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BEC transition of a weakly interacting ultracold Bose gas in a linear quadrupolar trap

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We discuss the thermal gas to Bose-Einstein Condensation (BEC) transition of an ultracold Bose gas in a linear quadrupolar trap with contact interatomic interactions within the Hartree-Fock (HF) approximation. We briefly review the theoretical framework of the thermodynamics of a gas confined by a non-uniform potential to show how mechanical equilibria must be formulated in term of generalized volume and pressure variables $\mathcal{V}$ and $\mathcal{P}$ that replace the usual volume and hydrostatic pressure of a uniform system. We solve for the density profile within HF as a function of temperature T and molar volume $v = \mathcal{V}/N$. With this information, we are able to calculate all the thermodynamic properties of the system and analyze the behavior of the gas through the BEC (superfluid) transition. We find that the transition is completely smooth, showing no sign of critical behavior. We emphasize how these predictions can be readily measured with the current experimental setups.

Keywords: Bose-Einstein Condensation in confined systems; weakly interacting ultracold gases; phase transitions.

En este trabajo discutimos la transición de gas térmico a la Condensación de Bose-Einstein (BEC) de un gas de Bose ultrafrío confinado en una trampa cuadrupolar lineal, considerando interacciones atómicas de contacto dentro de la approximación de Hartree-Fock (HF). Revisamos brevemente el marco teórico de la termodinámica de un gas confinado por un potencial no uniforme para mostrar cómo debe formularse el equilibrio mecánico en términos de variables generalizadas de volumen y presión $\mathcal{V}$ and $\mathcal{P}$, que reemplazan el volumen usual y la presión hidrostática de un sistema uniforme. Calculamos el perfil de densidad dentro de la aproximación HF como función de la temperatura T y el volumen molar generalizado $v = \mathcal{V}/N$. Con esta información podemos calcular todas las propiedades termodinámicas del sistema y analizamos el comportamiento del gas a través de la transición BEC (superfluido). Hallamos que la transición es completamente suave y que no muestra signos de comportamiento crítico. Enfatizamos cómo estas predicciones pueden ser medidas con los dispositivos experimentales actuales.

Descriptores: Condensación de Bose-Einstein en sistemas confinados; gases ultrafríos débilmente interactuantes; transiciones de fase.

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1. Introduction

Since the experimental realization of Bose-Einstein condensation (BEC) in gases of alkaline atoms [1-3], the theoretical efforts to fully understand the nature of the transition and the condensate itself have kept a vigorous pace [4-8]. Although the basic phenomenon of BEC may be illustrated with an ideal gas, it became clear very early on that the interatomic interactions play a predominant role in determining both the qualitative and the quantitative properties of the ultracold gases, especially for temperatures below the transition [5]. It was also proven experimentally that below BEC the gas is certainly superfluid, among other signatures, by the creation of vortices after rotation of the samples [9,10]. This last property makes the inclusion of interatomic interactions an essential requirement for the correct description of the phenomenon at hand. At the same time, it has also been determined that the gas is, or can be [11,12], placed within a weakly interacting regime. Even at this level, however, the statistical mechanics of the many-body states remains unsolvable and one has to resort to approximated schemes such as those proposed long ago by Bogoliubov [13], Gross [14], Pitaevskii [15] and even to older but tractable methods such as Hartree-Fock approximations [7]. The present contribution is within this last approach. The HF approximation has the virtue that it allows for a full determination of the thermodynamics of the gas, from above the BEC transition all the way down to zero temperature. Although it is not considered the best theory for dealing with a superfluid at very low temperatures, due to the fact that the elementary excitation spectrum shows a gap [7,13], HF is still very useful since it does take into account interatomic interactions and, being a mean-field theory, should give rise to a correct qualitative picture of a phase transition [16,17].

The additional property of the current ultracold gas is its confinement by non-uniform magnetic or optical external potentials. As a result of this property, the confined gas becomes inhomogeneous as well. This adds an interesting and novel challenge to the description of these systems because most of the theoretical tools have been developed for uniform fluids confined by rigid-wall vessels. Since most of the inhomogeneities of the trapped gases have turned out to be on macroscopic length scales, contrary to microscopic non-uniformities due to interfaces at phase coexistence states [17], schemes such as the local density approximation [18-20] have been very useful in extending uniform-gas calculations to inhomogeneous ones [5,7]. Nevertheless, this is not enough to describe the thermodynamic behavior of non-uniform systems. The main problem is that the mechanical properties of a uniform system, namely, the volume occupied by the gas and its hydrostatic pressure, cease to be thermodynamic variables for an inhomogeneous fluid confined by a non-uniform trap. The volume is not a variable since the volume of a trapped gas is unbounded and depends on the temperature. The hydrostatic pressure is at best a local quantity and, therefore, cannot describe the equilibrium state of the gas as a whole. This should not be surprising since volume and pressure are consequences of having rigid walls as a confinement. When the confinement is produced by a non-uniform external field $V_{ext}(\vec{r})$, this gives rise to its own equivalent mechanical variables "volume" and "pressure". This is the viewpoint that we have been advocating recently [21-27]: the usual volume and pressure are replaced by a generalized extensive volume $\mathcal{V}$ and a generalized intensive pressure $\mathcal{P}$, a unique pair for each external potential. The generalized volume turns out to be proportional to the mean volume that the gas occupies, and the generalized pressure is related to the mechanical equilibrium condition of the fluid (*i.e.* Pascal Law) in the same way as the hydrostatic pressure in a uniform fluid [21-24]. The underlying physics beneath the identification of these variables is the appropriate thermodynamic limit for each external potential. That is, for an external potential to confine a macroscopic number of particles, the potential itself must also be "macroscopic", which means that its energy level spacing should be much smaller than any excitation of the atoms or of the fluid, and certainly of the temperature.

The introduction of generalized volume and pressure not only yields the formal framework for describing non-uniform fluids, but it also serves as a powerful computational tool. This is due to a remarkable relationship between the generalized pressure and the inhomogenous particle density (or simply, density profile). That is, if knowledge is available of the characteristics of the trap (*i.e.* of the generalized volume), of the temperature of the gas and of its density profile, then the generalized pressure can be readily calculated. We recall that, precisely, it is the density profile that is mostly measured in the current experiments of ultracold gases [1-3,5,6]. Thus, direct measurement of the thermodynamics of these gases appears to be a realistic operation [25-27].

In the present article, making use of the generalized mechanical variables and the above considerations, we address the problem of an ultracold Bose gas confined by a linear quadrupolar trap [25], treating the interatomic interactions within a Hartree-Fock approximation [5,7,16]. We are able to calculate the full thermodynamics of the gas near and below the BEC (superfluid) transition. Among other properties, we focus our attention on results for the equation of state, heat capacity and the isothermal compressibility. Although HF is a mean-field scheme, and therefore, its predictions may fail near a second-order or critical phase transition, one expects in any case that it should show qualitatively correct behavior with precursors of the real features of the transition [28,29]. Our HF calculation show that the transition is completely smooth, showing no sign of being a critical second-order phase transition, as one could have expected from calculations in the ideal non-interacting case [8].

We proceed as follows. In the next section we briefly discuss the introduction of the generalized volume and pressure for a linear quadrupolar potential and the way they can be calculated. In Sec. 3 we present the Hartree-Fock calculation of the density profile for different thermodynamic conditions and show numerical results concerning different thermodynamic properties across the BEC transition. A section with Final Remarks concludes the paper.

2. Generalized volume and pressure for a linear quadrupolar potential

We consider N identical Bose atoms of mass m, with spin $s = 0$ or fully polarized in a given spin state [1-3], pairwise interacting and confined by an anisotropic linear quadrupolar potential,

$$H_N = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j} u(|r_{ij}|) + \sum_{i=1}^{N} |\vec{A} \cdot \vec{r}_i|. \tag{1}$$

The interatomic potential $u(|r_i - r_j|)$ shall be considered as a contact potential below.

As is well understood, the confinement by a non-uniform potential yields an inhomogeneous fluid. Under such general conditions, and as has been shown [21,23,24], the hydrostatic pressure and volume cease to be thermodynamic variables and these are replaced by the so-called generalized pressure and volume. To see how these arise, one may deal first with an ideal *classical* gas, *i.e.* $u(|r_i - r_j|) \equiv 0$. The canonical partition function is given by

$$Z(T, N, \mathcal{V}) = \frac{1}{N! \lambda_T^{3N}} \left(\zeta(T) \mathcal{V} \right)^N , \tag{2}$$

where $\lambda_T = h/(2\pi mkT)^{1/2}$ is the de Broglie thermal wavelength,

$$\mathcal{V} = \frac{1}{A_x A_y A_z} \tag{3}$$

is the generalized volume, and the function $\zeta(\beta)$ is defined by

$$\zeta(T)\mathcal{V} = \int e^{-\beta V_{ext}(\vec{r})} \, d^3r = 8\pi (kT)^3 \frac{1}{A_x A_y A_z}. \tag{4}$$

Helmholtz free energy is found with $F = -kT \ln Z$ and, after taking the limit $N \to \infty$, yields

$$F(N, T, \mathcal{V}) = -NkT \left(\ln \left[\frac{\mathcal{V}\zeta(T)}{N\lambda_T^3} \right] + 1 \right). \tag{5}$$

For the free energy per particle, F/N, to remain finite in the thermodynamic limit, $N \to \infty$, it is necessary that the "generalized" volume diverge, *i.e.* $\mathcal{V} \to \infty$, keeping the "density" $N/\mathcal{V}$ constant. We are assuming that not only can $\mathcal{V} = 1/A_x A_y A_z$ become arbitrarily large, but that each $A_i \to 0$ separately; that is, we are considering the trapped gas as macroscopic in the three spatial directions. The introduction of $\mathcal{V}$ as a *bona-fide* extensive thermodynamic variable result can be fully justified for an interacting system, classical or quantal [21,23,24] such that there exist an *intensive* conjugate variable to $\mathcal{V}$, called the generalized pressure, and given by

$$\mathcal{P} = -\left(\frac{\partial F}{\partial \mathcal{V}}\right)_{N,T}. \tag{6}$$

Here, $F = F(N, T, \mathcal{V})$ is Helmholtz free energy including interatomic interactions. By a simple calculation, one obtains that this quantity is related to the local particle density, or density profile $\rho(\vec{r})$, as

$$\begin{aligned}\mathcal{P} &= \frac{1}{3\mathcal{V}}\left\langle \sum_{i=1}^{N} \vec{r}_i \cdot \nabla_i |\vec{A}\cdot\vec{r}_i| \right\rangle \\ &= \frac{1}{3\mathcal{V}}\int \rho(\vec{r})\, \vec{r}\cdot\nabla|\vec{A}\cdot\vec{r}|\, d^3r,\end{aligned} \tag{7}$$

where the averages are performed in the corresponding ensemble. The last equality is one of our principal tools for calculating the thermodynamic properties of the system since it gives a direct way to calculate the generalized pressure with the sole knowledge of the external potential $V_{ext}(\vec{r}) = |\vec{A}\cdot\vec{r}|$, the density profile $\rho(\vec{r})$ and the temperature T. That is, the equation of state $\mathcal{P} = \mathcal{P}(\mathcal{V}/N, T)$ is a direct measurable quantity if knowledge of the density profile and temperature is available.

As has been shown before [21,23,24], the identification of the generalized pressure is not only a formal one but it also has a clear physical meaning: $\mathcal{P}$ for a non-uniform fluid confined by a given external potential plays the same thermodynamic role as the hydrostatic pressure p in a uniform fluid, since it is the quantity that bears the information that the fluid is in mechanical equilibrium.

We note that, with the above identification, the change in free energy is

$$dF = -SdT - \mathcal{P}d\mathcal{V} + \mu dN \tag{8}$$

with S the entropy and μ the chemical potential. As we shall see below, since the Hartree-Fock approximation, together with Ec. (7), yield $\mathcal{P} = \mathcal{P}(\mathcal{V}/N, T)$ and $\mu = \mu(\mathcal{V}/N, T)$, the free energy $F \equiv Nf(\mathcal{V}/N, T)$ can be reconstructed and, therefore, all the thermodynamic information becomes available.

3. Thermodynamics and BEC (superfluid) transition

We now turn our attention to the calculation of the thermodynamics of a weakly interacting Bose gas confined in a linear quadrupolar potential, $V_{ext}(\vec{r}) = |\vec{A}\cdot\vec{r}|$, within the Hartree-Fock approximation [5,7,16]. The Hamiltonian of the system is best described in its second quantized version,

$$H = \sum_n \epsilon_n a_n^\dagger a_n + U {\sum_{jklm}}' a_j^\dagger a_k^\dagger a_l a_m \tag{9}$$

where n and ϵ_n stand for the eigenstates and eigenvalues of the three-dimensional one-particle Hamiltonian in the presence of the external linear quadrupolar potential, $h_0 = \vec{p}^2/2m + |\vec{A}\cdot\vec{r}|$, and $a_n^\dagger$ and a_n are creation and annihilation operators. The "prime" in the second sum refers to the restrictions introduced by assuming an isotropic two-body potential. The coupling parameter is $U = 4\pi\hbar^2 a/m$, with m the atom mass and a the scattering length, assumed throughout to be positive [5].

The Hartree-Fock approximation is a self-consistent procedure that yields the density profiles of the thermal and the condensate densities, $\rho_{th}(\vec{r})$ and $\rho_0(\vec{r})$, in the form of the following set of equations [7,16]:

$$\begin{aligned}\rho_{th}(\vec{r}) = \frac{1}{\lambda_T^3} g_{3/2}\Bigg(\beta\Big[\mu - |\vec{A}\cdot\vec{r}| \\ - 2U\rho_{th}(\vec{r}) - 2U\rho_0(\vec{r})\Big]\Bigg)\end{aligned} \tag{10}$$

and

$$\rho_0(\vec{r}) = \frac{1}{U}\left(\mu - |\vec{A}\cdot\vec{r}| - 2U\rho_{th}(\vec{r})\right), \tag{11}$$

with the constraint that the number of particles is a given value N,

$$N = \int \rho_{th}(\vec{r})\, d^3r + \int \rho_0(\vec{r})\, d^3r. \tag{12}$$

In Eq. (10), $g_{3/2}(\alpha)$ is the usual Bose function $g_n(\alpha)$ for $n = 3/2$,

$$g_n(\alpha) = \frac{1}{n!}\int_0^\infty \frac{x^{n-1}dx}{e^{x-\alpha} - 1}. \tag{13}$$

The above equations have been derived within the local density approximation [18-20,24], which, in turn, is valid strictly in the thermodynamic limit, $N \to \infty$, $\mathcal{V} \to \infty$ with $N/\mathcal{V} =$ const. Therefore, its applicability to real systems should be restricted to those with a large number of particles, say $N \sim 10^6$ or larger; for smaller systems, finite size corrections may be required.

Note that Eq. (11) is to be understood to be valid for values when the right-hand-side is positive or zero. As a matter of fact, this is how the thermal to Bose-Einstein condensation (BEC) or superfluid transition is identified, *i.e.* given the temperature T, the transition occurs for the value of the chemical potential below which the condensate density $\rho_0(\vec{r})$ is different from zero. Equation (11) is the Gross-Pitaevskii equation in the thermodynamic limit where the kinetic energy term may be safely neglected. HF solutions do show superfluid behavior in the sense that the spectrum of the elementary excitations presents a density-dependent energy gap [7]. This, however, is known to be an incorrect dependence since at very low temperatures a superfluid should have gapless phonon-like Bogoliubov excitations [5,13]. Nevertheless, HF should be qualitatively correct for temperatures near the transition [16] since mean-field theories are known to correctly predict the order of the transition [17].

The solution to the above set of equations yields the density profile $\rho(\vec{r}) = \rho_0(\vec{r}) + \rho_{th}(\vec{r})$ and the chemical potential μ for given values of the temperature T and the generalized volume $v = \mathcal{V}/N$. Figure 1 shows typical density profiles above and below the transition. Knowing the profile, the value of the generalized pressure $\mathcal{P}(v, T)$ is found from Eq. (7) and, together with $\mu(v, T)$, one can further find the molar Helmholtz potential $f = F/N$ as $f(v, T) = -\mathcal{P}v + \mu$. From the free energy $f(v, T)$, all thermodynamic properties follow. The molar entropy is $s = (\partial f/\partial T)_v$ and, therefore, the specific heat is $c_v = T(\partial s/\partial T)_v$. From the generalized pressure, one can calculate the corresponding isothermal compressibility, $\kappa_T = -1/v(\partial\mathcal{P}/\partial v)_T$. The internal energy may be calculated with $e(v, T) = f(v, T) + Ts(v, T)$. Our results are summarized in Figs. 2 to 7. Note that we use units with $\hbar = 1$, $m = 1$ and $a = 1$. Therefore, lengths should be multiplied by a to get their actual value, energies by $\hbar^2/ma^2$, etc. It is interesting to note that, since the theory has only three "free" parameters, namely, $\hbar$, m and a, the predictions are "universal" for all bosonic gases within the weak interaction limit, since this reduces all the interatomic interactions to a single paramenter, the (positive) scattering length.

In all the figures we compare with the properties of an ideal gas, which can all be computed since the grand potential is exactly given by

$$\Omega(\mathcal{V}, T, \mu) = -8\pi\mathcal{V}kT\left(\frac{kT}{\lambda_T}\right)^3 g_{9/2}(\mu/kT), \tag{14}$$

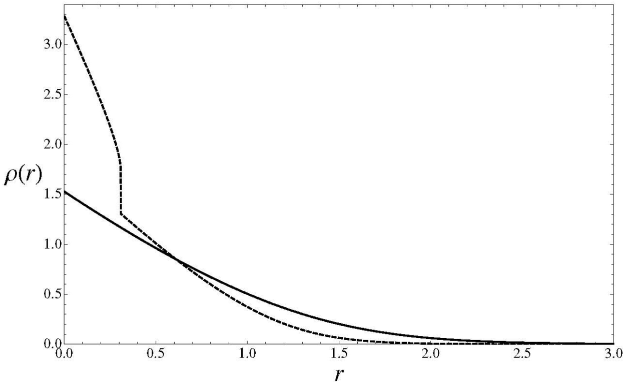

FIGURE 1. Typical density profiles $\rho(r)$ vs. r of a weakly interacting Bose gas confined by a linear quadrupolar potential in the HF approximation. Both belong to the same isochore $v = \mathcal{V}/N = 0.1$ but for two different temperatures. The solid line corresponds to a state with a temperature above the transition BEC (superfluid) temperature T_c^{HF} and the dotted for a temperature below it. Units are $\hbar = 1$, $m = 1$ and $a = 1$.

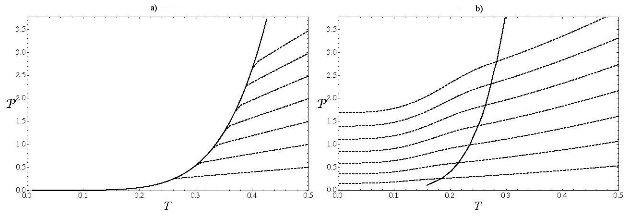

FIGURE 2. Phase diagram $\mathcal{P}-T$, (A) ideal non-interacting gas, (B) HF interacting gas. Several isochores ($\mathcal{V}/N =$ constant) are shown in dotted lines. The solid line shows the thermal gas to BEC transition. Note that the ideal transition temperature T_c^{id} is higher than the HF temperature T_c^{HF}, for a given isochore. Units are $\hbar = 1$, $m = 1$ and $a = 1$.

where $g_{9/2}(\mu/kT)$ is obtained from Eq.(13) with $n = 9/2$.

Figure 2 shows a few isochores ($v =$ const) of the equation of state $\mathcal{P}(v, T)$ comparing the ideal case, Fig. 2a, with the interacting Hartree-Fock approximation, Fig. 2b. We emphasize the following points. First, in the ideal case, the transition BEC line indicates that the pressure vanishes as $T \rightarrow 0$. That is, just as in the uniform case, the condensate exerts no pressure [30]. This is clearly changed once interactions are included: the pressure of the condensate is no longer zero, and even at $T = 0$, the interactions give rise to a remnant pressure. Second, the transition temperature, different for each isochore, is shifted down in the interacting case with respect to the ideal one. This downshift is in agreement with known results of more general theories for trapped gases [8]. Moreover, this effect is due to the interactions only and not related to finite size effects [5,31]. And, lastly, the transition line in the interacting case, as shall be further described below, marks a smooth thermal gas to superfluid transition, different from the ideal BEC transition, where discontinuities in the second derivatives of the free energy are encountered; in the interacting case, up to second derivatives – and it appears that at higher orders as well – the free energy is continuous.

Figures 3 and 4 show the entropy and the specific heat, both for the ideal and HF cases, as a function of temperature for a given isochore. In these and in all the subsequent figures, the isochore is $v = \mathcal{V}/N = 0.1$ and the transition temperatures are $T_c^{id} \approx 0.436$ for the ideal case and $T_c^{HF} \approx 0.306$ for HF, with units $\hbar = 1$, $m = 1$ and $a = 1$, showing the mentioned downshift. The transition temperatures are marked with an arrow. Perhaps the most interesting property of the specific heat in the HF approximation, Fig. 4, is that the transition temperature occurs at a (local) *minimum* rather than at a maximum, as is usually expected from the behavior of the ideal case and critical transitions [29]. From the behavior of the HF entropy and specific heat at BEC, one finds that the BEC (superfluid) transition is fully continuous. Thus, it shows signs of being neither a first-order nor a critical transition.

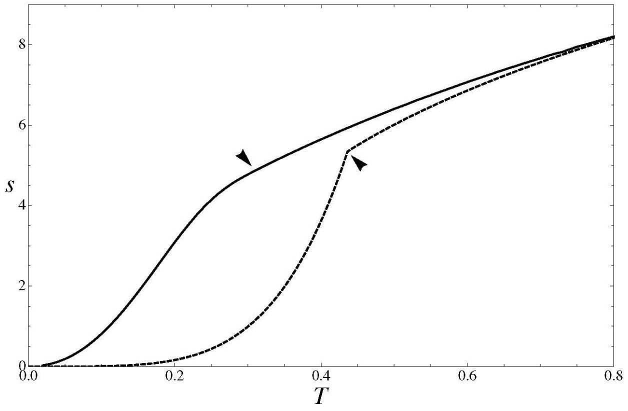

FIGURE 3. Molar entropy $s = S/N$ vs. temperature T for the isochore $v = 0.1$. The dotted line is the ideal non-interacting gas, the solid line the HF interacting gas. The BEC transition temperatures are marked with arrows, $T_c^{id} \approx 0.436$, $T_c^{HF} \approx 0.306$. See text for details. Units are $\hbar = 1$, $m = 1$ and $a = 1$.

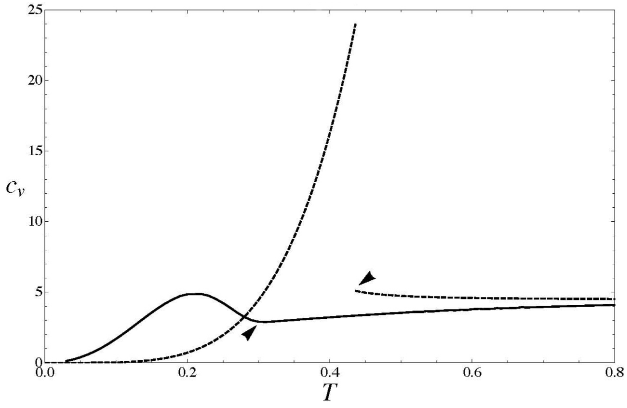

FIGURE 4. Specific heat at constant generalized (molar) volume c_v vs. temperature T for the isochore $v = 0.1$. The dotted line is the ideal non-interacting gas, the solid line the HF interacting gas. The BEC transition temperatures are marked with arrows, $T_c^{id} \approx 0.436$, $T_c^{HF} \approx 0.306$. Note that in the latter case, the transition does not occur at the maximum value of c_v but at a local *minimum*. See text for details. Units are $\hbar = 1$, $m = 1$ and $a = 1$.

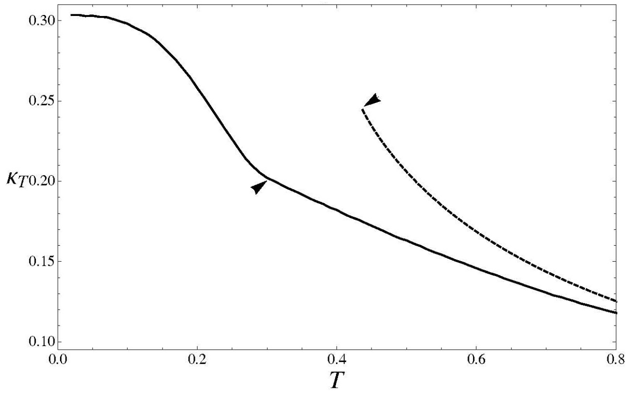

FIGURE 5. Isothermal compressibility κ_T vs. temperature T for the isochore $v = 0.1$. The dotted line is the ideal non-interacting gas, the solid line the HF interacting gas. The BEC transition temperatures are marked with arrows, $T_c^{id} \approx 0.436$, $T_c^{HF} \approx 0.306$. The ideal isothermal compressibility is not defined below T_c^{id}. See text for details. Units are $\hbar = 1$, $m = 1$ and $a = 1$.

Additional information on the nature of the transition is given by the isothermal compressibility κ_T, shown in Fig. 5 for the same isochore as above. We note first that the ideal κ_T is only shown for temperatures above T_c^{id}, and we next explain the underlying reason.

The ideal isothermal compressibility for the quadrupolar trapped gas, just as in the uniform case, is not defined below T_c^{id} since $(\partial \mathcal{P}/\partial v)_T = 0$. In the uniform case, this is usually considered to be a divergence of the isothermal compressibility below T_c^{id}, in apparent agreement with the anomalous behavior of the density fluctuations found at those temperatures; see Ref. 8 for a detailed discussion of this point. This behavior can be contrasted with that of an ideal gas in a harmonic trap below T_c^{id}, where the density fluctuations are found to be normal [32]. However, one can analyze the generalized pressure for the ideal gas in a harmonic trap [23] and find again that $(\partial \mathcal{P}/\partial v)_T = 0$ for $T < T_c^{id}$, where $\mathcal{V} = 1/\omega^3$ for an isotropic harmonic trap. In the present article we also find that the generalized pressure obeys $(\partial \mathcal{P}/\partial v)_T = 0$ below T_c^{id}. Therefore, based on the criterion of the divergence of the compressibilty, one could conclude that trapped ideal gases are also unstable below BEC, in contradiction with the mentioned stability results based on density fluctuations [8-32]. As we discuss below, there is really not a contradiction.

The minor point is that *below* BEC in an ideal 3D gas, the isothermal compressibility is no longer related to the density fluctuations. Such an expected and commonly used relationship arises from the fact that the entropy of a pure system, determined by the variables $(E, \mathcal{V}, N)$, is a concave function of two independent variables only; that is, since the entropy is an extensive quantity, it is of the form $S(E, \mathcal{V}, N) = N s(E/N, \mathcal{V}/N)$ with E/N and $\mathcal{V}/N$ the independent variables. The concavity of $s(E/N, \mathcal{V}/N)$ implies two stability conditions, the positivity of the specific heat and of the isothermal compressibility [33]. Now, below T_c^{id}, since the chemical potential remains constant, the number of particles is no longer an *independent* variable; rather, its value is determined by the equilibrium condition for given $\mathcal{V}$ and T, *i.e.* $N_{NC} = N_{NC}(\mathcal{V}, T)$ with N_{NC} the number of "thermal" particles not in the condensate. Thus, below T_c, the entropy depends on one independent variable only, say $S(E, \mathcal{V}) = \mathcal{V} s(E/\mathcal{V})$ with $E/\mathcal{V}$ the independent variable. Hence, the concavity of $s(E/\mathcal{V})$ has as a unique stability implication that the specific heat must be positive; there is no condition on the isothermal compressibility anymore. Therefore, the expression $(\partial \mathcal{P}/\partial v)_T = 0$ below T_c simply indicates that the (generalized) pressure depends on T but not on v; it bears no longer any relationship to the fluctuations of the density nor to the stability of the equilibrium state.

Returning to Fig. 5 for the HF case, one finds that all the previous discussion becomes irrelevant in the sense that the interatomic interactions smooth out any difficulty, and the isothermal compressibility becomes continuous at the transition and remains finite all the way down to $T = 0$. The fact that the compressibility continues to be defined below T_c^{HF}, in contrast to the ideal case, is due to the thermodynamic behavior of the chemical potential, shown in Fig. 6, where we find that it never becomes constant, such as in the ideal case. What is notorious in both figures, again, is the fact that the transition appears completely smooth, showing no sign of any "expected" type of phase transition, although indeed, there is a phase transition from a thermal gas to a BEC-superfluid gas.

We certainly understand that HF is a mean-field calculation and, as mentioned above, not the best description of a superfluid. However, mean-field theories typically yield incorrect quantitative results but do not change the order of the transition, as one learns from Landau-like theories [29]. The origin of the continuity of all the thermodynamic properties may be traced back to the emergence of the condensate fraction. This is exemplified in Fig. 7 where we compare the condensate fraction N_0/N of the ideal with the interacting case. Below T_c^{id}, the ideal condensate fraction is $N_0/N = 1 - (T/T_c^{id})^{9/2}$. Above T_c^{id}, $N_0/N = 0$. Thus, the transition in the ideal case has a discontinuity in the derivative. However, for the interacting HF case, as shown in Fig. 7, it appears that this transition is completely smooth, with no discontinuity or singularity at all. That is, the superfluid phase emerges smoothly from zero.

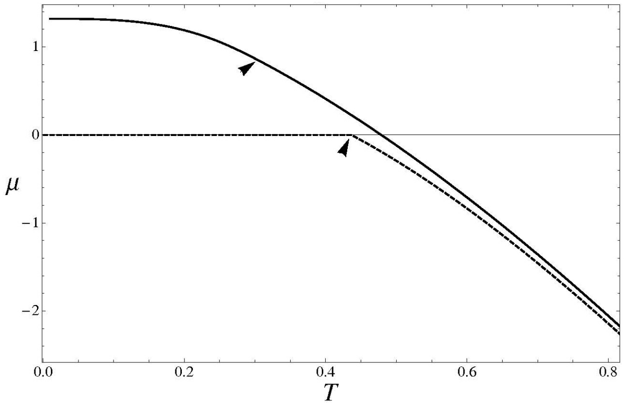

FIGURE 6. Chemical potential μ vs. temperature T for the isochore $v = 0.1$. The dotted line is the ideal non-interacting gas, the solid line the HF interacting gas. The BEC transition temperatures are marked with arrows, $T_c^{id} \approx 0.436$, $T_c^{HF} \approx 0.306$. Note that below T_c^{id}, the ideal chemical potential remains constant. See text for details. Units are $\hbar = 1$, $m = 1$ and $a = 1$.

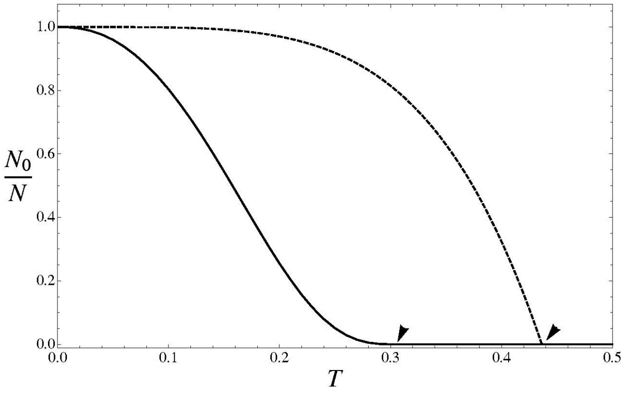

FIGURE 7. Condensate fraction N_0/N vs. temperature T for the isochore $v = 0.1$. the dotted line is the ideal non-interacting gas, the solid line the HF interacting gas. The BEC transition temperatures are marked with arrows, $T_c^{id} \approx 0.436$, $T_c^{HF} \approx 0.306$. Note that the derivative of the interacting HF curve is continuous at the transition. See text for details. Units are $\hbar = 1$, $m = 1$ and $a = 1$.

4. Final remarks

We have analyzed the thermodynamics and the BEC transition of a weakly interacting Bose gas confined by a linear quadrupolar potential $V_{ext}(\vec{r}) = |\vec{A} \cdot \vec{r}|$, in the Hartree-Fock approximation. To achieve this, we have made use of the proper mechanical thermodynamic variables, the generalized volume $\mathcal{V} = 1/A_x A_y A_z$, and its conjugate pressure $\mathcal{P}$. We emphasize that the latter can be calculated if knowledge of the density profile $\rho(\vec{r})$ is available. The HF approximation allows us to self-consistently find such a density profile together with the chemical potential μ in terms of given values of the temperature T and the molar volume $v = \mathcal{V}/N$. It is a simple exercise to show that all thermodynamics follows with this wealth of information.

We have focused our attention on the BEC (superfluid) transition that a Bose gas undergoes at low temperatures. From the equation of state $\mathcal{P} = \mathcal{P}(v, T)$ one finds that below the HF transition temperature $T < T_c^{HF}$, the condensate exerts pressure due to the interatomic interactions, in contrast to the ideal gas, where the condensate is thermodynamically inert. Further, for a given value of the volume v, $T_c^{HF} < T_c^{id}$, in agreement with general results on interacting gases [8]. The behavior of the entropy, heat capacity, chemical potential and isothermal compressibility indicate that the transition in the interacting HF case is completely smooth. We have mentioned that this is neither a common first-order nor a critical second-order phase transition. Moreover, the smoothness of the isothermal compressibility across the transition, see Fig. 5, indicates that there are no large fluctuations near the transition.

Since HF is a mean-field treatment, one may be inclined to suggest that the theory is not suitable for capturing critical behavior. However, we are puzzled by the clear result that, while the fluctuations may not be correctly accounted for, there is no evidence of a critical transition. We base this statement on the experience with Landau-like theories where mean-field may not be correct but it does not alter the order of the transition. This fact encourages us to improve our calculation, first, by including the proper role and statistical description of Bogoliubov modes [34], say, through the Popov approximation [5,7] and, next, by developing an analysis near the transition using the proper mechanical variables here used to search for evidence of critical behavior. On the other hand, however, if we believe in the HF results found here, namely, that the transition is smooth but not critical, this may indicate a kind of first-order transition without the possibility of phase separation. This does not appear to contradict well-known results from superfluidity behavior in ^{4}He [35] since the analysis of the transition discussed here should be valid for transitions, at very low temperatures, from the thermal gas phase to the superfluid phase; that is, very far from the critical λ-point and from the transition from superfluid to normal liquid. This study deserves much further research.

We finish our report by recalling that the measurement of the thermodynamic properties of these gases can be readily accomplished with the current experimental setups [25-27]. Hence, one should be able to test the behavior of the heat capacity and the isothermal compressibility found in this paper. We recall that the equation of state essentially requires knowledge of the trap, the temperature and the density profile, see Eq. (7). Incipient measurements have been performed and are under progress, see Ref. 25 for experimental details of the present quadrupolar trap. Certainly, below BEC, Majorana losses of particles at the center of the trap can occur [2] since in that region the external potential becomes zero. However, this may be avoided by slightly altering the potential around its center, making it different from zero [36], without substantially changing the overall form of the potential. Once the equation of state is found, the isothermal compressibility follows. As we have indicated before [24], the heat capacity can also be measured. The proposal is an adiabatic expansion or compression, namely a slow change of the confining potential parameters. After, say, an adiabatic expansion, $\Delta\mathcal{V} > 0$, the gas must cool down, $\Delta T < 0$. By measuring the ratio $\Delta\mathcal{V}/\Delta T$ and using the following identity, the molar specific heat can be obtained:

$$c_v = -T \left(\frac{\partial \mathcal{P}}{\partial T}\right)_v \left(\frac{\partial v}{\partial T}\right)_s , \qquad (15)$$

where knowledge of the equation of state is needed to evaluate the second factor on the right-hand side.

To conclude, we emphasize that the present analysis shows that the use of the appropriate mechanical variables is a useful and complementary tool for exploring and learning about the physics of gases confined by non-uniform traps.

Acknowledgments

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