Virial coefficients for Bose and Fermi trapped gases beyond the unitary limit: an S-Matrix approach

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We study the virial expansion for three-dimensional Bose and Fermi gases at finite temperature using an approximation that only considers two-body processes and is valid for high temperatures and low densities. The first virial coefficients are computed and the second is exact. The results are obtained for the full range of values of the scattering length and the unitary limit is recovered as a particular case. A weak coupling expansion is performed and the free case is also obtained as a proper limit.

The influence of an anisotropic harmonic trap is considered using the Local Density Approximation - LDA, Analytical results are obtained and the special case of the isotropic trap is discussed in detail.

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INTRODUCTION

The advances in experimental results and simulations on cold atoms require new methods for theorists to study these systems and explore similar ones. Analytical methods continue to be a powerful tool to explore these systems, although they generally provide approximate results, in comparison with numerical methods.

This work uses a formalism for Statistical Mechanics based on the S-Matrix. It provides an expression of the free energy at finite temperature and density built on an integral equation of the pseudo-energy with a kernel based on the logarithm of the 2-body S-matrix at zero temperature. This integral equation is quite similar to the Yang-Yang equations used in the Thermodynamical Bethe Ansatz - TBA.

The method is a “foam diagram” approximation which is valid for high temperatures and low densities and considers only contributions from two-body processes to the free energy. It is explained in and has been already used to study the thermodynamical and critical properties of quantum gases in two and three dimensions in the unitary limit and beyond the unitary limit in three dimensions. In the method was used to calculate the ratio of the viscosity to entropy density and the results were in well agreement with experimental data.

In it was shown how this method may be used to obtain the coefficients of the virial expansion for quantum gases and the first four virial coefficients were calculated in three dimensions in the unitary limit. The second coefficient provided by this method is exact and agrees with the result in. The third one in the unitary limit does not agree with the exact value obtained in where three-body processes were considered since the three-body processes are neglected in our approximation.

Since Feshbach Resonance experiments allow to adjust the scattering length to any finite value there is no reason to study only the unitary limit, in which the scattering length diverges. Here we calculate the first three virial coefficients for both Bose and Fermi gases in three dimensions for different values of the dimensionless ratio , where is the De Broglie thermal wave length and is the scattering length. The unitary limit results obtained in are recovered in the proper limit and also the free case where the scattering length is tuned to zero. For large positive scattering length molecules are formed and this is not considered in this work. However in the “upper branch” there are no molecules and our formalism may be applied. This situation is studied here because we consider the possibility that a Bose gas may stay in a metastable state before undergoing mechanical collapse.

Analytical expressions are obtained for a weak coupling expansion and they are compared to the previous results. The second virial coefficient is the only exact one (besides the first one) for the same reasons as in and this will be discussed here. Finally the influence of a harmonic trap on the virial coefficients will be studied using the Local Density Approximation (LDA) and analytic results will be obtained for the case of an anisotropic harmonic trap. The particular case of the isotropic trap will be discussed and some plots will be showed.

In the next section we present a brief summary of the formalism (for more details see), the actions of our physical systems, and the conventions used in this paper. In section III we derive the expression of the virial coefficients in terms of the two-body kernel of the theory in the foam diagram approximation in a different way than in. In section IV we obtain the first four virial coefficients of a Bose and a Fermi gas in three dimensions in terms of the ratio and discuss these results.

In section V we perform a weak coupling expansion and
obtain analytical expressions for the virial coefficients in this situation, then we compare these results with the previous ones obtained in section IV. In section VI we study the influence of a trap on the virial coefficients using the Local Density Approximation.

**FORMALISM AND CONVENTIONS**

The formalism developed in [16] allows one to write the exact free energy of the gas as:

$$ F = F_0 - \frac{1}{\beta} \sum_{N \geq 2} \frac{1}{N!} \int \left( \prod_{i=1}^{N} f_0(k_i) \right) \frac{d^3k_i}{(2\pi)^3} w_N(k_1, ..., k_N), $$

where $f_0(k)$ is a filling fraction and the $w_i$ are defined in terms of the connected elements of the imaginary part of the logarithm of the S-matrix. This is in agreement with what is expected from clustering properties of the S-matrix. The terms due to interactions may be expressed in terms of diagrammatic rules, as explained in [16].

The expression of the filling fraction is:

$$ f_0(k) = \frac{z}{z e^{\beta\epsilon(k)} - s}, $$

where $s$ is a statistical parameter (1 for bosons and -1 for fermions), $z = e^{\beta\mu}$ is the fugacity, $\mu$ is the chemical potential and $\beta = 1/T$ is the inverse of temperature (we always consider $\hbar = c = k_B = 1$). The free energy of the gas without interactions $F_0$, is given by:

$$ F_0 = -\frac{1}{\beta} \int \frac{d^3k}{(2\pi)^3} \left( 1 - s e^{\beta\epsilon(k)} \right). $$

We make use of an approximation in which only two-body processes are considered, the foam diagram approximation [16]. This approximation is reasonable for low densities and large temperatures.

Considering in [16] only the interaction terms represented by the foam diagrams is equivalent to write the following expression for the free energy:

$$ F = -\frac{1}{\beta} \int \frac{d^3k}{(2\pi)^3} \left[ -s \log(1 - se^{-\beta\epsilon}) - \frac{1}{2} \left( \frac{1}{e^{\beta\epsilon}} - s \right) \right], $$

where the pseudo-energy $\epsilon(k)$ is defined in terms of the particle number $n$ by

$$ n = \int \frac{d^3k}{(2\pi)^3} e^{\beta\epsilon(k)} - s. $$

The function $y(k)$ is defined by

$$ y(k) = e^{-(\beta\epsilon(k) + \mu - \frac{\hbar^2}{2m} k^2)}. $$

and satisfies the following integral equation:

$$ y(k) = 1 + \frac{\beta}{(2\pi)^3} \int d^3k' \frac{z e^{\frac{\hbar^2}{2m} k^2}}{1 - z e^{\frac{\hbar^2}{2m} k^2}} G_2(k, k'). $$

This integral equation arises from summing up the infinite number of foam diagrams.

In this paper we will work with three-dimensional gases. The Bose gas will be described by the following action:

$$ S = \int d^3x dt \left( i\phi^\dagger \partial_t \phi - \frac{\nabla \phi^2}{2m} - \frac{\sigma}{2} (\phi^\dagger \phi)^2 \right) $$

and the fermion gas by:

$$ S = \int d^3x dt \left( \sum_{\alpha = \uparrow, \downarrow} i\psi^\dagger_\alpha \partial_t \psi_\alpha - \frac{\nabla \psi_\alpha^2}{2m} - g\psi^\dagger_\uparrow \psi_\downarrow \psi_\uparrow \psi_\downarrow \right). $$

The conventions used here are the same as in [19]. The two-body kernel result for these actions may be expressed by:

$$ G_2(k, k') = -\frac{16\pi\sigma}{m (|k - k'|)} \arctan \left( \frac{mg\rho |k - k'|}{8\pi} \right), $$

where the factor $\sigma$ that appears in [19] is $\sigma = 1/2$ for fermions and $\sigma = 1$ for bosons. The renormalized coupling constant is given by:

$$ \frac{1}{g_R} = \frac{1}{g} + \frac{m\Lambda}{2\pi^2}, $$

where $\Lambda$ is the momentum cutoff introduced to regularize loop integrals. The scattering length is related to the renormalized coupling constant by:

$$ a = \frac{mg_R}{4\pi}. $$

For our system it can be shown [17, 18] that for $g_R \to \pm\infty$, the scattering length diverges, and there is a fixed point of the renormalization group in which the S-matrix is $S = -1$. This defines the so-called unitary limit. In the present work, the first virial coefficients will be obtained for any value of the scattering length and the unitary limit will be obtained in a particular limit.

**EXPRESSIONS FOR THE VIRIAL COEFFICIENTS IN THE FOAM DIAGRAM APPROXIMATION**

The virial coefficients $b_n$ may be defined by the following expression:

$$ F = -\frac{1}{\beta \lambda^2 F} \sum_{n=1}^{\infty} b_n z^n. $$
The scaling function for the density of particles will be defined by \( \mathcal{G} \)
\[
q = n\lambda^3_T, \tag{14}
\]
so remembering (13) and that \( n = -\frac{\partial P}{\partial n} \) one gets:
\[
q = \frac{1}{\lambda^3_T} \sum_{n=1}^{\infty} n b_n z^n. \tag{15}
\]
Substituting (5) in (14) and using (6), it is possible to expand \( q \) as:
\[
q = \left( \frac{1}{2\pi mT} \right)^{3/2} \int y(k) e^{-\frac{\beta k^2}{2m}} [1 + s y(k) e^{-\frac{\beta k^2}{2m}} + z^2 y^2(k) e^{-\frac{\beta k^2}{2m}} + ...] d^3k. \tag{16}
\]
Using (13) and (17) it is possible to expand \( y(k) \),
\[
y(k) = 1 + \frac{\beta}{(2\pi)^d} \int d^3k' G_2(k, k') z e^{-\frac{\beta k'^2}{2m}} (1 + s y(k') e^{-\frac{\beta k'^2}{2m}} + z^2 y^2(k') e^{-\frac{\beta k'^2}{2m}} + ...). \tag{17}
\]
Now, using (18) and (17) we can express the scaling function \( q \) in terms of the fugacity. Comparing to (15) one can then obtain expressions for the virial coefficients. The first three are:
\[
(2\pi mT)^{3/2} b_1 = \int d^3k e^{-\frac{\beta k^2}{2m}}, \tag{18}
\]
\[
2(2\pi mT)^{3/2} b_2 = s \int d^3k e^{-\frac{\beta k^2}{2m}} + \frac{\beta}{(2\pi)^3} \int d^3k d^3k' e^{-\frac{\beta k^2}{2m} - \frac{\beta k'^2}{2m}} G_2(k, k'), \tag{19}
\]
\[
3(2\pi mT)^{3/2} b_3 = \int d^3k e^{-\frac{3\beta k^2}{2m}} + s \frac{2\beta}{(2\pi)^3} \int d^3k d^3k' e^{-\frac{\beta k^2}{2m} - \frac{\beta k'^2}{2m}} G_2(k, k') + \frac{\beta s}{(2\pi)^3} \int d^3k d^3k' e^{-\frac{\beta k^2}{2m} - \frac{\beta k'^2}{2m}} G_2(k, k'). \tag{20}
\]
Because of the rotation symmetry \( G_2(k, k') = G_2(k', k) \) and we can group some terms, and also perform the integrals that do not depend on the kernel. This gives the simpler expressions:
\[
b_1 = 1, \tag{21}
\]
\[
2b_2 = \frac{s}{2\sqrt{2}} + \frac{\beta}{(2\pi)^3} (2\pi mT)^{3/2} \int d^3k d^3k' e^{-\frac{\beta k^2}{2m} - \frac{\beta k'^2}{2m}} G_2(k, k'), \tag{22}
\]
\[
3b_3 = \frac{3s}{3\sqrt{2}} + \frac{3\beta s}{(2\pi)^3} (2\pi mT)^{3/2} \int d^3k d^3k' e^{-\frac{\beta k^2}{2m} - \frac{\beta k'^2}{2m}} G_2(k, k'). \tag{23}
\]
The above derivation of these expressions is slightly different than the one in [19], since it is not necessary to consider each diagram and find its contributions to the virial coefficients. The method presented in this paper automatically considers the foam diagram approximation because of the use of the integral equation (17), the fact that the results here are in agreement with [19] shows the consistency of the formalism presented in [16].

THE RESULTS FOR THE FIRST VIRIAL COEFFICIENTS

Substituting the kernel (11) in equations (21), (22), and performing the angular parts of the integrals, it is possible to write the first virial coefficients in terms of the ratio \( \alpha = \frac{\lambda}{\sqrt{\pi}T} \). The results are the following:
\[
b_1 = 1 \tag{24}
\]
\[
b_2 = \frac{s\sqrt{2}}{8} - \frac{2\sqrt{2}\sigma}{\pi^2} \int_0^{\infty} v e^{-\frac{v^2}{2\alpha}} \arctan \left( \frac{v}{\alpha} \right) dv, \tag{25}
\]
\[
b_3 = \frac{3\sqrt{2}}{27} - \frac{16\sqrt{3}s}{9\pi^2} \int_0^{\infty} v e^{-\frac{v^2}{2\alpha}} \arctan \left( \frac{v}{\alpha} \right) dv. \tag{26}
\]
In the unitary limit, the above integrals can be performed analytically [19]. For a finite scattering length \( a \), the integrals can only be done numerically.

The second virial coefficient as a function of \( \alpha \) is plotted in Figure 1 for bosons and in Figure 2 for fermions, Figures 3 and 4 show the third virial coefficient for bosons and fermions respectively. The values of these coefficients in the free case and in the unitary limit are also indicated in these figures with dotted and dashed lines respectively and one sees they are recovered in the proper limits \( a \to 0 \) and \( a \to \infty \). Note that both \( b_2 \) and \( b_3 \) flip sign as one passes through the unitary limit and the scattering length changes from \( +\infty \) to \( -\infty \).

The figures [1] [2] [3] and [4] show that the second and third virial coefficients are bounded by the values of the unitary
FIG. 1: (Color Online): Second virial coefficient against the ratio between the thermal wave length and the scattering length: \( b_2 \times \alpha = \frac{\lambda}{a} \) for bosons (black). The values of the unitary limit (\( \alpha \rightarrow 0^{\pm} \)) obtained in [19] are represented by the dashed (blue) lines and the value of the free case (\( g = 0 \Rightarrow \alpha \rightarrow \pm \infty \)) is represented by the dotted (red) line.

FIG. 2: (Color Online): Second virial coefficient against the ratio between the thermal wave length and the scattering length: \( b_2 \times \alpha = \frac{\lambda}{a} \) for fermions (black). The values of the unitary limit (\( \alpha \rightarrow 0^{\pm} \)) obtained in [19] are represented by the dashed (blue) lines and the value of the free case (\( g = 0 \Rightarrow \alpha \rightarrow \pm \infty \)) is represented by the dotted (red) line.

FIG. 3: (Color Online): Third virial coefficient against the ratio between the thermal wave length and the scattering length: \( b_3 \times \alpha = \frac{\lambda}{a} \) for bosons (black). The values of the unitary limit (\( \alpha \rightarrow 0^{\pm} \)) obtained in [19] are represented by the dashed (blue) lines and the value of the free case (\( g = 0 \Rightarrow \alpha \rightarrow \pm \infty \)) is represented by the dotted (red) line.

FIG. 4: (Color Online): Third virial coefficient against the ratio between the thermal wave length and the scattering length: \( b_3 \times \alpha = \frac{\lambda}{a} \) for fermions (black). The values of the unitary limit (\( \alpha \rightarrow 0^{\pm} \)) obtained in [19] are represented by the dashed (blue) lines and the value of the free case (\( g = 0 \Rightarrow \alpha \rightarrow \pm \infty \)) is represented by the dotted (red) line.

limit case (when \( \alpha \rightarrow 0 \), the dashed lines) in the foam diagram approximation. When \( g \rightarrow 0^{\pm} \Rightarrow \alpha \rightarrow \pm \infty \) (the dotted lines), the free case is always recovered as expected. The exact results for the values of the second coefficient in the unitary limit are also properly recovered for Bose and Fermi gases [19, 22–24]. The expression [25] for fermions (\( s = -1, \sigma = \frac{1}{2} \)) is the same as the exact one obtained in [24], up to an integration by parts, thus our results for the second virial coefficient are exact for the hole spectrum of \( \alpha \), as expected from our formalism.

The results in the unitary limit for the third coefficient obtained in [19] are recovered as expected. As discussed previously, they differ from the exact ones from [24] since the three-body processes are not considered in our approximation. As the ratio \( \alpha \) increases, the interaction effects decrease and our results should become closer to the correct ones. The Figure 4 indeed shows that for \( \alpha \) sufficiently large the results obtained in [24] are nearly recovered.

WEAK COUPLING EXPANSION

Expressions [24] and [25] give the virial coefficients in terms of the ratio \( \alpha = \frac{\lambda}{a} \). In this section we perform
an expansion for large values of $\alpha$, which means that $\sqrt{T gR} << 1$. Since the temperature can not be too small because we are under the foam diagram approximation, the coupling constant $gR$ should be very small in order for this expansion be valid.

One can simply expand the arc-tangent function in expressions (25) and (26) in a Taylor series, truncate it to the first degree term of $1/\alpha$, and perform the integrals analytically. Performing this expansion, one obtains

$$b_2 = \frac{s \sqrt{2}}{8} - \frac{2\sigma}{\alpha}$$

and

$$b_3 = \frac{\sqrt{2}}{27} - \frac{\sqrt{2}\sigma s}{\alpha}.$$  (28)

Figure 5 shows the second virial coefficient for bosons against $\alpha$ in the weak coupling approximation and the numerical result obtained in the latest section, Figure 6 does the same for the fermionic situation and Figures 7 and 8 do the same for the third coefficient of bosons and fermions respectively. It is easy to see that the curves corresponding to equations (27) and (28) and the ones obtained numerically integrating the expressions (25) and (26), shown in figures 5, 6, 7 and 8 are almost indistinguishable for $|\alpha| > 4$.

**VIRIAL COEFFICIENTS FOR TRAPPED GASES**

In order to study the influence of a harmonic trap for quantum gases it is possible to use the local density approximation (LDA). The LDA may be used if one ignores the variation of thermodynamic quantities due to density gradients [33, 34]. In our formalism this means that one can replace the chemical potential by $\mu \rightarrow \mu - V(r)$, giving a free energy $F(r)$ that depends on $r$. The final free energy will be given by: $F = \int F(r) d^3r$.

We know that the virial coefficients are related to the free energy by equation (13). Therefore, in the LDA approximation, expression (13) becomes:

$$F = -\frac{1}{\beta \lambda^3} \sum_{n=1}^{\infty} b_n \left( \int e^{-\beta n V(r)} d^3r \right) z^n.$$  (29)

Comparing (29) to (13) one sees that the presence of the trap changes the virial coefficients in the following way.

FIG. 5: (Color Online): Second virial coefficient against the ratio between the thermal wave length and the scattering length: $b_2 \times \alpha = \frac{4}{\lambda T a}$ for bosons (black). The dashed (red) line shows the same result obtained with the expression of the weak coupling expansion.

FIG. 6: (Color Online): Second virial coefficient against the ratio between the thermal wave length and the scattering length: $b_2 \times \alpha = \frac{4}{\lambda T a}$ for fermions (black). The dashed (red) line shows the same result obtained with the expression of the weak coupling expansion.

FIG. 7: (Color Online): Third virial coefficient against the ratio between the thermal wave length and the scattering length: $b_2 \times \alpha = \frac{4}{\lambda T a}$ for bosons (black). The dashed (red) line shows the same result obtained with the expression of the weak coupling expansion.
under the LDA approximation:

\[ b_n \rightarrow b_n \int e^{-\beta n V(r)} d^d r. \]  \hfill (30)

Considering an anisotropic harmonic trap

\[ V(r) = \sum_{i=1}^{d} \left[ \frac{w_i r_i^2}{2} \right] - \log A \]

, we obtain

\[ b_n \rightarrow b_n A^n \left( \frac{2\pi}{\beta w} \right)^{\frac{d}{2}} \cdot \left[ \prod_{i=1}^{3} w_i \right]^{-\frac{1}{2}}. \]  \hfill (31)

In particular, if the trap is isotropic, \( w_1 = w_2 = \ldots = w_d = w \), we arrive at the following result:

\[ b_n \rightarrow b_n A^{\frac{n}{\alpha}} \left( \frac{2\pi}{\beta w n} \right)^{\frac{d}{2}}. \]  \hfill (32)

One sees that for \( A = 1 \) and \( w \) given by the fundamental Matsubara frequency \( \frac{2\pi}{\beta} \), the first virial coefficient \( b_1 \) does not change in the presence of the harmonic isotropic trap. In the following figures we plot the ratios \( b'_n / b_n \) for \( n = 2, 3, 4 \), where ‘ means the presence of the harmonic isotropic trap, as a function of \( w \) for \( A = T = 1 \), and also as a function of \( T \) for \( w = 1 \), \( A = 0.5 \) and \( A = 2 \).

Expressions (31) and (32) show that the virial coefficients decrease monotonically with the frequencies of the trap as Figure 8 illustrates for the isotropic case. When \( A = 1 \) the virial coefficients increase with the temperature as a power law. When \( A \neq 1 \) an exponential behavior should be considered also. For \( A \leq 1 \) the virial coefficients vanish as the temperature comes close to zero and for \( A > 1 \) the virial coefficients diverge when \( T \to 0^+ \) as shown in Figure 9. In every situation the virial coefficients increase with the temperature as a power law for large temperature. We included results on the 4-th virial coefficient, using formulas that were obtained in [19] extended to non-zero \( \alpha \), but not included in this paper.
CONCLUSIONS

The first virial coefficients of a bosonic and a fermionic gas were obtained as functions of the ratio of the thermal wave length to the scattering length $\alpha = \frac{\lambda}{a}$ in the foam diagram approximation. The results obtained in $[22]$ are recovered when $\alpha \to 0^+$ as expected and one also recovers the free case when $\alpha \to \pm \infty$.

The second virial coefficients are exact and the unitary limit values for the fermionic case agree with the results of $[22]$ as is explained in $[19]$. The third coefficient is not exact since the foam diagram approximation neglects 3-body interactions, however it becomes very close to the correct value when the absolute value of the ratio $\alpha$ is large.

A weak coupling expansion was performed and analytical expressions for the virial coefficients were obtained for large values of $|\alpha|$. The weak coupling expansion is in close agreement with the results we obtained for any $\alpha$ when $|\alpha| > 4$.

The influence of an anisotropic harmonic trap was also considered under the Local Density Approximation and analytical expressions were obtained, and also specialized to an isotropic trap. The authors acknowledge financial support from CNPq, CAPES, and FAPERJ.

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