On the higher virial coefficients of a unitary Fermi gas

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Third and higher order quantum virial coefficients require the solution of the corresponding quantum many-body problem. Nevertheless, in an earlier paper (Phys. Rev. Lett. 108, 260402 (2012)) we proposed that the higher-order cluster integrals of a dilute unitary fermionic gas may be approximated in terms of the two-body cluster, together with an appropriate suppression factor. Although not exact, this ansatz gave a fair agreement up to fugacity $z \approx 6$ with the experimentally obtained equation of state. The objective of the present note is to give some physical arguments in favor of this ansatz.

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Experimentally, it is feasible to adjust the interatomic interaction in a gas using Feshbach resonance [1, 2]. When this is adjusted such that the two atoms are just shy of binding (scattering length $\to \pm \infty$), the gas is called unitary. In recent times, there has been considerable experimental activity on obtaining the thermodynamic properties of a unitary fermionic gas [3–6]. It was proposed long back that the two-body cluster integral that is most sensitive to the interaction between the atoms may be expanded in a power series of $z$ and written as

$$
\Omega - \Omega^{(0)} = -\tau Z(\beta) \sum_{l=2}^{\infty} (\Delta b_l) z^l.
$$

(1)

The grand potential of the ideal Fermi gas is denoted by $\Omega^{(0)}$, and is given by $\Omega^{(0)} = -\tau Z(\beta) f_{\nu/2}(z)$, where $f_{\nu}(z)$ is the usual Fermi integral [13]

$$
f_{\nu}(z) = \frac{1}{\Gamma(\nu)} \int_0^\infty dy \frac{y^{(\nu-1)}}{1+z^{-1}e^y}.
$$

(2)

In Eq. (1), $Z(\beta)$ is the one-body partition function, and $\Delta b_l$ is the $l$-particle interaction part of the cluster integral. For an untrapped gas in volume $V$, we have $Z(\beta) = 2(V/\lambda)$, where spin degeneracy of 2 is included and $\lambda = (2\pi\hbar^2/\beta m)^{1/2}$ is the thermal wave length. For a unitary gas, the interaction part of the cluster integrals $\Delta b_l$’s are temperature independent in the high temperature limit. Even though the virial expansion (1) for the interaction part converged well even for large $z$, such was not the case for the statistical part $\Omega^{(0)}$. Therefore its exact form by computing the Fermi integral was used, rather than its fugacity expansion. From Eq. (1), we see that the interaction part of the grand potential requires a knowledge of $\Delta b_l$’s. We proceed to obtain these assuming that its major contribution is coming from two-body physics. It was assumed in Ref. [11] that at unitarity, $\Delta b_l$ could be obtained from $\Delta b_2$ by applying an appropriate suppression factor. We emphasize that the temperature-independent $\Delta b_l$’s at unitarity were obtained only when the quantum expressions were taken to the high temperature limit. There is some justification, then, in doing a semiclassical analysis by imposing the Pauli principle to the interaction bonds. This has a huge effect on the counting of bonds. For example, consider the three-body problem. On applying the Pauli principle, we see that the linked cluster triangle diagram linking all three particles with interaction bonds is not allowed. This is because two spin-up identical atoms cannot interact at zero-range in the relative $s$-state.

To understand the suppression factor due to Pauli principle, consider a cluster with $l$ fermionic atoms. Choose any one of
them as a test particle, interacting pairwise with the fermions in the remaining \((l-1)\)-particle cluster. Our objective is to examine how the two-body bonds involving the test particle with the rest may get suppressed due to the Pauli blocking. Let \(N_{(l-1)}\) denote the number of two-body pairs in a cluster with \((l-1)\) fermions. To illustrate with the simplest example, let \(l=3\). For this case \(N_{(l-1)}=(l-1)(l-2)/2=1\), and the test particle sees only one pair, as shown in Fig. 1. In Fig. 1(a) we assume that the test particle has spin up, and the pair consists of one spin-up and the other spin-down particle. Since the interaction is a zero-range (s-state) potential, the pair consists of one spin-up and the other spin-down particle. Since the Pauli principle gives an effective repulsive effect, in contrast to the attractive potential at unitarity, we expect the \(\Delta b_l\)’s to be of opposite signs to \(b_l^{(0)}\)’s.

Using these reasonings, we write down the equation for the net suppression factor.

\[
\Delta b_l = (-)^l \frac{(\Delta b_2)}{2^{N_{(l-1)}}}, \quad l \geq 2.
\]

In the above, as stated earlier, \(N_{(l-1)}=(l-1)(l-2)/2\) is the number of pairs in a cluster with \((l-1)\) fermions. For \(l=2\), \(N_1=0\), and Eq. (3) is an identity. Since \(\Delta b_2 = \frac{1}{\sqrt{2}}\) is known analytically [15], all the higher virial coefficients can be found using our Eq. (3). The third virial coefficient has been calculated very accurately [16, 17] up to 12 decimal figures to be \(-0.3551\ldots\). Our formula gives \(\Delta b_3 = -\frac{1}{2 \sqrt{2}} = -0.3536\ldots\). For \(l=4\), we get \(\Delta b_4 = 
\]

\[
\frac{1}{3 \sqrt{2}} = 0.088\ldots\], to be compared with the value based on measurements, \(0.096 \pm 0.015\) [3].

The alternating signs in Eq. (3) are borne out by experimental data, up to at least \(l=8\). Using Eq. (1), we get

\[
\frac{\Delta P}{P^{(0)}} = \frac{\sum_{l=2}^{\infty} (\Delta b_l) z^l}{f_{3/2}(z)},
\]

FIG. 1. (Color online) Interactions in three-particle clusters. Effective two-particle interactions between the test particle and the pair are indicated by the dashed line connecting the particles.

FIG. 2. (Color online) Four-particle cluster. A test particle effectively sees three pairs.

FIG. 3. (Color online) Incremental pressure as a function of fugacity. The numbers labelling the curves indicate the maximum \(l\)-value that is included in the sum of Eq. (4). The curves with \(l = 9, 10, 20\) show no discernible difference. The inset has a logarithmic horizontal scale indicating a range of \(z\) values from 0.2 to 10. The tic mark corresponds to \(z = 1\). The experimental data is taken from Ref. [3].
where \( P \) is the pressure of the interacting gas, and \( P^{(0)} \) the pressure of an ideal Fermi gas at the same value of \( z \), and in the same volume. In the above equation, \( \Delta P = P - P^{(0)} \) shows that a positive \( \Delta b_l \) increases the pressure from its ideal value, whereas a negative \( \Delta b_l \) decreases it. This is seen clearly in Fig. 3, where the incremental contribution to the pressure is shown by taking the upper limit in the summation of \( l \) at \( l = 2, 3, 4, \ldots \) etc. In the curve labelled 3, for example, only the contributions from \( \Delta b_2 \) and \( \Delta b_3 \) are included. The alternating signs \((-1)^l\) ensure that the virial series for the EOS follows the experimental points closely. It is evident from Fig. 3 that the series converges since terms involving \( l > 9 \) do not change the sum.

We note that in general the \( l \)-body quantum problem has to be solved in order to obtain the cluster integral \( \Delta b_l \). We have argued, however, that in the high temperature limit of a dilute unitary gas, the main contribution to the \( l \)-body cluster comes from two-body physics. It is essential to go to the high temperature limit where the virial coefficients are temperature independent, and semiclassical arguments may be made. The qualitative physical arguments led us to propose Eq. (3). Since it is able to match the experimental data well, this presentation may encourage others to do a more quantitative derivation of the equation.

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