2, \ldots, \eta_j, \ldots\rangle$ is the reservoir state with η_1 quanta in the first oscillator, η_2 in the second, etc., and the summation excludes the ground state.

Inserting Eq. (6) into Eq. (7), we convert the sum over reservoir states to an integral, and note that oscillators for which $\omega_j \simeq \nu_k$ dominate. Hence, slowly varying quantities such as the density of states factor W_j, matrix elements g_{jk}, and Bose factors η_j may be evaluated at $j = k$. The resulting integration over ω_j yields a temporal delta function, since $\int d\omega_j \exp i(\nu_k - \omega_j)(t-t') = 2\pi\delta(t-t')$, and the master equation becomes Markovian. We further note that the reservoir is only weakly coupled to the Bose gas and take the reservoir oscillators and the excited states of the Bose gas to be populated according to equilibrium statistical mechanics. Proceeding along these lines we find

$$\dot\rho_{n_0,n_0} = -K_{n_0}(n_0+1)\rho_{n_0,n_0} + K_{n_0-1}n_0\rho_{n_0-1,n_0-1} - H_{n_0}n_0\rho_{n_0,n_0} + H_{n_0+1}(n_0+1)\rho_{n_0+1,n_0+1}. \quad (8)$$

The cooling and heating coefficients K_{n_0} and H_{n_0} are given by $K_{n_0} = \sum_k 2\pi W_k g_k^2 \langle \eta_k + 1\rangle \langle n_k\rangle_{n_0}$ and $H_{n_0} = \sum_k 2\pi W_k g_k^2 \langle \eta_k\rangle \langle n_k + 1\rangle_{n_0}$, where $\langle \eta_k\rangle$ is the average occupation number of the kth heat bath oscillator as in Eq. (11), and $\langle n_k\rangle_{n_0}$ is the average number of atoms in the kth excited state, given n_0 atoms in the condensate. We evaluate K_{n_0} and H_{n_0} in varying degrees of rigor. One of the most illuminating is to note that for the bulk of the excited states the factors $\langle n_k + 1\rangle$ and $\langle \eta_k + 1\rangle$, as they appear in H_{n_0} and K_{n_0}, can be replaced by unity. For simplicity, we take $2\pi W_k g_k^2 = \kappa$; in later work k dependence will be presented.

Then the heating term is approximately

$$H_{n_0} \simeq \kappa \sum_k \langle \eta(\epsilon_k)\rangle = \kappa \sum_{\ell,m,n} \frac{1}{e^{\beta \hbar\Omega(n+\ell+m)} - 1} \equiv \mathcal{H} .$$

In the weak trap limit $\mathcal{H} \simeq \kappa (k_B T/\hbar\Omega)^3 \zeta(3)$, where $\zeta(3)$ is the Riemann zeta function, and Ω is the trap frequency.

Likewise, the cooling term in Eq. (8) is governed by the total number of excited state bosons,

$$K_{n_0} \simeq \kappa \sum_k \langle n_k\rangle_{n_0} = \kappa(N - n_0). \tag{9}$$

The preceding suggests new ways to motivate the critical temperature for small N. By writing the equation of motion for $\langle n_0\rangle$ from Eq. (8), using $\mathcal{H}$ in the weak trap limit, and (9) for K_{n_0}, we find

$$\langle \dot{n}_0\rangle = \kappa \left[N\langle n_0\rangle - \langle n_0^2\rangle - \zeta(3)\left(\frac{k_B T}{\hbar\Omega}\right)^3 \langle n_0\rangle \right]. \tag{10}$$

We may obtain T_c in two ways.

Proceeding dynamically, we note that, near T_c, $\langle n_0\rangle \ll N$, and we may neglect $\langle n_0^2\rangle$ compared to $N\langle n_0\rangle$. Then Eq. (10) becomes $\langle \dot{n}_0\rangle = \kappa[N - \zeta(3)(k_B T/\hbar\Omega)^3]\langle n_0\rangle$. We now define the critical temperature (in analogy with the laser threshold) such that cooling (gain) equals heating (loss) and $\langle \dot{n}_0\rangle = 0$ at $T = T_c$; this yields $T_c = [\hbar\Omega/k_B)(N/\zeta(3)]^{1/3}$.

Alternatively, from a statistical mechanical point of view, we may define T_c as the temperature at which $\langle n_0\rangle$ vanishes when neglecting fluctuations. That is, replacing $\langle n_0^2\rangle \simeq \langle n_0\rangle^2$ in Eq. (10), the steady state solution is $N - \langle n_0\rangle = \zeta(3)(k_B T/\hbar\Omega)^3$; and $\langle n_0\rangle$ vanishes when $T_c = [\hbar\Omega/k_B)(N/\zeta(3)]^{1/3}$.

In terms of T_c, the heating rate is then $H_{n_0} = \kappa N(T/T_c)^3$. Inserting this and (9) for K_{n_0} into Eq. (8) yields Eq. (1). For other potentials [18], the sum in $\mathcal{H}$ changes and the results will be presented elsewhere.

When we do not go to the weak trap limit, but keep the entire sum in H_{n_0}, we have

$$\tilde{\rho}_{n_0,n_0} = \frac{1}{\tilde{Z}_N} \mathcal{H}^{-n_0} \frac{N!}{(N - n_0)!}. \tag{11}$$

Equation (11) is plotted for a 3D oscillator trap in Fig. 2, as is the distribution from the (1997) papers of Wilkens, Weiss, Grossmann, and Holthaus (WWGH) [8]. We conclude that the simple analytic (but approximate) expression (11) describes the ground state quite well even for $N = 100$. Numerical analysis shows that, for $N \gtrsim 10^5$, ρ_{n_0,n_0} and $\tilde{\rho}_{n_0,n_0}$ given by Eqs. (2) and (11) converge; for $N \simeq 10^2$, their peaks differ by some 10%.

For small N, the critical temperature should now be redefined by modifying Eq. (10) so that $\zeta(3)(k_B T/\hbar\Omega)^3 \to \mathcal{H}$, and then the modified critical temperature $\tilde{T}_c$ is defined by $\mathcal{H}(\tilde{T}_c) = \sum\{[\exp(\hbar\Omega)(\ell + m + n)/k_B\tilde{T}_c] - 1\}^{-1} = N$, in agreement with Ketterle and van Druten [19].

We remark in closing that, as for the laser, Eq. (1) implies a coupled hierarchy of moment equations which are useful in analysis of the time evolution; we find

$$\frac{d}{dt}\langle n_0^\ell\rangle = \sum_{i=0}^{\ell-1} \binom{\ell}{i} \Bigg\{ \langle n_0^{i+1}\rangle \kappa N \left[1 - (-1)^{\ell-1-i}\left(\frac{T}{T_c}\right)^3 \right] + \langle n_0^i\rangle \kappa N - \kappa[\langle n_0^{i+2}\rangle + \langle n_0^{i+1}\rangle] \Bigg\}. \tag{12}$$

Equation (12) can be solved numerically when a proper truncation scheme is devised. This has been carried out in Ref. [20]. See the inset of Fig. 1 for the present problem. When truncating the third moment, only $\langle \dot{n}_0\rangle$ and $\langle \dot{n}_0^2\rangle$ are involved (i.e., $M = 2$ in the inset of Fig. 1); and the truncation prescription is $\langle n_0^3\rangle = [2\langle n_0^2\rangle^{1/2} - \langle n_0\rangle]^3$.

The present paper is largely devoted to equilibrium questions, and such results are relatively insensitive to the details of the model. For example, Eq. (2) should describe

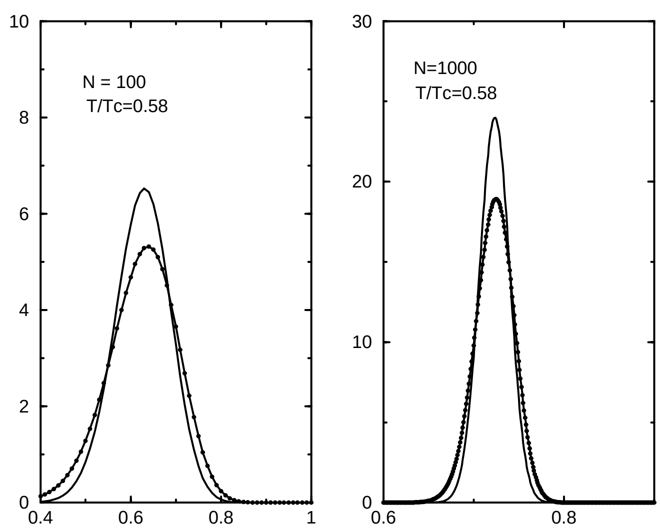

FIG. 2. Equation (11) (solid line) for probability of having n_0 bosons in ground state of 3D harmonic trap compared with WWGH (dot-dashed line), for 100 and 1000 atoms with $T/T_c = 0.58$, vertical axis: $N \times \rho_{n_0,n_0}$ and horizontal axis n_0/N for both graphs.

N atoms in a harmonic trap at steady state reasonably well. However, the dynamics of evaporative cooling is conceptually different from the present heat bath model. The present model would be rather closer to the dilute He^4 gas in porous gel experiments [3] in which phonons in the gel would play the role of the heat bath. Nevertheless, a master equation having the form of Eq. (8) would be expected for any cooling mechanism, and the structure of Eq. (1) has a certain aesthetic appeal.

In summary, (i) We derive a master equation for the cooling of N bosons towards the ground state via energy exchange with a "phonon" heat bath, which incorporates the N particle constraint in a simple and natural fashion. In the weak trap limit the master equation takes an aesthetically pleasing form. The steady state solution yields a simple analytic expression for (ii) the N boson state function Z_N, (iii) the ground state boson statistics ρ_{n_0,n_0}, and (iv) a quasiprobability density for the order parameter Δ in terms of a Ginzburg-Landau free energy deriving from the fact that the N particle constraint introduces a nonlinear effective interaction. (v) Simple analytic expressions are obtained for $\langle n_0 \rangle$ and Δn_0^2. (vi) A new "derivation" of the critical temperature valid for small N is developed dynamically and statistically. (vii) Time dependence relevant to experiments such as the porous gel/He^4 experiments can be obtained via laser calculational techniques.

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