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Bose–Einstein Condensation in a Harmonic Trap: Effect of Interactions on T_c

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For a harmonically trapped dilute Bose gas with uniformly repulsive interactions which is assumed to satisfy a certain condition on the extensivity of fluctuations, I find on upper bound on the condensate fraction f. If BEC is defined by the condition that $f > \text{const.}\, N^{-\alpha}$, $\alpha < 1/2$, I argue that in the limit $N \to \infty$, $V_o \to 0$, $NV_o \to \text{const.}$ where V_o is the space integral of the potential, the interactions cannot increase the critical temperature over that of the noninteracting gas.

KEY WORDS: Bose–Einstein condensation; harmonic traps; interaction effects; critical temperature.

Since the attainment$^{(1,2)}$ in 1995 of Bose–Einstein condensation (BEC) in magnetically confined dilute atomic alkali gases, a topic which has attracted considerable interest (see, e.g., refs. 3 and 4) is the effect of the interactions which exist in such a gas on the transition temperature T_c and by implication on the fraction $f(T)$ of the atoms which is condensed at any given temperature T. The general belief is that if the gas in question is sufficiently dilute, the interactions may be modeled by a pseudopotential of the form

$$V_{\text{eff}}(\mathbf{r}) = \frac{4\pi\hbar^2}{M}\, a_s\, \delta(\mathbf{r}) \tag{1}$$

where M is the mass of the atoms and a_s is the s-wave scattering length, which may have either sign. (For a discussion of the justification of Eq. (1), see, e.g., ref. 5, Section IV.C.) It is almost universally believed that when a_s

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is negative the system is unstable (or at best metastable) against collapse in real space: see, e.g., ref. 6. I will not be further interested in this case here.

In the case of a repulsive interaction ($a_s > 0$) and for atoms moving freely in three-dimensional space, a number of recent papers have used some form of the perturbation theory or numerical technique to calculate the effect of the interactions on T_c; the almost uniform conclusion of these papers[3] (though cf. ref. 7) is that in the dilute limit T_c is *increased* above the noninteracting-gas transition temperature $T_c^{(0)}$, with the increase ΔT_c being given by a formula of the form

$$\Delta T_c / T_c^{(0)} = C(n^{1/3} a_s) \tag{2}$$

where n is the density; different authors obtain values for the positive numerical constant C which span an order of magnitude. Perhaps the easiest way to understand the positive sign of the right-hand side of Eq. (2) is to note that, because of the Bose statistics, in the simplest (Hartree–Fock) approximation the interaction energy of two condensed atoms is half that of either two non-condensed ones or a condensed and a non-condensed atom (see, e.g., ref. 5, Section IV.D); thus, at the Hartree–Fock level there is a term in the energy proportional to $-a_s f^2$. Although such a term would have no effect on T_c in a simple mean-field theory of the phase transition, it seems reasonable that once one goes beyond this the effect would be to favor BEC, i.e., to raise T_c over its noninteracting-gas value $T_c^{(0)}$.

A previous paper[8] by the present author (hereafter referred to as I) investigated the question: Given a ("true") interatomic potential $V(\mathbf{r})$ which is positive for all $\mathbf{r}$, can one place an upper bound (other than that which follows from Hohenberg's[9] lemma or a generalization[10] thereof) on the condensate fraction f as a function of T? In I such a bound is indeed obtained, subject to a single assumption about the extensivity of fluctuations in the condensate number; for the special case $T = T_c^{(0)}$ it gives the inequality (Eq. (16) of I)

$$f(T_c^{(0)}) \leqslant A(nV_o / kT_c^{(0)})^{1/3}, \qquad A \approx 2.2 \tag{3}$$

where V_o is the space integral of $V(\mathbf{r})$. If in the case of a realistic alkali gas we are content to replace the true interatomic potential (which in general is not everywhere positive) by the pseudopotential (1), the right-hand side of (3) is proportional to $(n^{1/3} a_s)^{1/3}$.

In the real-life experiments which observe BEC, the system is almost always confined by a potential, either magnetic or laser-derived or both, which can be treated to a good approximation as that of a three-dimensional harmonic oscillator, and the results obtained for the free-space case need to be appropriately generalized. In the following I will consider for simplicity the case of an isotropic potential with classical harmonic frequency ω_o, but the results are straightforwardly generalized. In the case of a noninteracting Bose gas, the transition temperature $T_c^{(0)}$ is a function of N:(11)

$$T_c^{(0)} = KN^{1/3}\hbar\omega_o/k_B \tag{4}$$

where the constant K tends to approximately 0.94 in the limit $N \to \infty$. For the interacting case with two-body interaction $V(r)$, I shall follow the usual convention in parametrizing the interaction by the two-body s-wave scattering length a_s. Then for $a_s \neq 0$ we need to decide what limiting process most closely corresponds to the "thermodynamic limit" $N \to \infty, V \to \infty$, $N/V \to$ const. in the free-space case. If we require that the groundstate energy should be proportional to N in the limit $N \to \infty$, then we must allow a_s to tend to zero with increasing N in such a way that the quantity $g \equiv Na_s$ tends to a constant:

$$N \to \infty, \qquad a_s \to 0, \qquad Na_s \to g \equiv \text{const.} \tag{5}$$

This then has the consequence that the form of the Gross–Pitaevskii (GP) equation for the condensate wave function $\varphi_o(\mathbf{r})$ (or the associated order parameter $\sqrt{N}\,\varphi_o(r)$) is independent of N. Very recently, Lieb and Seiringer(12) have shown that in the limit defined by Eq. (5) (actually for a more general potential) BEC takes place into the GP groundstate $\varphi_o(r)$ with 100% amplitude (i.e., the depletion is zero). It is remarkable that this is the first rigorous proof of the existence of BEC in any continuum model with short-range interactions; for the 3D free-space case, by contrast, BEC has been established(13) only within the framework of perturbation theory.

In the remainder of this note I shall consider the effects of the interactions on the transition temperature $T_c^{(0)}(N)$ in the limit defined by (5), or more precisely by (5) with a_s replaced by the space integral V_o of $V(\mathbf{r})$. As in I, I shall assume a "true" potential $V(\mathbf{r})$ which is short-ranged and positive for all $\mathbf{r}$ and corresponding to a (positive) two-body scattering length a_s which I will use, in the next paragraph only, as a convenient parametrization of its strength. We immediately note that in addition to the effect noted above for the free-space case, which would be expected if anything to increase T_c, the interactions may be expected(14) to have a second effect with the opposite sign: they will tend to decrease the density at the origin, and since for the noninteracting gas (in the limit $N \to \infty$) $T_c^{(0)}$ is proportional to the $2/3$ power of this central density, we would expect the effect to decrease T_c.

We may make a simple dimensional estimate of these two effects, starting from the fact that the maximum density $\rho_m^{(0)}$ (i.e., the density at the origin) of the noninteracting gas at $T_c^{(0)}$) is proportional to $N(m\omega_0^2/kT_c^{(0)})^{3/2} \sim N^{1/2}$ (cf. Eq. (4)). Thus the former effect should give, from Eq. (4), $\Delta T_c \sim \rho_m^{(0)\,1/3} a_s T_c^{(0)} \sim N^{1/2} a_s$, and since the mean field at the origin is $\sim \rho_m^{(0)} a_s$ and competes with the thermal energy $kT_c^{(0)}$, the latter effect should give $\Delta T_c \sim (\delta\rho_m/\rho_m^{(0)})\, T_c^{(0)} \sim (\rho_m^{(0)} a_s/T_c^{(0)}) \cdot T_c^{(0)} \rho_m^{(0)} \sim \rho_m^{(0)} a_s$, which is also proportional to $N^{1/2} a_s$. (Alternatively, one can say that both effects on the relative shift $\Delta T_c/T_c^{(0)}$ are of the order $N^{1/6} a_s/a_{ho}$, where $a_{ho} \equiv (\hbar/m\omega_0)^{1/2}$: cf. the more quantitative calculation of the second effect in ref. (14)). Thus the effects are comparable, but both vanish in the limit (5). The rest of this paper is effectively an attempt to make (part of) this conclusion more persuasive.

I will use the technique described in I to argue that provided we are prepared to accept a definition of BEC which is a very slight modification of the conventional one, and make the assumption (hereafter called assumption A) specified by Eq. (2) of I, namely that the fluctuations of the condensate fraction are proportional to $N^{-1/2}$ in the limit $N \to \infty$, then the quantity ΔT_c cannot be greater than zero in the limit defined by (5). The argument proceeds by first establishing, as in I, an upper limit on the fraction $f(T{:}N)$ of condensed particles, and then using this in conjunction with our slightly modified definition of BEC to set an upper limit on ΔT_c which vanishes in the specified limit.

The derivation of an upper bound on $f(T{:}N)$ parallels fairly closely that used in I for the free-space case, and I omit most of the details. It is convenient to choose the zero of single-particle energy at the groundstate value for a single particle in the well, namely $3\hbar\omega_o/2$. We first write the obvious inequality for the actual free energy $F(N,T)$ of the interacting gas:

$$F(N,T) \leqslant F_o(N,T) + \langle V \rangle_o \, (N,T) \tag{6}$$

where F_o is the free energy of the corresponding noninteracting gas and $\langle V \rangle_o$ is the expectation value of the interaction energy calculated using the noninteracting-gas density matrix. The next step is to obtain a *lower* bound on $F(N,T)$ by considering the state obtained by removing all the condensed particles while leaving the rest intact (see I for details). As argued in I, this process does not change the entropy, and cannot increase the single-particle energy (since the single-particle energy associated with the condensate wave function $\varphi_0(\mathbf{r})$ must be at least $3\hbar\omega_0/2$). Finally, if we consider the state (density matrix) so obtained as a variational ansatz for the equilibrium state of the noninteracting gas with $N(1-f)$ atoms, the interaction energy of this system (zero!) cannot be greater than the (positive) value it had for the original interacting gas. Consequently, since the ansatz so obtained obviously cannot yield a lower free energy than $F_o(N(1-f), T)$, the free energy obtained by the standard textbook density matrix of the noninteracting gas, we obtain the lower bound

$$F(N,T) \geqslant F_o(N(1-f),T) \tag{7}$$

(In the above argument the complications arising from the fact that our ansatz is in general not an eigenstate of total particle number are similar to those arising in the free-space case, which were discussed in I; it is to deal with these complications that we need to make assumption A.). Finally, combining (6) and (7), we obtain (cf. I, Eq. (5))

$$F_o(N(1-f),T) - F_o(N,T) \leqslant \langle V \rangle_o \, (N,T) \tag{8}$$

Since F_o is a decreasing function of N, Eq. (8) is an implicit bound on the condensate function $f(N,T)$, which I believe is rigorous given assumption A.

We now set $T \geqslant T_c^{(0)}(N)$ and consider the two sides of Eq. (8). At this point it is convenient to assume that the error involved in replacing sums over the discrete single-particle states by integrals over energy weighted with the density of states $\rho(\epsilon) = \epsilon^2/6(\hbar\omega_o)^3$ is of relative order $N^{-\beta}$, $\beta > 0$, and hence can be neglected in what follows. With this assumption (hereafter referred to as assumption B) the argument for a lower bound on the left-hand side of (8) runs closely parallel to that given in the appendix of I, but is simpler since we can substitute the inequality $e^{-n\tilde{\mu}} \geqslant 1 - n\tilde{\mu}$ directly into the analog of Eq. (A.2) of I, and evaluate the sums over n as they stand. Thus we obtain for the quantity $\tilde{\mu} \equiv -\mu/kT$ the inequality

$$\zeta(2)\, \tilde{\mu}/\zeta(3) \geqslant \epsilon'' \equiv 1 - \left(\frac{T_c^0}{T}\right)^3 \tag{9}$$

We choose some value $T' \equiv (1+\delta)\, T_c^{(0)}$ of $T, \delta > 0$. Then it is clear that for $T_c^{(0)} \leqslant T \leqslant T'$ the inequality (9) implies

$$-\mu(N,T) \geqslant \frac{3\kappa\zeta(3)}{\zeta(2)} \left(T - T_c^{(0)}(N)\right) \tag{10}$$

where $\kappa(\delta) \equiv (1 - \frac{1}{(1+\delta)^3})/3\delta$. (Not surprisingly, in the limit $\delta \to 0$ the inequality (9) reduces to an equality). Finally, since $T_c^{(0)}(N)$ is an increasing function of N, we find

$$F_o(N(1-f),T) - F_o(N,T) \geqslant Nf(3\kappa\zeta(3)/\zeta(2))(T - T_c^{(0)}(N)) \tag{11}$$

Now consider the RHS of Eq. (8). Let $\rho_o(\mathbf{r} : N, T)$ be the density distribution of the noninteracting gas and $\rho_m^{(0)}(N, T)$ its maximum value, and write as above V_o for the space integral of $V(r)$. Then we evidently have

$$\langle V \rangle_o \leqslant \iint d\mathbf{r}\, d\mathbf{r}'\, V(\mathbf{r}-\mathbf{r}')\, \rho_o(\mathbf{r})\, \rho_o(\mathbf{r}') \leqslant NV_o \rho_m^{(0)}(N, T) \tag{12}$$

where the first inequality follows from the fact that since $V(\mathbf{r})$ is specified to be everywhere positive the "Fock" term in the interaction energy cannot exceed the "Hartree" one (cf. Eq. (6) of I). At this point I shall again, in the interests of a compact presentation, assume, essentially on dimensional grounds, that $\rho_m^{(0)}(N, T)$ is given in the limit $N \to \infty$ by the expression

$$\rho_m^{(0)}(N, T) = \lambda N (m\omega_o^2/kT)^{3/2} \leqslant \lambda' N^{1/2} a_{ho}^{-3} \tag{13}$$

where $a_{ho} \equiv (\hbar/m\omega_o)^{1/2}$ is, up to a factor, the zero-point diplacement of an atom in the oscillator potential and the quantities λ and $\lambda' \equiv (0.94)^{-3/2}\lambda$ are dimensionless constants which we could (but do not need to) calculate (call this assumption C). Finally, combining Eqs. (8), (11)–(13) and denoting the numerical constant $\lambda'\zeta(2)/3\kappa\zeta(3)$ by σ_o, we obtain the inequality

$$f(N, T) \leqslant N^{1/2} \sigma_o V_o a_{ho}^{-3} (T - T_c^{(0)})^{-1} \tag{14}$$

Now in the present notation the limit analogous to Eq. (5) corresponds to $N \to \infty$, $V_o \to 0$, $NV_o \to g'\hbar\omega_o a_{ho}^3$, where g' is a dimensionless constant (the dimensional parameters are chosen to be $\hbar\omega_o$ and a_{ho}^3 only for definiteness: they could be any N-independent quantities). Thus (14) reduces to

$$f(N, T) \leqslant N^{-1/2} \sigma_o g'\hbar\omega_o / (T - T_c^{(0)}(N)) \tag{15}$$

If now we are prepared to refine our definition of BEC to the statement that f exceeds some small quantity ϵ, where ϵ is either a constant or decreases with N as $N^{-\alpha}, \alpha < 1/2$, we immediately see from (15) that $\Delta T_c(N)$ tends to zero as $N \to \infty$. Thus our claim is proved: in the limit $N \to \infty$, $V_o \to 0$, $NV_o \to$ const., repulsive interactions cannot enhance T_c.

The above conclusion rests on three assumptions (A)–(C). (B) and (C) are relatively trivial and I believe could almost certainly be removed by a more elaborate calculation should the incentive to do so arise. The assumption (A) is more serious: just as in I, we need to assume that the (statistical and quantum) fluctuations of the condensate fraction f are of relative order $N^{-1/2}$ in the limit $N \to \infty$. Because of the rather unusual nature of the limit taken in (5), this is perhaps not quite so overwhelmingly plausible as for the free-space case discussed in I; nevertheless I believe it makes sense to assume it for our purposes. I note also that the numerical coefficient appearing on the RHS of the inequality (14) is certainly not the minimum attainable; e.g., one could improve it by using in place of $\langle V \rangle_o$ in Eq. (6) the value of $\langle V \rangle$ calculated in the Hartree–Fock approximation. However, in the present context the extra work involved does not appear justified by the comparatively minor improvement which would result.

In the case of a realistic interatomic potential $V(\mathbf{r})$, which is not in general everywhere positive, the above argument fails. The situation then parallels that in the free-space case discussed in I: *Provided* we are content to assume that the relevant dynamics is adequately parametrized by the pseudopotential (1), the inequality (14) (and hence the final result of the paper, with $V_o \rightarrow a_s$) follows, with g' now given by the expression $4\pi N a_s / a_{ho}$. However, one may question the plausibility of the replacement (1) in the case where the limit (5) is obtained by adjusting the details of the potential so that $a_s \rightarrow 0$ while $V(r)$ stays in general finite, and in any event conclusions based on (1) cannot be regarded as possessing the same degree of persuasiveness as our main conclusion.

The rather modest result obtained in this note suggests at least three obvious questions. First, is it possible to prove rigorously that for large but finite values of N the correction to T_c in a harmonic trap from repulsive inter-particle interactions is negative (if indeed it is: cf. ref. 15)? Secondly, is it possible to supplement the result obtained above by establishing that in the relevant limit interactions not only cannot increase T_c, but cannot decrease it either? Thirdly—a question which is perhaps more subjective—is the limit specified by Eq. (5) really the "interesting" one for the finite-temperature properties, and if not, what should we replace it with? If for example we choose to let $N^{1/2} V_0$ rather than $N V_0$ tend to a constant as $N \rightarrow \infty$, so as to preserve a constant value of the mean field at the origin at $T_c^{(0)}$, then it is clear that the inequality (14) no longer leads to the conclusion that $\Delta T_c \rightarrow 0$ in the limit $N \rightarrow \infty$; however, in view of (4) the *relative* shift $\Delta T_c / T_c^{(0)}$ can still be argued to tend to zero. These questions are left for possible future research.

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[2] I take this opportunity to note a minor typographical error in this paper, which in no way affects the conclusions: the left-hand side of the inequality (1) should read $f/(1-f)^{2/3}$.