λ-Transition to the Bose-Einstein Condensate

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We study Bose-Einstein condensation of comparatively small numbers of atoms trapped by a three-dimensional harmonic oscillator potential. Under the assumption that grand canonical statistics applies, we derive analytical expressions for the condensation temperature, the ground state occupation, and the specific heat capacity. For a gas of N atoms the condensation temperature is proportional to $N^{1/3}$, apart from a downward shift of order $N^{-1/3}$. A signature of the condensation is a pronounced peak of the heat capacity. For not too small N the heat capacity is nearly discontinuous at the onset of condensation; the magnitude of the jump is about $6.6\,Nk$. Our continuum approximations are derived with the help of the proper density of states which allows us to calculate finite-N-corrections, and checked against numerical computations.

I. Introduction

Very recently, Anderson, Ensher, Matthews, Wieman, and Cornell [1] succeeded in cooling a dilute gas of ^{87}Rb down to the nanokelvin regime and observed the onset of Bose-Einstein condensation at 170 nK, finally obtaining a condensate consisting of merely 2 000 atoms. Independently, Bradley et al. [2] reported the condensation of about 100 000 ^{7}Li atoms.

When the total number of particles is that small, the question arises whether there really is a sharp phase transition to the condensate state. In other words, is there still a reasonably well defined transition temperature, or is the onset of condensation completely blurred? How does the heat capacity for these small samples of matter vary with temperature?

Besides the small number of particles, there is a second feature which distinguishes experimental reality from the common textbook paradigm of the condensation of a free Bose gas: atoms that are stored in a trap do not move freely, but inevitably feel the confining potential. Typical trap potentials [3, 4] can be described, to a good approximation, by the potential of a three-dimensional harmonic oscillator. In general, the oscillator potential is anisotropic. The quantum state that can be occupied by the condensate is the oscillator ground state. Bose-Einstein condensation in a harmonic potential had been considered already in 1950 by de Groot, Hooyman, and ten Seldam [5], who found that the heat capacity shows a discontinuity at the onset of condensation (see Fig. 6 in [5]). This result was later confirmed by Bagnato, Pritchard, and Kleppner [6]. However, the discontinuity develops only in the unphysical limit of an infinite number of trapped particles. To which extent does the discontinuity survive in the regime of physically accessible particle numbers? Will the discontinuity be washed out, or should experimentalists, who endeavour to measure the heat capacity of a dilute atomic vapor near the onset of Bose-Einstein condensation, expect to find a still "practically discontinuous" heat capacity?

These are the questions that we will try to answer in the present paper. We will investigate, both analytically and numerically, Bose-Einstein condensation of a comparatively small number of ideal Bosons confined by the potential of a harmonic oscillator. Since both the system's heat capacity and the condensation temperature are primarily determined by the number of accessible quantum states, it is clear that particular attention will have to be paid to obtaining a good description of the density of states. Within the grand canonical framework, we will show that the specific heat capacity below the condensation temperature is *enhanced* above the level attained for very large particle numbers, whereas the condensation temperature *decreases*. When the total number of particles is small, then the condensate fraction turns out

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to be substantially *reduced* for temperatures slightly below the onset of condensation. Nevertheless, the heat capacity shows a quite pronounced temperature dependence in the transition region, even for systems consisting of merely a few thousand particles. An attempt to measure the heat capacity of a dilute gas of Bosons at the onset of Bose-Einstein condensation should, therefore, definitely be worthwhile.

The above statements will be substantiated, and made more precise, in the following two technical sections. We will first derive expressions for the ground state population and the condensation temperature, and demonstrate the accuracy of our formulae by comparison with numerical computations. We will then consider the heat capacity, again presenting analytical and numerical results. In the final fourth section we discuss some relevant orders of magnitude and compare Bose-Einstein condensation in a harmonic trap to the condensation of a gas of free Bosons.

II. Bose-Einstein Condensation of a Few Thousand Particles

We study a system of N noninteracting Bosons moving in the potential of a three-dimensional harmonic oscillator. We assume N to be of order 10^3 or 10^4, say, so that we are dealing not with a macroscopic but rather with a mesoscopic sample of matter. Denoting the three oscillator frequencies by ω_1, ω_2, and ω_3, the single-particle energies read

$$E_{n_1 n_2 n_3} = \hbar(\omega_1 n_1 + \omega_2 n_2 + \omega_3 n_3) + E_0 \, , \quad (1)$$

where $n_i = 0, 1, 2, \ldots \; (i = 1, 2, 3)$, and

$$E_0 = \frac{\hbar}{2}(\omega_1 + \omega_2 + \omega_3) \quad (2)$$

is the zero-point energy. We assume that grand canonical statistics applies, so that one control parameter is the system's temperature T. The chemical potential μ is then determined from the requirement that the sum over the occupation probabilities of all states yields the total number of particles:

$$N = \sum_{n_1 n_2 n_3} \frac{1}{\exp[\beta E'_{n_1 n_2 n_3} + \beta(E_0 - \mu)] - 1} \, , \quad (3)$$

where $E'_{n_1 n_2 n_3} = E_{n_1 n_2 n_3} - E_0$ and $\beta = 1/kT$. Such sums have been evaluated by de Groot et al. [5] with the help of a technique dating back to Fowler and Jones [7]. We choose a different strategy: we replace discrete summations by integrations, and account for finite-N-effects by employing the proper density of states, similar to the procedure applied in [8] to a Bose gas confined by a cubic container. As we will show, this approach combines technical simplicity with high accuracy. By merely computing standard integrals, one obtains precise estimates for the magnitude of finite-N-corrections, even for particle numbers as small as 10^3.

The desired density $\rho(E)$ can be obtained from the number $\nu(E)$ of states for which $\hbar(\omega_1 n_1 + \omega_2 n_2 + \omega_3 n_3)$ is less than or equal to a given energy E. Finding $\nu(E)$ is equivalent to computing the number of points of a rectangular lattice with lattice constants $\hbar\omega_i$ $(i = 1, 2, 3)$ which fall inside, or on the surface of, the simplex $\{x_1 \geq 0, x_2 \geq 0, x_3 \geq 0, x_1 + x_2 + x_3 \leq E\}$. Therefore, $\nu(E)$ can roughly be estimated by dividing the volume of that simplex, which is $E^3/6$, by the volume of the "energy unit cell", which is $\hbar\omega_1 \cdot \hbar\omega_2 \cdot \hbar\omega_3$. Introducing the geometric mean Ω of the oscillator frequencies,

$$\Omega = (\omega_1 \omega_2 \omega_3)^{1/3} \, , \quad (4)$$

we find $\nu(E) \approx E^3/(6\hbar^3\Omega^3)$, hence

$$\rho(E) \approx \frac{1}{2} \frac{E^2}{(\hbar\Omega)^3} \, . \quad (5)$$

But this approximation, which would be sufficient for an analysis of the large-N-case [5, 6], is not accurate enough for our purposes. Its deficiency becomes obvious if we consider the special case of an isotropic harmonic oscillator, i.e., $\omega_1 = \omega_2 = \omega_3 = \Omega$, and ask for the number $\nu_=(E)$ of states for which $\hbar\Omega(n_1 + n_2 + n_3)$ is *exactly* equal to E. If $E/\hbar\Omega$ is an integer, then $\nu_=(E)$ is equal to the number of ways in which $E/(\hbar\Omega) = n_1 + n_2 + n_3$ can by partitioned into a sum of three integers (including zero). This number is $\binom{E/\hbar\Omega + 2}{2}$, i.e.,

$$\nu_=(E) = \frac{1}{2}\left(\frac{E}{\hbar\Omega}\right)^2 + \frac{3}{2}\frac{E}{\hbar\Omega} + 1 \, . \quad (6)$$

Otherwise $\nu_=(E) = 0$. Thus, in the isotropic case the triple sum (3) reduces to a single sum:

$$N = \sum_{n=0}^{\infty} \frac{n^2/2 + 3n/2 + 1}{\exp[\beta\hbar\Omega n + \beta(E_0 - \mu)] - 1} \, . \quad (7)$$

Obviously, the right hand side of (6) equals $\rho(E)\cdot\Delta E$ for $\Delta E = \hbar\Omega$. Hence, a better approximation than (5) to the density of states is given by

$$\rho(E) = \frac{1}{2}\frac{E^2}{(\hbar\Omega)^3} + \gamma\frac{E}{(\hbar\Omega)^2}\,, \tag{8}$$

with $\gamma = 3/2$ for an *isotropic* harmonic oscillator. For an *anisotropic* oscillator the argument which led to (6) fails. When the three lattice constants do not coincide, the determination of the exact number of lattice points inside a simplex is, in fact, linked to a difficult number-theoretical problem [9]. We adopt a more pragmatical philosophy here: there should be a correction proportional to $E/(\hbar\Omega)^2$ to the density (5) also in the anisotropic case, and its coefficient γ can be found numerically by counting the number of lattice points inside the energy simplex, subtracting $E^3/(6\hbar^3\Omega^3)$, and averaging over a suitable energy range. Numerical calculations [10] have shown that (8) can be regarded as an effective parametrization of the density of states in the general, anisotropic case; the value of γ then tends to be slightly larger than 3/2.

Replacing $\hbar(\omega_1 n_1 + \omega_2 n_2 + \omega_3 n_3)$ by a continuous variable E, and using the density (8) to convert summation over the quantum numbers n_1, n_2, n_3 to integration over E, (3) becomes

$$\begin{aligned} N &= N_0 + \frac{1}{2}\frac{1}{(\hbar\Omega)^3}\int_0^\infty \frac{E^2\mathrm{d}E}{\exp[\beta(E+E_0-\mu)]-1} \\ &+ \frac{\gamma}{(\hbar\Omega)^2}\int_0^\infty \frac{E\mathrm{d}E}{\exp[\beta(E+E_0-\mu)]-1}\,. \end{aligned} \tag{9}$$

As in the familiar case of an ideal Bose gas in the absence of external potentials [11, 12], the ground state occupation N_0 has to be treated separately, since it can become large, of order N, when the chemical potential μ approaches the ground state energy E_0.

Incorporating E_0 into our definition of the fugacity z,

$$z = \exp[\beta(\mu - E_0)]\,, \tag{10}$$

and introducing the Bose-Einstein functions [12]

$$g_n(z) = \frac{1}{\Gamma(n)}\int_0^\infty \frac{x^{n-1}\,\mathrm{d}x}{z^{-1}e^x - 1}\,, \tag{11}$$

(9) can be written more compactly as

$$N = N_0 + \left(\frac{kT}{\hbar\Omega}\right)^3 g_3(z) + \gamma\left(\frac{kT}{\hbar\Omega}\right)^2 g_2(z)\,. \tag{12}$$

The conversion of the sum (3) into this expression is justified only if the number of appreciably populated states is sufficiently large, i.e., if the temperature T is large compared to the ground state temperature E_0/k. If this condition is not satisfied, only a few terms contribute to the sum, so that it has to be evaluated as it stands.

Now we can apply standard arguments [11, 12]: Since the ground state occupation number is given by $N_0 = 1/(z^{-1} - 1)$, we have

$$z = \frac{N_0}{N_0 + 1}\,, \tag{13}$$

hence $0 \le z < 1$. The expansion

$$g_n(z) = \sum_{\ell=1}^{\infty}\frac{z^\ell}{\ell^n} \tag{14}$$

shows that the functions $g_n(z)$ are bounded by $g_n(1) = \zeta(n)$ in this interval, with $\zeta(x)$ denoting the Riemannian zeta function. In particular, $\zeta(3) \approx 1.202057$ and $\zeta(2) = \pi^2/6$ are both finite. Therefore, in order to satisfy (12) at low temperatures, the ground state population N_0 must necessarily become large, i. e., the system exhibits Bose-Einstein condensation.

A condensation temperature T_C can now be introduced as follows. At sufficiently low temperatures, where the ground state population N_0 is large, the approximation $z \approx 1$ holds, and (12) becomes

$$N_0 = N - \left(\frac{kT}{\hbar\Omega}\right)^3\zeta(3) - \gamma\left(\frac{kT}{\hbar\Omega}\right)^2\zeta(2)\,. \tag{15}$$

We then *define* T_C as that temperature where, according to this equation, the ground state population N_0 should become zero. Rearranging (15) with $N_0 = 0$ yields

$$T_C = \frac{\hbar\Omega}{k}\left(\frac{N}{\zeta(3)}\right)^{1/3}\left[1 - \gamma\frac{\zeta(2)}{N}\left(\frac{kT_C}{\hbar\Omega}\right)^2\right]^{1/3}. \tag{16}$$

Thus, if the number of particles is very large, Bose-Einstein condensation occurs at the temperature

$$T_0 = \frac{\hbar\Omega}{k}\left(\frac{N}{\zeta(3)}\right)^{1/3} . \tag{17}$$

If, however, the number of particles is such that $N^{-1/3}$ is not negligible compared to unity, we find a downward shift of the condensation temperature of order $N^{-1/3}$:

$$T_C \approx T_0\left[1 - \frac{\gamma\zeta(2)}{3\zeta(3)^{2/3}}\cdot\frac{1}{N^{1/3}}\right] . \tag{18}$$

The relative shift of T_C with respect to T_0 is given by

$$\frac{T_C - T_0}{T_0} \approx -0.485\,\gamma\,N^{-1/3} . \tag{19}$$

For $N = 2\,000$ particles, for example, the magnitude of the relative shift is about 6%.

It must be emphasized that there is a certain arbitrariness in the definition of the condensation temperature T_C. We have chosen to extrapolate (15) from temperatures well below the onset of condensation (where the approximation $z = 1$ is valid) to the temperature regime where N_0 becomes small (where it is not). The error introduced into (12) by setting z equal to unity for $T < T_C$ is of order $(kT/\hbar\Omega)^3/N_0$. For temperatures only slightly below T_C, where the ground state population N_0 is still very small compared to N, this approximation error is large compared to the error that results from the conversion of the discrete sum (3) into its continuum version (12). In the vicinity of T_C, that conversion error is a few $kT/(\hbar\Omega)$. If one requires that the approximation error remains smaller than the conversion error, one has to exclude a temperature interval around T_C of order $N^{-1/3}$ from the analysis.

Instead of extrapolating (15), one could also define the typical condensation temperature as that temperature where the chemical potential μ (which is negative for high temperatures, and approaches the positive ground state energy E_0 for very low temperatures) crosses zero. This arbitrariness in the definition of T_C again reflects, of course, the finiteness of the particle number. The onset of condensation does not occur at a sharply defined temperature, as it would in the unphysical limit $N \to \infty$, but is smeared out over a temperature interval of order $N^{-1/3}$. The following numerical studies will show, however, that (18) actually describes the onset of condensation quite well.

In order to demonstrate the accuracy of our analytical results, and to study the Bose gas even for temperatures close to T_C, we evaluate the discrete sum (3) numerically, *without* the approximation $z = 1$. Rather, the chemical potential μ is determined iteratively to such a precision that the right hand side of (3) reproduces the preassigned particle number N with a relative error of less than 10^{-5}. The limit of the achievable accuracy is set mainly by roundoff errors.

Figure 1 depicts the relative ground state population N_0/N as function of the normalized temperature T/T_0 for a gas of $N = 2\,000$ ideal Bosons moving in the potential of an isotropic harmonic oscillator with $\Omega = 300\,\mathrm{s}^{-1}$. For these parameters, the ground state temperature E_0/k is 3.437 nK; the characteristic temperature T_0 is less than an order of magnitude higher: $T_0 = 27.153$ nK. Moreover, $T_C = 0.942\,T_0$. Inserting the definition (17) of T_0 into (15), our result for the ground state population below T_C can be written as

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_0}\right)^3 - \gamma\frac{\zeta(2)}{\zeta(3)^{2/3}}\frac{1}{N^{1/3}}\left(\frac{T}{T_0}\right)^2 . \tag{20}$$

The dashed line in Fig. 1 shows the ground state population for N very large (i.e., $N_0/N = 1 - (T/T_0)^3$ below T_0), the full line shows the prediction of (20) for $N = 2\,000$, and the diamonds indicate data computed

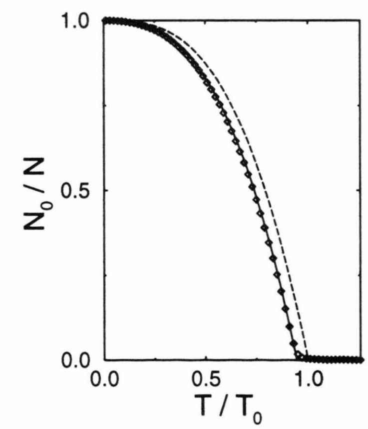

Fig. 1. Relative ground state population N_0/N versus reduced temperature T/T_0 for $N = 2\,000$ ideal Bosons confined by an isotropic harmonic oscillator potential with frequencies $\omega_i = 300\,\mathrm{s}^{-1}$ $(i = 1,2,3)$. The full line corresponds to (20), the diamonds are numerically computed data points. For comparison, the dashed line shows the ground state population for the large-N-case.

numerically for this particle number. The intersection of the full curve with the abscissa $N_0/N = 0$ yields T_C/T_0. As expected, the numerical data show a smooth onset of the condensation at temperatures slightly above T_C, but their overall agreement with (20) is impressive.

Figure 2 then shows the ground state population at temperatures slightly below T_0 for N very large (dashed line), $N = 20\,000$ (circles), and $N = 2\,000$ (diamonds), again for an isotropic oscillator with the same frequency as above. In addition, we show results (triangles) for an anisotropic oscillator with $\omega_1 = \omega_2 = 300\,\mathrm{s}^{-1}$ and $\omega_3 = \sqrt{8} \cdot 300\,\mathrm{s}^{-1}$, so that the frequency ratios are identical with those of the TOP trap used in the recent experiments [1, 4]. (The acronym TOP stands for "time-averaged, orbiting potential".) In this case $\gamma \approx 1.8$, so that the corrections to the limit of very large particle numbers are even larger than for the isotropic oscillator potential, where $\gamma = 1.5$.

The good agreement between the numerical and the analytical data underlines the importance of the term proportional to γ in the density of states (8). It is also remarkable that a continuum approximation can give accurate results even if the ground state temperature E_0/k and the condensation temperature T_C differ by less than an order of magnitude, as in the above numerical example.

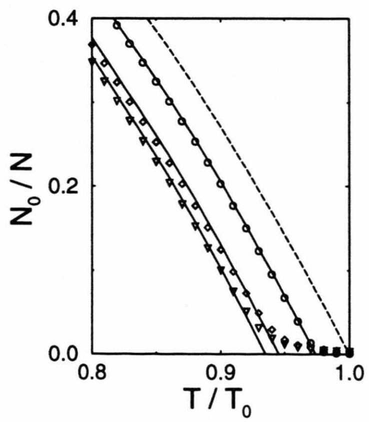

Fig. 2. Numerically computed ground state population in the vicinity of T_0 for an isotropic oscillator with $\omega_i = 300\,\mathrm{s}^{-1}$ ($i = 1, 2, 3$) and $N = 20\,000$ (circles) and $N = 2\,000$ (diamonds). The triangles correspond to an anisotropic oscillator with $\omega_1 = \omega_2 = 300\,\mathrm{s}^{-1}$ and $\omega_3 = \sqrt{8} \cdot 300\,\mathrm{s}^{-1}$, for $N = 2\,000$. In all three cases the full lines show the prediction of (20); the dashed line shows the ground state occupation for very large N.

Figure 3 displays the fugacity $z = \exp[\beta(\mu - E_0)]$ versus temperature, for $N = 20\,000$ (full line) and $N = 2\,000$ Bose particles (dashed) in an isotropic oscillator potential. This figure confirms once more that the onset of condensation ($z \to 1$) is shifted to temperatures lower than T_0 if the number of particles is merely mesoscopically large, and that the onset of condensation remains fairly well defined. It should also be noted that already for $T/T_0 \approx 2$ one is close to the classical limit. Then $g_n(z) \approx z$ and thus $z \approx \zeta(3)(T/T_0)^{-3}$, corresponding to $\beta(\mu - E_0) \approx 0.184 - 3\ln(T/T_0)$.

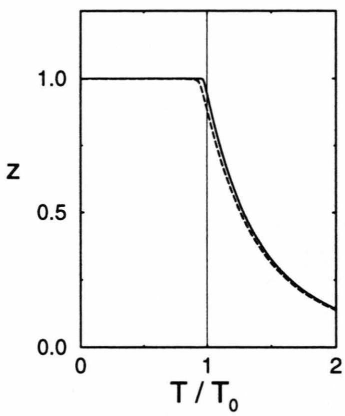

Fig. 3. Fugacity z (see (10)) for $N = 20\,000$ (full line) and $N = 2\,000$ noninteracting Bosons (dashed) in an isotropic harmonic oscillator potential.

III. The Temperature Dependence of the Heat Capacity

The logarithm of the grand partition function for N ideal Bosons confined by a harmonic potential is

$$\ln \mathcal{Z} = -\sum\nolimits_{n_1 n_2 n_3} \ln(1 - \exp[\beta(\mu - E_0 - \hbar(\omega_1 n_1 + \omega_2 n_2 + \omega_3 n_3))]). \tag{21}$$

Again employing the density of states $\rho(E)$ and proceeding in complete analogy to the derivation of (12), one obtains the continuum approximation

$$\ln \mathcal{Z} = \left(\frac{kT}{\hbar\Omega}\right)^3 g_4(z) + \gamma \left(\frac{kT}{\hbar\Omega}\right)^2 g_3(z) - \ln(1 - z), \tag{22}$$

where the last term on the right hand side is the contribution of the ground state, $\ln(1+N_0)$. Using the identity

$$kT^2\left(\frac{\partial}{\partial T}\ln \mathcal{Z}\right)_{z,\Omega} = U - NE_0, \tag{23}$$

which can be verified easily, one finds the mean energy U:

$$\begin{aligned} U - NE_0 = 3kT\left(\frac{kT}{\hbar\Omega}\right)^3 g_4(z) \\ + 2\gamma kT\left(\frac{kT}{\hbar\Omega}\right)^2 g_3(z). \end{aligned} \tag{24}$$

The heat capacity C of the system (for fixed oscillator frequencies) then follows by differentiating with respect to temperature,

$$C = \left(\frac{\partial U}{\partial T}\right)_{N,\Omega}. \tag{25}$$

To evaluate C we use the same approximations as in the previous section, i.e., we assume that $z=1$ below T_C and $N_0 = 0$ above T_C, with the implicit understanding that these approximations are inconsistent in a vicinity of T_C of order $N^{-1/3}$.

The heat capacity for temperatures below T_C, denoted as $C_<$, can be computed easily:

$$C_< = 12k\left(\frac{kT}{\hbar\Omega}\right)^3 \zeta(4) + 6\gamma k\left(\frac{kT}{\hbar\Omega}\right)^2 \zeta(3); \tag{26}$$

or, using (17),

$$\frac{C_<}{Nk} = 12\frac{\zeta(4)}{\zeta(3)}\left(\frac{T}{T_0}\right)^3 + 6\gamma\zeta(3)^{1/3}\frac{1}{N^{1/3}}\left(\frac{T}{T_0}\right)^2. \tag{27}$$

We will denote the heat capacity pertaining to the case of very large N by $C^{(\infty)}$. When the number of particles can be considered as large, and the temperature approaches T_0 (i.e., the exact condensation temperature for this case) from below, the specific heat approaches the value

$$\left.\frac{C_<^{(\infty)}}{Nk}\right|_{T_0-} = 12\frac{\zeta(4)}{\zeta(3)} \approx 10.805. \tag{28}$$

The calculation of $C_>$, the heat capacity above T_C, is more involved. Employing the identity

$$\frac{d}{dz}g_n(z) = \frac{1}{z}g_{n-1}(z), \tag{29}$$

one obtains from (24)

$$\begin{aligned} C_> = 12k\left(\frac{kT}{\hbar\Omega}\right)^3 g_4(z) + 6\gamma k\left(\frac{kT}{\hbar\Omega}\right)^2 g_3(z) \\ + \left[3kT\left(\frac{kT}{\hbar\Omega}\right)^3 g_3(z) \right. \\ \left. + 2\gamma kT\left(\frac{kT}{\hbar\Omega}\right)^2 g_2(z)\right]\frac{1}{z}\frac{\partial z}{\partial T}. \end{aligned} \tag{30}$$

The T-derivative of the fugacity z (at fixed Ω) can be found by differentiating the equation for the particle number, (12), with respect to temperature, again using (29):

$$\frac{1}{z}\frac{\partial z}{\partial T} = -\frac{3}{T}\cdot\frac{g_3(z) + (2\gamma\hbar\Omega/3kT)\,g_2(z)}{g_2(z) + (\gamma\hbar\Omega/kT)\,g_1(z)}; \tag{31}$$

hence

$$\frac{T_0}{z}\frac{\partial z}{\partial T} = -\frac{3T_0}{T}\cdot\frac{g_3(z) + \frac{2\gamma T_0}{3T}\left(\frac{\zeta(3)}{N}\right)^{1/3} g_2(z)}{g_2(z) + \frac{\gamma T_0}{T}\left(\frac{\zeta(3)}{N}\right)^{1/3} g_1(z)}. \tag{32}$$

In this way, we finally arrive at

$$\begin{aligned} \frac{C_>}{Nk} = 12\left(\frac{T}{T_0}\right)^3\frac{g_4(z)}{\zeta(3)} + \frac{6\gamma}{N^{1/3}}\left(\frac{T}{T_0}\right)^2\frac{g_3(z)}{\zeta(3)^{2/3}} \\ + \left[3\left(\frac{T}{T_0}\right)^4\frac{g_3(z)}{\zeta(3)} \right. \\ \left. + \frac{2\gamma}{N^{1/3}}\left(\frac{T}{T_0}\right)^3\frac{g_2(z)}{\zeta(3)^{2/3}}\right]\frac{T_0}{z}\frac{\partial z}{\partial T}. \end{aligned} \tag{33}$$

Before discussing this expression, it is again useful to consider first the case of a very large particle number. Then $(T/T_0)^3 = \zeta(3)/g_3(z)$, and one finds

$$\frac{C_>^{(\infty)}}{Nk} = 3\left[4\frac{g_4(z)}{g_3(z)} - 3\frac{g_3(z)}{g_2(z)}\right]. \tag{34}$$

In the high-temperature limit the fugacity is small. The Bose-Einstein functions $g_n(z)$ can then simply be approximated by z, see (14), so that $C_>^{(\infty)}$ approaches the classical value $3Nk$, as it should. On the other hand, when T approaches the condensation temperature T_0 we have

$$\left.\frac{C_>^{(\infty)}}{Nk}\right|_{T_0+} = 3\left[4\frac{\zeta(4)}{\zeta(3)} - 3\frac{\zeta(3)}{\zeta(2)}\right] \approx 4.228. \quad (35)$$

Comparing with (28), one sees that $C^{(\infty)}$ is discontinuous at T_0 [5, 6]. The jump is rather large, namely

$$\frac{\Delta C^{(\infty)}}{Nk} = 9\frac{\zeta(3)}{\zeta(2)} \approx 6.577\,. \quad (36)$$

This is quite different from the signature which is characteristic for the onset of Bose-Einstein condensation in the absence of a trap potential: the heat capacity of a gas of free, noninteracting Bosons exhibits merely a kink in the thermodynamic limit [11, 12], but remains continuous. Figure 4 compares the heat capacity of an ideal gas of free Bosons in the thermodynamic limit with that of a very large number of harmonically trapped particles.

The equations (27) and (33) now allow us to study how the heat capacity is modified when the number of particles can not be considered as very large. First of all, with $g_n(z) \approx z$ for $T \to \infty$, it follows from (32) that

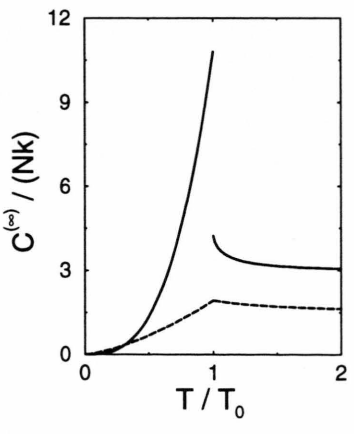

Fig. 4. Heat capacity of a very large number of noninteracting Bosons confined by a harmonic oscillator potential (full line), compared to the heat capacity of an ideal gas of free Bosons in the thermodynamic limit (dashed). Note the pronounced λ-shape of the curve for trapped particles, reminiscent of the specific heat of ^{4}He near the transition to superfluidity.

$$\frac{T_0}{z}\frac{\partial z}{\partial T} \to -\frac{3T_0}{T} \quad (37)$$

in the high-temperature limit. Equation (33) then yields

$$C_> \approx 3k\left(\frac{kT}{\hbar\Omega}\right)^3 z\,, \quad (38)$$

and (12) gives

$$\left(\frac{kT}{\hbar\Omega}\right)^3 z \approx N\,. \quad (39)$$

Thus, for $T \to \infty$ also the full expression (33) correctly reduces to the classical result, $C_> \approx 3Nk$.

The other limit, $T \to T_C$ or $z \to 1$, is more interesting. When the fugacity approaches unity, then $g_1(z)$ diverges, since $g_1(1) = \zeta(1) = \infty$ is the harmonic series, see (14). Therefore (32) yields

$$\frac{T_0}{z}\frac{\partial z}{\partial T} \to 0 \quad (40)$$

for $z \to 1$. But then, (27) and (33) reveal that both $C_<$ and $C_>$ approach the same value for $T \to T_C$: for any finite N the specific heat at the onset of the Bose-Einstein condensation is continuous, but the transition range shrinks with increasing N, its relative width being of order $N^{-1/3}$. Strictly speaking, these statements are not fully borne out by our analysis, since, as repeatedly emphasized, both (27) and (33) are not valid in the immediate vicinity of T_C. If one nevertheless takes these two equations at face value even for $T \to T_C$, one obtains an approximation to the specific heat that is continuous at T_C, but has a discontinuous derivative. A more accurate treatment (which would have to abandon the two approximations $z = 1$ for $T < T_C$, and $N_0 = 0$ for $T > T_C$) would show that the specific heat capacity varies continuously and smoothly at the onset of condensation.

We obtain the precise temperature dependence of the heat capacity for systems with comparatively small particle numbers by numerically computing the mean energy U by discrete summation, and differentiating with respect to temperature. Figure 5 shows the result for $N = 2\,000$ particles in an isotropic harmonic potential. Diamonds indicate numerically computed data points, the heavy line shows the heat capacity for very large N, and the thin line corresponds to the predictions of (27) and (33), respectively. For the

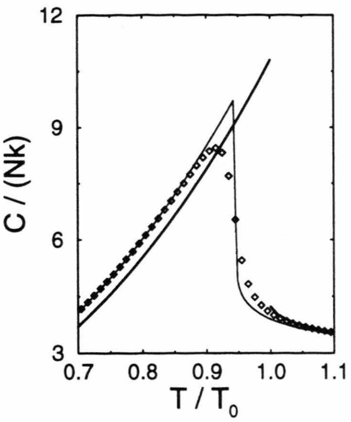

Fig. 5. Numerically computed heat capacity of a system of $N = 2\,000$ noninteracting Bosons moving in the potential of an isotropic harmonic oscillator (diamonds), and the prediction of eqs. (27) and (33) (thin line). Note that these approximate equations are not valid in the immediate vicinity of T_C/T_0, where the thin line has a discontinuous derivative. The heavy line shows the heat capacity for the large-N-case.

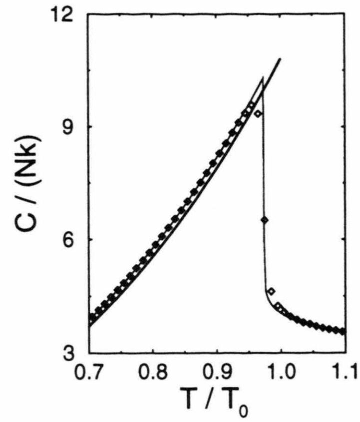

Fig. 6. As Fig. 5, but for $N = 20\,000$ noninteracting Bosons.

sake of clarity, the graphs corresponding to $C_<$ and $C_>$ have been drawn without omitting the vicinity of T_C, even though they are not valid there. The analytical formulae overestimate the change of the heat capacity and underestimate the width of the transition regime: the finite-N-corrections smoothen the transition. Only for particle numbers above 10^6 is the relative width of the transition regime below 1%. (We remark that the most convenient way to evaluate the formidable looking equation (33) numerically is to consider the fugacity z as the fundamental variable, and to obtain the relation $T(z)$ by inverting the cubic equation (12) with the help of the Cardanic formula).

Three observations deserve to be mentioned. First, (27) provides an excellent description of the enhancement of the heat capacity $C_<$ (as compared to $C_<^{(\infty)}$), which results from the enhancement of the actual density of states (8) above the naive estimate (5). Second, the temperature T_C falls in the middle of the interval where the heat capacity drops smoothly from its maximum to its value at T_0. Third, even though there are merely 2 000 particles, the variation of the heat capacity with temperature is fairly pronounced; the maximum at $T = 0.92\,T_0$ is roughly $2.8 \cdot 3Nk$.

Figure 6 finally shows the corresponding data for $N = 20\,000$. Now the enhancement of the heat capacity below T_C is smaller, as it should, since the relative importance of the term proportional to γ in the density (8) decreases with increasing energy. The drop in the vicinity of T_C is already quite sharp. To an experimentalist, who can only take a limited number of data points, such a drop might already appear as a discontinuity.

IV. Discussion: free versus trapped Bosons

One is accustomed to discussing the condensation of an ideal, free Bose gas in the thermodynamic limit [11, 12]. However, the recent experimental progress [1, 2] forces us to reshape our image of Bose-Einstein condensation: the trap volumes are small, the extension of the ground state wave function is merely of the order of a few μm, and the number of particles is limited. Let us take, for example, an isotropic trap with frequency $\Omega = 300\,\mathrm{s}^{-1}$ and depth $T_{\mathrm{trap}} = 100\,\mu\mathrm{K}$. Supposing that the condensation temperature must be *at least* one order of magnitude below T_{trap} (two orders might be more realistic), one finds that the number of particles should not exceed $N_{\mathrm{max}} \approx 10^{11}$ (or $N_{\mathrm{max}} \approx 10^8$ for the more pessimistic estimate). Moreover, the volume is no control parameter. In such a situation conventional thermodynamics, which relies on the distinction of extensive and intensive quantities, no longer applies.

The different statistical ensembles can no longer be considered as equivalent. We have adopted the grand canonical point of view, which requires that both an energy reservoir *and* a particle reservoir is coupled to the trapped Bose gas. Within the grand canonical ensemble, the mean-square fluctuations $\langle(\delta N_E)^2\rangle$ of the population $\langle N_E\rangle$ of a state with energy E are given by $\langle N_E\rangle + \langle N_E\rangle^2$ for a bosonic system. Hence, at temperatures well below T_C the fluctuations of the ground state occupation number become comparable to the total mean particle number N. This might not adequately describe an experiment where a *fixed* number of atoms condenses in a trap. In general, it will depend on the specific experimental conditions whether a microcanonical, a canonical, or a grand canonical approach is most appropriate.

Nevertheless, there are several practically important aspects of our results. First of all, even if there are merely a few thousand Bose particles in a harmonic trap, this number is already close enough to the large-N-case to preserve essential features of a sharp phase transition at the onset of Bose-Einstein condensation. The occupation of the ground state by a mesoscopic number of particles starts at a (seen with the eyes of an experimentalist) reasonably well defined temperature T_C, and the system's heat capacity exhibits a distinct drop at T_C.

Although the formulae for the large-N-case already can yield reasonable estimates, the corrections caused by the effective enhancement of the density of states can be quite substantial. For example, if there are $N = 20\,000$ particles in an isotropic harmonic trap, the estimate for the condensate fraction N_0/N at $T/T_0 = 0.9$ would be $N_0/N \approx 1-(0.9)^3 = 0.271$ if one disregards the finite-N-corrections proportional to γ, whereas the evaluation of the proper Eq. (20), which includes these corrections, gives $N_0/N \approx 0.206$. That is, according to the naive estimate the condensate should consist of roughly 5420 atoms, but this number would actually be by 1300 atoms smaller — and the difference would be even larger in the case of the TOP trap [4], where $\gamma \approx 1.8$ instead of 1.5. Such differences appear to be too large to be ignored in experiments which aim at probing the condensate, such as experiments which search for coherent condensate oscillations in double-well potentials [13].

A mesoscopic particle number can be large enough to cause a sudden variation of the heat capacity at T_C. It is essential to note that the very same number can still be small enough to justify, at least as a first step, the neglection of particle-particle interactions, i.e., the use of the ideal gas approximation. Take a sample of $N = 20\,000$ ^{87}Rb atoms trapped by an isotropic harmonic potential with $\Omega = 300\,\mathrm{s}^{-1}$, as in some of our numerical examples. The extension of the ground-state wave function is given by the oscillator length

$$L_\Omega = \sqrt{\frac{\hbar}{M\Omega}}\,, \tag{41}$$

where M is the mass of the atoms. Thus, at temperatures close to zero the N Bosons, occupying the ground state, will be confined to a volume of order L_Ω^3. That gives a particle density $n \approx 5 \cdot 10^{21}\,\mathrm{m}^{-3}$. Now the (positive) s-wave scattering length of ^{87}Rb is about 46 Å [14]; hence $na^3 \approx 5 \cdot 10^{-4}$. In contrast to the case of liquid ^{4}He, where $na^3 \approx 0.2$, it should then be possible to account for interactions among the atoms by low-order perturbation theory, and even the ideal gas approximation itself should provide a fair description of the real system's properties.

One question remains to be answered. How is the criterion for the onset of Bose-Einstein condensation of harmonically trapped particles related to the corresponding criterion for a free Bose gas in a box? If there is no external potential, the condensation temperature for a gas of N ideal Bosons (of mass M) confined to a volume $V = L^3$ is

$$T_0^{(\mathrm{free})} = \frac{2\pi\hbar^2}{ML^2k}\left(\frac{N}{\zeta(3/2)}\right)^{2/3} \tag{42}$$

in the thermodynamic limit [11, 12]. In terms of the particle density $n = N/L^3$ and the thermal wavelength

$$\lambda(T) = \frac{2\pi\hbar}{\sqrt{2\pi MkT}}\,, \tag{43}$$

the condition for Bose-Einstein condensation can be expressed as

$$n\lambda_0^3 = \zeta(3/2) \approx 2.612\,, \tag{44}$$

where $\lambda_0 = \lambda(T_0^{(\mathrm{free})})$: on the average, there should be about 2.6 particles in a cube with sidelength λ_0.

A trapped Bose gas, on the other hand, is inhomogeneous; its density n depends on the position in the trap: it decreases strongly with increasing distance from the center. *If* a "quasihomogeneous" approximation holds for a harmonically trapped ideal Bose gas, i.e., if the trap potential (and hence the density) remains almost constant on a length scale corresponding to the thermal wavelength of a free particle at the approximate condensation temperature

$$T_0 = \frac{\hbar\Omega}{k}\left(\frac{N}{\zeta(3)}\right)^{1/3}\,, \tag{45}$$

then the particles in the center of the trap may be considered as nearly free, not feeling the potential, and the criterion (44) remains approximately valid, with n denoting the maximum density in the trap center, and λ_0 denoting the thermal wavelength at T_0 [6, 15].

But it is evident that this quasihomogeneous approximation can only be viable when the number of trapped particles is large: large numbers N are necessary to get high T_0, which, in turn, result in the required small $\lambda(T_0)$. Now the characteristic length scale for the variation of the trap potential is the oscillator length (41), and the ratio of the termal wavelength of a (hypothetical) free particle at T_0 and the oscillator length turns out to be

$$\frac{\lambda(T_0)}{L_\Omega} = \sqrt{2\pi}\,\zeta(3)^{1/6}\,N^{-1/6}\,. \tag{46}$$

Hence, the regime of validity of the quasihomogeneous approximation, and therefore of the criterion (44), is restricted to particle numbers such that $2.6 \cdot N^{-1/6}$ is small compared to unity. If that condition is not satisfied — and it is certainly not for $N = 2\,000$ or $N = 20\,000$, even $N = 10^6$ is not a large number in this respect — then the thermal wavelength looses its physical meaning, and the relevant length scale becomes the oscillator length L_Ω.

In summary, Bose-Einstein condensation of a mesoscopic number of particles in a harmonic trap shows several attractive features. On the one hand, a thermodynamic limit does not exist and corrections to the large-N-case must be taken into account; on the other, the transition to the condensate state is not too blurred. Most interestingly, the temperature dependence of the specific heat capacity in the transition region bears strong resemblance to the specific heat of liquid ^{4}He at the famous "λ-point". But whereas particle-particle interactions are believed to play a decisive role in the case of ^{4}He, the "λ" appears for *trapped* Bosons even if their interactions with each other are negligible.

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