Universal Equation of State of a Unitary Fermionic Gas

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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.

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Feshbach resonance makes it possible to adjust the strength of the interatomic interaction in a neutral atomic gas. When the scattering length goes to $\pm\infty$, there is no length scale left other than the average interparticle 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 $T_c/T_F = 0.167(13)$.

In this Letter—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 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 $\Omega(\beta, \mu)$ is defined as $\Omega = -\tau \ln \mathcal{Z}$, where $\tau = k_B T = 1/\beta$ and $\mathcal{Z}$ is the grand canonical partition function. Furthermore, $\Omega = -PV$, and may be expressed in a power series of fugacity $z = \exp(\beta\mu)$, where μ is the chemical potential. The grand potential $\Omega = -\tau Z_1(\beta) \sum_{l=1}^{\infty} b_l z^l$, where $Z_1(\beta)$ is the one-body partition function, and b_l is the l-particle cluster integral. For an untrapped gas in volume V, we have $Z_1(\beta) = 2(V/\lambda^3)$, where spin degeneracy of 2 is included and $\lambda = (2\pi\hbar^2\beta/m)^{1/2}$ is the thermal wavelength. For a harmonic oscillator (HO) trap in three dimensions, $Z_1(\beta) = 2/(\hbar\omega\beta)^3$. 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 $\Omega^{(0)}$, we obtain the interaction part of the EOS as

$$\Omega - \Omega^{(0)} = -\tau Z_1(\beta) \sum_{l=2}^{\infty} (\Delta b_l) z^l, \tag{1}$$

where $\Delta b_l = b_l - b_l^{(0)}$. Note that $b_1 = b_1^{(0)} = 1$, and cancels out on taking the difference.

Consider now the special role played by Δb_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 that the pair interaction will be operative only between singlet pairs. One finds that [9] $\Delta b_2 = (2\sqrt{2}) \times \frac{1}{2}(\Delta Z_2)$, where the factor $2\sqrt{2}$ arises from the c.m. motion, ΔZ_2 is the relative two-body partition function, and the "suppression factor" $\frac{1}{2}$ 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 $\Delta Z_2 = \frac{1}{2}$, yielding $\Delta b_2 = \frac{1}{\sqrt{2}}$ for such a system. What about the Δb_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 Δb_l for $l > 2$ should be expressible in terms of (Δb_2) with an appropriate suppression factor. Viewing an 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 $2^{\mathcal{N}_{(l-1)}}$, where $\mathcal{N}_{(l-1)} = (l-1)(l-2)/2$ is in general the number of pairs in a cluster with $(l-1)$ fermions. Thus, our basic ansatz is

$$\Delta b_l = (-)^l \frac{(\Delta b_2)}{2^{\mathcal{N}_{(l-1)}}}, \qquad l \geq 2. \tag{2}$$

For $l = 2$, $\mathcal{N}_1 = 0$, and Eq. (2) is an identity. The alternating sign $(-)^l$ in the above equation was put in to keep the number fluctuation $(\Delta N)^2/\bar{N} = \sum_l l^2 b_l z^l / \sum_l l b_l z^l$ from growing to a very large value with z, where $(\Delta N)^2 = \overline{N^2} - \bar{N}^2$ 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, a similar relationship between the third and second virial coefficients has 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 nontrivial.

With this ansatz,

$$\Omega - \Omega^{(0)} = -\tau Z_1(\beta)(\Delta b_2) \sum_{l=2}^{\infty} (-)^l \frac{z^l}{2^{\mathcal{N}_{(l-1)}}}. \tag{3}$$

Experimentally [2,5,15], it is the quantity $h(\zeta) = \Omega/\Omega^{(0)}$ that is extracted, where $\zeta = 1/z$. This is given by

$$h(\zeta) = 1 + (\Delta b_2) \frac{\sum_{l=2}^{\infty} (-)^l (\zeta)^{-l} / 2^{\mathcal{N}_{(l-1)}}}{\tilde{\Omega}^{(0)}}. \tag{4}$$

In a homogeneous gas with a spin degeneracy of 2,

$$\tilde{\Omega}^{(0)} = \frac{2}{\sqrt{\pi}} \int_0^{\infty} \sqrt{t} \ln(1 + z e^{-t}) dt.$$

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, Δb_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 Δb_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 Δb_4 as quoted in Ref. [17] is of a different sign and magnitude from that quoted in Ref. [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 HO, Eq. (4) is modified to [2,5]

$$h(\zeta) = 1 + (\Delta b_2) \sum_{l=2}^{\infty} \frac{(-)^l}{(l)^{3/2}} \frac{\zeta^{-l}}{2^{\mathcal{N}_{(l-1)}}} / \tilde{\Omega}^{(0)}, \tag{5}$$

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

We are now ready to compare our predictions given by Eq. (4) for the homogeneous gas and Eq. (5) for the HO with experimental data. In Fig. 1, $h(\zeta) - 1$ for the homogeneous unpolarized gas [as given by our Eq. (4)] is plotted against ζ.

The crosses on the plot are the ENS experimental data as found by Nascimbène *et al.* [2]. The authors quote that h and ζ are accurate to within 6 percent. It will be seen from this figure that the series given by our Eq. (4) is in good agreement with the data down to $\zeta \approx 0.2$. To put the agreement in perspective, the same data are plotted as a function of $z = 1/\zeta$ in Fig. 2, along with the behavior of the EOS, including virial coefficients 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 Δb_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 [2]—rather than 0.088 given by our ansatz. Note that the $h(\zeta)$ has been calculated in [6] within Padé approximation and including up to Δb_3. Despite deviation from ENS data for $\zeta < 1$, they obtain surprisingly good

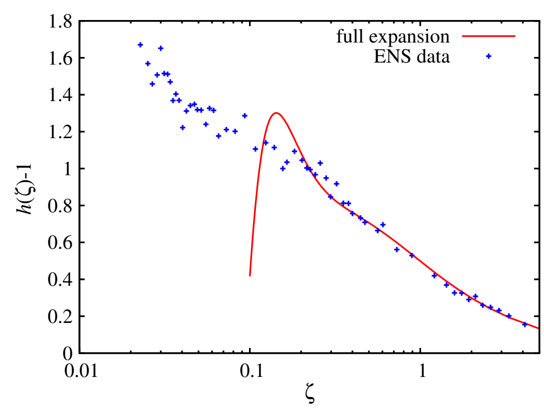

FIG. 1 (color online). The function $h(\zeta) - 1$ for the untrapped unitary Fermi gas [from Eq. (4)] as a function of ζ. The crosses represent the experimental data presented by Nascimbène *et al.* [2] in their Fig. 3(a).

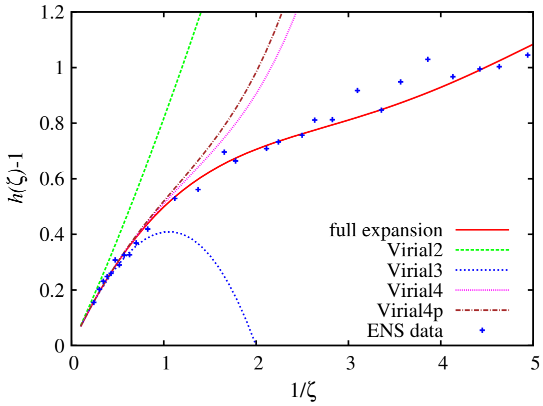

FIG. 2 (color online). The universal function $h(\zeta) - 1$ for the untrapped Fermi gas plotted as a function of the fugacity $1/\zeta$. The 2nd, 3rd, and 4th virial expansions are also shown. The 4th-order expansion (labelled "Virial4p") has $\Delta b_4 = 0.096$. The experimental data are the same as in Fig. 1.

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 Eq. (5). (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 when the truncated predictions from previous work are compared with our result. The range of applicability of the virial series (5) is now extended fourfold to $z \approx 10$.

It should be noted that the series given in Eqs. (4) and (5) converge for any value of z. However, the range of validity of the sum depends on the maximum value of l as seen from Figs. 2 and 4 for free gas and HO, respectively. The first few terms make a significant difference but the importance of Δb_l for $l > 8$ is minimal even at $z = 5$. The series gets saturated by the first twenty terms, which is denoted as "full expansion" in all the figures.

Encouraged by the agreement with $h(z)$, even deep into region $z > 1$ where the normal virial expansion is not expected to work, we next compare our predictions for the recently measured data on compressibility, heat capacity, and pressure by the MIT group [7]. Following their notation, we write $\beta P = f_P(X)/\lambda^3$, where P is the pressure, $X = \ln z = \beta\mu$, and $f_P(X)$ is the universal function given by

$$f_P(X) = 2\left(f_{5/2}[\exp(X)] + \sum_{l=2}^{\infty} \Delta b_l \exp(lX)\right). \qquad (6)$$

The first term in the bracket is the contribution due to the ideal Fermi gas, and is the standard Fermi-Dirac integral [18]. All thermodynamic quantities can now be expressed in terms of this universal function and its derivatives. (See Ref. [7].) Specifically, we have pressure and compressibility normalized by their zero temperature values, P_0, κ_0, given by

$$\tilde{p} = \frac{P}{P_0} = \frac{5T}{2T_F}\frac{f_P(X)}{f'_P(X)}; \qquad \tilde{\kappa} = \frac{\kappa}{\kappa_0} = \frac{2T_F}{3T}\frac{f''_P(X)}{f'_P(X)}, \qquad (7)$$

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 $C_V/Nk_B = \frac{15}{4}\frac{f_P(X)}{f'_P(X)} - \frac{9}{4}\frac{f'_P(X)}{f''_P(X)} = \frac{3T_F}{2T} \times (\tilde{p} - 1/\tilde{\kappa})$, $S/Nk_B = \frac{5}{2}\frac{f_P(X)}{f'_P(X)} - \ln(z)$. 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 to compare them with the respective experimental data of Ku *et al* [7].

In the light of our earlier remarks (see Fig. 1), these comparisons are limited to z values less than 4.95, corresponding to $T/T_F > 0.22$. Figure 5 shows the variation of the pressure, entropy, and heat capacity as a function of T/T_F. The agreement with experimental data improves

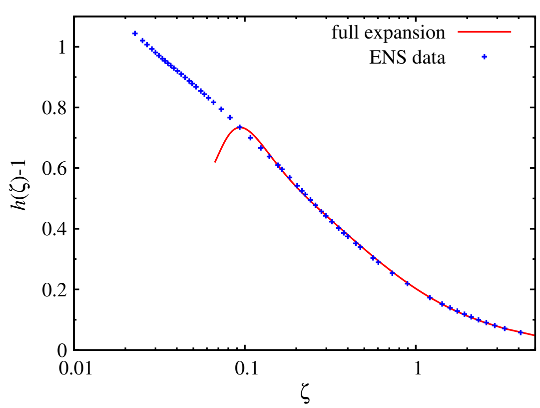

FIG. 3 (color online). The universal function $h(\zeta) - 1$ for fermions in a harmonic trap as a function of ζ, Eq. (5). The crosses represented the experimental data presented in Fig. 6 of Hu *et al.* [5].

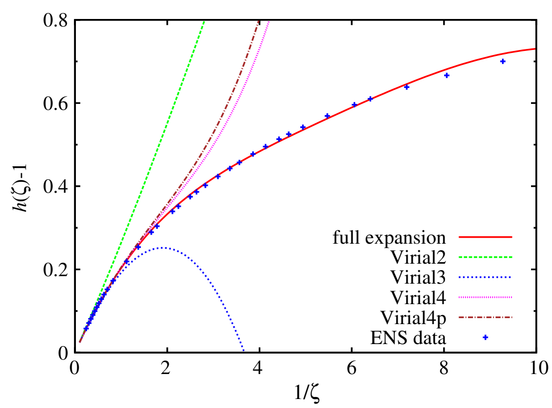

FIG. 4 (color online). The universal function of trapped fermions $h(\zeta) - 1$ as a function of fugacity. See Eq. (5). Virial4p is the 4th-order virial expansion with $\Delta b_4 = 0.096$. The experimental data are the same as in Fig. 3.

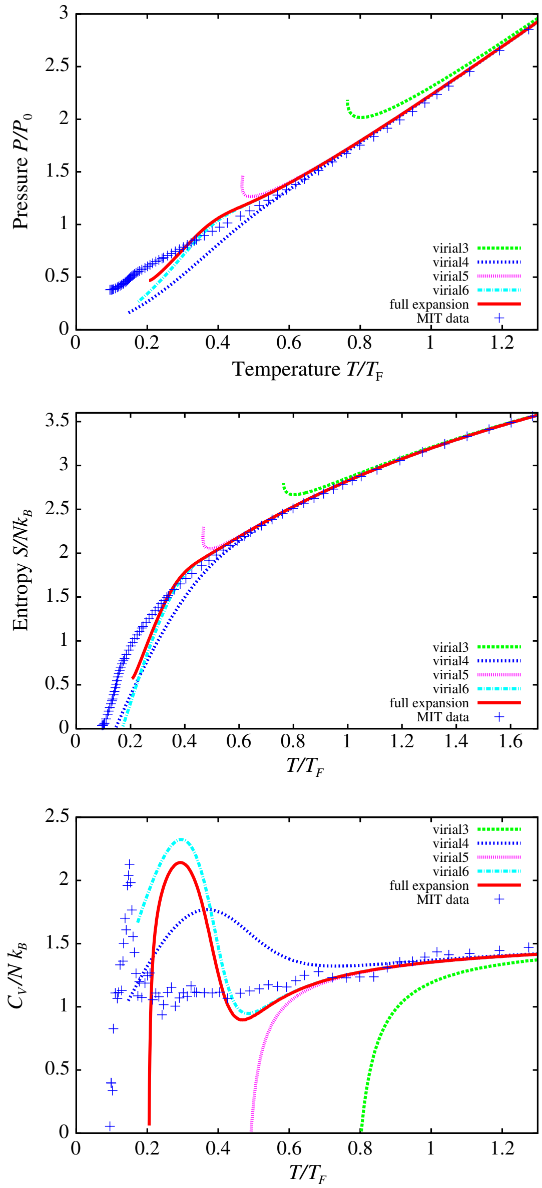

FIG. 5 (color online). Reduced pressure (top), entropy (middle), and heat capacity (bottom) shown as a function of T/T_F for the untrapped unitary Fermi gas. The experimental data are taken from Ku *et al.* [7].

noticeably as the higher Δb_l's are included. The agreement for the pressure and entropy hold to $T/T_T = 0.3$, 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 show. 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

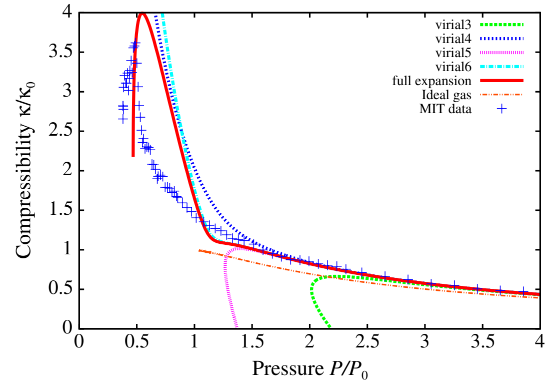

FIG. 6 (color online). Reduced compressibility shown as a function of reduced pressure for the untrapped unitary Fermi gas. The experimental data are taken from Ku *et al.* [7].

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 (Δb_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.

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