

## Equation of state for a trapped quantum gas: remnant of zero-point energy effects

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2016 New J. Phys. 18 023014

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## PAPER

## Equation of state for a trapped quantum gas: remnant of zero-point energy effects

## OPEN ACCESS

## RECEIVED

7 July 2015

## REVISED

22 October 2015

## ACCEPTED FOR PUBLICATION

23 November 2015

## PUBLISHED

29 January 2016

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P C M Castilho<sup>1</sup>, F J Poveda-Cuevas<sup>1</sup>, J A Seman<sup>2</sup>, R F Shiozaki<sup>1</sup>, G Roati<sup>3</sup>, S R Muniz<sup>1</sup>, D V Magalhães<sup>4</sup> and V S Bagnato<sup>1</sup><sup>1</sup> Instituto de Física de São Carlos, Universidade de São Paulo, C.P. 369, 13560-970 São Carlos, SP, Brazil<sup>2</sup> Instituto de Física, Universidad Nacional Autónoma de México Apartado Postal 20-364, 01000 México, D. F. México<sup>3</sup> INO-CNR and LENS, Università di Firenze, 50019 Sesto Fiorentino, Italy<sup>4</sup> Escola de Engenharia de São Carlos, Universidade de São Paulo, São Carlos 13566-590, BrazilE-mail: [patricia.cmcastilho@gmail.com](mailto:patricia.cmcastilho@gmail.com)**Keywords:** Bose–Einstein condensate, trapped gases, thermodynamics**Abstract**

The study of the thermodynamic properties of trapped gases has attracted great attention during the last few years and can be used as a tool to characterize such clouds in the presence of other phenomena. Here, we obtain an equation of state for a harmonically trapped Bose–Einstein condensate taking the limit of  $T \rightarrow 0$  by means of global thermodynamic variables. These variables allow us to explore limits in which the standard thermodynamics are not defined. Our results are taken in the high density limit, and the extrapolation for  $N \rightarrow 1$  is done later. Even in this situation, we qualitatively observe the well known existence of a zero-point energy for harmonic potentials in which the determination of conjugated variables is limited by the quantum nature of the system.

**1. Introduction**

The macroscopic manifestation of quantum phenomena has been widely studied, especially, in superfluid helium [1–3], superconductors [4–6], and ultracold gases [7–9]. In this context, quantum fluids are especially interesting from the standpoint of thermodynamics because, at low temperatures, they exhibit a macroscopic occupation of the ground state of energy [10] and a continuous phase transition [11, 12] with consequences in the macroscopic observables. Particularly, ultracold gases have been gaining importance in recent decades thanks to their large versatility and the high level of control of their important parameters. In such systems, in both classical or quantum regimes, a main characteristic is the spatial inhomogeneity due to the confining potential. Normally, in dealing with a Bose–Einstein condensate (BEC) of trapped atoms with a nonhomogeneous density distribution of particles, the equation of state relating the usual conjugated thermodynamic variables, pressure and volume, is derived with the help of the local density approximation (LDA) method [13–15]. In this context, the atomic cloud is divided in infinitesimal volumes of constant density ( $n(\mathbf{r})$ ) and a defined local pressure ( $P$ ). The BEC phase transition can be studied by building up the  $P \times n$  phase diagram from the infinitesimal volumes with different densities as if each of them were individual systems. Besides, this strange assumption and the loss of information in the atomic density profile, the LDA method cannot be applied in situations in which there are abrupt changes in the density as it occurs in the presence of vortices. To contour these problems, we based the thermodynamic description of the trapped BEC in terms of global generalized variables [16–18].

Historically, the natural way to approach a many particle system is to treat it in terms of quantum mechanics and then to take the thermodynamic limit since the thermodynamic study of systems in the quantum limit is not an easy task. In particular, situations in which quantum effects are appreciable, such as the Lamb shift [19], the Casimir effect [20], or the Higgs field [21], cannot be treated in a trivial form. These phenomena are defined in different contexts, but they share one point in common: they are consequences of the existence of a *zero point*

energy. The global thermodynamic approach allows exploring limits in the total quantum regime, allowing the use of macroscopic variables to observe effects in the quantum limit.

In this paper, we present a relation between global ‘pressure’ and ‘volume’ for a harmonically trapped condensate of  $^{87}\text{Rb}$  atoms near zero temperature. In recent publications [22–24], we have introduced an alternative method to describe the thermodynamic properties of a heterogeneous trapped (classical or quantum) gas. Briefly, considering an ideal gas confined by a harmonic trapping potential with frequencies  $(\omega_x, \omega_y, \omega_z)$ , the critical temperature for condensation ( $T_c$ ), the number of particles ( $N$ ), and the confinement, in terms of  $\bar{\omega} = (\omega_x \omega_y \omega_z)^{1/3}$ , are related through  $k_B T_c \approx 0.94 \hbar \bar{\omega} N^{1/3}$  [25]. This relation implies that, on taking the thermodynamic limit as  $N \rightarrow \infty$ , one needs  $1/\bar{\omega}^3 \rightarrow \infty$  in order to preserve  $T_c$  constant. The quantity  $N/(1/\bar{\omega}^3)$  plays the role of a density parameter, which leads to the definition of  $\mathcal{V} = 1/\bar{\omega}^3$  as the global *volume parameter* [16, 17]. In fact,  $\mathcal{V}$  is an extensive variable, and its intensive conjugated variable is defined as the *pressure parameter*  $\Pi$ . This pressure parameter is fully determined by the trapping potential and the atomic density distribution  $n(\mathbf{r})$ . The expressions for both conjugated parameters are defined as

$$\mathcal{V} = \frac{1}{\omega_x \omega_y \omega_z}, \quad (1)$$

$$\Pi = \frac{m}{3\mathcal{V}} \int d^3r n(\mathbf{r})(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2). \quad (2)$$

The relation between  $\Pi$  and  $\mathcal{V}$  constitute the equation of the state for the trapped gas.

## 2. Experimental setup

The BEC of  $^{87}\text{Rb}$  atoms is obtained in a hybrid trap composed of a magnetic quadrupole trap (MQT) and an optical-dipole trap (ODT) [26]. At low temperatures, this trap gives a harmonic potential with frequencies  $\omega_{x,z} = \sqrt{\frac{4U_0}{mw_0^2}}$  due to the optical confinement and  $\omega_y = \sqrt{\frac{\mu_B B'_x}{2m|z_0|}}$  due to the magnetic field gradient, where  $U_0$  is the optical potential depth,  $m$  is the atomic mass,  $w_0$  is the dipole trap beam waist,  $\mu_B$  is the Bohr magneton,  $B'_x$  is the field gradient along its main axis ( $x$  axis), and  $z_0$  is the relative position of the MQT and ODT centers along the gravity direction. Therefore, the volume parameter can be varied simply by changing the ODT laser power  $P$ , and its characterization was done by measuring the trapping frequencies for different values of  $P$ . The error in this measurement is small (typically around 1.5%) resulting in a small error for the determination of  $\mathcal{V}$ .

After combining radio-frequency and pure optical evaporative cooling processes, we produce a BEC with about  $N = 5 \times 10^5$  atoms, condensate fraction ( $N_0/N$ ) running from 80% to zero, and temperature ( $T$ ) ranging from 50 to 400 nK. These parameters can be changed by applying small modifications to the evaporation processes. Once the BEC is produced, the confinement is turned off, and an absorption image of the cloud is recorded on a CCD camera after 21 ms of free expansion. From this image, we obtain the 2D density profile that allows the determination of  $N$ ,  $N_0/N$ , and  $T$  of the atomic cloud by fitting a bimodal function composed of Gaussian and Thomas–Fermi (TF) distributions. By assuming the cylindrical symmetry of the trap ( $\omega_x \simeq \omega_z$ ), the 3D density profile of the expanded cloud is determined. The *in situ* 3D density profile  $n(\mathbf{r})$  is recovered separately for the thermal and condensate parts by considering a virial theorem and by applying the Castin–Dum regression procedure [27], respectively. Once the *in situ* density profile is obtained, the pressure parameter is calculated by means of equation (2).

## 3. Results

We have conducted experiments in five different volume parameters:  $\mathcal{V}_1 = 0.6 \times 10^8 \text{ s}^3$ ,  $\mathcal{V}_2 = 1.0 \times 10^8 \text{ s}^3$ ,  $\mathcal{V}_3 = 1.6 \times 10^8 \text{ s}^3$ ,  $\mathcal{V}_4 = 3.0 \times 10^8 \text{ s}^3$ , and  $\mathcal{V}_5 = 27 \times 10^8 \text{ s}^3$ . A typical pressure parameter curve as a function of temperature for fixed  $\mathcal{V}$  and  $N$  is shown in figure 1. The critical temperature  $T_c$  is identified by the presence of an inflection point on the  $\Pi$  versus  $T$  diagram. While the pressure parameter for the thermal cloud ( $T > T_c$ ) presents a linear behavior given by the adapted ideal gas relation  $\Pi = Nk_B T/\mathcal{V}$ , below  $T_c$  the curve is closer to a  $T^4$  dependence, which is typical for bosonic massless particles [17, 28]. The behavior of the pressure parameter versus temperature is equivalent to the graph presented by Ensher *et al* [29] showing the energy release per particle of the condensed cloud as a function of temperature. The reason for this similarity is due to the fact that  $\Pi\mathcal{V}$  is the total internal energy as measured in [23]. The extrapolation of the curve for  $T < T_c$  allows for identifying the pressure parameter on the condition where  $T \rightarrow 0$ ,  $\Pi_0(N)$ . Equivalent curves were obtained for different numbers of atoms at each  $\mathcal{V}$  in order to investigate the behavior of  $\Pi_0(N)$ . More than 600 images were taken for each value of  $\mathcal{V}$  varying  $N$ ,  $T$ , and  $N_0/N$ , and a statistical treatment involving averages of similar images was done during the analysis. Figure 2 shows the curve of  $\Pi_0(N)$  versus  $N$  for the same volume parameter of

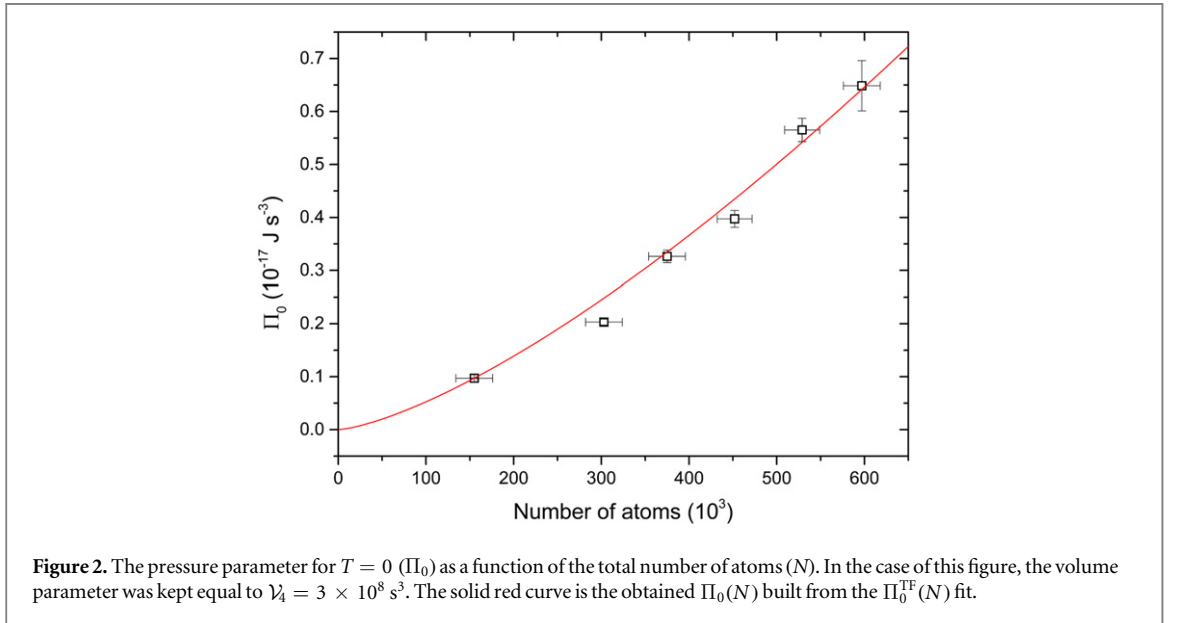
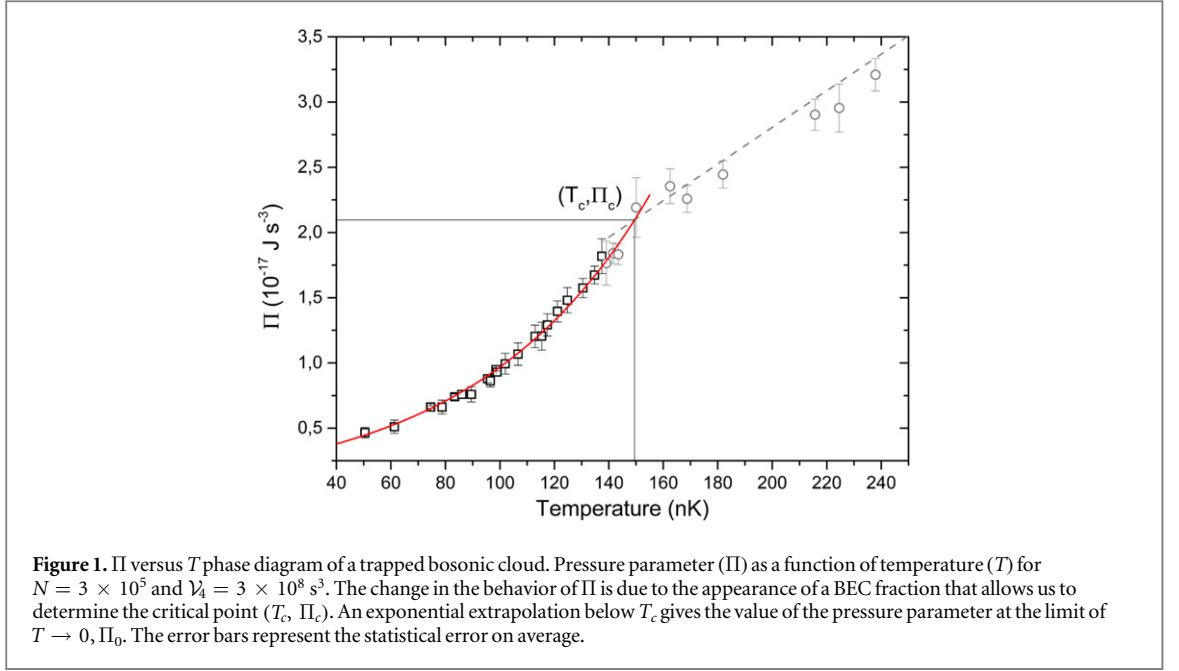
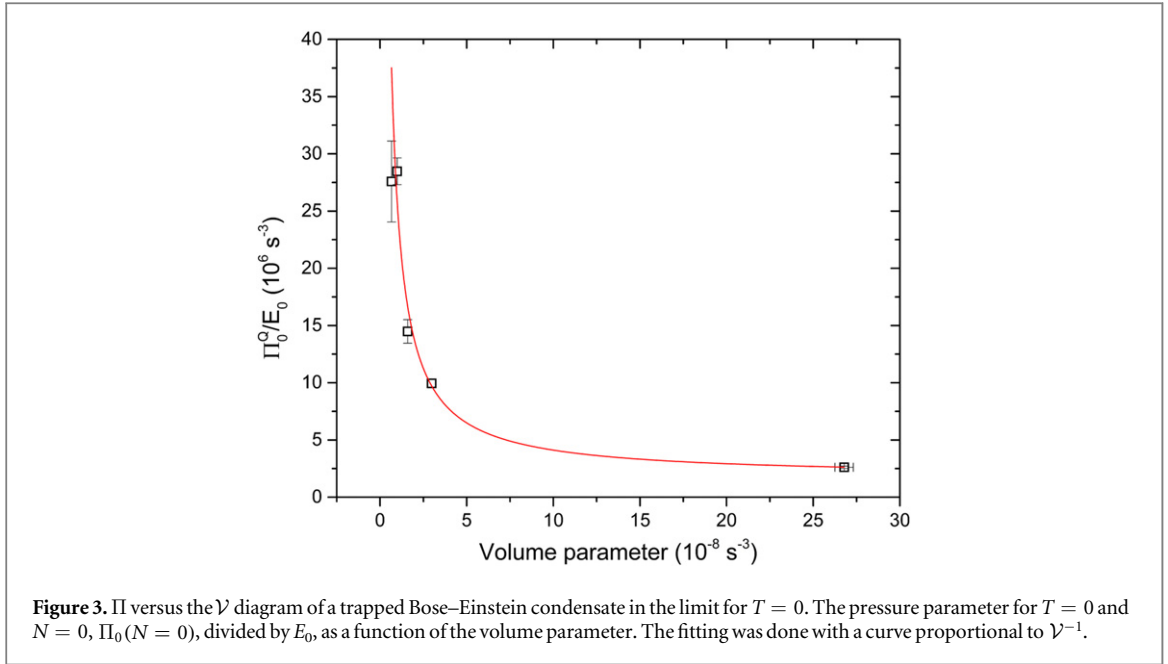


figure 1. We observe that, as the number of atoms decreases,  $\Pi_0(N)$  also decreases reaching a lower limit value of  $\Pi_0^Q$  when the number of atoms is extrapolated to unity.  $\Pi_0^Q$  is a quantum physical constant with no classical equivalent, and its experimental observation represents one of the main results of this paper. The value of  $\Pi_0^Q$  was obtained for each studied volume parameter, and the final diagram showing the dependence of  $\Pi_0^Q$  with  $\mathcal{V}$  is presented in figure 3.

A first theoretical approximation to obtain the expected value for the pressure parameter as  $T \rightarrow 0$  can be done considering the TF approximation in addition to the expressions for the condensate fraction  $N_0/N \simeq 1 - (T/T_c)^3$  [25] and for the critical temperature, valid for an ideal gas. The analytic expression obtained from equation (2) with such considerations is then given by

$$\Pi^{\text{TF}} = \frac{m}{21} \left( \frac{15\hbar^2 a_s}{m^2} \right)^{2/5} \left\{ \frac{N}{\mathcal{V}} - \left( \frac{k_B T}{0.94} \right)^3 \right\}^{7/5}. \quad (3)$$

In the limit of  $T \rightarrow 0$ ,  $\Pi_0(N)$  will depend only on the  $s$ -wave scattering length of the atomic cloud  $a_s$  and on its total number of atoms as follows in the equation below:



$$\Pi_0^{\text{TF}} \equiv \Pi^{\text{TF}}(T \rightarrow 0) = \frac{m}{21} \left( \frac{15\hbar^2 a_s}{m^2} \right)^{2/5} \left( \frac{N}{\mathcal{V}} \right)^{7/5}. \quad (4)$$

The TF approximation is valid only when the interaction dominates the kinetic energy term on the Hamiltonian of the system. Therefore, in the limit of  $N \rightarrow 0$ , equation (4) also goes to zero. For a large number of atoms ( $> 5 \times 10^5$  atoms), the validity of equation (4) has been demonstrated [22] but, as the number decreases, some deviations can be observed. This is mostly due to the fact that the TF approximation is not a good choice for a small number of atoms when the pressure parameter tends to the zero-point energy limit deviating from the expected zero value as  $N \rightarrow 0$ .

In the classical picture, the relation between  $\Pi$  and  $\mathcal{V}$  is proportional to the temperature of the system, and, in the case of  $T \rightarrow 0$ , the product  $\Pi \cdot \mathcal{V}$  vanishes [30]. Dealing with trapped quantum systems, one would expect that this relation should change since the minimum possible energy at  $T = 0$  is no longer zero.

A theoretical estimation of  $\Pi_0^Q$  can be made by taking into account the fact that the limit of  $N \rightarrow 1$  represents a system in which the interactions vanish and one can consider a single particle state in order to describe it. The ground state of the system corresponds to the ground state of a single particle trapped in a harmonic oscillator. Therefore, we consider the density profile given by

$$n_0(\mathbf{r}) = |\Psi(\mathbf{r})|^2 = \left( \frac{m\bar{\omega}}{\pi\hbar} \right)^{3/2} e^{-m(\omega_x x^2 + \omega_y y^2 + \omega_z z^2)/\hbar}. \quad (5)$$

Finally, by inserting equation (5) into equation (2), one obtains  $\Pi_0^Q$  as a function of  $\mathcal{V}$  and the ground state energy of a single particle  $E_0 = \frac{1}{2}(\omega_x + \omega_y + \omega_z)\hbar$  as follows:

$$\Pi_0^Q = \frac{1}{3} \frac{E_0}{\mathcal{V}}, \quad (6)$$

showing that the state equation is limited by the ground state energy of the system. It is interesting to note that this pressure parameter at the limit of zero temperature is equivalent to the pressure obtained for a gas of photons in a box ( $P_{\text{photons}} \sim \text{energy density}/3$ ). This is somehow not surprising because an ideal gas of bosons in a harmonic trap below the critical temperature is equivalent to a massless gas of bosons. Evidences of such similarities were found while observing  $\Pi$  versus  $T$  that results in  $\Pi \propto T^4$  at  $T < T_c$ , such as for a photon gas [17]. Such a point has also been indicated in [28].

As part of our discussion, we should clarify the method used to extract  $\Pi_0^Q$  from the data in figure 2. The regime we are working with is dominated by interactions (TF regime), and it cannot provide a good extrapolation for low atom numbers. We, therefore, consider that at  $T = 0$  the BEC atomic density is composed of two parts:  $n_{\text{TF}}(\mathbf{r})$  from the TF regime and  $n_{\text{Gauss}}(\mathbf{r})$  for the low atom number limit in which the interactions do not play an important role any longer. For each number of atoms at any volume parameter, the total density is given by  $n(\mathbf{r}) = \alpha n_{\text{TF}}(\mathbf{r}) + (1 - \alpha) n_{\text{Gauss}}(\mathbf{r})$  with

$$n_{\text{TF}}(\mathbf{r}) = \frac{15}{8\pi} \frac{N_0}{R_x R_y R_z} \max \left[ \left( 1 - \frac{x^2}{R_x^2} - \frac{y^2}{R_y^2} - \frac{z^2}{R_z^2} \right), 0 \right] \text{ and} \quad (7)$$

where  $R_i = \sqrt{\frac{2\mu}{m\omega_i^2}}$  are the TF radii and  $n_{\text{Gauss}}(\mathbf{r}) = N\bar{n}_0(\mathbf{r})$ , which has the same form of equation (5) but frequency values obtained from the TF fitting to our experimental data. The parameter  $\alpha$  is number dependent and should vary between 0, for low atom numbers, and 1, at high numbers, keeping a smooth transition between these extremes. In this sense, we proposed the following relation:

$$\alpha(N) = 1 - e^{-\frac{N}{N_a}}, \quad (8)$$

where  $N_a$  is the number above which the density starts to be predominantly given by the TF limit. With these definitions,

$$\Pi_0(N) = \alpha \Pi_0^{\text{TF}}(N) + (1 - \alpha) \Pi_0^{\text{Gauss}}(N), \quad (9)$$

and our experimental data could be appropriately fitted by the TF term. From this fit, we extracted the value of  $\mathcal{V}$  which then is used to calculate  $\Pi_0^Q = \Pi_0(N = 1)$ . In this way, we find the parameters of the best Gaussian density that would represent our system at low atom numbers. This was done for each volume parameter in order to be able to build the graph of figure 3. The fitting resulted in  $\frac{\Pi_0^Q}{E_0} = 0.2 \frac{1}{\mathcal{V}}$ , which is remarkably close to the expected value from equation (6). Figure 3 dependence indicates clearly that  $\Pi_0^Q$  and  $\mathcal{V}$  cannot be simultaneously zero, not even at  $T = 0$ , providing a remanent of the uncertainty principle for these two conjugated macroscopic thermodynamic quantities [31–34].

## 4. Conclusions

Pressure and volume constitute a very useful pair of independent variables to determine the state of a thermodynamic system. Equivalent with pairs of conjugated variables that, in the quantum limit, obey an uncertainty relation [31–34], it is somehow expected as an analogous constraint between pressure and volume [30, 35]. The preceding demonstration reveals ideas for the thermodynamic variables quite equivalent to the ones observed due to the uncertainty relation that compromises momentum and position (kinetic and potential energy) to generate the ground state energy of a system [36]. The fact that an equivalent compromise can exist between pressure and volume for a confined gas near absolute zero temperature is totally different from what is expected in traditional classical thermodynamics. Situations in which the equation of state is limited by the basic concepts of quantum mechanics open up a complete new window of possibilities for investigating quantities, such as susceptibilities, phase diagrams, and the construction of fully quantum thermodynamic machines, possibly demonstrating extreme conditions for the well established field of thermodynamics.

## Acknowledgments

We sincerely thank K. M. Farias for all the experimental support. We acknowledge financial support from FAPESP, CNPq, CAPES, and LENS.

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