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Observation of Bose-Einstein condensation in an atomic trap in terms of macroscopic thermodynamic parameters

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To overcome the difficulties in defining pressure for a gas confined in an inhomogeneous trap, we define single macroscopic parameters that behave like pressure and volume. We measure the phase diagram of a ^{87}Rb Bose gas in a harmonic trap in terms of those macroscopic parameters obtained from the spatial distribution of atoms. Considering the relevant variables such as the trap potential $\mathcal{V} = (\omega_x\omega_y\omega_z)^{-1}$, number of atoms N, and temperature T, a parameter $\Pi = \Pi(N,\mathcal{V},T)$ is introduced to characterize the overall macroscopic pressure of the system. We construct the phase diagram (Π vs T) identifying the main features related to the Bose-Einstein condensation (BEC) transition in a trapped gas. A thermodynamic description of the phase transition based on purely macroscopic parameters provides us with a description that does not need the local-density approximation. This procedure can be used to explore different aspects related to BEC such as the nature of the phase transition in a trapped gas.

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I. INTRODUCTION

Experiments with cold gases are normally performed in traps that result in spatially inhomogeneous samples [1–5]. In such cases, the phase diagram for the transition from condensate to noncondensate phases becomes difficult to express using quantities that apply mostly for homogeneous systems such as pressure and volume. Part of the problem can be solved if one relies on a local-density approximation (LDA), where characterization of a nonuniform fluid, at a given spatial position, is obtained by considering local quantities, which in turn determine bulk properties. Since the phenomena observed, such as Bose-Einstein condensation (BEC), occur at a macroscopic level in a nonuniform trap, the description would be more appropriate if the overall characterization of the system could be achieved based on macroscopic thermodynamic parameters, which should depend on other thermodynamic variables such as temperature, number of particles, and properties of the confining potential.

Recently, several papers have explored macroscopic quantum phenomena based on measurements of thermodynamic properties. Horikoshi *et al.* [6] used a force balance equation to create a state equation, which allows one to determine local quantities of a Fermi gas at unitarity. Ho and Zhou [7] proposed an algorithm to obtain the phase diagram and thermodynamic quantities of the corresponding bulk system by analyzing the density profile of trapped gases. Equivalent concepts were also used by Nascimbène *et al.* [8] to explore thermodynamics of a Fermi system.

In a recent work quantum turbulence (QT) was demonstrated as a tangled configuration of quantized vortices in a Bose-Einstein condensate of ^{87}Rb atoms [9]. In this case, QT is mainly determined by the spatial distribution as well as modifications of the hydrodynamic properties. Nevertheless, a proper way to identify turbulence in the superfluid could be through the variation of the overall thermodynamic pressure. As in normal fluids, the phenomenon of turbulence must be followed by a drop in pressure [10]. However, there are intrinsic difficulties associated with the determination of pressure in a sample of turbulent BEC. Because of the strong local fluctuations it is not appropriate to use a LDA. Therefore, an alternative macroscopic quantity related to pressure but resulting from the overall integration within the sample would be better for characterizing QT in a trapped atomic superfluid.

In this work we consider a different way to describe the phase diagram for the BEC transition using a single macroscopic parameter to characterize the inhomogeneous system. This approach is based on concepts introduced in Refs. [4,11–13] and it is applied to experimentally analyze the BEC transition for a harmonically trapped ^{87}Rb gas. However, the employed ideas are quite general and can be applied for any trapped system.

II. DEFINING MACROSCOPIC PARAMETERS

In choosing macroscopic parameters analogous to pressure and volume for inhomogeneous systems, we have required that in the case of a homogeneous system those choices represent the real pressure and volume. We start by considering the relevant macroscopic parameters to be used. The thermodynamic state of a gas trapped in a macroscopic harmonic potential is naturally characterized by the trapped number of atoms N, the temperature T, and parameters that determine the confining potential. In a uniform gas, apart from the temperature and number of particles, the mechanical variable that specifies the thermodynamic state of the system is the volume V that the sample occupies. Since a gas confined in a harmonic trap does not have a well-defined volume, one can use an alternative variable that yields analogous information regarding its size. Considering the harmonic potential $V_{\rm ext}(\vec{r}) = \frac{1}{2}m(\vec{\omega}\cdot\vec{r})^2$, with

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$\vec{\omega} = (\omega_x, \omega_y, \omega_z)$, it turns out that in a first approximation the size of the system is given by $r^{*3} \approx (k_B T/m\omega^2)^{3/2}$. Thus, apart from constants and other independent thermodynamic variables, this allows us to identify $\mathcal{V} \equiv 1/\omega^3$ as the volume parameter, where $\omega^3 = \omega_x\omega_y\omega_z$. This variable plays the role of the actual volume in a harmonically trapped fluid. In fact, long ago, de Groot *et al.* [14], and later Bagnato *et al.* [15] and others [16–18], demonstrated that $\mathcal{V}$ is the correct thermodynamic quantity to determine the thermodynamic limit ($N \to \infty$, $\mathcal{V} \to \infty$ but $N/\mathcal{V} \to$ const). The volume parameter should not be identified with the real volume of the system. In fact, it does not even have units of volume. However, it presents the most relevant property, which is the extensive thermodynamic quality [11–13].

Therefore, we take the collection $(N,T,\mathcal{V})$ as the independent thermodynamic variables that specify the state of the system. Any other thermodynamic property of the confined gas in this case can be expressed as a function of those variables. In a homogeneous fluid the phase diagram may be expressed in terms of the equation of state $p = p(N,T,V)$, with p the hydrostatic pressure. For inhomogeneous fluids, since the state is given in terms of the volume parameter, we also define a pressure parameter Π such that the equation of state becomes now $\Pi = \Pi(N,T,\mathcal{V})$. Analogously to the volume parameter, Π is not an actual hydrostatic pressure, although it does retain characteristics of a pressure, as we argue now. We start by evaluating the Helmholtz free energy

$$F(N,T,\mathcal{V}) = -k_B T \ln \mathrm{Tr} e^{-\beta H}, \tag{1}$$

where $H = K + U_{\mathrm{int}} + V_{\mathrm{ext}}$ is the Hamiltonian of the system composed by the kinetic energy $K = \sum_i \frac{p_i^2}{2m}$, the internal energy $U_{\mathrm{int}} = \sum_{i<j} U(r_{ij})$, and the external harmonic potential $V_{\mathrm{ext}} = \sum_i \frac{1}{2}m(\omega_x^2 x_i^2 + \omega_y^2 y_i^2 + \omega_z^2 z_i^2)$. One can show [11] that in this case, the quantity $\mathcal{V} = (\omega_x\omega_y\omega_z)^{-1}$ is an extensive parameter in order to preserve the necessary extensive character for the Helmholtz free energy. The pressure parameter is defined as the intensive variable conjugated to $\mathcal{V}$, that is,

$$\Pi \equiv -\left(\frac{\partial F}{\partial \mathcal{V}}\right)_{N,T}. \tag{2}$$

We note that while Π has neither units of pressure nor $\mathcal{V}$ units of volume, the product $\Pi\mathcal{V}$ still has units of energy. Since Π is an intensive thermodynamic variable, its dependence on $(N,T,\mathcal{V})$ must be of the form $\Pi = \Pi(N/\mathcal{V},T)$. Thus, in keeping with the analogy, we shall call $N/\mathcal{V}$ the density parameter. From the above definition of Π, without resorting to a LDA, a very useful and general expression can be derived [11–13]:

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

where $n(\vec{r})$ is the inhomogeneous density profile of the gas averaged over quantum or thermodynamic fluctuations. Since both $n(\vec{r})$ and the confining potential are measurable quantities, Π can be readily determined. While $\vec{r}$ is a microscopic variable, the pressure parameter resulting from the overall integration in all space occupied by the atoms is actually a macroscopic quantity. With the equation of state $\Pi = \Pi(N/\mathcal{V},T)$, the phase diagram for the transition can be fully described based on measured macroscopic quantities of the global system, without the necessity of considering the corresponding local uniform system as done with the LDA.

Additional insight into the physics of Π can be gained by noticing the additional identity [12]

$$\Pi\mathcal{V} = \int p(\vec{r}) d^3r, \tag{4}$$

showing that the pressure parameter Π is actually proportional to the integral of the local hydrostatic pressure $p(\vec{r})$ over all space. To obtain this result we need to remember that mechanical equilibrium in the fluid is determined by the balance of local forces, namely, $\vec{\nabla} p(\vec{r}) + n(\vec{r})\vec{\nabla} V_{\mathrm{ext}}(\vec{r}) = 0$. By using Eq. (3), the integration of the virial of these forces $\vec{r}\cdot\vec{f}$ leads to Eq. (4). A similar mechanical equilibrium argument has also been used by Horikoshi *et al.* [6].

III. EXPERIMENTAL SYSTEM AND MEASUREMENTS

To measure the quantities involved in Eq. (3) across BEC transition we have used an experimental setup composed of a double magneto-optical trap (MOT) and a quadrupole–Ioffe-configuration (QUIC) type of trap. The system has been described in detail elsewhere [19]. In brief, we collect 10^9 ^{87}Rb atoms in a MOT, producing a sample at approximately 100 μK. After a population transfer to the $|2,2\rangle$ hyperfine state, the sample is used to load a QUIC magnetic trap. While trapped, a rf-induced evaporation is applied to obtain quantum degeneracy. The trapping potential is harmonic with frequencies $\omega_x = \omega_0$ and $\omega_y = \omega_z = 9\omega_0$, where $\omega_0 = 2\pi \times 23$ Hz. The characterization of the sample is done by absorption imaging it on a CCD camera after a 15-ms time of flight. We typically produce BEC samples containing $(1–7)\times 10^5$ atoms.

Each acquired image is fitted with a bimodal distribution composed of a Gaussian and an inverted parabola (Thomas-Fermi distribution), which represent, respectively, the thermal cloud and the condensate part. The quality of the images in our experiment allows good fittings, which are necessary for two reasons. First, the absorption image gives us a two-dimensional profile from which it is impossible to determine the three-dimensional one without assumptions. Second, since we have a time-of-flight image, we need the fitting parameters of the expanded cloud to determine the *in situ* profile $n(\vec{r})$ used to calculate Π through Eq. (3). For the thermal part and the condensate part, the *in situ* profile is obtained by considering a ballistic expansion and by applying the theory developed by Castin and Dum [20], respectively. From those fittings, the temperature T, the number of condensed atoms N_0, and the total number of atoms N are obtained. Finally, by using Eq. (3) we obtain the pressure parameter Π.

For the experiment reported here we have kept the trap frequencies fixed, that is, $\mathcal{V}$ = constant. The temperature and number of atoms were varied by controlling the evaporative cooling final frequency and the time of evaporation [19]. Since our experiment is supposed to test the equation of state, we should perform experiments including the variation of $\mathcal{V}$ (trapping potential frequencies). However, with our present experimental system this is a very hard task. Variations on the trapping frequencies cause a displacement of the potential minimum as well as the evaporation conditions. The use of

an optical trap instead of a full magnetic QUIC one would be more appropriate for this purpose.

IV. RESULTS AND DISCUSSION

We have performed about 300 runs of the experiment and grouped the results with a similar number of particles for different temperatures. In the first group the number of particles varies 33% around the average value of 1.2×10^5 atoms. In the second group the variation is 21% in 2.4×10^5 atoms and for the other three groups the number of particles varies less than 10% around the respective average. Therefore, the data in each group were considered as belonging to an isodensity (practically the same number of particles) for all temperatures. Since we are expressing $\Pi = \Pi(N/\mathcal{V}, T)$, the experiment corresponds to the investigation of the isodensities Π vs T, while the density parameter $N/\mathcal{V}$ remains constant in each group. The results of this experiment are shown in Fig. 1. For a fixed density parameter we observe two different regions of behavior as T decreases. First, for high temperatures, Π has an almost linear dependence on both T and $N/\mathcal{V}$ (which is the prediction of an ideal Bose gas above BEC), until an abrupt change takes place, and the decrease of Π with T becomes faster than linear. This change of behavior characterizes the critical temperature $T_c = T_c(N/\mathcal{V})$ where BEC takes place. This change was also detected in the corresponding density profiles, that is, those below T_c showed the characteristic peak of the condensate. The lines used to connect the points in Fig. 1 are empirical fittings. Above T_c the data were fitted by a linear function and below T_c exponential functions were used. The critical point (Π_c, T_c) for each density parameter was determined by the crossing point of these lines for each isodensity. Following the definition of Π from Eq. (2) and considering the fact that for $T > T_c$ the density clouds are very well fitted by a Gaussian profile, the mentioned linear dependence is expected. That is, if one considers the Bose distribution of particles in the noninteracting approximation

$$\Pi \approx \frac{N k_B T}{\mathcal{V}} \frac{g_4(z)}{g_3(z)} \quad \text{(ideal gas)} \tag{5}$$

and

$$N \approx \mathcal{V} \left(\frac{k_B T}{\hbar}\right)^3 g_3(z) \quad \text{(ideal gas)}, \tag{6}$$

with $g_n(z)$ the Bose function and $z = \exp(\mu/k_B T)$ the fugacity, the deviation from linearity of Π, in T and $N/\mathcal{V}$, is rather small since $1 \geqslant g_4(z)/g_3(z) \geqslant 0.9$. Even if Hartree-Fock corrections are included [11], the dependence of Π on T remains very close to linear for $T > T_c$. Below T_c, the behavior of Π is intrinsically related to the superfluid nature of the gas, depending very strongly now on the magnitude of the interparticle interaction. That is, if the interparticle interactions played no role, all the curves below T_c in Fig. 1 would lie on the top of each other, as expected for an ideal gas.

From Fig. 1 one can determine the critical points and extract the phase diagram Π vs T shown in Fig. 2, where the critical line Π_c vs T_c separates the thermodynamic states into two domains, one where the fluid is fully thermal and the other where there is a superposition of a Bose condensate fluid with a thermal component. The curve Π_c vs T_c represents what is expected to be a continuous phase transition [18] between a normal gas and a superfluid in an interacting Bose fluid confined by a harmonic trap. This curve has a shape that recalls the celebrated ^{4}He phase diagram separating the superfluid from the normal fluid phase. For completeness we have reproduced in Fig. 3 the adopted diagram for ^{4}He [21,22] equivalent to Fig. 2. Compared to ^{4}He there are a few peculiarities related to the present system that we address below. If the gas were ideal one should obtain $\Pi_c \sim T_c^4$ at the transition line; however, a logarithmic plot reveals that a simple law $\Pi T^\gamma = \text{const}$ is not obeyed for γ constant. The exponent becomes larger as the temperature decreases. This feature, as well as those discussed below, is certainly due to

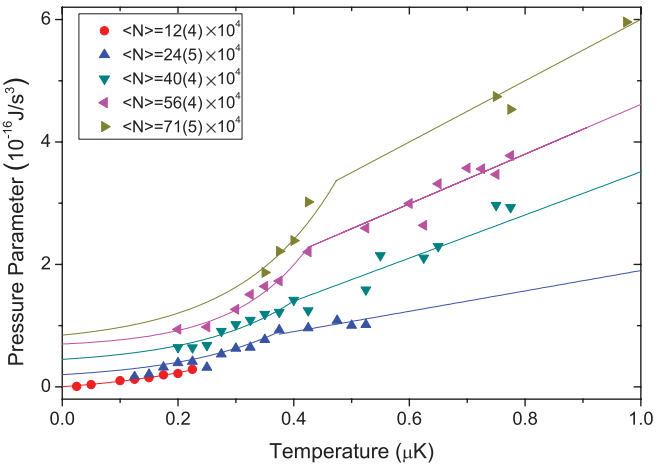

FIG. 1. (Color online) Pressure parameter Π as a function of temperature T for different constant numbers of particles N, crossing their corresponding critical temperature $T_c(N/\mathcal{V})$. Solid lines are fittings with empirical functions. Above T_c the data were fitted by a linear function and below T_c exponential functions were used. From the fittings we have extracted the value of Π at $T = 0$.

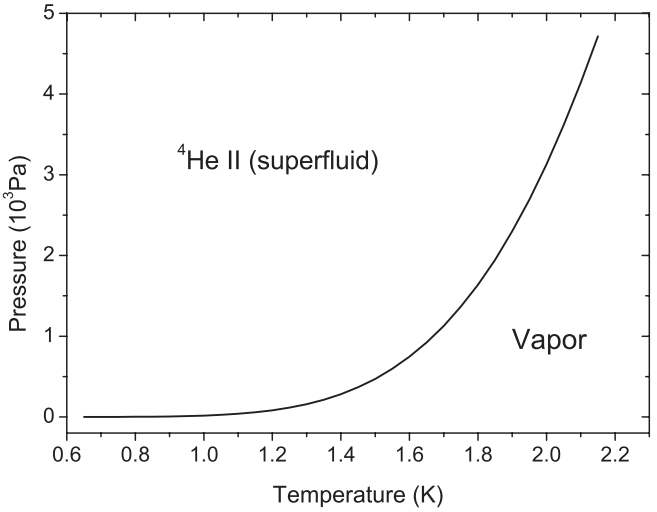

FIG. 2. Phase diagram presenting the critical points Π_c vs T_c. The BEC transition line separates the two phases: purely thermal cloud and thermal cloud plus condensate.

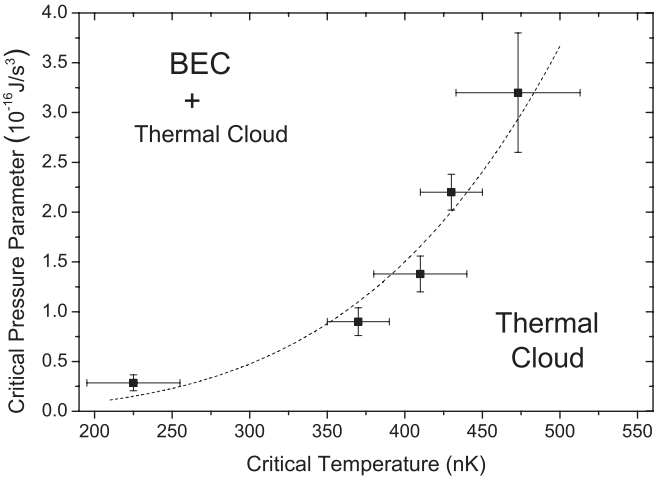

FIG. 3. Saturated vapor pressure versus temperature for ^{4}He from Refs. [21,22]. The curve divides the superfluid and the normal fluid regions.

the influence of interactions below T_c and to the presence of the confining potential.

Returning to Fig. 1, we now analyze data for each isodensity curve (density parameter constant) for temperatures below T_c. These points are presented in Fig. 4. Note that higher isodensity curves produce higher pressure parameter values at a given temperature. This appears as expected from an overall analysis of these variables in harmonic [11] and linear quadrupolar [13] traps using the Hartree-Fock approximation. The extrapolation of the experimental points in Fig. 4, represented by the solid lines, allows the determination of $\Pi_0 = \Pi(N/\mathcal{V}, T = 0)$, the zero-temperature pressure parameter, which depends on the pure condensate density without the presence of the thermal component. At $T = 0$, the Thomas-Fermi approximation (TFA) works on its best conditions. Therefore, by using the

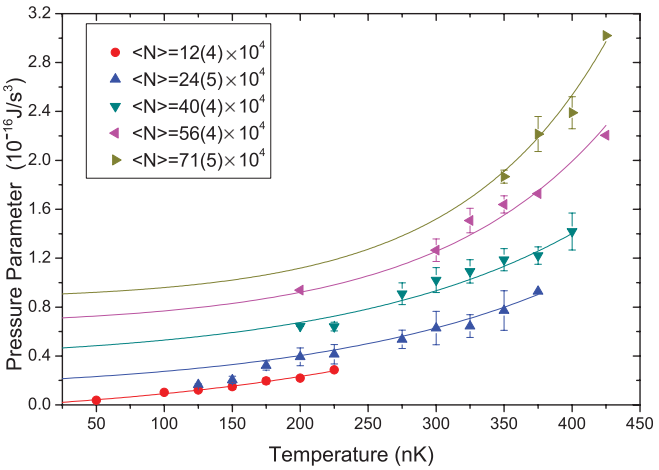

FIG. 4. (Color online) Detail of pressure parameter dependence on temperature for different fixed numbers of particles $\Pi = \Pi(N/\mathcal{V}, T)$ in the BEC region. The extrapolation of the experimental points allows for the determination of the pressure parameter at $T = 0$.

TFA and LDA [16,17] and assuming a cloud of N interacting atoms with scattering length a, Eq. (3) at $T = 0$ yields

$$\Pi_0 = \tfrac{1}{7}(15\hbar^2 a\sqrt{m})^{2/5}(N\omega_r^2\omega_z)^{7/5}. \quad (7)$$

It is found then that at $T = 0$ the pressure parameter scales with the number of particles (keeping $\mathcal{V}$ fixed) as $\Pi_0 \sim N^\delta$. A log-log plot of the values found from Fig. 4 yields the value $\delta = 1.5^{+0.3}_{-0.2}$, well within the expected value 1.4 predicted by the TFA. The use of expression (7) together with the data presented in Fig. 4 allows the determination of the scattering length, fully based on global thermodynamic quantities. We have obtained for the scattering length the value $a = 94 \pm 32$ Å, which is a bit higher than the real value of approximately 50 Å [23]. Naturally, as the temperature decreases we have less data for a high number of atoms, which is intrinsically related to the evaporation process. The absence of experimental points at lower temperatures makes the determination of Π_0 subjected to a higher imprecision. This is associated with the discrepancy of values for the scattering length.

As with standard pressure and volume in uniform fluid systems, the variables Π and $\mathcal{V}$ provide us with a macroscopic thermodynamic description of the fluid without the necessity of relying on the LDA. Because of the physical connection between the parameters $(\Pi, \mathcal{V})$ with (p, V), the phase diagram reveals interesting macroscopic features not yet considered along the phase transition for the formation of a superfluid atomic phase in a trap.

It is interesting to compare the phase diagram Π vs T of Fig. 2 to the corresponding diagram for the superfluid transition of ^{4}He in Fig. 3. Nevertheless, we also insist on the profound differences between considering a local picture and a global or thermodynamic one of a confined system. If studies were made of local variables only, the phase diagram obtained would refer to the bulk system and the transition line would not yield the information of the occurrence of BEC in the trapped gas. That is, knowledge of the bulk phase diagram solely does not allow a direct calculation of the phase diagram of the inhomogeneous trapped gas. One first needs full knowledge of the number particle density $n = N/V$ and hydrostatic pressure p of the homogeneous gas as a function of both chemical potential μ and temperature T, i.e., $n(\mu, T)$ and $p(\mu, T)$. Then, using the LDA with the harmonic potential, a reconstruction of the phase diagram Π vs T such as in Fig. 1 could be made. However, BEC occurs in the trapped inhomogeneous gas and this information is succinctly contained in the phase diagram of Figs. 1 and 2.

The use of a single macroscopic thermodynamic parameter $\Pi = \Pi(N/\mathcal{V}, T)$ to describe the phase transition will allow us to go further in many aspects. One of the main motivations is the possibility of making a thermodynamic description for turbulent phenomena in atomic superfluids held in traps. Analyses comparing the variation of Π when turbulence occurs remain a goal for further experiments.

V. CONCLUSION

To summarize, we have demonstrated the use of a single macroscopic thermodynamic quantity to describe the BEC

in an inhomogeneous system. The ability to describe an inhomogeneous quantum gas via macroscopic parameters creates a means to access other thermodynamic quantities proper of the trapped gas that cannot be accessed using local variables within the LDA. It can be shown that the heat capacity may be obtained by full knowledge of the equation of state $\Pi = \Pi(N/\mathcal{V}, T)$ and by independent temperature measurements of adiabatic changes of the volume parameter [13]. This last aspect requires a variation in the trap frequencies and an optical trap seems more appropriate than a magnetic QUIC one, as used in the present experiments.

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