PHYSICAL REVIEW E **78**, 061129 (2008)

Thermodynamics of trapped gases: Generalized mechanical variables, equation of state, and heat capacity

Nadia Sandoval-Figueroa[*] and Víctor Romero-Rochín[†]
Instituto de Física, Universidad Nacional Autónoma de México, Apartado Postal 20-364, 01000 México, Distrito Federal Mexico

(Received 6 May 2008; revised manuscript received 7 October 2008; published 24 December 2008)

We present the full thermodynamics of an interacting fluid confined by an arbitrary external potential. We show that for each confining potential, there emerge "generalized" volume and pressure variables $\mathcal{V}$ and $\mathcal{P}$, that replace the usual volume and hydrostatic pressure of a uniform system. This scheme is validated with the derivation of the virial expansion of the grand potential. We discuss how this approach yields experimentally amenable procedures to find the equation of state of the fluid, $\mathcal{P}=\mathcal{P}(\mathcal{V}/N,T)$ with N the number of atoms, as well as its heat capacity at constant generalized volume $C_{\mathcal{V}}=C_{\mathcal{V}}(\mathcal{V},N,T)$. With these two functions, all the thermodynamics properties of the system may be found. As specific examples we study weakly interacting Bose gases trapped by harmonic and by linear quadrupolar potentials within the Hartree-Fock approximation. We claim that this route provides an additional and useful tool to analyze both the thermodynamic variables of an ultracold trapped gas as well as its elementary excitations.

DOI: 10.1103/PhysRevE.78.061129 PACS number(s): 05.70.−a, 03.75.Hh, 03.75.Ss

I. INTRODUCTION

The intense experimental and theoretical activity in the field of quantum ultracold trapped gases [1–24] has largely stimulated first principles analysis of the physics of these inhomogeneous systems. In particular, the calculation of density profiles has turned out to be of fundamental importance since it is one of the main measurable quantities in the recent experiments. From the density profile several thermodynamic quantities can be obtained, such as the number of particles and the temperature. However, because the hydrostatic pressure is a local quantity and the volume of the system cannot be rigorously defined, the use of thermodynamics as a tool to analyze and characterize such trapped gases has been of limited application. For instance, important properties and quantities such as the equation of state of the fluid or its heat capacities, are lacking. As we discuss here, those properties can be extracted from the knowledge of the density profile and other simple properties of the trapped gases.

The main purpose of this paper is to emphasize the fact that the thermodynamics of trapped systems must be reformulated in terms of the appropriate mechanical variables that, for lack of a better name, we shall call generalized pressure $\mathcal{P}$ and volume $\mathcal{V}$. That is, the usual hydrostatic pressure p and the volume V of a fluid contained in a vessel of rigid walls are no longer thermodynamic variables for a fluid confined by an external inhomogeneous field $V_{\text{ext}}(\vec{r})$. As mentioned above, in the presence of an arbitrary confining potential, the pressure of the fluid becomes a local variable $p=p(\vec{r})$ and the volume is strictly undefined. As we shall show there is a "new" and unique pair of variables $\mathcal{P}$ and $\mathcal{V}$ that replace the usual ones, p and V. We shall illustrate these variables with specific examples. This result has already been pointed out for a gas trapped in a harmonic potential [16–18] and incipient comparisons have been made with experiments in ultracold Na gases [25–27] showing its potential usefulness. However, we believe the main point has not been fully appreciated, namely, the fact that a different set of thermodynamics variables must be used for a given external confining potential. We proceed here to fill this gap, deducing the virial expansion for the grand potential in the grand canonical ensemble for an arbitrary external potential, valid for classical and quantum fluids, either ideal or with pairwise interatomic interactions. Extensions to three-or higher-body interactions may be further considered. We discuss the physical meaning of the generalized pressure and its relevance regarding the equation of state of the fluid, i.e., $\mathcal{P}=\mathcal{P}(\mathcal{V}/N,T)$ with N the number of molecules or atoms in the fluid and T the temperature. This finding should have immediate practical applications since all the thermodynamic properties, especially phase transitions, can be quantitatively described and certainly visualized in the corresponding phase diagram. We emphasize the fact that the generalized pressure can be very simply measured or calculated once the particle density profile $\rho(\vec{r})$ is known. This procedure has already been exploited in the analysis of experimental data of trapped Na ultracold gases in quadrupolar [25] and in harmonic traps [26,27]. As a further step, we propose a simple and independent experiment that, in addition to the knowledge of the equation of state, allows for the determination of the heat capacity at constant generalized volume $\mathcal{V}$, $C_{\mathcal{V}}$. This experiment should be easily performed in the currently confined ultracold gases. To the best of our knowledge there are no measurements of such a heat capacity. It is a simple exercise to show that knowledge of the equation of state $\mathcal{P}=\mathcal{P}(\mathcal{V}/N,T)$ and the heat capacity $C_{\mathcal{V}}=C_{\mathcal{V}}(N,\mathcal{V},T)$ suffices to know all the thermodynamics of a pure fluid. We need not overemphasize the fact that the quantitative features of the latter quantities are direct consequences of the interatomic interactions and of the collective excitations of the fluid.

As a corollary of our analysis we shall show that the so-called "local density approximation" (LDA) follows within the appropriate thermodynamic limit of the confining potentials. Our results are in agreement with rigorous proofs

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[*] nadia@fisica.unam.mx

[†] Corresponding author.; romero@fisica.unam.mx

of LDA for classical systems [28,29] and quantum systems [30] as well; these works have been largely overlooked in the current literature of ultracold gases, but are very relevant since they show that, under the appropriate conditions, LDA is an exact procedure. The validity of LDA is expected, and certainly widely used, because in the trapped gases the main nonuniformity appears at macroscopic length scales due to the presence of the confining external field. That is, the latter must be "macroscopic" in order to trap a large number of particles. For macroscopic potentials this equivalently means that the energy-level separations of the external potential are much smaller than the typical atomic and collective excitations [1–11]. Although LDA has been used in essentially all current works on ultracold gases that yield density profiles, its validity is mostly assessed on these physical grounds. Thus, it is reassuring to find that the virial expansion when applied to confined quantum fluids yields LDA as well. As we shall discuss, however, care must be taken when using it. That is, LDA can be directly used for the grand potential density, the entropy density, and the particle density, but not so for the internal energy and other free energy densities, among other possible thermodynamic quantities. That is, while it gives a procedure to calculate thermodynamic properties of a confined inhomogeneous fluid, it does not imply that the local states of the trapped fluid are thermodynamic states of the corresponding homogenous fluid.

To show the usefulness of the general framework we have introduced, we devote a section to analyze a confined weakly interacting Bose gas as a particular and relevant example. We study gases confined by harmonic and by linear quadrupolar traps within the Hartree-Fock approximation. We calculate the phase diagram $\mathcal{P}$-T and the heat capacity at constant volume. Based on these properties, a brief discussion on the nature of the normal gas to superfluid transition is presented. It is found that the transition is completely smooth but with no trace of critical behavior.

II. THERMODYNAMIC VARIABLES OF TRAPPED GASES

The system consists of N identical atoms or particles of mass m with Hamiltonian

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

We assume additive pairwise potentials but the analysis may be extended to arbitrary interatomic interactions. The external potential $V_{\rm ext}(\vec{r})$ confines the system. To serve this purpose, it should have at least one minimum and must obey that $V_{\rm ext}(\vec{r}) \to \infty$ for $|\vec{r}| \to \infty$. For rigid-wall containers it is customary not to write the potential; here, we include it as $V_{\rm ext}(\vec{r})=0$ if $\vec{r}$ is within the volume V enclosed by the rigid walls and $V_{\rm ext}(\vec{r})=\infty$ if $\vec{r}$ is outside of it. Typical examples of traps of atomic gases are $V_{\rm ext}(\vec{r})=(1/2)m(\vec{\omega}\cdot\vec{r})^2$, a harmonic potential, such as in Ref. [1], and $V_{\rm ext}(\vec{r})=|\vec{A}\cdot\vec{r}|$, a linear quadrupolar potential [25]; but one can consider any confining potential such as a Pöschl-Teller [31] $V_{\rm ext}(\vec{r})=V_0/\cos^2(\vec{\gamma}\cdot\vec{r})$ for $|x| \leq \pi/2\gamma_x$ and analogously for y and z. This last case serves as an example of a potential that, in addition to a generalized volume, introduces an additional intensive variable, namely, V_0. We write these potentials to exemplify the appropriate thermodynamic variables as well as the thermodynamic limit for each case.

To illustrate how the generalized variables emerge and how the thermodynamic limit is to be taken, we shall deal here first with a classical ideal gas. Further below, we shall treat an interacting fluid and we shall verify the correctness of the identification of the variables given here. Consider, therefore, a system given by the Hamiltonian (1) with no interatomic interactions, i.e., $u(|r_{ij}|)\equiv 0$. Assume the system is in thermodynamic equilibrium at temperature T. The canonical partition function is

$$Z(T,N,\mathcal{V}) = \frac{1}{h^{3N}N!}\int d^{3N}p \int d^{3N}r \times \exp\left[-\beta\sum_{i=1}^{N}\left(\frac{\vec{p}_i^{\,2}}{2m} + V_{\rm ext}(\vec{r}_i)\right)\right], \tag{2}$$

where $\beta=1/kT$. We assume the external confining potential to be of the form $V_{\rm ext}=V_{\rm ext}(x/l_x, y/l_y, z/l_z, \eta)$ where the quantities l_i do not necessarily have units of length and η stand for other parameters that we assume to remain constant throughout. Integration of the partition function yields

$$Z(T,N,\mathcal{V}) = \frac{1}{N!\lambda_T^{3N}}[\zeta(\beta)\mathcal{V}]^N, \tag{3}$$

where $\lambda_T=h/(2\pi mkT)^{1/2}$ is de Broglie thermal wavelength, $\mathcal{V}=l_xl_yl_z$ is the generalized volume, and the function $\zeta(\beta)$ is defined by

$$\zeta(\beta)\mathcal{V} = \int e^{-\beta V_{\rm ext}(\vec{r})}d^3r. \tag{4}$$

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

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

For the free energy per particle, F/N, to remain finite in the thermodynamic limit, $N\to\infty$, it must be required that the "generalized" volume diverges, i.e., $\mathcal{V}\to\infty$, keeping constant the "density" $N/\mathcal{V}$. As it will be fully justified below, $\mathcal{V}$ is an extensive thermodynamic variable. The generalized volume certainly is proportional to the actual average volume that the system occupies, $\bar{V}\sim\zeta(\beta)\mathcal{V}$. This average volume, however, is not an independent thermodynamic variable since it depends on the temperature. Moreover, it is not a correct variable since the actual volume that the system occupies is, in fact, unbounded. Nevertheless, the thermodynamic limit $\mathcal{V}\to\infty$ indeed implies that the volume of the system becomes arbitrarily large.

For the particular external potentials here considered one finds $\mathcal{V}=V$ for rigid walls, $\mathcal{V}=1/\omega_x\omega_y\omega_z$ for the harmonic potential, $\mathcal{V}=1/A_xA_yA_z$ for the quadrupolar potential, and $\mathcal{V}=1/\gamma_x\gamma_y\gamma_z$ for the Pöschl-Teller potential. Likewise, we find $\zeta(\beta)=1$ for rigid walls, $\zeta(\beta)=(2\pi/\beta m)^{3/2}$ for the harmonic potential, $\zeta(\beta)=8\pi/\beta^3$ for the quadrupolar potential, and

$\zeta(\beta)=4\pi\int_{-\pi/2}^{\pi/2}x^2\exp(-\beta V_0/\cos^2 x)dx$ for the Pöschl-Teller potential. For the harmonic case, it has been known for quite a long time that the thermodynamic limit is the one here presented [32]. As we shall see, while the role of the generalized volume is completely analogous to that of the usual volume in homogeneous systems, the thermodynamic properties of the different confined fluids show very strong variations on their temperature dependences due to the function $\zeta(\beta)$.

For purposes of presentation we have assumed that the fluids under study are effectively three dimensional. That is, we suppose that in the three spatial dimensions the trap becomes macroscopic. It is clear that the theory can be adjusted to deal with (quasi-) two- and one-dimensional systems. For this to occur, the trap must be spatially very tight in one or two directions, which also implies that the fluid thermal excitations in those directions are smaller than the trap energy levels in the same direction; thermodynamic behavior can only exist in the remaining directions. This is the case for the very recent studies on the Berezinskii-Kosterlitz-Thouless transition in quasi-2D harmonic traps in clouds of ^{87}Rb [33,34] and ^{23}Na gases [35], and where a generalized area and pressure can be defined.

As it will be fully justified below with the virial expansion for an interacting gas confined in an arbitrary potential, the generalized volume is a bona-fide extensive variable. Therefore, there exists an intensive variable, conjugate to the volume $\mathcal{V}$, that we call the generalized pressure $\mathcal{P}$ 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

$$\mathcal{P}=\frac{1}{3\mathcal{V}}\left\langle \sum_{i=1}^{N}\vec{r}_i\cdot\vec{\nabla}_i V_{\text{ext}}(\vec{r}_i)\right\rangle=\frac{1}{3\mathcal{V}}\int \rho(\vec{r})\vec{r}\cdot\vec{\nabla}V_{\text{ext}}(\vec{r})d^3r, \tag{7}$$

where in the first line the average is performed in the corresponding ensemble and in the second line we have introduced the density profile $\rho(\vec{r})$. The last equality is a remarkable formula since it gives rise, with the sole knowledge of the density profile $\rho(\vec{r})$ and the temperature T, to a direct route for the calculation of the generalized pressure and, hence, to the equation of state of the fluid, $\mathcal{P}=\mathcal{P}(\mathcal{V}/N,T)$. We recall that the density profile may be known from exact or approximate calculations, or directly from experiments. In Sec. V we shall use this result for the calculation of the phase diagram of a confined interacting Bose gas within the Hartree-Fock approximation. We note that the expression (7) is valid for any external potential, including the rigid-wall case. It is interesting to note that for the latter case, such an identification of the hydrostatic pressure serves to be used in the so-called virial theorem to find the well-known expression relating the pressure to the two-body density correlation function [36]. Here, we find that Eq. (7) yields a direct calculational tool for the generalized pressure. Thus, for inhomogeneous systems knowledge of the one-body density suffices.

It is important to point out that the identification of the generalized pressure is not only a formal one but it has a clear physical meaning. From the thermodynamic definition of $\mathcal{P}$, Eqs. (6) and (7), one sees that the product $\mathcal{P}\mathcal{V}$ equals (1/3) of (minus) the virial of the external force. Hence, one can recall that mechanical equilibrium in a fluid is given by Pascal law,

$$\vec{\nabla}\cdot\tilde{P}(\vec{r})=-\rho(\vec{r})\vec{\nabla}V_{\text{ext}}(\vec{r}), \tag{8}$$

where $\tilde{P}(\vec{r})$ is the pressure tensor of the fluid. One expects the pressure tensor to be a local quantity, $\tilde{P}(\vec{r})=p(\vec{r})\tilde{1}$, where $\tilde{1}$ is the unit tensor and $p(\vec{r})$ is the local hydrostatic pressure, barring phase-separated states within the confined fluid. By calculating the virial of the right-hand side of Eq. (8), and after integrating by parts, one finds

$$\int \text{Tr}\,\tilde{P}d^3r=\int d^3r\rho(\vec{r})\vec{r}\cdot\vec{\nabla}V_{\text{ext}}(\vec{r})=3\mathcal{P}\mathcal{V}. \tag{9}$$

That is, $\mathcal{P}$ for a nonuniform fluid confined by a given external potential plays the same thermodynamic role as the hydrostatic pressure p in a uniform fluid: It is the quantity that bears the information that the fluid is in mechanical equilibrium.

To obtain the thermodynamics of a pure system the knowledge of the free energy as a function of two independent variables is needed. Thus, in addition to the equation of state, one needs another quantity. This may be the heat capacity at constant generalized volume. As we now show, the measurement of the heat capacity $C_{\mathcal{V}}$ should also be achievable within the current experimental setups. We propose here how to measure it by means of adiabatic compressions and expansions. We note first that the ultracold trapped gases are actually isolated and confined by magnetic or optical traps [1–11]. Therefore, a slow change of the confining potential, namely, of the generalized volume $\mathcal{V}$, should give rise to an increase or decrease of the temperature T depending on whether the fluid is compressed or expanded. Since the generalized volume and temperature are measurable in the current experiments, the quantity $(\partial\mathcal{V}/\partial T)_{N,S}$ can, therefore, be calculated. The corresponding heat capacity can then be evaluated using the following thermodynamic relationship:

$$C_{\mathcal{V}}=-T\left(\frac{\partial \mathcal{P}}{\partial T}\right)_{\mathcal{V},N}\left(\frac{\partial \mathcal{V}}{\partial T}\right)_{N,S}. \tag{10}$$

We note that previous knowledge of the equation of state is needed for the calculation of the second factor on the right-hand side of (10). However, the measurements of the equation of state and of the quantity $(\partial\mathcal{V}/\partial T)_{N,S}$ correspond to two different sets of experiments.

III. VIRIAL EXPANSION FOR ARBITRARY CONFINING POTENTIALS

With the identification of the generalized variables and the corresponding thermodynamic limit in hand, we now turn to the general problem of an interacting gas, classical or quantum. We extend the analysis described in the texts by Mayer and Mayer [37], ter Haar [38] and Blatt [39]. Again, we assume the system is in thermodynamic equilibrium at temperature T and we analyze it in the grand canonical ensemble. We thus consider a chemical potential μ whose value may be found by imposing a given number of particles N. The grand potential is given by

$$\Omega = -kT \ln \sum_{N=0}^{\infty} e^{\beta\mu N}\, \mathrm{Tr}'\, e^{-\beta H_N}, \tag{11}$$

where

$$\mathrm{Tr}'\, e^{-\beta H_N} = \frac{1}{h^{3N} N!} \int d^{3N}r \int d^{3N}p e^{-\beta H_N}, \tag{12}$$

if the system is classical, and

$$\mathrm{Tr}'\, e^{-\beta H_N} = \frac{1}{N!}\sum_P \epsilon^P \int d^{3N}r \langle \vec{r}_1,\vec{r}_2,\ldots,\vec{r}_N | e^{-\beta H_N} | \vec{r}_{1P},\vec{r}_{2P},\ldots,\vec{r}_{NP}\rangle, \tag{13}$$

if the system is quantum. The sum is over all permutations of $1,2,\ldots,N$ and $\epsilon = \pm 1$ for bosons or fermions.

To find the virial expansion, Eq. (11) is first rewritten as [37–39]

$$-\beta\Omega = \sum_{n=1}^{\infty} e^{\beta\mu n} \frac{1}{n!} I_n, \tag{14}$$

where the functions I_n are given by

$$I_n = \begin{cases} \dfrac{1}{h^{3n}} \displaystyle\int d^{3n}r \int d^{3n}p U_n(\vec{r}_1,\vec{p}_1;\ldots;\vec{r}_n,\vec{p}_n), \\ \displaystyle\int d^{3n}r U_n(\vec{r}_1,\ldots,\vec{r}_n) \end{cases} \tag{15}$$

for classical and quantum systems, respectively, and where the Ursell functions are given by the hierarchy: First order,

$$U_1(1) = W_1(1), \tag{16}$$

second order,

$$U_2(1,2) = W_2(1,2) - U_1(1)U_1(2), \tag{17}$$

third order,

$$\begin{aligned} U_3(1,2,3) = W_3(1,2,3) &- U_1(1)U_2(2,3) - U_1(2)U_2(1,3) \\ &- U_1(3)U_2(1,2) - U_1(1)U_1(2)U_1(3), \end{aligned} \tag{18}$$

and so on, and

$$W_n(1,2,\ldots,n) = \begin{cases} e^{-\beta H_n}, \\ \displaystyle\sum_P \epsilon^P \langle \vec{r}_1,\vec{r}_2,\ldots,\vec{r}_n | e^{-\beta H_n} | \vec{r}_{1P},\vec{r}_{2P},\ldots,\vec{r}_{nP}\rangle \end{cases} \tag{19}$$

for classical and quantum systems, respectively.

The problem of the virial expansion reduces to find the value of each contribution I_n in the thermodynamic limit, taking into account the interactions among the atoms or molecules. This is what we do now for a general confining external potential $V_{\mathrm{ext}}(\vec{r})$. We proceed by systematically calculating I_n order by order and then generalize it to I_n. We did so from I_1 to I_4. Since the calculations are quite lengthy, though straightforward, we explicitly present in the Appendix the case I_2 only. Next we discuss the results.

The calculation of I_1 is very simple and it turns out that, in the thermodynamic limit, the classical and quantum cases give the same result,

$$I_1 = \begin{cases} \dfrac{1}{h^3} \displaystyle\int d^3p \int d^3r e^{-\beta H_1}, \\ \displaystyle\int d^3r \langle \vec{r} | e^{-\beta H_1} | \vec{r} \rangle, \end{cases} \tag{20}$$

where the one-particle Hamiltonian H_1 is given by

$$H_1 = \frac{\vec{p}^2}{2m} + V_{\mathrm{ext}}(\vec{r}). \tag{21}$$

In the limit, one finds

$$I_1 = \frac{1}{\lambda_T^3} \zeta(\beta) \mathcal{V} \tag{22}$$

for both classical and quantum cases.

In the Appendix we show the explicit calculation of I_2. That analysis suffices to see how to find I_n. The key is in the separation of center of mass and relative coordinates. This change of variables is generally, $\vec{R} = \frac{1}{n}(\vec{r}_1 + \vec{r}_2 + \cdots + \vec{r}_n)$, $\vec{r}^{(1)} = \vec{r}_1 - \vec{r}_2$, $\vec{r}^{(2)} = \vec{r}_2 - \vec{r}_3, \ldots, \vec{r}^{(n-1)} = \vec{r}_{n-1} - \vec{r}_n$, with their canonical conjugate momenta.

In both the classical and quantum cases, the main assumption is the same, namely, that one must take the thermodynamic limit $\mathcal{V} \to \infty$. This allows us to make the approximation,

$$V_{\mathrm{ext}}(\vec{r}_1) + V_{\mathrm{ext}}(\vec{r}_2) + \cdots + V_{\mathrm{ext}}(\vec{r}_n) \approx n V_{\mathrm{ext}}(\vec{R}), \tag{23}$$

where $(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_n)$ are to be given in terms of the variables $(\vec{R},\vec{r}^{(1)},\vec{r}^{(2)},\ldots,\vec{r}^{(n-1)})$ by the above transformation. This approximation separates the center-of-mass motion from the relative ones. The former is always quasiclassical and its contribution to I_n is proportional to $\zeta(n\beta)\mathcal{V}/\lambda_T^{3n}$, while the contribution from the relative coordinates yields the virial coefficients b_n; these can be classical or quantum, but they are the same for any external potential. That is, we find

$$I_n = \frac{\mathcal{V}}{\lambda_T^{3n}} \zeta(n\beta) b_n. \tag{24}$$

The validity of the above procedure, in the classical case, reduces to require that the intermolecular potential must vanish for lengths $r \gg \sigma$, with σ the range of such a potential. Additionally, the interaction must be "short range," namely, decaying faster than $1/r^3$, otherwise the virial coefficients b_n do not exist [37,40]. In the quantum case and for high temperatures, the range of the relative variables $\vec{r}$ is bounded due to presence of the potential $u(r)$ and the validity has the same limitations as in the classical case. At low temperatures the bound is set up by either the thermal de Broglie wavelength or the scattering length a [41]. If the gas behaves as an ideal one, the relevant length is de Broglie wavelength. In any case, as long as the relative coordinates remain bounded by a finite quantity, however large, one can take the limit of very large volumes, $\mathcal{V}\rightarrow\infty$, and implement the thermodynamic limit just as in the classical case.

Summarizing, we find that in the thermodynamic limit the grand potential can be written in general as

$$\Omega = -kT\mathcal{V}\sum_{n=1}^{\infty}\frac{e^{\beta n\mu}}{n!}\frac{\zeta(n\beta)}{\lambda_T^{3n}}b_n(T), \tag{25}$$

where quantum or classical virial coefficients should be used; in both cases $b_1=1$. Expression (25) for the grand potential is one of the main results of this paper. It is the virial expansion for arbitrary confining potentials. The number of particles N and the entropy S can be calculated from (minus) the partial derivatives of Ω with respect to μ and T, respectively. Ω, N, and S are found to be homogeneous first-order functions of $\mathcal{V}$, and this implies that $\mathcal{V}$ must be an extensive variable and justifies the thermodynamic limit as used above. From the expression $\Omega=-\mathcal{P}\mathcal{V}$, the generalized pressure is read off (25). Strictly speaking, the expression for Ω is an expansion in the fugacity $z=\exp(\beta\mu)$. The actual virial expansion of the pressure $\mathcal{P}$, as a power series in the generalized density $N/\mathcal{V}$, may be found from inverting $N=N(V,\mu,T)$ to yield $\mu=\mu(N/\mathcal{V},T)$, and substitute into $\mathcal{P}=\mathcal{P}(\mu,T)$.

Note that the most important difference of the grand potential between a given arbitrary external potential and the homogeneous case is the function $\zeta(\beta)$ rather than the generalized volume $\mathcal{V}$. The latter enters in the same way for any potential, including the rigid-walls case; that is, it gives rise to the intensive quantities formed between the extensive variables N, S, E, etc., and $\mathcal{V}$, and that remain finite in the thermodynamic limit, i.e., $N/\mathcal{V}$, $S/\mathcal{V}$, $E/\mathcal{V}$, etc. However, as it is well known from calculations in external potentials, the temperature dependence of the thermodynamic variables is very different and unique for each external potential. This difference is contained in the function $\zeta(\beta)$. This will be exemplified in the next section.

To illustrate the use of Eq. (25), we apply it to an ideal quantum gas. From the analysis in the Appendix and their corresponding value for third and fourth orders, one finds that the virial coefficients are given by

$$b_n^{(0)} = \epsilon^{n+1}\frac{n!}{n^{5/2}}\lambda_T^{3(n-1)}. \tag{26}$$

The grand potential for an ideal quantum gas can, thus, be written as

$$-\beta\Omega = \frac{\mathcal{V}}{\lambda_T^3}\sum_{n=1}^{\infty}e^{n\beta\mu}\zeta(n\beta)\frac{\epsilon^{n+1}}{n^{5/2}}. \tag{27}$$

This formula can be directly compared with the corresponding ones for, say, the rigid walls potential $\mathcal{V}=V$ and $\zeta(n\beta)=1$, or the harmonic potential $\mathcal{V}=1/\omega^3$ and $\zeta(n\beta)=(2\pi kT/nm)^{3/2}$. The "textbook" formulas for these potentials are [42]

$$-\beta\Omega = \frac{V}{\lambda_T^3}\frac{1}{\Gamma(5/2)}\int_0^{\infty}\frac{x^{3/2}dx}{e^{x-\beta\mu}-\epsilon} \tag{28}$$

for rigid walls, and

$$-\beta\Omega = \left(\frac{kT}{\hbar\omega}\right)^3\frac{1}{\Gamma(4)}\int_0^{\infty}\frac{x^3dx}{e^{x-\beta\mu}-\epsilon} \tag{29}$$

for a three-dimensional (3D) isotropic harmonic potential. Expansion of the integrals of these last two equations in powers of $e^{\beta\mu}$ yield the virial expansion, Eq. (27).

IV. A COMMENT ON THE "LOCAL DENSITY APPROXIMATION"

The exactness, or validity, of the "local density approximation" follows right away from the corresponding expressions for Ω, N, and S, as given by Eq. (25). Consider the rigid-wall external potential, $\mathcal{V}=V$ and $\zeta(n\beta)=1$. We can thus define the grand potential per unit volume $\omega(\mu,T)=\Omega/V$, the number of particles per unit volume (particle density) $\rho(\mu,T)=N/V$, and the entropy per unit volume $s(\mu,T)=S/V$. We now consider the same system but confined by an external potential $V_{\text{ext}}(\vec{r})$. We can find its thermodynamic properties by implementing the "local density approximation:" Take ω, ρ, and s of the homogenous case and make those functions per unit volume to be their "local" densities $\omega(\vec{r})$, $\rho(\vec{r})$, and $s(\vec{r})$, in the presence of the given external potential, by replacing the chemical potential μ by the "local" chemical potential $\mu_{\text{local}}(\vec{r})=\mu-V_{\text{ext}}(\vec{r})$. It turns out that integration of $\omega(\vec{r})$, $\rho(\vec{r})$, and $s(\vec{r})$ over all space yield the exact expansions for Ω, N, and S, in the presence of $V_{\text{ext}}(\vec{r})$, as given by Eq. (25) and its derivatives. That is, one finds that LDA procedure gives rise to exact results. It is important to point out, however, that the validity of LDA is independent of the convergence of the virial expansion. The validity of LDA for classical and quantum systems in the thermodynamic limit was rigorously proved in Refs. [28–30], respectively.

The above description does show that in the thermodynamic limit the system is locally homogenous and that "locally" actually means in length scales large compared with those of interatomic interactions. It is in this latter connection that LDA is largely used without the need of further justification. There is a warning, however, that must be raised when using LDA. It may appear that if one is able to find any thermodynamic variable q for a homogenous system and express it in terms of the chemical potential μ and temperature T, namely $q=q(\mu,T)$, its local counterpart when in the presence of an external potential $V_{\text{ext}}(\vec{r})$ is simply $q(\vec{r})=q(\mu_{\text{local}}(\vec{r}),T)$. This, in general, is incorrect; its is strictly justified for Ω/V, N/V, and S/V only. It is incorrect, for instance, for the internal energy and other free energies, except Ω, as well as for other functions such as heat capacities. This statement can be verified by using expression (25) for the grand potential of a confined fluid. Thus, the fact that the system is locally homogeneous does not imply that the local states of the confined fluid are thermodynamic states of the corresponding homogeneous system, i.e. $q_{\mathrm{local}}(\vec{r}) \neq q[\mu_{\mathrm{local}}(\vec{r}),T]$ in general.

V. EQUATION OF STATE AND HEAT CAPACITY OF WEAKLY INTERACTING BOSE GASES

The chief importance of correctly identifying the generalized pressure and volume, resides in its use as a tool to characterize a given system. For the simple case of a one-component gas and for a fixed interatomic interaction, there are only two independent thermodynamic variables, say, the temperature T and the molar, or per particle, generalized volume $v=\mathcal{V}/N$. Therefore, at least two further functions of these variables should be measured or calculated independently, in order to obtain the full thermodynamics of the system. We choose the equation of state $\mathcal{P}=\mathcal{P}(v,T)$ and the specific heat at constant generalized volume $C_{\mathcal{V}}/N=c_v(v,T)$. As we have explained in Sec. II, these two quantities should be very easily measured in the current experiments of ultracold gases.

Both as an example of the use of the generalizad variables and because of the relevance to current experiments and theory dealing with ultracold trapped gases, we now turn our attention to the calculation of the equations of state and heat capacities of weakly interacting Bose gases confined by harmonic and linear quadrupolar potentials, $V_{\mathrm{ext}}(\vec{r})=(1/2)m(\vec{\omega}\cdot\vec{r})^2$ and $V_{\mathrm{ext}}(\vec{r})=|\vec{A}\cdot\vec{r}|$, within the Hartree-Fock (HF) approximation [13,42,43]. First, we write the Hamiltonian in a second quantized version and consider a contact interatomic potential,

$$H=\sum_n \epsilon_n a_n^\dagger a_n + U{\sum_{jklm}}' a_j^\dagger a_k^\dagger a_l a_m, \tag{30}$$

where n and ϵ_n stand for the eigenstates and eigenvalues of the three-dimensional one-particle Hamiltonian in the presence of the external potential. $a_n^\dagger$ 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 positive throughout. This form of the interaction is appropriate for gases at low temperatures [13,42].

The Hartree-Fock approximation yields a self-consistent calculation for the density profiles of the thermal and the condensate densities, $\rho_{th}(\vec{r})$ and $\rho_0(\vec{r})$, that leads to the following set of equations [43]:

$$\rho_{th}(\vec{r})=\frac{1}{\lambda_T^3}g_{3/2}\{\beta[\mu-V_{\mathrm{ext}}(\vec{r})-2U\rho_{th}(\vec{r})-2U\rho_0(\vec{r})]\} \tag{31}$$

and

$$\rho_0(\vec{r})=\frac{1}{U}[\mu-V_{\mathrm{ext}}(\vec{r})-2U\rho_{th}(\vec{r})], \tag{32}$$

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

$$N=\int \rho_{th}(\vec{r})d^3r+\int \rho_0(\vec{r})d^3r. \tag{33}$$

In Eq. (31), $g_{3/2}(\alpha)$ is the usual Bose function $g_n(\alpha)$ for $n=3/2$. Equation (32) is to be understood valid for values when the right-hand side is positive or zero. As a matter of fact, this is how the normal 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 (32) is the Gross-Pitaevskii equation in the thermodynamic limit where the kinetic energy term may be safely neglected. The above set of equations suffers essentially from the fact that it does not consider the expected Bogoliubov excitations at very low temperatures. However, it should be fine for temperatures near the transition [43].

As it is clear from the above set of equations, their solution yields the density profile $\rho(\vec{r})$ and the chemical potential μ for given values of the temperature T and the generalized volume $v=\mathcal{V}/N$. The value of 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 $f(v,T)=-\mathcal{P}v+\mu$. The molar entropy $s=(\partial f/\partial T)_v$ follows and, therefore, the specific heat $c_v=T(\partial s/\partial T)_v$. Our results are summarized in Figs. 1–4.

Figures 1 and 2 show a few isochores (v=const) of the equation of state for both external potentials, comparing the ideal case with the interacting HF approximation. Note that although the generalized pressures are quantitatively different, even with different units, their qualitative behavior is essentially the same. We make the following comments. First, in the ideal case the transition BEC line indicates that the pressure vanishes as $T\to 0$. That is, just as in the uniform case [40], the condensate exerts no pressure. 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 of the transition temperature is in agreement with results of more general theories of trapped Bose gases [15]. Moreover, this is an effect due solely to the interactions and not related to finite size effects [13,44]. Last, the transition line in the interacting case, as shall be further described below, marks a smooth normal gas to superfluid transition, different to BEC where discontinuities in the second derivatives of the free energy are encountered; in the interacting case, up to second derivatives—and appears that to higher order as well—the free energy is continuous.

In Figs. 3(a) and 3(b) we show the specific heat as a function of temperature, for a given isochore, for both potentials. Again the qualitative behavior is the same. Once more, we see that the transition temperature in the interacting case, marked with an arrow, is lower than that of the ideal case. But more interestingly, one finds that at the transition temperature the specific heat does not show its maximum value, but rather it is a (local) minimum, and that the transition is continuous. Thus, it shows sign of being neither a first order

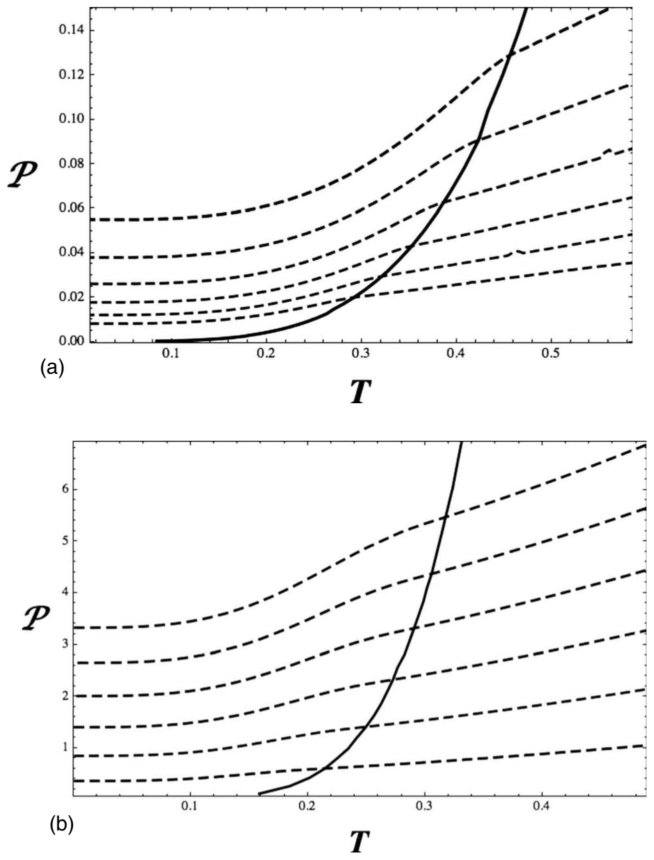

FIG. 1. Phase diagram $\mathcal{P}$-T of a weakly interacting Bose gas confined by a harmonic trap (a) and by a linear quadrupolar potential (b). Several isochores ($\mathcal{V}/N$=constant) are shown with dotted lines. The solid line shows the normal gas to superfluid (BEC) transition. Compare with Fig. 2, the ideal case. In the latter the BEC transition line occurs at higher temperatures than in the interacting case. Note also that in the interacting case, below the transition temperature, the condensed phase exerts pressure. Units are $\hbar=1$, $m=1$, and $a=1$.

nor a critical transition. We understand that the present is a mean-field calculation and, as mentioned above, perhaps 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. The origin of the continuity of all the thermodynamic properties may be traced back to the behavior of the condensate fraction. This is exemplified in Fig. 4 where we compare the condensate fraction N_0/N of the ideal with the interacting case. Below T_c, the ideal condensate fraction is $N_0/N=1-(T/Tc)^{3/2}$ for the uniform case, $N_0/N=1-(T/T_c)^3$ for the harmonic trap, and $N_0/N=1-(T/T_c)^{9/2}$ for the linear quadrupolar potential. Above T_c, $N_0/N=0$. Thus, the transition in the ideal case has a discontinuity in the derivative. However, for the interacting case, as shown in Fig. 4, there appears that this transition is completely smooth, with no discontinuity or singularity at all.

Preliminar comparisons with experiments performed in ^{23}Na gases trapped in a harmonic potential [27] indicate that below T_c the role of the interactions is still underestimated by HF, yielding a calculated generalized pressure lower than the experimental one. We believe this is due to the fact that HF elementary excitations are not the expected ones. An improvement using better theories, that include the proper role and statistical description of Bogoliubov modes [45] and/or including the Popov approximation [13,42], is certainly desirable. Nevertheless, these initial experiments do show the usefulness of the knowledge of the equation of state, not only for purposes of characterization, but clearly as an additional tool to learn about the elementary excitations of ultracold gases.

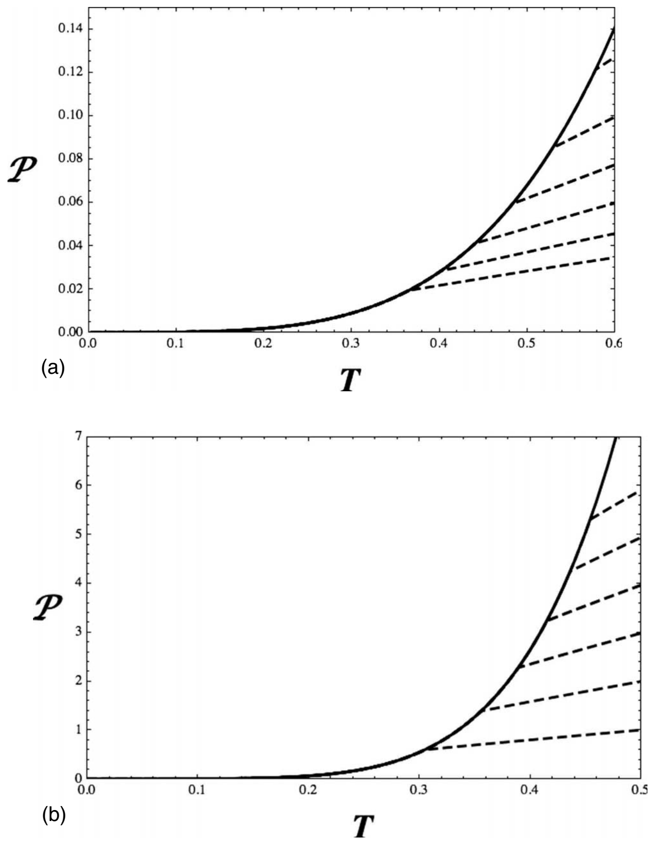

FIG. 2. Phase diagram $\mathcal{P}$-T of an ideal Bose gas confined by a harmonic trap (a) and by a linear quadrupolar potential (b). Several isochores ($\mathcal{V}/N$=constant) are shown with dotted lines. The solid line shows the BEC transition. See caption of Fig. 1 for further details.

VI. FINAL REMARKS

As a final comment, we emphasize that the use of the generalized thermodynamic variables here presented should lead to correct results by simply following the rules of thermodynamics, without necessarily resorting to a local picture. It is clear to us that for this to be useful one needs, first, to change the usual intuition on volume and hydrostatic pressure to their generalized counterparts and, second, to provide examples where these variables lead to new insights. To show how this approach serves to fully study and characterize a confined system, we have studied the BEC (superfluid) transition in a weakly interacting Bose gas trapped by two different potential. We would like to emphasize that such an

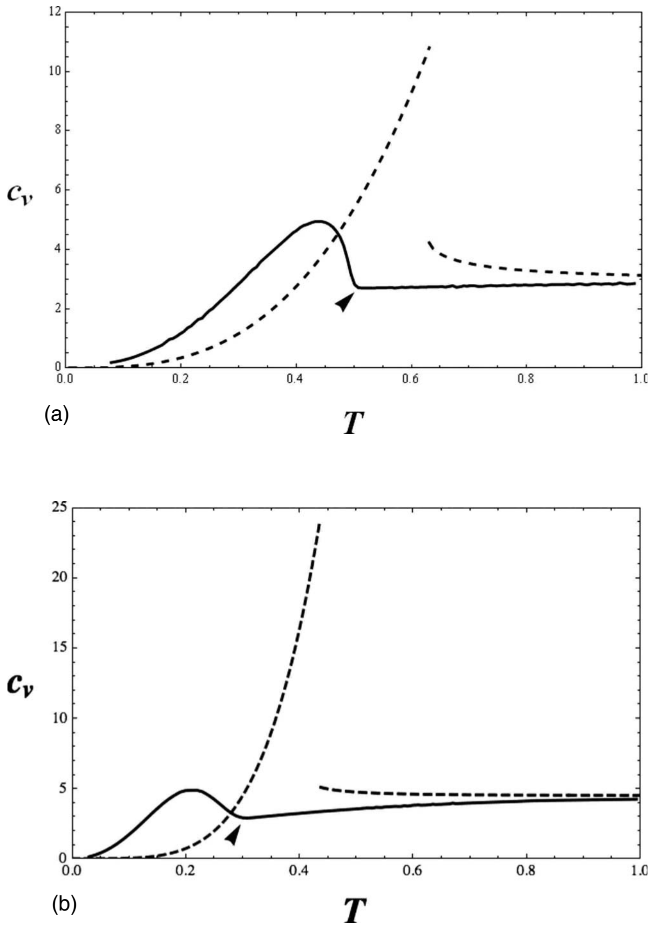

FIG. 3. Specific heat at constant generalized (molar) volume c_v vs temperature T for a gas confined by a harmonic trap (a) and by a linear quadrupolar potential (b). The dotted line is the ideal case and the solid line is the weakly interacting Bose gas. The transition temperature in the interacting case is marked with an arrow. Note that while in the ideal case the heat capacity is discontinuous at the transition temperature, it appears that in the interacting case it is completely continuous. Further, in the latter case, the transition does not occur at the maximum value of c_v but at its minimum. Units are $\hbar=1$, $m=1$, and $a=1$.

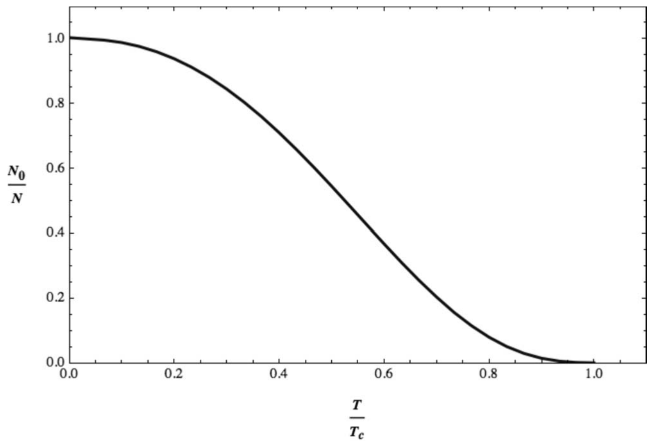

FIG. 4. Condensate fraction N_0/N as a function of temperature T for an interacting Bose gas confined by a linear quadrupolar trap. Note that the derivative of the curve is continuous at the transition. See text for details. Units are $\hbar=1$, $m=1$, and $a=1$.

analysis is possible because of the identification of the proper variables. It is our belief that the measurement of the equation of state and the heat capacity in terms of the generalized thermodynamic variables offers a complementary and useful tool for the analysis of ultracold trapped fluids.

Although much has been learned with use of LDA, we have indicated that care must be taken when using it. This should be more notorious when dealing with phase-separated fluids where it is not clear if LDA suffices for their description since the interfacial widths of the phase boundaries are expected to be of the order of the range of the intermolecular interactions [36]. This situation appears to be the case for the states found recently in trapped gases of ^{6}Li atoms [8,9,11], where it is found that the confined fluid phase separates into a superfluid and a normal paramagnetic gas, showing clearly an interfacial phase boundary. There are differing theoretical studies of whether LDA should be enough or if "surface tension" terms should be included [19–21]. In general, for such inhomogeneous states, one should not expect a local picture to be valid across the interface; the thermodynamic potentials are indeed expected to be nonlocal on the density profiles.

ACKNOWLEDGMENTS

Work supported by UNAM DGAPA IN-114308. We thank an anonymous referee for bringing to our attention Refs. [28–30].

APPENDIX: DERIVATION OF I_2

In this Appendix we provide the derivation of the second-order contribution to the virial expansion.

Classical case. From Sec. III we find that I_2 in the classical case is given by

$$I_2 = \frac{1}{h^6}\int d^3p_1 \int d^3r_1 \int d^3p_2 \int d^3r_2 e^{-\beta H_2} - \frac{1}{h^6}\left(\int d^3p_1 \int d^3r_1 e^{-\beta H_1}\right)\left(\int d^3p_2 \int d^3r_2 e^{-\beta H_1}\right) \tag{A1}$$

with H_2 given by Eq. (1) for $N=2$. We make the change of variables to center of mass and relative coordinates,

$$\vec{R} = (\vec{r}_1 + \vec{r}_2)/2 \quad \text{and } \vec{r} = \vec{r}_1 - \vec{r}_2, \tag{A2}$$

with their canonical momenta $\vec{P}$ and $\vec{p}$. Thus,

$$I_2 = \frac{1}{h^6}\int d^3P \int d^3R \int d^3p \int d^3r e^{-\beta H^{(2)}_{\mathrm{c.m.}}} e^{-\beta \mathcal{H}_2} - \frac{1}{\lambda_T^6}\int d^3R \int d^3r e^{-\beta\{V_{\mathrm{ext}}[\vec{R}+(\vec{r}/2)]+V_{\mathrm{ext}}[\vec{R}-(\vec{r}/2)]\}} \tag{A3}$$

where the center-of-mass Hamiltonian is

$$H^{(2)}_{\mathrm{c.m.}} = \frac{\vec{P}^2}{2(2m)} + V_{\mathrm{ext}}\left(\vec{R} + \frac{\vec{r}}{2}\right) + V_{\mathrm{ext}}\left(\vec{R} - \frac{\vec{r}}{2}\right) \tag{A4}$$

and the two-particle relative-coordinates one is

$$\mathcal{H}_2 = \frac{\vec{p}^2}{2(m/2)} + u(r). \tag{A5}$$

The integrals over the momenta yield $1/\lambda_T^6$. Notice, however, that the integrals over $\vec{R}$ depend strongly on $\vec{r}$, even for particles confined in a rigid vessel of volume V. In such a case, the boundary terms couple the integrals. We rewrite I_2 as follows:

$$I_2 = \frac{1}{\lambda_T^6}\int d^3R \int d^3r e^{-\beta\{V_{\mathrm{ext}}[\vec{R}+(\vec{r}/2)]+V_{\mathrm{ext}}[\vec{R}-(\vec{r}/2)]\}} f(r), \tag{A6}$$

where we have introduced the Mayer function $f(r)=e^{-\beta u(r)}-1$. Here we provide the important step: The function $f(r)$ vanishes for distances r longer than the range of the intermolecular potential σ, i.e., the value of r is bounded, $r \leqslant \sigma$. Hence, in the thermodynamic limit, in which the external potential becomes "shallower" and "shallower" and the volume of the system larger and larger, we can set

$$V_{\mathrm{ext}}\left(\vec{R} + \frac{\vec{r}}{2}\right) + V_{\mathrm{ext}}\left(\vec{R} - \frac{\vec{r}}{2}\right) \approx 2V_{\mathrm{ext}}(\vec{R}). \tag{A7}$$

This is the thermodynamic limit. Therefore,

$$I_2 = \frac{1}{\lambda_T^6}\int d^3 R e^{-2\beta V_{\mathrm{ext}}(\vec{R})}\int d^3 r f(r) = \frac{\mathcal{V}}{\lambda_T^6}\zeta(2\beta) b_2, \tag{A8}$$

where we have identified the classical second virial coefficient b_2. Thus, the well-known bound is that the intermolecular potential must vanish for lengths $r \gg \sigma$. Clearly, it must be "short-range" interaction (faster than $1/r^3$), otherwise b_2 does not exist.

Quantum case. Again, from the expressions in Sec. III, one finds

$$I_2 = \int d^3r_1 \int d^3r_2 (\langle \vec{r}_1,\vec{r}_2|e^{-\beta H_2}|\vec{r}_1,\vec{r}_2\rangle + \epsilon\langle \vec{r}_1,\vec{r}_2|e^{-\beta H_2}|\vec{r}_2,\vec{r}_1\rangle) - \int d^3r_1 \langle \vec{r}_1|e^{-\beta H_1}|\vec{r}_1\rangle \int d^3r_2 \langle \vec{r}_2|e^{-\beta H_1}|\vec{r}_2\rangle, \tag{A9}$$

where $\epsilon = \pm 1$ for bosons or fermions. The derivation follows essentially the same steps as in the classical case. First, one performs the same change of variables as in Eq. (A2) to rewrite I_2. Then, the thermodynamic limit may be taken by separating the center-of-mass motion from the relative one. It can be realized that for high temperatures the range of the variable $\vec{r}$ is bounded due to presence of the potential $u(r)$. At low temperatures the bound is set up by either the thermal de Broglie wavelength or the scattering length a. Therefore, as long as r remains bounded by a finite quantity, however large, one can take the limit of very large volumes, $\mathcal{V} \to \infty$, and implement the thermodynamic limit just as in the classical case. One finds

$$I_2 = \frac{\mathcal{V}}{\lambda_T^6}\zeta(2\beta) b_2, \tag{A10}$$

formally identical with its classical counterpart, formula (A8), but with the quantum second virial coefficient

$$b_2 = 2^{3/2}\lambda_T^3 \int d^3r (\langle \vec{r}|e^{-\beta\mathcal{H}_2}|\vec{r}\rangle + \epsilon\langle \vec{r}|e^{-\beta\mathcal{H}_2}|-\vec{r}\rangle - \langle \vec{r}|e^{-\beta p^2/2(m/2)}|\vec{r}\rangle), \tag{A11}$$

where $\mathcal{H}_2$ is given by Eq. (A5). As a rule, in the thermodynamic limit the center-of-mass motion is always quasiclassical [40]. The expression for the quantum second virial coefficient above can be seen to be the correct one by comparing, for instance, with the expression given in Ref. [40]. For slow collisions, the relevant ones for ultracold gases, b_2 depends on the scattering length and this may become quite large near a Feschbach or potential resonance. The formulas here derived may then be not applicable very near such a point, called the unitarity limit, but as it has been shown [22] this may be expected since in such a limit the system behaves as if near a critical point. We add that the description of the scattering energies near resonances is valid for interatomic potentials $u(r)$ that decay at least as $1/r^3$ [41].

To end this Appendix, we calculate b_2 for an ideal quantum gas, i.e., for $u(r)=0$. One finds the so-called "exchange" contribution to the second virial coefficient,

$$b_2^{(0)} = \epsilon\frac{1}{2^{3/2}}\lambda_T^3. \tag{A12}$$

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