Measuring the heat capacity in a Bose-Einstein condensation using global variables

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Phase transitions are well understood and generally followed by the behavior of the associated thermodynamic quantities, such as in the case of the λ-point superfluid transition of liquid He, which is observed in its heat capacity. In the case of a trapped Bose-Einstein condensate, the heat capacity cannot be directly measured. In this work, we present a technique capable of determining the global heat capacity from the density distribution of a weakly interacting gas trapped in an inhomogeneous potential. This approach represents an alternative to models based on the local density approximation. By defining a pair of global conjugate variables, we determine the total internal energy and its temperature derivative, the heat capacity. We then apply the technique to a trapped ^{87}Rb BEC, and a λ-type transition dependent on the atom number is observed, and the deviations from the noninteracting, ideal gas case are discussed. Finally, we discuss the chances of using this method to study the heat capacity at $T \to 0$.

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I. INTRODUCTION

The heat capacity is one of the fundamental quantities containing information about the nature of a given phase transition. The remarkable discontinuity in the heat capacity near the superfluid transition (λ point), observed in liquid He, was considered one of the most important properties to be well understood, and the quest to understand it brought theoretical proof that Bose-Einstein condensation (BEC) does take place in a liquid such as the superfluid He, please see Refs. [1,2], and the references therein.

Even before the experimental observation of a BEC in trapped dilute gases [3–5], predictions of the heat capacity in such systems were made [6], and soon after its realization a measurement was performed by means of the kinetic energy of the expanded cloud [7]. In the two last decades there were many theoretical papers discussing this topic [8–12], but quite few experimental studies have investigated the heat capacity behavior in trapped gases. The lack of reliable methods to measure the total internal energy of these ultracold samples explain such discrepancy. Recently, the interest in heat capacity measurements has come back, motivated by the characterization of quantum degenerate gases at the unitary limit, where a strong correlated system is studied [13]. The understanding of the behavior of a strong interacting ensembles of quantum particles is a real challenge to the modern physics [14,15].

The majority of the heat capacity measurements made in trapped quantum degenerate gases have relied on local density approximation (LDA) [13,16] theoretical models. However, LDA is not valid when the correlation length is comparable to the cloud typical sizes. In particular, in a standard BEC at the critical temperature, there exists a finite shell, centered at the critical points, within which LDA fails as discussed in Ref. [17]. In addition, LDA is not valid when there are topological defects, such as vortices and vortex tangles, closely spaced and spread over the cloud [18].

In this paper we introduce a technique to measure the global heat capacity at "constant volume," $C_{\mathcal{V}}$. We have applied this newly developed approach, based on global thermodynamic variables [19,20], instead of LDA. The technique was used to measure $C_{\mathcal{V}}$ across the BEC transition of a ^{87}Rb BEC confined in a harmonic magnetic trap. We start by presenting the theoretical background of our method, followed by a short description of the experimental setup, and finally we present and discuss the main results.

II. GLOBAL VARIABLE ANALYSIS AND HEAT CAPACITY

In a recent publication [21], we studied the BEC transition in a harmonically trapped ^{87}Rb sample in terms of the new global thermodynamic parameters introduced in Refs. [19,20]. We built a phase diagram split in two domain regions: (i) a pure thermal gas; and (ii) a mixture of condensate and thermal fractions. By considering a collection of global variables $(N,T,\mathcal{V})$, where $\mathcal{V} = 1/\omega^3$ is defined as the *volume parameter*, and $\omega = (\omega_x\omega_y\omega_z)^{\frac{1}{3}}$ is the geometric mean of the trapping frequencies, we defined $\Pi(N,T,\mathcal{V})$ as the *pressure parameter*, which corresponds to the hydrostatic pressure of the system. In fact, Π is the conjugate variable to $\mathcal{V}$, i.e.,

$$\Pi = -\left(\frac{\partial F}{\partial \mathcal{V}}\right)_{N,T} \tag{1}$$

for the Helmholtz free energy $F = F(N,T,\mathcal{V})$. In this context, Π is obtained as [19,20]

$$\Pi = \frac{2}{3\mathcal{V}}\int n(\vec{r})\,\frac{1}{2}m(\vec{\omega}\cdot\vec{r})^2\,d^3r, \tag{2}$$

which can be determined by knowing the number density distribution $n(\vec{r})$ and the confining harmonic frequencies $\omega = (\omega_x\omega_y\omega_z)^{\frac{1}{3}}$. It is important to stress that Eq. (2) is valid in the thermodynamic limit $N \to \infty$ and $\mathcal{V} \to \infty$ $(\omega \to 0)$, which means that (i) finite number effects are not taken into

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account, and (ii) $\hbar\omega$ must be much smaller than any other energy scale. Also it is worth noting that Eq. (2) is written for a harmonic trapping potential, but the method is general and may be applied to an arbitrary shaped trap potential [20].

As a function of the global extensive parameter $\mathcal{V}$ and its intensive conjugate Π, one can show that the internal energy of a harmonically trapped thermal cloud and pure BEC are, respectively [22], $U_{\text{th}} = 3\Pi\mathcal{V}$ and $U_0 = \frac{5}{2}\Pi\mathcal{V}$. These expressions can be found starting from the virial theorem. The first is the expected result for a noninteracting gas held in a three-dimensional (3D) harmonic oscillator potential. And the second results from a contact interaction potential combined with the Thomas-Fermi approximation. Therefore it is valid to separate the thermal and condensed fractions to determine the total internal energy

$$U = 3\Pi_{\text{th}}\mathcal{V} + \tfrac{5}{2}\Pi_0\mathcal{V} = 3\Pi\mathcal{V} - \tfrac{1}{2}\Pi_0\mathcal{V}, \tag{3}$$

where the total *pressure parameter* is also considered as the sum of the two components $\Pi = \Pi_{\text{th}} + \Pi_0$. Then the heat capacity, at constant *volume parameter*, can be written as $C_{\mathcal{V}} = (\frac{\partial U}{\partial T})_{N,\mathcal{V}}$. By assuming $\frac{\partial \Pi_0}{\partial T} \ll \frac{\partial \Pi}{\partial T}$, the last term in Eq. (3) can be neglected. In fact, this assumption is in very good agreement with our experimental data where $|\frac{\partial \Pi_0}{\partial T}/\frac{\partial \Pi}{\partial T}| < 0.1$ even at the lowest temperature values of $T/T_c \approx 0.1$. Therefore, we finally find that a good approximation is given by

$$C_{\mathcal{V}} = \frac{3}{\omega^3}\left(\frac{\partial \Pi}{\partial T}\right)_{N,\omega}, \tag{4}$$

meaning that the heat capacity can be directly determined by measuring the equation of state $\Pi(N/\mathcal{V},T)$ as shown in Ref. [21].

Soon after the production of the first experimental BEC by the JILA group, an attempt to map the heat capacity was carried out, taking into account the balance between the internal energy and the kinetic energy released during the free fall [7]. In that paper, the overall scaled energy per particle is obtained as a function of the temperature. Above the critical temperature the linearity of the energy with temperature indicates the Maxwell-Boltzmann classical limit. The data around the critical temperature suggest a change in the energy balance, indicating a jump in the heat capacity. The value extracted from the data is lower than that expected for an ideal gas, but in good agreement with that predicted by a finite number corrected, ideal gas theory [8].

From the theoretical point of view, the heat capacity near the phase transition has been derived using different approaches [8–11] in the presence or the absence of interactions. For particles confined in a harmonic potential, the calculations presented similar results. In this work, we will use, as a reference, the original calculation presented by the authors of Ref. [6], that is, a Bose gas with a large number of particles and negligible interactions. In this picture, the heat capacity $C_{\mathcal{V}}$ evolves presenting a λ-shaped curve across the BEC transition for a harmonically trapped Bose gas. It displays a steep change in the $C_{\mathcal{V}}$ values, near the critical temperature. By defining $C_{\mathcal{V}}^- \equiv C_{\mathcal{V}}(T_c^-)$, $C_{\mathcal{V}}^+ \equiv C_{\mathcal{V}}(T_c^+)$, and $\Delta C_{\mathcal{V}} = C_{\mathcal{V}}^- - C_{\mathcal{V}}^+$, the $C_{\mathcal{V}}$ peak value is found, just below the critical temperature, as $\frac{C_{\mathcal{V}}^-}{Nk_B} = 12\frac{\zeta(4)}{\zeta(3)}(\approx 10.8)$, and shall quickly change around T_c by $\frac{\Delta C_{\mathcal{V}}}{Nk_B} = 9\frac{\zeta(3)}{\zeta(2)}(\approx 6.6)$ [6,8]. These theoretical results are general and valid for arbitrary oscillator frequencies. The presence of weak interactions would produce minor changes on $C_{\mathcal{V}}$ very near the critical temperature when compared to the ideal Bose gas case, while keeping its overall shape [7,11,12].

The resemblance to the liquid ^{4}He heat capacity, near the λ point, is clear [23], as well as its rapid change around T_c, in the limit of large N. This qualitative characteristic was predicted by different theories whether considering finite number effects [8,10] and interactions [11] or not [6]. However, for an ideal Bose gas in the large number limit, the values of $C_{\mathcal{V}}^+$, $C_{\mathcal{V}}^-$, and $\Delta C_{\mathcal{V}}$ scale linearly with the number of atoms. In fact, the interactions are predicted to change the $C_{\mathcal{V}}$ behavior by rounding off the peak existing just below the critical temperature, as discussed by Giorgini *et al.* [11].

III. EXPERIMENTAL DESCRIPTION, RESULTS, AND DISCUSSION

The experimental system comprises a double magneto-optical trap (MOT) and a quadrupole-Ioffe configuration (QUIC) magnetic trap. Details about the system are described in previous publications [24]. A combination of laser cooling and RF-evaporative cooling allows to obtain a BEC containing 2–8 $\times 10^5$ ^{87}Rb atoms. The trap frequencies are $\omega_x = 2\pi \times 23$ Hz for the weak axis, and $\omega_y = \omega_z = 2\pi \times 207$ Hz for the most confining directions. A full characterization of the condensate is performed by first recording an absorption image with a CCD camera, after 15 ms of free expansion. The data were fitted using a bimodal atomic distribution (condensate and thermal fractions as a sum of a Thomas-Fermi and a Gaussian profiles, respectively), and we assume cylindrical symmetry for the trapping potential to rebuild the complete 3D distribution, i.e., the Gaussian widths and the Thomas-Fermi radii, as well as the respective error values, which account for deviations from both the ideal Gaussian assumption and the Thomas-Fermi approximation.

The fittings also promptly provide the temperature values and both the condensate and thermal number of atoms. Then the *in situ* distribution is determined by assuming a ballistic expansion of the thermal cloud, and then rescaling backwards the characteristic parabolic shape of the BEC expansion, as demonstrated in Refs. [25–27]. For the BEC fraction, simple analytical expressions are known for an elongated cigar-shaped trap [25]. Finally, the full 3D density distribution $n(\vec{r})$ is inserted in Eq. (2), and the parameter Π is obtained. Finite temperature corrections to the Thomas-Fermi (TF) expansion fits of our samples were neglected. We estimate that these corrections would slightly change the value of Π, on the order of 1% or less.

The heat capacity is determined as follows. First, we derive the equation of state $\Pi = \Pi(N/\mathcal{V},T)$ by taking data in a constant volume trap potential ($\mathcal{V}$ constant). The acquired data sets presenting similar number of atoms N are grouped. We then plot isodensity parameter curves (i.e., curves at constant density parameter $N/\mathcal{V}$), Π versus T, for different average number of atoms $\langle N\rangle$, as shown in Fig. 1. Second, above T_c, we take the data points presenting no measurable condensed fractions and assume them as pure thermal clouds. Under these conditions, the linear behavior of Π versus T is well known as a result of the dominant Gaussian distribution [19].

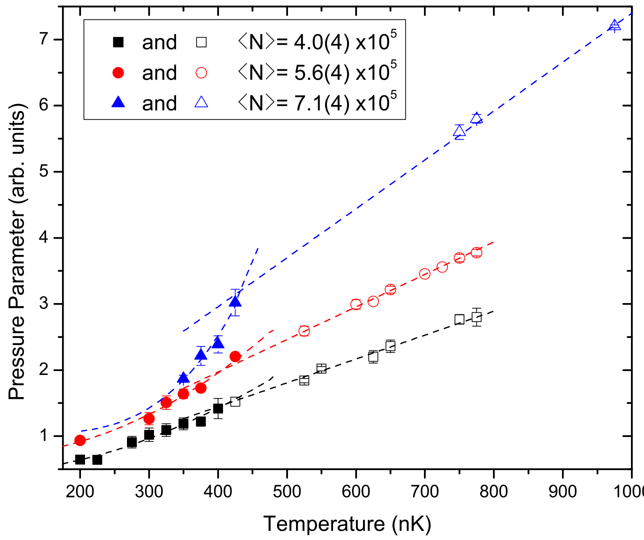

FIG. 1. (Color online) *Pressure parameter* as a function of temperature for three different averaged particle number $\langle N \rangle$. For each $\langle N \rangle$, the crossing between a linear fitting for thermal points (open symbols) and the interpolation or extrapolation of points with measurable condensate fraction (solid symbols) determines the critical point.

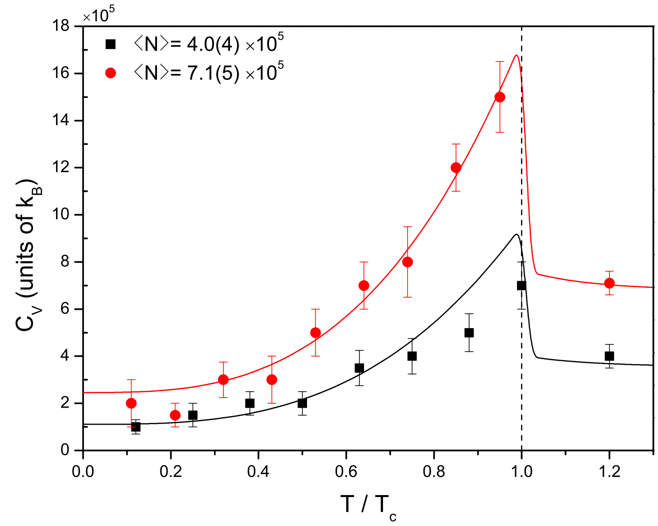

FIG. 2. (Color online) The heat capacity versus the reduced temperature is plotted around the condensation temperature T_c for two different atom numbers. The experimental points are extracted from diagram of Fig. 1, via Eq. (4). The lines result from Eqs. (10) and (14) [8], where N is the only adjustable parameter.

We fitted a line to the data above T_c, which, by means of Eq. (4), directly yields the constant value for the heat capacity expected for high temperatures. For the data below T_c, we performed a numerical interpolation (extrapolation) over the raw data and generated a set of extra points in between. Then, we performed a numerical differentiation to determine the heat capacity. Uncertainties in the derivative were determined from different possible interpolations according to the uncertainties in the values of Π.

The evolution of the heat capacity as a function of the reduced temperature is plotted in Fig. 2, for two different atom numbers. From there, one may note the steep change in the measured heat capacity near the critical temperature T_c. The lines result from the direct application of Eqs. (10) and (14), derived in Ref. [8], computing the heat capacity across T_c. We did use the measured frequencies of our QUIC trap to determine the typical level spacing $\hbar\omega/k_B \approx 5$ nK and the zero point energy $E_0/k_B \approx 10$ nK. The absolute values, as well as the steep change in the heat capacity are expected to be number dependent. The measured $C_\mathcal{V}$ is in very good agreement with the finite-N theory for BECs held in harmonic traps [8], as shown in Fig. 2. Therefore, one may conclude that the finite-N corrections, included in the theory [8], already contain the essential features shown by our results.

The choice of testing the results with the noninteracting model is based on the discussions presented by Giorgini *et al.* [11]. They concluded that the inclusion of the two-body interactions shall be more pronounced just in a small temperature region, very near T_c. The end result would be a rounded off curve joining the values just near T_c. It would also be very interesting to carefully study the effects of the two-body interactions in temperatures ranging from 0.8 to $1.0T/T_c$ (see Fig. 15 in Ref. [11]). In doing so, one would be able to map the rounded off curve joining the two regimes. In any case, we are confident that the method used here is reliable and robust to treat the acquired experimental data, regardless of the absolute accuracy achieved.

The heat capacity evolves, starting from zero, with increasing values proportional to the third power of the reduced temperature, that is, $C_\mathcal{V}^- \propto (T/T_0)^3$, peaking around 0.9 and $0.98T_c$. Very close to T_c a steep jump takes place while it goes from $C_\mathcal{V}^-$ to $C_\mathcal{V}^+$. Right above the critical temperature, a slow decrease with the temperature is observed in $C_\mathcal{V}^+$. And, at high temperatures, the heat capacity approaches the temperature-independent behavior expected for the noninteracting Bose gas $3k_BN$. This interesting general shape of the heat capacity is accepted in the literature [7] as a property of a second-order phase transition. Thus, the investigation of the heat capacity steep change in a trapped gas, near T_c, is very significant to the overall understanding of the phase transition itself, especially for nonhomogeneous density distributions.

Figures 3(b) and 3(c) present $C_\mathcal{V}$ as a function of the trapped atoms number measured across T_c. In Fig. 3(a), the difference $\Delta C_\mathcal{V} = C_\mathcal{V}(T_c^-) - C_\mathcal{V}(T_c^+)$ is plotted, measured just below or above T_c. We observed a small departure from the linear dependence as the number of trapped of atoms increases [Fig. 3(a)]. We believe this might be related to the atomic interactions. On the other hand, the behavior of the heat capacity of a thermal gas (above T_c) is quite linear, in very good agreement with the standard theoretical result: $3k_B/N$.

In Fig. 4, we plot the normalized heat capacity, $C_\mathcal{V}/Nk_B$, versus the reduced temperature, T/T_c for two different averaged number of atoms, $\langle N \rangle$. For an ideal Bose gas, in the limit of large number of atoms, the $C_\mathcal{V}/Nk_B$ shows the typical, $\langle N \rangle$-independent, curve (dashed blue line). The weakly interacting BEC data deviates from the universal curve in an intermediate range, below and the critical temperature. We found that $C_\mathcal{V}/Nk_B$ presents larger values for smaller $\langle N \rangle$, in agreement with the theory [8,11]. The effect of downshifting

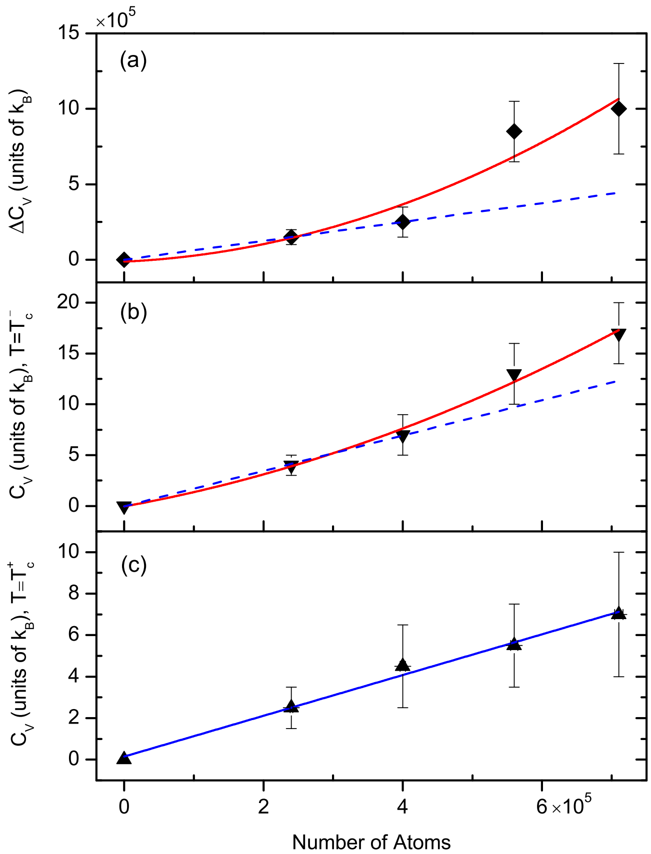

FIG. 3. (Color online) Dependence of the heat capacity around the critical temperature on the total number of atoms: (a) the $\Delta C_{\mathcal{V}}$ jump, (b) $C_{\mathcal{V}}(T_c^-)$, and (c) $C_{\mathcal{V}}(T_c^+)$. Dashed line is the theoretical result for a weakly interacting, large N, case and solid lines are only eye guides.

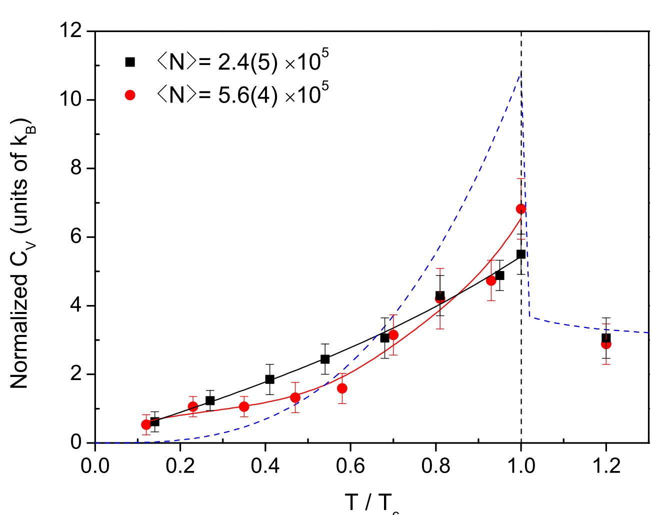

FIG. 4. (Color online) The normalized heat capacity versus the average number of atoms $\langle N \rangle$ as a function of reduced temperature (T/T_c) for two different $\langle N \rangle$. Solid lines are interpolations of the data. The blue dashed line is the theoretical curve for the finite-N corrected, large N case.

the $C_{\mathcal{V}}$ at large N may seem a bit surprising at first, but according to the theoretical models presented on Refs. [8,11], it comes from the finite-N correction. Indeed, the effect is reversed since the $C_{\mathcal{V}}$ correction for lower N results in larger $C_{\mathcal{V}}$ values due to the factor proportional to $(T/T_c)^2 N^{-1/3}$ (see Eq. (10) in Ref. [8]). We believe that, close to the zero temperature limit $T \to 0$, it will be theoretically allowed for the heat capacity to undergo an "energy gap" behavior [28], which is beyond the scope of this work.

Our method of measuring Π relies on the ability to indirectly determine the *in situ* number density, after some time of flight [21]. The data processing may introduce small shifts in the absolute values, which would be important in a more accurate study of $C_{\mathcal{V}}/Nk_B$ at the low-temperature limit, as well as near the critical temperature.

It is important to point out that the ability to directly acquire the *in situ* number density would overcome the reconstruction procedure innate limitations. Generally, it would be best to be able to determine the 3D density distribution without relying on any fitting. In addition, the interactions do not play any role on limiting the global variables theory validity. Thus, the experimental method here presented and discussed for determining the heat capacity would certainly stand valid in strongly interaction regimes [13].

IV. CONCLUSION

We have developed an alternative technique for determining the global heat capacity of a nonhomogeneous, harmonically trapped gas, which does not assume LDA. By using new macroscopic conjugate variables (*volume* and *pressure parameters*), presented in recent publications [19,21], we were able to determine both the internal energy and the heat capacity $C_{\mathcal{V}}$ at constant *volume parameter*. We have then successfully applied this technique to measure the heat capacity across the BEC transition of a ^{87}Rb Bose gas. A steep $C_{\mathcal{V}}$ curve was observed, in the vicinity of the critical temperature T_c, in close similarity to the λ point in liquid ^{4}He [23]. Moreover, the evolution of $C_{\mathcal{V}}$ near T_c suggests an interplay of the mean-field interactions. We point out three interesting phenomena to be studied in a narrow temperature region, near T_c: (ii) its absolute value downshift; (ii) the $C_{\mathcal{V}}$ peak round off; and (iii) the larger values of the normalized $C_{\mathcal{V}}$ for lower N in a relatively broad temperature range below T_c. It is important to remark that the second effect was theoretically predicted, but not yet measured. The third is shown in Fig. 4, which, to the best of our knowledge, stands as the first reported experimental observation. Finally, we have briefly discussed the relevance of measuring $C_{\mathcal{V}}$ in trapped BECs across the critical temperature, which, together with the three phenomena above mentioned, may prompt further investigation and future experiments.

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