

Equation of State of an Interacting Bose Gas Confined by a Harmonic Trap: The Role of the “Harmonic” Pressure

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A gas of interacting atoms confined by a three dimensional anisotropic harmonic potential is studied. It is shown that there appear “new” thermodynamic variables instead of the usual pressure and volume: the latter is replaced by (the inverse of) the cube of the geometric average of the oscillator frequencies of the trap, and the former by the harmonic pressure responsible for the mechanical equilibrium of the fluid in the trap. We discuss the origin and physical meaning of these quantities and show that the equation of state of the gas is given in terms of these variables. The equation of state of a cold gas of interacting Bose atoms in the Hartree-Fock approximation is presented. We indicate how the harmonic pressure can be measured in current experiments.

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The current experimental activity in the field of cold bosonic atoms [1–11] has prompted a review and development of novel theoretical tools to gain a better understanding of the thermodynamics of these systems. Toward this end, both theoretical [12–16] and experimental work [6–11] have been devoted to the elucidation of the temperature dependence and structure of the condensed fraction of atoms, the energy and heat capacity, and the release energy in time-of-flight measurements. Very recently, Gerbier *et al.* [11] have performed a detailed study of those thermodynamic properties in ^{87}Rb . However, little attention has been paid to the equation of state (EOS) *per se*. The purpose of this Letter is to contribute to filling this gap. As we shall indicate below, the EOS can be readily measured in current experiments.

We believe that the EOS has not been fully explored due to the fact that the volume and the usual pressure are no longer thermodynamic variables in a fluid confined by an external potential different from rigid walls. In other words, most of our thermodynamic intuition is developed with the use of pressure and volume as given thermodynamic variables and we tend to lose sight that these are appropriate only in systems contained in vessels. The current cold gases are not of this type. They are confined by a potential that interacts with the gas *everywhere*, not only at the walls, and this results in the gas becoming nonuniform. As a consequence, one reaches the conclusion that the pressure is neither uniform everywhere and the mechanical equilibrium condition is expressed, then, in terms of the *local* pressure tensor and the external force [17–19].

Thermodynamics, however, is a theory that deals with a few *global* variables. As we show here, one can deduce the role of (the inverse of) the cube of the geometric average of the frequencies of a harmonic trap as the *extensive* thermodynamic variable analogous to the volume. Then, one finds that there exists an *intensive* variable, conjugate to the

previous one, that plays an analogous role to the hydrostatic pressure in the sense that it is responsible for the mechanical equilibrium of the fluid with itself and with the external force of the trap. We shall refer to the inverse of the cube of the geometric average of the frequencies as the “harmonic volume” $\mathcal{V} = \omega^{-3}$ and to its conjugate variable as the “harmonic pressure” \mathcal{P} . These identifications allow us to construct the equation of state of these fluids, namely $\mathcal{P} = \mathcal{P}(N/\mathcal{V}, T)$. We shall also refer to $\rho = N\omega^3$ as the “harmonic” density.

The system we consider is a fluid (classical or quantum) of N identical particles of mass m , in thermodynamic equilibrium at temperature T , confined by a harmonic anisotropic trap of frequencies ω_1 , ω_2 , and ω_3 , with $\omega = (\omega_1\omega_2\omega_3)^{1/3}$ the geometric average frequency. If there is an interaction among the particles, we shall consider it to be pairwise additive via a short-range potential $v(|\vec{r}_i - \vec{r}_j|)$, with scattering length a . We shall concentrate mainly on bosonic systems but the general results apply to fermionic systems as well.

To motivate the introduction of the new variables, let us analyze first the case of N noninteracting bosons. By working in the grand canonical ensemble, the grand potential is found to be

$$\Omega(\mu, T, \omega) = -kT \left(\frac{kT}{\hbar\omega} \right)^3 g_4(\alpha), \quad (1)$$

where $\alpha = \mu/kT$, and μ is the chemical potential. $g_n(\alpha)$ are the Bose functions [20]. With this potential we can readily calculate the number of particles N , the internal energy E , and the entropy S as functions of μ , T , ω ;

$$N = \left(\frac{kT}{\hbar\omega} \right)^3 g_3(\alpha), \quad (2)$$

$$E = 3kT \left(\frac{kT}{\hbar\omega} \right)^3 g_4(\alpha), \quad (3)$$

and

$$S = k \left(\frac{kT}{\hbar\omega} \right)^3 [4g_4(\alpha) - \alpha g_3(\alpha)]. \quad (4)$$

These are the same formulas found by using a different approach [12] and already discussed in Refs. [16,21].

That ω is a bona fide thermodynamic variable can be simply verified by imagining an *adiabatic* change of the frequency of the trap at constant N : from Eqs. (2) and (4) one finds that $(T/\omega)^3$ is an adiabatic invariant and, therefore, a change in ω results in a change in temperature. Now, N , E , S , and Ω must be extensive. Hence, since T and μ are intensive, one finds by simple inspection of the previous formulas that ω^{-3} must also be extensive. In a harmonic potential the available volume for the gas is infinite. However, at a given temperature, the gas will mostly occupy a volume of the order of $(kT/m\omega^2)^{3/2}$, namely, proportional to ω^{-3} . Thus, the harmonic volume $\mathcal{V} = \omega^{-3}$ does make physical sense as a ‘‘volume’’ since small frequencies imply large actual volumes and vice versa. Notice an important point from the formula for N , Eq. (2): because that equation is rigorously exact only in the *thermodynamic limit*, such a limit must be $N \rightarrow \infty$, $\omega \rightarrow 0$, but $N\omega^3 \rightarrow \text{constant}$. This result will be used below. The role of the thermodynamic limit in the present form was originally pointed out by de Groot *et al.* [22] and has already been discussed by several authors; see Ref. [16] and references therein.

If \mathcal{V} is an extensive variable, then, there must be an intensive variable conjugate to it. This is

$$\mathcal{P} = - \left(\frac{\partial \Omega}{\partial \mathcal{V}} \right)_{T,\mu} = \frac{(kT)^4}{\hbar^3} g_4(\alpha); \quad (5)$$

manifestly an intensive variable [21]. It is clear that $\Omega = -\mathcal{P}\mathcal{V}$, in full analogy to a gas confined by rigid walls [20]. The physical meaning and significance of the harmonic pressure \mathcal{P} is given further below. A simple but very illuminating result is the classical limit of the above formulas [20], one finds $\mathcal{P}\mathcal{V} = NkT$, the equation of state of an ideal classical gas.

We now turn our attention to a fluid *with* interactions. The thermodynamics of the system is found by calculating, say, the Helmholtz free energy,

$$F(T, N, \omega^{-3}) = -kT \ln \text{Tr} e^{-\beta H}, \quad (6)$$

where we have already written ω^{-3} as the corresponding extensive variable. $H = K + U_{\text{int}} + V_{\text{ext}}$ is the Hamiltonian of the system with $K = \sum_i \vec{p}_i^2 / 2m$ the total kinetic energy, $U_{\text{int}} = \sum_{i < j} u(r_{ij})$ the interaction energy among the particles, and $V_{\text{ext}} = \sum_i (1/2)m(\omega_1^2 x_i^2 + \omega_2^2 y_i^2 + \omega_3^2 z_i^2)$ the external potential. One can show [23] that in the *thermodynamic limit* described above, $N\omega^3$ must be intensive in order for F to be extensive. That is, only in such a limit the Helmholtz free energy can be written as $F(N, \omega^3, T) = Nf(N\omega^3, T)$. Since N is exten-

sive by definition and F must be extensive then $\mathcal{V} = \omega^{-3}$ is extensive. The argument can be extended to any short-range multiple particle-particle interaction potential.

The harmonic pressure, conjugate to \mathcal{V} , is thus

$$\mathcal{P} = - \left(\frac{\partial F}{\partial \mathcal{V}} \right)_{N,T} = \frac{2}{3} \omega^3 \langle V_{\text{ext}} \rangle, \quad (7)$$

where the second line follows from using Eq. (6), and the average is taken over the corresponding (quantum or classical) canonical ensemble. Expression (7) for the harmonic pressure will prove to be very useful for experimental and calculational purposes. In order to grasp the physical meaning of \mathcal{P} we make use, first, of the virial theorem of classical and quantum mechanics. This yields $\langle V_{\text{ext}} \rangle = \langle K \rangle - \frac{1}{2} \langle \sum_i \vec{r}_i \cdot \frac{\partial U_{\text{int}}}{\partial \vec{r}_i} \rangle$, which, when substituted into Eq. (7) gives

$$\mathcal{P} = \frac{2}{3} \omega^3 \langle K \rangle - \frac{\omega^3}{3} \langle \sum_i \vec{r}_i \cdot \frac{\partial U_{\text{int}}}{\partial \vec{r}_i} \rangle. \quad (8)$$

If the system is classical, the first term in the right-hand side equals $N\omega^3 kT$, the classical ideal gas harmonic pressure. Equation (8) is a remarkable formula. It is *formally identical* to the virial equation of the hydrostatic pressure if one changes ω^{-3} by the volume V of a fluid confined by rigid walls [18]. Again, in the thermodynamic limit described above, it can be shown that the harmonic pressure is intensive depending only on T and $\rho = N/\mathcal{V} = N\omega^3$. This is the equation of state of the fluid, $\mathcal{P} = \mathcal{P}(\rho, T)$.

To show that \mathcal{P} is the variable responsible for mechanical equilibrium, we recall first that in a *nonuniform* fluid the pressure is no longer a constant neither isotropic. Instead, the mechanical equilibrium of the fluid is given in terms of the pressure tensor [24]. The condition for mechanical balance is

$$\nabla \cdot \tilde{P}(\vec{r}) = \vec{f}(\vec{r}), \quad (9)$$

where \tilde{P} is the pressure tensor of the fluid and \vec{f} is the external force per unit of volume. The latter is generated by the trap and it is given by $\vec{f}(\vec{r}) = -n(\vec{r})m(\omega_1^2 x\hat{i} + \omega_2^2 y\hat{j} + \omega_3^2 z\hat{k})$, where $n(\vec{r})$ is the local particle density of the fluid. By taking the scalar product of both sides of Eq. (9) with \vec{r} , integrating over all space and using Eq. (7) [see Eq. (11) below], one finds,

$$\mathcal{P} = \omega^3 \int d^3r \frac{1}{3} \text{Tr} \tilde{P}(r). \quad (10)$$

The physical meaning of the harmonic pressure is clear now. It is the integral of the invariant of the pressure tensor that is identified as the ‘‘pressure’’ in fluid mechanics [24]. For a uniform system confined within rigid walls, $(1/3) \text{Tr} \tilde{P} = p$, the hydrostatic pressure. That is, the harmonic pressure is not only the formal analog of the hydrostatic pressure in a uniform fluid but it has also the same physical meaning: it is the force that the fluid exerts against

itself and against the trap in order to reach mechanical equilibrium. That the harmonic pressure \mathcal{P} does not have units of force per unit of area is irrelevant, just as the harmonic volume \mathcal{V} does not have units of volume; what matters is that their product, as with any pair of thermodynamic canonical conjugate variables, does have units of energy.

The harmonic pressure, remarkably, is much more easily measurable than its hydrostatic counterpart. This can be seen from Eq. (7), by recasting it as,

$$\mathcal{P} = \frac{2}{3} \omega^3 \int d^3r n(\vec{r}) \left(\frac{1}{2} m (\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2) \right). \quad (11)$$

In current experiments with cold atoms the main quantity that it is measured is the particle density $n(\vec{r})$ [1–11]. Thus, the experimental elucidation of the equation of state of these gases could be done right away.

As can be seen from the virial expression Eq. (8), the harmonic pressure strongly depends on the interatomic collisions. In what follows, we shall consider a gas of cold bosonic atoms in a self-consistent Hartree-Fock (HF) approximation [15,25–28]. This description takes into account the presence of the thermal cloud below the Bose-Einstein condensation (BEC) transition and it has been found to be in good agreement with experimental

data [11]. As we can see from Eq. (11), we only need to know the particle density profile $n(\vec{r})$ in order to calculate the harmonic pressure. The HF approximation yields such a profile as the sum of the thermal component $n_{\text{th}}(\vec{r})$ plus the condensed fraction density $n_0(\vec{r})$. The thermal part is found self-consistently as [25]

$$n_{\text{th}}(\vec{r}) = \frac{1}{\lambda_T^3} g_{3/2}(\beta[\mu - V_{\text{eff}}(\vec{r})]), \quad (12)$$

where λ_T is the thermal de Broglie wavelength. The effective potential is given by

$$V_{\text{eff}}(\vec{r}) = V_{\text{ext}}(\vec{r}) + 2Un_0(\vec{r}) + 2Un_{\text{th}}(\vec{r}), \quad (13)$$

and the condensed particle density is found from

$$Un_0(\vec{r}) = \mu - V_{\text{ext}}(\vec{r}) - 2Un_{\text{th}}(\vec{r}) \quad (14)$$

when the right-hand side is positive and it is zero otherwise. In the above expressions $U = 4\pi\hbar^2 a/m$ is the mean-field coupling constant. The above equations can be solved with the restriction that the total number of particles is $N = \int [n_0(\vec{r}) + n_{\text{th}}(\vec{r})] d^3r$. Figures 1–3 summarize the EOS of this fluid, $\mathcal{P} = \mathcal{P}(\rho, T)$. We use dimensionless units in terms of the mass of the atoms m , Planck's constant \hbar , and the scattering length a , assumed to be positive. This

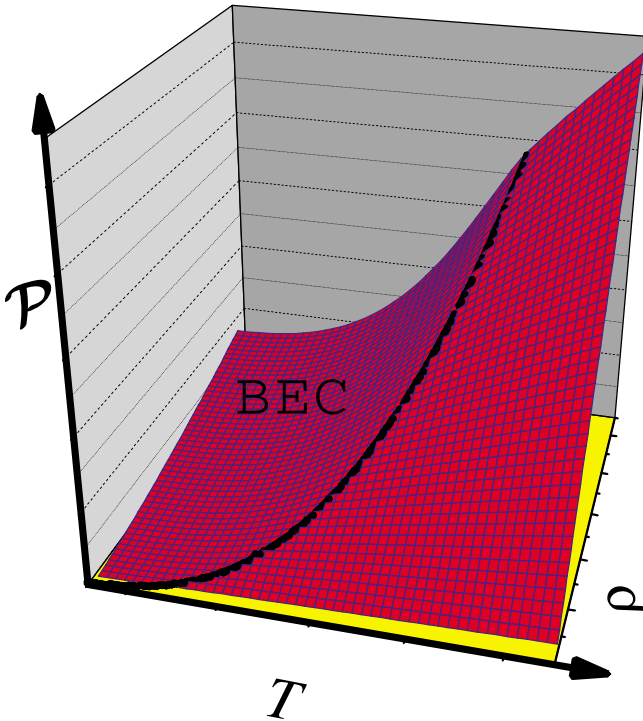


FIG. 1 (color online). Equation of state $\mathcal{P} = \mathcal{P}(\rho, T)$ for an interacting Bose gas in the Hartree-Fock approximation. The BEC transition and the BEC region are indicated. The intervals are $0.001 \leq T \leq 0.01$, $10^{-8} \leq \rho \leq 10^{-6}$ ($\rho = N\omega^3$), and $10^{-11} \leq \mathcal{P} \leq 10^{-8}$ in reduced units. These intervals correspond to gases with $0.3 \leq \eta \leq 0.7$.

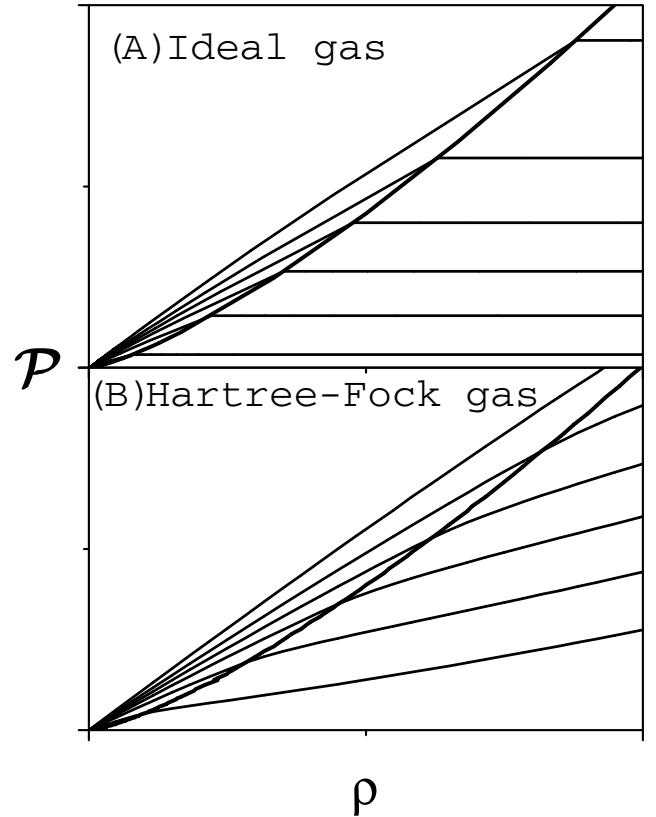


FIG. 2. Isotherms \mathcal{P} vs ρ . The intervals are $0 \leq \mathcal{P} \leq 4 \times 10^{-9}$, $0 \leq \rho \leq 6 \times 10^{-7}$. (a) Ideal gas. (b) Hartree-Fock gas.

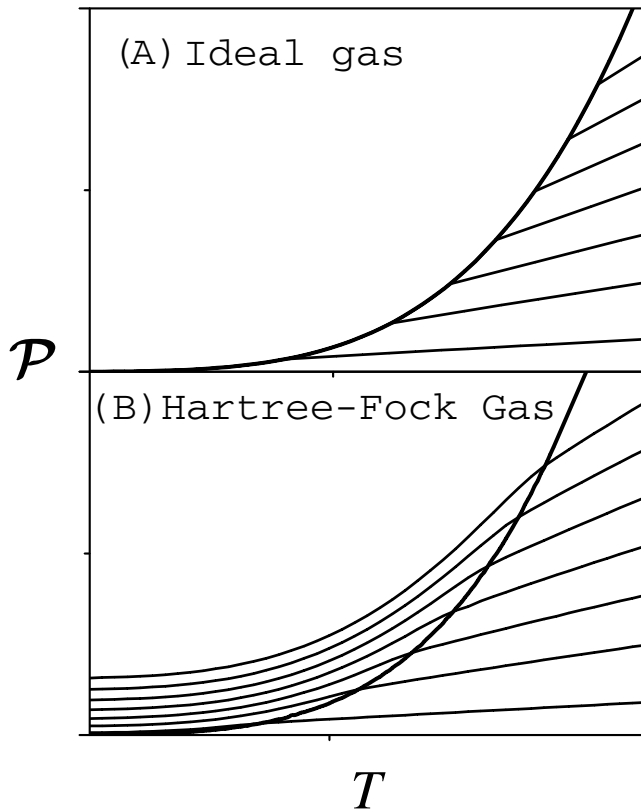


FIG. 3. Isochores \mathcal{P} vs T . The intervals are $0 \leq \mathcal{P} \leq 10^{-8}$, $0 \leq T \leq 0.01$. (a) Ideal gas. (b) Hartree-Fock gas.

choice of units can be cast in terms of the scaling parameter $\eta = \mu[N_0 = N]/kT_c^0$, introduced by Giorgini *et al.* [15], with N_0 the number of atoms in the condensate and T_c^0 the critical temperature of the corresponding ideal gas at the same harmonic density $\rho = N\omega^3$. The fragment of the EOS that we present in the figures goes from $\eta \approx 0.2$ to $\eta \approx 0.7$. The current experiments with alkaline atoms [6–11] lie within this interval. For instance, $\eta \sim 0.3$ – 0.4 in Ref. [7], while $\eta \approx 0.49$ in Ref. [11]. The interatomic interactions in these intervals cannot be neglected. Figure 1 is the surface $\mathcal{P} = \mathcal{P}(\rho, T)$. We have indicated the curve of the BEC transition found when the condensed fraction becomes different from zero. In Figs. 2 and 3 we show the isotherms \mathcal{P} vs ρ and the isochores \mathcal{P} vs T both for the HF and the ideal cases [see Eq. (5)]. The main observation, quantitatively measurable, is that contrary to the ideal case, the condensed fraction of *interacting* atoms plays a thermodynamic role. That is, in the ideal case the condensed fraction exerts no pressure (just as in the usual BEC in a box). Thus, the role of the interactions is not only to shift the value of the critical temperature (at a given harmonic density), as it has been extensively verified, but the interactions also allow the atoms in the condensed phase to participate in the process of mechanical equilibrium. From Fig. 2 we see that the pressure continues to grow above the BEC transition as the density is increased,

while from Fig. 3 we find that the pressure saturates to a value different from zero as the temperature vanishes.

With the knowledge of the harmonic pressure and volume, the number of particles and the chemical potential, and the internal energy and temperature, the thermodynamics of these systems is fully determined since the entropy is given by $TS = E + \mathcal{P}\mathcal{V} - \mu N$.

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- [1] M. H. Anderson *et al.*, *Science* **269**, 198 (1995).
- [2] K. B. Davis *et al.*, *Phys. Rev. Lett.* **75**, 3969 (1995).
- [3] C. C. Bradley, C. A. Sackett, and R. G. Hulet, *Phys. Rev. Lett.* **78**, 985 (1997).
- [4] M. R. Matthews *et al.*, *Phys. Rev. Lett.* **83**, 2498 (1999).
- [5] C. Orzel *et al.* *Science* **291**, 2386 (2001).
- [6] M. O. Mewes *et al.*, *Phys. Rev. Lett.* **77**, 416 (1996).
- [7] J. R. Ensher *et al.*, *Phys. Rev. Lett.* **77**, 4984 (1996).
- [8] D. J. Han *et al.*, *Phys. Rev. A* **57**, R4114 (1998).
- [9] B. P. Anderson and M. A. Kasevich, *Phys. Rev. A* **59**, R938 (1999).
- [10] F. Schreck *et al.*, *Phys. Rev. Lett.* **87**, 080403 (2001).
- [11] F. Gerbier *et al.*, *Phys. Rev. A* **70**, 013607 (2004).
- [12] V. Bagnato, D. E. Pritchard, and D. Kleppner, *Phys. Rev. A* **35**, 4354 (1987).
- [13] H. Shi and W.-M. Zheng, *Phys. Rev. A* **56**, 1046 (1997); *Phys. Rev. A* **56**, 2984 (1997).
- [14] A. Minguzzi, S. Conti, and M. P. Tosi, *J. Phys. Condens. Matter* **9**, L33 (1997).
- [15] S. Giorgini, L. P. Pitaevskii, and S. Stringari, *Phys. Rev. A* **54**, R4633 (1996); *Phys. Rev. Lett.* **78**, 3987 (1997).
- [16] F. Dalfovo *et al.*, *Rev. Mod. Phys.* **71**, 463 (1999).
- [17] J. K. Percus, in *The Liquid State of Matter: Fluids, Simple and Complex*, edited by E. W. Montroll and J. L. Lebowitz (North-Holland, Amsterdam, 1982).
- [18] J. S. Rowlinson and D. Widom, *Molecular Theory of Capillarity* (Clarendon, Oxford, 1982).
- [19] V. Romero-Rochín and J. K. Percus, *Phys. Rev. E* **53**, 5130 (1996).
- [20] L. Landau and L. Lifhitz, *Statistical Physics* (Pergamon, Oxford, 1980), Part 1.
- [21] V. Romero-Rochín and V. S. Bagnato, in *Developments in Mathematical and Experimental Physics*, edited by A. Macias, F. Uribe, and E. Diaz (Kluwer, New York, 2003), Vol. B.
- [22] S. R. de Groot, G. J. Hooyman, and C. A. Ten Seldam, *Proc. R. Soc. London A* **203**, 266 (1950).
- [23] L. E. Díaz-Sánchez and V. Romero-Rochín (to be published).
- [24] L. Landau and L. Lifhitz, *Fluid Mechanics* (Pergamon, Oxford, 1959).
- [25] V. V. Goldman, I. F. Silvera, and A. J. Leggett, *Phys. Rev. B* **24**, R2870 (1981).
- [26] D. A. Huse and E. D. Siggia, *J. Low Temp. Phys.* **46**, 137 (1982).
- [27] J. Oliva, *Phys. Rev. B* **39**, 4197 (1989).
- [28] A. Griffin, *Phys. Rev. B* **53**, 9341 (1996).