The universal equation of state of a unitary fermionic gas

R.K. Bhaduri, 1 W. van Dijk, 1,2 and M. V. N. Murthy 3

1Department of Physics and Astronomy, McMaster University, Hamilton, Ontario L8S 4M1, Canada
2Physics Department, Redeemer University College, Ancaster, Ontario L9K 1J4, Canada
3The Institute of Mathematical Sciences, Chennai 600113, India

(Dated: December 21, 2013)

It is suggested that for a fermi gas at unitarity, the two-body bond plays a special role. We propose an equation of state using an ansatz relating the interaction part of the l-body cluster to its two-body counterpart. This allows a parameter-free comparison with the recently measured equation of state by the ENS group. The agreement between the two over a range of fugacity (z < 5 for a homogeneous gas, and z < 10 for the trapped gas) leads us to perform the calculations of more sensitive quantities measured recently by the MIT group.

Feshbach resonance makes it possible to adjust the strength of the inter-atomic interaction in a neutral atomic gas. When the scattering length goes to ±∞, there is no length scale left other than the average inter-particle distance and the thermal wavelength (assuming a zero-range interaction). The gas is then termed “unitary” and its properties are universal when expressed in appropriate dimensionless units at all scales whether the system is fermionic or bosonic. 1 Recent accurate measurements by the ENS group 2, 3 and the Tokyo group 4 have confirmed the universal nature of the equation of state (EOS) of a gas of neutral fermionic atoms, and have given fresh impetus to its theoretical understanding 5, 6. More recently, direct measurements by the MIT group 7 of the isothermal compressibility κ, pressure P, and heat capacity C V /Nk B for a unitary gas have revealed the superfluid transition at Tc/T F = 0.167(13).

In this paper, keeping in mind the fundamental nature of the two-particle bond at unitarity, we propose a description of the unitary gas as consisting of singlet pairs, in terms of which all higher order clusters are expressed. The resulting Equation of State (EOS) extends the agreement with the ENS data 2, 3 on the grand potential over a much larger range of fugacity z than expected. However, this description breaks down for z > 5 for the homogeneous gas (and z > 10 for the harmonically trapped gas). For the homogeneous gas, z = 5 corresponds to a temperature T/T F = 0.22, below which the proposed EOS cannot be trusted. We calculate, with our higher virial coefficients, the pressure, compressibility and heat capacity of the homogeneous gas to compare with the MIT data 5. The calculation of these quantities is a stringent test since they require higher moments of the virial expansion. We find that inclusion of the higher virial coefficients yields agreement with the MIT data for pressure and entropy down to T/T F = 0.3, and the compressibility and heat capacity to T/T F = 0.6.

To set the stage for the proposed universal EOS, we briefly recapitulate the virial expansion of a two-component interacting homogeneous fermi gas 8. The grand potential Ω(β, μ) is defined as Ω = −τ ln Z, where τ = k B T = 1/β and Z is the grand-canonical partition function. Furthermore Ω = −PV, and may be expressed in a power series of fugacity z = exp(βμ), where μ is chemical potential. The grand potential Ω = −τZ 1(β) ∑l≥1 b l z l , where Z 1(β) is the one-body partition function, and b l is the l-particle cluster integral. For an untrapped gas in volume V, we have Z 1(β) = 2V/λ 3, where spin degeneracy of 2 is included and λ = (2πh 2 β/m) 1/2 is the thermal wave length. For a harmonic oscillator (HO) trap in three dimensions, Z 1(β) = 2/(hωβ) 3. For a unitary gas, the cluster integrals b l’s are also temperature independent in the high-temperature expansion. Subtracting from Ω the ideal part of the grand potential Ω(0) we obtain the interaction part of the EOS as

Ω − Ω(0) = −τZ 1(β) ∑l≥2 (∆b l ) z l ,

where ∆b l = b l − b l(0). Note that b 1 = b 1(0) = 1, and cancels out on taking the difference.

Consider now the special role played by ∆b 2 of the two-particle cluster at unitarity. In such a gas, the spin-up fermions have a tendency to pair up with the spin-down fermions because the short-range interaction potential is on the verge of producing zero-energy bound states. The Feshbach resonance being in the relative s-state, ensures the pair interaction to be operative only between singlet pairs. One finds that 8, 9 ∆b 2 = (2√2) × 1/4(∆Z 2), where the factor 2√2 arises from the CM motion, ∆Z 2 is the relative two-body partition function, and the “suppression factor” 1/4 arises from the fact that only half of the N particles can interact in a spin-balanced two-component Fermi gas. Note that [10] at unitarity ∆Z 2 = 1 2, yielding ∆b 2 = 1 4 for such a system. What about the ∆b l’s for the l-body clusters that appear in Eq. (1)? Keeping in mind that the unitary gas may be looked upon as a system consisting of forming and dissolving two-body pairs, we conjecture that for the scale invariant system, the ∆b l for l > 2 should be expressible in terms of (∆b 2) with an appropriate suppression factor. Viewing a l-body cluster as one particle interacting with the rest from a cluster of (l − 1) paired particles, we assume that the suppression factor is given by 2N(l−1), where N(l−1) = (l − 1)(l − 2)/2 is in general the number of pairs in a cluster with (l − 1) fermions. Thus our basic ansatz is

∆b l = (−1) l (1/2)N(l−1), l ≥ 2.

For l = 2, N 1 = 0, and Eq. (2) is an identity. The alternating sign (−1) l in the above equation was put in to keep the number fluctuation (∆N) 2/ N = ∑l l 2b l z l / ∑l l b l z l not to grow.
to a very large value with \( z \), where \((\Delta N)^2 = \overline{N^2} - \overline{N}^2\) is the number fluctuation, proportional to the isothermal compressibility \([11]\). A large value of the compressibility would lead to a vanishing monopole excitation which is a signature of instability \([12]\).

Although our description of the higher virial coefficients in terms of the second may seem to be very different from the conventional one, similar relationship between the third and second virial coefficients have been found in anyons which is also a scale invariant system \([13, 14]\). This is obtained by demanding that the divergences in the three-body clusters cancel by similar divergences in two-body clusters in the high temperature limit. A formal derivation for arbitrary \( l \) for the unitary gas appears to be non-trivial.

With this ansatz,

\[
\Omega - \Omega^{(0)} = -\tau Z_1(\beta)(\Delta b_2) \sum_{l=2}^{\infty} (-)^l \frac{z^l}{2^{N_l(l-1)}} .
\]

(3)

Experimentally \([2, 3, 15]\), it is the quantity \( h(\zeta) = \Omega/\Omega^{(0)} \) that is extracted, where \( \zeta = 1/z \). This is given by

\[
h(\zeta) = 1 + (\Delta b_2) \sum_{l=2}^{\infty} (-)^l \frac{\zeta^{-l}}{2^{N_l(l-1)}} .
\]

(4)

In a homogeneous gas with a spin-degeneracy of 2,

\[
\tilde{\Omega}^{(0)} = \frac{2}{\sqrt{\pi}} \int_0^{\infty} \sqrt{t} \ln(1 + ze^{-t}) \; dt.
\]

It is worth noting that using Eq. (2) with \( \Delta b_2 = 1/\sqrt{2} \), we obtain \( \Delta b_3 = -1/2\sqrt{2}, \Delta b_4 = 1/8\sqrt{2}, \Delta b_5 = -1/64\sqrt{2}, \) etc. Numerically \( \Delta b_3 \) is known to great accuracy, it was calculated up to 8 decimal figures in \([16]\) and has now been improved to 12 decimal figures \([17]\). Our ansatz for the third virial coefficient differs from the numerically computed value in the third decimal and as such cannot be exact. However, as we shall see the agreement with EOS data is unaffected by such fine differences in \( \Delta b_3 \). It is also estimated \([2]\) that \( \Delta b_4 \approx 0.096 \pm 0.015 \), and is consistent with our prediction within the error bars. It should be mentioned that \( \Delta b_4 \) as quoted in \([17]\) is different sign and magnitude from \([2]\) and our value. This however destroys the agreement with the data from the ENS group.

Before confronting the experimental data, we note that for a gas trapped in a three-dimensional harmonic oscillator (HO), Eqs. (4) is modified to \([2, 3]\)

\[
h(\zeta) = 1 + (\Delta b_2) \sum_{l=2}^{\infty} \frac{(-)^l}{l^{3/2}} \zeta^{-l} \tilde{\Omega}^{(0)} ,
\]

(5)

and \( \tilde{\Omega}^{(0)} = \frac{1}{2} \int_0^{\infty} t^2 \ln(1 + ze^{-t}) \; dt \). The additional suppression factor of \( 1/l^{3/2} \) in Eq. (5) was derived in \([16]\) assuming a local fugacity in a HO potential.

We are now ready to compare our predictions given by Eq. (4) for the homogeneous unpolarized gas, as given by our Eq. (4), is plotted against efficiencies up to the fourth order, as was done by Hu et al. \([5]\).

We see that such a truncated series could match the data to about \( z \approx 1.7 \). Our series \([4]\) extends this to about \( z \approx 5 \). This also underlines the importance of higher-order virial coefficients \( \Delta b_l \)'s for \( l > 4 \), despite their rapidly diminishing values. For the curve labelled Virial4p we set \( \Delta b_4 = 0.096 \), the estimated value \([3]\), rather than 0.088 given by our ansatz.
Note that the \( h(\zeta) \) has been calculated in \[6\] within Pade approximation and including up to \( \Delta b_3 \). Despite deviation from ENS data for \( \zeta < 1 \), they obtain surprisingly good agreement for energy and entropy per particle down to \( T/T_F = 0.16 \).

We now turn to the ENS measurement for the trapped unitary unpolarized gas, as extracted by Hu et al. \[5\], and compare with our result. The range of applicability of the virial series \((5)\) is now extended fourfold to \(\zeta \approx 0.1\) (See Fig. 3). Here the convergence of the virial series is faster as expected, and the agreement is remarkably good down to \(\zeta \approx 0.1\). Figure 4 shows this clearly.

\[\begin{align*}
\bar{\rho} &= \frac{P}{P_0} = \frac{5T}{2T_F} f_P(X), \\
\kappa &= \frac{\kappa_0}{\kappa} = \frac{2T_F}{3T} f_P''(X). 
\end{align*}\]

where \( T/T_F = 4\pi/[3\pi^2 f_P'(X)]^{2/3} \) is the dimensionless temperature scale and the prime denotes a derivative with respect to \(X\). The heat capacity at constant volume and entropy are given by \(C_V/Nk_B = 15 f_P(X)/f_P'(X) - 4 f_P''(X)/f_P'(X) = \frac{3T_F}{2T} (\bar{\rho} - 1)/\kappa, S/Nk_B = \frac{5}{2} f_P'(X) - \ln(z)\). The above expressions allow one to calculate the relevant quantities either as a function of fugacity \(z\) or temperature \(T/T_F\) using the virial expansion given by Eq. \((6)\) and compare with the respective experimental data of Ku et al.

In the light of our earlier remarks (see Fig. 1), these comparisons are limited to \(z\) values less than \(4.95\), corresponding to \(T/T_F > 0.22\). Fig. 5 shows the variation of the pressure, entropy, and heat capacity as a function of \(T/T_F\). The agreement with experimental data improves noticeably as the higher \(\Delta b_l\)'s are included. The agreement for the pressure and entropy hold to \(T/T_F = 0.3\), indicating that the first moments of the virial expansion are good.This is not the case for the second moments, however, as the plots for heat capacity vs \(T/T_F\) shows. The theoretical plots start deviating appreciably from the data for \(T/T_F < 0.6\). The same behavior is seen in Fig. 6 where the compressibility is plotted as a function of pressure (in reduced variables). It is interesting to note that despite these deviations, a peak in the compressibility of about the right magnitude appears in the theoretical curve, though at a higher value of \(P/P_0\) or \(T/T_F\). Though tempting, we are reluctant to interpret this as indicative of the onset of superfluidity in view of the inaccuracy of the virial description in this range of temperature or pressure.

We conclude that the high-temperature virial expansion, in conjunction with our ansatz, can match the EOS over a significantly larger range of fugacity, corresponding to about \(T/T_F \approx 0.3\) for the homogeneous gas. Our ansatz (given by
Eq. (2) resulted from the picture of a unitary fermi gas as a dynamic collection of singlet pairs, and assumed that \((\Delta b_2)\) determines the higher virial coefficients. The resulting success of this picture may point to some truth in this conjecture, and poses a challenge for deeper understanding.

We thank S. Nascimbène, H. Hu and M. Ku for sharing the experimental data for the ideal and trapped fermion gas. We thank S. Das Gupta for helpful discussions. WvD acknowledges financial support from the Natural Sciences and Engineering Research Council of Canada, and MVN acknowledges the hospitality of Department of Physics and Astronomy, McMaster University where part of this work was done.

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