An upper bound on the condensate fraction in a Bose gas with weak repulsion

Anthony J Leggett
Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, IL 61801-3080, USA
E-mail: aleggett@uiuc.edu

New Journal of Physics 3 (2001) 23.1–23.6 (http://www.njp.org/)
Received 18 July 2001, in final form 22 November 2001
Published 19 December 2001

Abstract. For a spinless Bose gas moving in three-dimensional free space with an interaction \(V(r)\) which is everywhere positive, I show that the condensate fraction \(f\) is bounded above by an expression parametrized by the quantity \(nV_0/kT_c(0) \equiv \eta\), where \(n\) is the density, \(V_0\) the space integral of the interaction potential and \(T_c(0)\) the critical temperature of the corresponding noninteracting gas. The only assumption needed is that fluctuations in the interacting system have the standard extensivity properties. In particular, for \(T = T_c(0)\) the upper bound on \(f\) is proportional to \(\eta^{1/3}\), while for \(\eta^{1/3} \ll 1 - T_c(0)/T \ll 1\) it is proportional to \(\eta/(1 - (T_c(0)/T)^{3/2})^2\).

The phenomenon of Bose–Einstein condensation (BEC), in which the maximum eigenvalue of the single-particle density matrix is a finite fraction \(f\) of the total particle number \(N\) in the thermodynamic limit, is believed to be ubiquitous at low temperatures in not-too-dense systems of particles obeying Bose statistics and with a repulsive (or zero) interaction. Despite this widespread belief, rigorous theorems on the existence of BEC and/or the magnitude of \(f\) are few and far between [1]. Many years ago, Gavoret and Nozières [2] proved the existence of BEC at \(T = 0\) for any system for which perturbation theory starting from the free Bose gas converges, but were unable to say anything about the magnitude of \(f\) or the transition temperature \(T_c\). The only system with short-range interactions for which the existence of BEC has been rigorously established, even at \(T = 0\), is the lattice gas with repulsive interactions at exactly half-filling [3]. (In the case of a lattice gas with all sites equally coupled, both Toth [4] and Penrose [5] have established the existence of a transition to the BEC state at finite temperature.) In the negative direction, the famous theorem of Hohenberg [6] precludes the existence of BEC in the thermodynamic limit at any finite temperature in \(d\)-dimensional free space for \(d \leq 2\). It may be less universally appreciated that for three-dimensional free space Hohenberg’s lemma
(equation (18) of his paper [6]), while imposing no restriction on the transition temperature $T_c$ as such, places an upper bound on the condensate fraction $f$ as a function of $T$:

$$\frac{f^{2/3}}{(1-f)} \leq \gamma(T_c^{(0)}/T) \quad \gamma \equiv [(3\zeta(3/2)/4)\pi^{1/2}]^{2/3} \approx 2.3$$  \hfill (1)

where $T_c^{(0)}$ is the transition temperature of the noninteracting gas of the same mass and density $n$. Using an improved version of the lemma, Roepstorff [7] was able to obtain a slightly tighter upper limit which replaces $\gamma$ in equation (1) by 2. The bound (1) (or the improved version of [7]) is completely independent of the strength and even the sign of the interparticle interactions; however, while it is nonvacuous for any value of $T$, for $T \sim T_c^{(0)}$ the limit on $f$ is quite weak ($f \lesssim 0.8$). Finally, I note that Penrose [8] obtained an upper limit for the condensate fraction at zero temperature, $f(0)$, for a hard-core Bose gas in terms of the fraction of the volume occupied by the hard cores, and Pitaevskii [9] has established a more general upper limit on $f(0)$ in terms of the excitation spectrum (see also [10]); not surprisingly, this limit tends to 1 as the slope of the $k \to 0$ spectrum (thus, presumably, the strength of the (effective) interaction) tends to zero.

The purpose of this paper is to establish a second upper bound on $f(T)$ which in certain regimes is stronger than (1), and in particular, for $T \gtrsim T_c^{(0)}$, tends to zero with the strength of the (repulsive) interaction [11]$.^\dagger$

I consider a system of $N$ identical spinless bosons moving freely (i.e. in zero external potential) in a volume $\Omega$, impose the standard periodic boundary conditions and take the thermodynamic limit $N, \Omega \to \infty$, $N/\Omega \to \text{constant} \equiv n$. The wave function of the lowest single-particle state is then simply a constant, $\Omega^{-1/2}$, and corresponds to zero kinetic energy; I denote the creation operator for this state by $a_0^+$, and write $N_0 \equiv a_0^+ a_0$. Then the condensate fraction $f$ is defined$^\ddagger$ as $\langle N_0 \rangle / N$, where for any operator $\hat{Q}$ we define $\langle \hat{Q} \rangle \equiv \text{Tr} \hat{Q} \hat{\rho}$ where $\hat{\rho}$ is, here and below, the true $N$-body density matrix of the interacting system. An assumption which will be essential in the argument below is that in the thermodynamic equilibrium state of the interacting system the fluctuations in $N_0$ have the usual behaviour as regards extensivity in the thermodynamic limit; more formally, that we can bound the probability $P(N_0)$ of finding a given eigenvalue of $N_0$ different from the average $\langle N_0 \rangle$ by the inequality

$$P(N_0) \leq \zeta \exp(-(N_0 - \langle N_0 \rangle)^2/KN)$$  \hfill (2)

where $\zeta$ and $K$ tend to constants of order 1 in the thermodynamic limit. While the inequality (2) is actually false for the noninteracting gas below $T_c$, it is overwhelmingly plausible that for any system with finite (repulsive; cf. below) interactions it should hold. Concerning the interparticle interaction potential $V(r)$, I assume

$$V(r) \geq 0 \quad \text{everywhere}$$  \hfill (3)

and define

$$V_0 \equiv \int V(r) \, d^3r.$$  \hfill (4)

$^\dagger$ The motivation for emphasizing this feature is the fact that most perturbation calculations seem to indicate that the effect of a repulsive interaction is to raise $T_c$, with the increase tending to zero with the strength of the repulsion. See e.g. [11].

$^\ddagger$ For pedagogical simplicity I make, here, the usual assumption that condensation occurs in the state $k = 0$ (only). However, it is clear that the ensuing argument carries through for condensation into an arbitrary single-particle state or set of states.
Then, subject to assumptions (2) and (3), I shall establish the following inequality:

\[ F_0(N(1 - f), \Omega, T) - F_0(N, \Omega, T) \leq NnV_0 \]

(5)

where \( F_0(N, \Omega, T) \) is the free energy of the corresponding noninteracting gas. Equation (5) is an implicit bound on \( f \) (cf. below) and is the central result of this note; note that in the limit \( V_0 \to 0 \) it is compatible (as an equality) with the known thermodynamics of the noninteracting Bose gas.

The demonstration of the inequality (5) proceeds via the establishment of upper and lower bounds on the free energy \( F(N, \Omega, T) \) of the interacting system. Let \( \hat{H}_0 \) denote the kinetic energy operator, and let \( k \) label the plane-wave states which are eigenstates of \( \hat{H}_0 \). Then an upper limit on \( F \) follows straightforwardly from the Peierls–Bogoliubov inequality (see e.g. [12]†), namely

\[ F(N, \Omega, T) \leq F_0(N, \Omega, T) + \frac{1}{2} \left( NnV_0 + \Omega^{-1} \sum_{k \neq k'} V_{k-k'} \langle n_k \rangle \langle n'_k \rangle \right) \leq F_0(N, \Omega, T) + NnV_0 \]

(6)

where in the second step we used the fact that in view of equation (3) we have \( V_{k-k'} \leq V_0 \).

The derivation of a lower bound on \( F \) is a little more tricky; it relies on the fact that \( F \) cannot be less than the free energy of a noninteracting gas at the same \( T \) and \( \Omega \) but with a total particle number \( N(1 - f) \); otherwise we could construct a trial density matrix for the latter system which does better than the standard form \( \hat{\rho}_0 \equiv Z^{-1} \exp(-\beta \hat{H}_0) \). To see this, define an operator \( \hat{Y} \) by its matrix elements in the basis where \( \hat{N}_0 \) is diagonal, as follows:

\[ \hat{Y} \equiv (\hat{n}_0)^{\hat{N}_0}(\hat{N}_0)!^{-1/2}. \]

(7)

In words, \( \hat{Y} \) removes all the particles in the condensate while leaving the rest untouched. Note that while the operator \( \hat{Y} \) is obviously nonunitary (in fact does not even possess an inverse), nevertheless when operating on a manifold of given fixed total particle number \( N \) it preserves the orthonormality of the many-particle states. Because the actual \( N \)-particle density operator of the interacting system in general fails to commute with \( \hat{N}_0 \), the density matrix \( \hat{\rho}' \) defined (with \( \hat{Y}' \) the Hermitian conjugate of \( \hat{Y} \)) by

\[ \hat{\rho}' \equiv \hat{Y} \hat{\rho} \hat{Y}'^+ \]

(8)

in general corresponds to a superposition of states with different total particle number; however, since all physical operators such as the kinetic energy commute with \( \hat{N} \), in evaluating the expectation values of such operators it is adequate to replace the superposition by the corresponding mixture. Note that in view of equation (2), the fluctuations, in the ensemble defined by \( \hat{\rho}' \), in the ‘final’ value of \( N_f \) of \( \hat{N} \) around its expectation value \( N(1 - f) \) are a negligible fraction of the latter in the thermodynamic limit; in fact, if \( \text{Prob}' \) denotes the probability in the ensemble defined by \( \hat{\rho}' \), then the probability \( \text{Prob}'(N_f) \) is given in terms of the \( P(N_0) \) defined in equation (2) by

\[ \text{Prob}'(N_f) = P(\langle N_0 \rangle + N_f - N(1 - f)). \]

(9)

We now regard the density matrix \( \hat{\rho}' \) defined in equation (8) as a trial density matrix for a noninteracting gas with variable total number of particles, and consider the corresponding free energy \( F_0 \). It is immediately clear that the kinetic energy and (because of the orthonormality-preserving property of the operator \( \hat{Y} \)) the entropy are identical to those of the interacting system, \( \dagger \) In equation (3) of this reference, put \( \mathcal{H}_0 \) and \( \mathcal{H}_1 \) equal to the kinetic and potential energies respectively.

New Journal of Physics 3 (2001) 23.1–23.6 (http://www.njp.org/)
while from equation (3) the potential energy (zero!) cannot have increased. Consequently we reach the conclusion that the free energy of the noninteracting system described by $\hat{\rho}'$ cannot exceed $F(N, \Omega, T)$.

There remains one final, rather delicate step. Consider the problem of constructing the optimum density matrix for a mixture of states of the noninteracting gas with different $N_f$, with the probability of a given $N_f$ being given by equation (9); note that the problem is as it were posed in the context of the macrocanonical ensemble, so we do not assume a priori a grand canonical distribution. It is clear that the solution is a mixture of the $N_f$-particle macrocanonical noninteracting gas density matrices with weights $\text{Prob}f(N_f)$, and from equations (9) and (2) it is then clear that, to within terms whose relative contribution vanishes in the thermodynamic limit, the associated free energy is just $F_0(N(1 - f), \Omega, T)$ (note that this statement is true whether or not $T > T_c(0)$). Thus, the free energy of the state described by $\hat{\rho}'$ cannot lie below $F_0$, and since we already saw that it cannot exceed $F(N, \Omega, T)$, we conclude that $F(N, \Omega, T)$ is bounded below by $F_0(N(1 - f), \Omega, T)$. Combining this result with the inequality (6), we arrive at equation (5).

Before examining the implications of equation (5) for the quantity $f$ itself, it is worth noting (with a view to possible future developments) that (5) is actually a special case of a more general inequality, which can be proved by a slight modification of the above argument in which the upper bound on $F$ is relative to $F_0$ replaced by the exact relation and the actual mean value $\langle V \rangle$ of the potential is kept in the lower bound:

$$F_0(N(1 - f), \Omega, T) - F_0(N, \Omega, T) \leq \Delta K$$

where $K = \langle H_0 \rangle - TS$ ($S =$ entropy) and the notation $\Delta \phi(N, \Omega, T)$ represents the value of $\phi$ in the true (interacting) system relative to that in the corresponding noninteracting gas.

To turn the inequality (5) into an explicit upper bound on the condensate function $f$, we need a lower bound on the quantity $\bar{\mu} \equiv -\mu_0/kT$, where $\mu_0(N', \Omega, T) \equiv \partial F_0/\partial N'$ is the chemical potential of the noninteracting gas of $N'$ particles. For $T \leq T_c(0)(N') = (2\pi/[\zeta(3/2)]^{2/3})(N'/V)^{2/3}$ ($h = m = 1$), we clearly have $\bar{\mu} = 0$, while for $T \geq T_c(0)(N')$ it is shown in the appendix that $\bar{\mu}$ is bounded as a function of the quantity $\epsilon'(N', \Omega, T) \equiv 1 - (T_c(0)(N')T)^{3/2}$ by the inequality

$$\bar{\mu}(\epsilon') \geq \alpha \epsilon'^2 \quad \alpha_0 \approx 0.3.$$ (11)

I will consider here only the case of $T \geq T_c(0)(N)$, where $N$ is the actual number of particles in the system of interest (the opposite case involves even messier algebra and is less interesting). Then using the standard relation (above) between $T_c(0)(N')$ and $N'$ and using (11), we can bound the LHS of (5) by an integral over $\epsilon'$ and find after some algebra the result

$$F_0(N(1 - f), \Omega, T) - F_0(N, \Omega, T) \geq NkT\alpha_0 \left\{ \frac{1}{3} \epsilon'^2 (1 - \epsilon)^2 + \epsilon(1 - \epsilon) f^2 + \epsilon f \right\}$$

where $\epsilon \equiv \epsilon(N)$. Substituting (12) into (5), we find the implicit bound

$$\frac{1}{3} \epsilon'^2 (1 - \epsilon)^2 + \epsilon(1 - \epsilon) f^2 + \epsilon f \leq \alpha_0^{-1} \eta T_c(0)/T$$

where

$$\eta \equiv nV_0/kT_c(0) \quad \epsilon \equiv 1 - (T_c(0)/T)^{3/2}.$$ (14)

Using standard results [13] for the solution of cubic equations we can obtain from (13) the explicit bound

$$f \leq \frac{\epsilon}{1 - \epsilon} \left\{ 1 + \frac{3(\eta/\epsilon_0)(T_c(0)/T)(1 - \epsilon)}{\epsilon^3} \right\}^{1/3}.$$ (15)

New Journal of Physics 3 (2001) 23.1–23.6 (http://www.njp.org/)
In particular, for \( T = T_c(0) \) we have

\[
f \leq \left( \frac{3\eta}{\alpha_0} \right)^{1/3}
\]

while for \( \eta^{1/3} \ll \epsilon \ll 1 \) the bound (15) reduces approximately to

\[
f \leq \frac{\eta}{\alpha_0} \epsilon^{-2}.
\]

The above results are not directly applicable to the system of most experimental interest, namely dilute atomic alkali gases in a harmonic trap, both because we cannot assume that condensation occurs in the lowest-single-particle state of the noninteracting system and because the actual interatomic potential by no means satisfies equation (3). To take the latter point first, it is clear, to the extent that the standard approximation of replacing the true potential by a pseudopotential proportional to the s-wave scattering length remains valid for this problem, that one recovers (15) for the free-space problem with \( a_s > 0 \), with \( V_0 \) replaced as usual by \( 4\pi \hbar^2 a_s/m \); thus at \( T_c(0) \) the condensate fraction would be bounded above by an expression proportional to \( (n a_s^3)^{1/9} \). The former complication seems more serious, and I have not at the time of writing succeeded in generalizing the argument to a trap geometry.

Finally, I note that if a lower limit could be found on the actual potential energy relative to the Hartree–Fock value, it might well be possible to improve the bound (15) considerably. However, even with such an improvement it looks unlikely that an agreement of the above form will yield a bound on the transition temperature \( T_c \), as distinct from the condensate fraction \( f(T) \).

**Acknowledgments**

This work was supported by the National Science Foundation under grant No NSF-DMR-99-86199. I am grateful to Gordon Baym for pointing out an error in the first version of the manuscript, and to a referee for calling my attention to the explicit form (15) of the general bound.

**Appendix. The chemical potential of a noninteracting Bose gas for \( T > T_c \)**

The purpose of this appendix is to derive an analytic lower bound on the (positive) quantity \( \tilde{\mu} \equiv -\mu/kT \) in a noninteracting Bose gas as a function of the variable \( \epsilon \equiv 1 - (T_c(0)/T)^{3/2} \), for \( T > T_c(0) \). (For \( T \leq T_c(0) \), \( \tilde{\mu} \) is of course zero in the thermodynamic limit.)

The formula for the total particle number \( N \equiv n\Omega \) as a function of \( T \) and \( \tilde{\mu} \) is given for \( T \geq T_c(0) \) by the usual sum over the Bose distribution. Taking the thermodynamic limit and using the limiting value of the resulting integral for \( T \to T_c(0) \) (\( \tilde{\mu} \to 0 \)) to eliminate \( n \) in favour of \( T_c(0) \), we can rewrite the formula in the form

\[
1 - I(\tilde{\mu})/I(0) \equiv q(\tilde{\mu}) = \epsilon
\]

where the function \( I(\tilde{\mu}) \) is given by the expression

\[
I(\tilde{\mu}) \equiv \sum_{n=1}^{\infty} n^{-3/2} \exp(-n\tilde{\mu}).
\]
To establish the needed result we use the inequality $e^{-x} \geq 1 - x$ and set $\ell \equiv \text{int}(\tilde{\mu}^{-1})$ (int $\equiv$ integral part of); then we can write

$$I(\tilde{\mu}) \geq \sum_{n=1}^{\ell} n^{-3/2}(1 - n\tilde{\mu})$$

and hence, since $I(0) \equiv \zeta(3/2)$,

$$q(\tilde{\mu}) \leq (\zeta(3/2))^{-1} \left\{ \sum_{n=\ell+1}^{\infty} n^{-3/2} + \tilde{\mu} \sum_{n=1}^{\ell} n^{-1/2} \right\}.$$  \hspace{1cm} (A.4)

Since the summands in the brackets are decreasing functions of $n$, an upper limit on the RHS of (A.4) can be obtained by replacing them respectively by integrals from $\tilde{\mu}^{-1} - 1$ to $\infty$ and from 0 to $\tilde{\mu}^{-1} - 1$. In this way we obtain the inequality

$$q(\tilde{\mu}) \leq (4/\zeta(3/2))(1 - \tilde{\mu}/2) \left( \frac{\tilde{\mu}}{1 - \tilde{\mu}} \right)^{1/2} \leq (4/\zeta(3/2)) \left( \frac{\tilde{\mu}}{1 - \tilde{\mu}} \right)^{1/2}. \hspace{1cm} (A.5)$$

Substituting (A.5) into (A.1), solving for $\tilde{\mu}$ and taking into account that from its definition the maximum possible value of $\epsilon$ is 1, we find

$$\tilde{\mu} \geq \alpha_0 \epsilon^2 \quad \alpha_0 \equiv \frac{\zeta^2(3/2)/16}{1 + \zeta^2(3/2)/16} \approx 0.3$$

which is the result needed in the text.

References

[1] Lieb E H 1999 Physica A 263 491
[2] Gavoret J and Nozières P 1964 Ann. Phys., NY 28 349
[3] Kennedy T, Lieb E H and Shastry S 1988 Phys. Rev. Lett. 61 2582
[4] Toth B 1990 J. Stat. Phys. 61 749
[5] Penrose O 1991 J. Stat. Phys. 63 761
[6] Hohenberg P C 1967 Phys. Rev. 158 383
[7] Roepstorff G 1978 J. Stat. Phys. 18 191
[8] Penrose O 1964 Phys. Lett. 11 224
[9] Pitaevskii L P 1987 Pis. Zh. Eksp. Teor. Fiz. 45 149 (Engl. transl. 1987 JETP Lett. 45 185)
[10] Pitaevskii L P and Stringari S 1991 J. Low Temp. Phys. 85 377
[11] Baym G, Blaizot J-P, Holzmann M, Laloe F and Vautherin D 1999 Phys. Rev. Lett. 83 1703
[12] Griffiths R B 1964 J. Math. Phys. 5 1815, section 2
[13] Abramowitz M and Stegun I A (ed) 1964 Handbook of Mathematical Functions (New York: Dover) section 3.8.2