Comment on "Numerical analysis of Bose–Einstein condensation in a three-dimensional harmonic oscillator potential," by Martin Ligare [Am. J. Phys. 66 (3), 185–190 (1998)]—An extension to anisotropic traps and lower dimensions

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(Received 8 June 2001; accepted 24 August 2001)

[DOI: 10.1119/1.1412649]

In a recent article in this journal[1] I pointed out that the harmonic oscillator potential used to model most experiments on Bose–Einstein condensation of atomic gases simplifies the numerical analysis. In this note I extend my previous analysis to allow for anisotropic confining potentials. This extension yields a better comparison with real experiments (which are performed in anisotropic confining potentials), but another benefit is the added generality which allows the study of Bose–Einstein condensation in systems whose atoms' motion is limited to one and two dimensions in severely anisotropic traps.

It should be noted that for systems with a finite number of particles, such as those studied in Ref. 1 and in this Comment, there is no true critical temperature, which can be defined only in the limit of an infinite system. However, the systems under investigation exhibit rapid increases in the fraction of particles in the ground state when the temperature is lowered sufficiently and also exhibit rapid changes in the heat capacity. The effective condensation indicated by the calculations of this paper is consistent with more detailed numerical and analytical studies of condensation in harmonic and anharmonic traps.[2]

The occupation number of bosons in a distinct single-particle state with energy ϵ_l at a temperature parametrized by $\beta = 1/kT$ is given by the Bose–Einstein distribution,

$$n_l = \frac{1}{Ce^{\beta\epsilon_l} - 1}, \tag{1}$$

where C is a constant determined by the normalization condition that the sum of the occupation numbers of all states is equal to the total number of particles N. (The constant C can be written in terms of the chemical potential μ as $C = e^{-\beta\mu}$.)

For the isotropic harmonic oscillator potential considered in Ref. 1, the possible single-particle energies are given by

$$E = (j_x + j_y + j_z + \tfrac{3}{2})\hbar\omega, \tag{2}$$

where j_x, j_y, and j_z are all non-negative integers. (In what follows, the energy scale will be rezeroed, and the term giving the zero-point energy of the oscillator will be dropped.) Simple combinatoric arguments show that there are $(m+2) \times (m+1)/2$ linearly independent states with energy $m\hbar\omega$, so that the normalization condition becomes

$$\sum_{m=0}^{\infty} \frac{(m+2)(m+1)}{2(Ce^{m\hbar\omega\beta} - 1)} = N. \tag{3}$$

MATHEMATICA was used in Ref. 1 to solve Eq. (3) numerically for C, and then used to evaluate Eq. (1) to determine the occupation numbers.

For the anisotropic harmonic oscillator potential the frequencies characterizing the confinement along the x, y, and z axes are not equal. I make the simplifying assumption that the frequencies are all integer multiples of some common frequency ω, so that the energies of the single-particle states are

$$\begin{aligned} E &= j_x(p\hbar\omega) + j_y(q\hbar\omega) + j_z(r\hbar\omega) \\ &= (j_z p + j_y q + j_z r)\hbar\omega, \end{aligned} \tag{4}$$

where p, q, and r are all non-negative integers. If $p = q = 1$ and $r > 1$, the potential confines particles more tightly in the z direction than in the x and y directions. States with $j_z > 0$ can be frozen out at temperatures much below $kT = r\hbar\omega$, and the particles are effectively confined to two-dimensional motion in the x–y plane at these temperatures. (This freezing-out of states can occur well above the Bose–Einstein condensation temperature.) If $r = 1$ and $p = q > 1$, the particles are effectively confined to one-dimensional motion along the z axis for large enough values of p and low enough temperatures. Confinement to lower dimensionality affects the Bose–Einstein transition temperature and the nature of the phase transition itself.

The techniques used in Ref. 1 require a single modification for an anharmonic oscillator: The factor giving the multiplicity of the states with a given energy must be changed. The new multiplicities have algebraic expressions in terms of the "floor" function $F(x)$ giving the largest integer that is less than a given input. [In MATHEMATICA $F(x)$ is the Floor[x] function.]

For $p = q = 1$ and $r > 1$, the number of distinct states with energy $m\hbar\omega$ is given by

$$n_1(m,r) = [F(m/r) + 1][m + 1 - \tfrac{1}{2} r F(m/r)], \tag{5}$$

and for $r = 1$ and $p = q > 1$, the number of distinct states is given by

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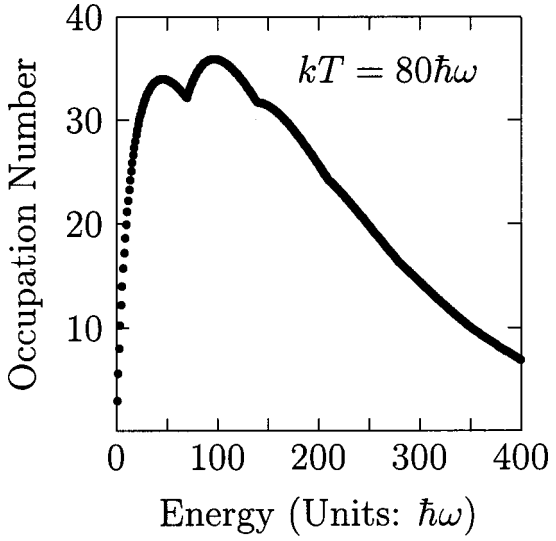

Fig. 1. The occupation numbers of single-particle states in an anisotropic harmonic oscillator potential for 10 000 particles. The particles are relatively strongly confined in the z direction; the energy of the single-particle states is given by $E=(j_x+j_y+70j_z)\hbar\omega$. The temperature is given by $kT=80\hbar\omega$, which is above the transition temperature.

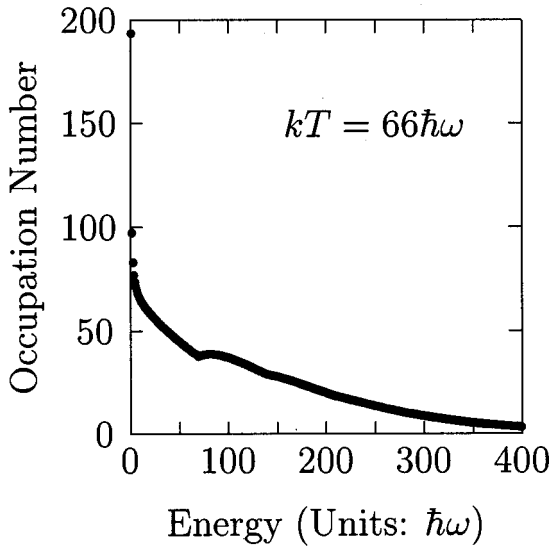

Fig. 2. The occupation numbers of single-particle states of an anisotropic harmonic oscillator potential for 10 000 particles, at the onset of Bose–Einstein condensation. The data are for the same confining potential illustrated in Fig. 1, but the temperature has been lowered to $kT=66\hbar\omega$. Note the relatively large occupation of the state with $E=0$.

$$n_2(m,p)=\tfrac{1}{2}[F(m/p)+1][F(m/p)+2]. \tag{6}$$

The functions n_1 or n_2 replace the factor $(m+1)(m+2)/2$ in the calculation of the normalization sum. A discussion of the derivation of these formulas is left to a footnote.[3]

It is easy to monitor several physical properties as the effective dimensionality of the system is changed by adjusting the integer multipliers, $\{p,q,r\}$. The examples presented in the figures are for the case in which the confinement along the z axis is "strong," leading to two-dimensional confinement in the $x-y$ plane (that is, $p=q=1$ and $r>1$). I illustrate the effect of the anisotropy on (i) the occupation numbers for temperatures above the effective condensation temperature, (ii) the value of the condensation temperature, and (iii) the value of the exponent parametrizing the ground state occupation number below the condensation temperature.

Figure 1 illustrates the occupation numbers for the states of the anisotropic oscillator trap with $p=q=1$ and $r=70$ at temperature given by $kT=80\hbar\omega$. This potential confines particles much more tightly along the z axis than in the plane perpendicular to this axis. The calculations assume that there are 10 000 particles in the trap. At this temperature the anisotropy of the trap is evident in the abrupt change in the occupation numbers at states with energies that are multiples of $70\hbar\omega$; at these energies the multiplicity of states changes as the range of accessible j_z quantum numbers changes. Bose–Einstein condensation has not yet occurred at this temperature. (For the conditions of Fig. 1, the value of the normalization constant is $C=1.341$. Inclusion of 2000 terms. in the normalization sum ensures that the states that are ignored have mean occupation numbers less than 10^{-6}.)

Figure 2 shows the occupation numbers for the same trapping potential as in Fig. 1, but at a slightly lower temperature given by $kT=66\hbar\omega$. The relatively large number of particles occupying the ground state is an indication of the onset of Bose–Einstein condensation. In the isotropic potential considered in Ref. 1 the onset of condensation occurs at a much lower temperature ($kT=19.3\hbar\omega$). (For the conditions of Fig. 2, $C=1.005\,17$, and as the temperature is reduced, C becomes even closer to 1.)

Calculations for an extremely anisotropic trap with $p=q=1$ and $r=1000$ show condensation of particles in the ground state at temperatures below $kT=78\hbar\omega$. In this case the particles are effectively confined to two dimensions. An approximation similar to that done in Appendix B of Ref. 1, but using the continuum density of states for a two-dimensional oscillator, $\epsilon d\epsilon/(\hbar\omega)^2$, gives an approximate transition temperature of $kT^*=\sqrt{6N/\pi^2}\hbar\omega$. For 10 000 par-

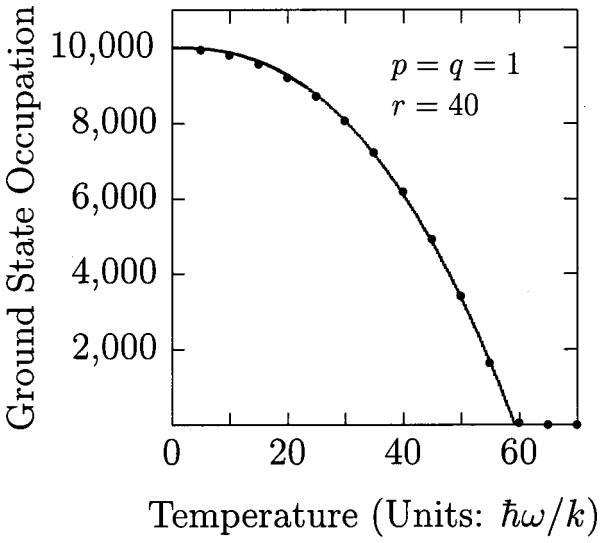

Fig. 3. The number of particles in the ground state of an anisotropic harmonic oscillator potential as a function of temperature. The points are the results of calculations for 10 000 particles in a potential with relatively strong confinement along the z axis; the energy of the single-particle states is given by $E=(j_x+j_y+40j_z)$. The curve is a fit of the data to the form of Eq. (7). The fit yields values of $kT^*=59.4\hbar\omega$ and $\nu=2.41$. These values lie between those predicted for two- and three-dimensional confinement.

ticles this approximation gives a transition temperature of $kT^*=77.97\hbar\omega$, in very good agreement with the numerical results.

Below the condensation temperature T^*, the fraction of particles occupying the ground state for several physical systems can be approximated with the functional form

$$\frac{N_0}{N_{\text{total}}}=1-\left(\frac{T}{T^*}\right)^{\nu}, \tag{7}$$

where the value of the parameter ν depends on the physical system. This works well for free particles in three dimensions ($\nu=1.5$), particles in an isotropic three-dimensional harmonic oscillator confining potential ($\nu=3$), and particles confined in a two-dimensional oscillator trap ($\nu=2$).[2] This functional form also gives a good approximation for the ground-state fraction for the anisotropic traps investigated in this Comment. Figure 3 shows a fit to a function with the form of Eq. (7) for 10 000 particles confined in a trap with $p=q=1$ and $r=40$. This trap is not anisotropic enough to be considered fully two dimensional, but the effects of the anisotropy are very evident in the observed transition temperature of $kT=59.4\hbar\omega$, and the exponent $\nu=2.41$. For 10 000 particles, all values of the parameter r (a measure of the strength of the confinement along the z axis) give very good fits to Eq. (7), with ν and T^* varying smoothly from the theoretical values for two and three dimensions.

Similar results can be obtained for potentials that strongly confine the particles to one dimension by changing the multiplicity factor from n_1, Eq. (5), to n_2, Eq. (6). It is also easy to study the heat capacity near the transition temperature as the effective dimensionality of the system changes. The results of this simple numerical technique agree well with analytical approximations which account for the finite number of particles and the anisotropy of the trap.[2]

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[3] Consider m units of energy $\hbar\omega$. For $p=q=1$ and $r>1$, these m units must be partitioned between the two "small"-energy modes (excitations along the x and y axes), and the "large"-energy mode (excitation along the z axis). There are $m+1$ ways to arrange the energy units with no energy in the large-energy mode, $m-r+1$ ways to arrange the energy units with one excitation of the large-energy mode, etc. The largest possible number of excitations in the large-energy mode is $F(m/r)$, so the multiplicity is $n_1=(m+1)+(m-r+1)+\cdots+(m-rF(m/r)+1)$. Summing the $F(m/r)+1$ terms in this expression gives Eq. (5). For $r=1$ and $p=q>1$, there is only one way to arrange the energy units with no excitation in the two large-energy modes, two ways to arrange the energy units with one excitation in a large-energy mode, three ways to arrange the energy with two excitations in large-energy mode, etc. The largest possible number of excitations in the large-energy modes is $F(m/p)$, so the multiplicity is $n_2=1+2+3+\cdots+(F(m/p)+1)$, which when summed gives Eq. (6).

Comment on "Space–time exchange invariance: Special relativity as a symmetry principle," by J. H. Field [Am. J. Phys. 69 (5), 569–575 (2001)]

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(Received 22 June 2001; accepted 13 September 2001)

[DOI: 10.1119/1.1417533]

A recent paper by Field[1] presents an interesting reformulation of special relativity based on the postulates of space–time exchange (STE) invariance and spatial homogeneity. It is shown that for the standard configuration of frames S and S' (in one dimension, for convenience) these postulates lead to the transformation[1]

$$x'=\gamma(v)(x-vt), \tag{1}$$

$$t'=\gamma(v)\left(t-\frac{vx}{V^2}\right), \tag{2}$$

where v is the velocity of S' relative to S, $\gamma(v)=(1-v^2/V^2)^{-1/2}$, and V is a universal parameter that remains to be determined. Equations (1) and (2) are known as the V^2-Lorentz transformation (V^2-LT) to distinguish them from the usual Lorentz transformation.[2]

The purpose of this comment is to suggest that a comparison of the STE symmetry approach with the derivation and discussion of the V^2-LT presented by Rindler[2] would also be helpful to students. The following could be noted.

(1) STE is defined as $x\leftrightarrow Vt$ and $x'\leftrightarrow Vt'$, where V is a parameter.[1] By contrast, the treatment in Ref. 2 is based on the relativity principle (RP) which uses the exchanges $x\leftrightarrow x'$, $t\leftrightarrow t'$, and $v\rightarrow -v$. Thus STE transforms Eqs. (1) and (2) into each other, whereas the exchange used in the RP transforms Eqs. (1) and (2) into their inverses.

(2) In STE, the parameter V and two of its properties (real and universal) enter at the beginning of the discussion. In the RP approach, the parameter V^2 is defined in terms of the unknown coefficient $\gamma(v)$ appearing in Eqs. (1) and (2) and

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