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The third virial coefficient of a two-component unitary Fermi gas across an Efimov-effect threshold

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Abstract – We consider a mixture of two single-spin-state fermions with an interaction of negligible range and infinite s -wave scattering length. By varying the mass ratio α across $\alpha_c \simeq 13.6069$ one can switch on-and-off the Efimov effect. We determine analytically the third cluster coefficient of the gas. We show that it is a smooth function of α across α_c since, unexpectedly, the three-body parameter characterizing the interaction is relevant even on the non-Efimovian side $\alpha < \alpha_c$.

Introduction. – A powerful theory tool in the statistical physics of interacting quantum systems is the so-called cluster or virial expansion, where the thermodynamic potentials are expanded in powers of the small degeneracy parameter [1]. Whereas the second cluster coefficient b_2 had a known general expression since the 1930s [2], it has been a long-lasting challenge to determine the third cluster coefficient b_3 explicitly. Starting from the late 1950s, analytical results for b_3 have been obtained for the two-body hard-core model, the archetype of non-resonant interactions where the s -wave scattering length a is at most of the order of the interaction range, in the form of expansions in powers of a small parameter λ/a [3] or a/λ [4], where λ is the thermal de Broglie wavelength.

Interest in b_3 was reactivated by recent experimental breakthrough with cold atoms: long-lived spin 1/2 Fermi gases can be prepared in the resonantly interacting regime ($|a| \gg$ interaction range) via Feshbach resonances [5]. This motivated numerical calculation of b_3 in maximally interacting, unitary limit $1/a=0$, with the harmonic regulator technique of [6] as done in [7], or with diagrams [8]. Due to scaling invariance in the unitary limit, b_3 is just a number, and via a precise measurement of the gas equation of state [9, 10], its predicted value was confirmed [10].

Physics is richer when the Efimov effect [11] sets in: the continuous scaling invariance is broken, there appears a length scale R_t characterizing the interaction, the three-body parameter, and there exists an infinite number of trimer states with an asymptotically geometric spectrum. The third cluster coefficient b_3 becomes a function of temperature. In a spinless bosonic gas with zero-range inter-

actions, it was determined analytically [12]. Within the three-body hard-core model that fixes R_t [13], Quantum Monte Carlo simulations have confirmed this analytical prediction and have shown that the third order cluster expansion can provide a good description of the gas down to the liquid-gas transition [14], exemplifying its usefulness.

The problem is even more intriguing when a system parameter allows to switch on-and-off the Efimov effect, as in the two-component Fermi gas with adjustable mass ratio. For two identical fermions and a distinguishable particle, there is an Efimov effect if the fermion-other particle mass ratio α exceeds $\alpha_c = 13.6069 \dots$ [11, 15]. Up to now, the calculation of b_3 is numerical and limited to $\alpha < \alpha_c$ [16]. Strikingly it predicts that b_3 has an infinite derivative at $\alpha = \alpha_c$. As b_3 is a coefficient in the grand potential Ω , this would imply a singular derivative of Ω as a function of α , i.e. a first order phase transition, subsisting at arbitrarily low phase space density, i.e. at temperatures T arbitrarily higher than the Fermi temperature T_F , contrarily to common expectations for phase transitions. The present work determines b_3 analytically and solves this paradox.

The cluster expansion. – We consider a mixture of two fully polarized fermionic species, with single particle masses m_1 and m_2 , with no intraspecies interaction and a purely s -wave interspecies interaction, of negligible range and infinite scattering length (unitary limit). At thermal equilibrium in a cubic box, the total pressure P admits in the thermodynamic limit the cluster expansion

$$\frac{P\lambda_r^3}{k_B T} = \sum_{(n_1, n_2) \in \mathbb{N}^2} b_{n_1, n_2} z_1^{n_1} z_2^{n_2} \quad (1)$$

where z_i are fugacities $\exp(\beta\mu_i)$, $\lambda_r = [2\pi\hbar^2/(m_r k_B T)]^{1/2}$ is the thermal de Broglie wavelength associated to the reduced mass $m_r = m_1 m_2 / (m_1 + m_2)$ and temperature T , $\beta = 1/(k_B T)$, μ_i is the chemical potential of species i , and \mathbb{N} is the set of all non-negative integers.

To determine the cluster coefficients b_{n_1, n_2} one can use the harmonic regulator trick [6]: one rather assumes that the system is at thermal equilibrium in an isotropic harmonic trap, with the same trap frequency ω for the two species, and one considers the cluster expansion of $(-\Omega)/(k_B T Z_1)$ in powers of z_1 and z_2 , with Ω the grand potential and Z_1 the single particle partition function in the trap. When $\omega \rightarrow 0$, the corresponding coefficients have a limit B_{n_1, n_2} that one can relate to b_{n_1, n_2} [6, 7, 16]:

$$B_{n_1, n_2} = \left(\frac{m_r}{n_1 m_1 + n_2 m_2} \right)^{3/2} b_{n_1, n_2} \quad (2)$$

We study $B_{2,1}$ as a function of the mass ratio $\alpha = m_1/m_2$.

Case $\alpha < \alpha_c$: 0-parameter zero-range model. – The cluster coefficient $B_{2,1}$ can be deduced from the partition functions of up to three bodies in the trap, that is from the n -body energy spectra for $n \leq 3$. In the unitary limit, the interspecies interaction is described by the Bethe-Peierls binary contact condition on the wavefunction, which leads to a separable three-body Schrödinger equation in internal hyperspherical coordinates [11] even in a harmonic trap [17–19]. The hyperangular part of the problem can be solved in position space [11] or in momentum space [20]: the corresponding real eigenvalue s^2 (that will serve as a separability constant) obeys the transcendental equation $\Lambda_l(s) = 0$ of explicit expression [21]¹

$$\Lambda_l(s) = \cos \nu + \frac{1}{\sin \nu} \int_{\frac{\pi}{2}-\nu}^{\frac{\pi}{2}+\nu} d\theta P_l \left(\frac{\cos \theta}{\sin \nu} \right) \frac{\sin(s\theta)}{\sin(s\pi)} \quad (3)$$

with $l \in \mathbb{N}$ the angular momentum, P_l a Legendre polynomial, $\nu = \arcsin \frac{\alpha}{1+\alpha}$ the mass angle. We call $(u_{l,n})_{n \in \mathbb{N}}$ the positive roots of Λ_l , sorted in increasing order. There is no complex root for $\alpha < \alpha_c$. The hyperradial part of the wavefunction, after multiplication by R^2 , solves an effectively bidimensional Schrödinger equation:

$$EF = -\frac{\hbar^2}{2M} \left(F'' + \frac{1}{R} F' \right) + \left(\frac{\hbar^2 s^2}{2MR^2} + \frac{1}{2} M \omega^2 R^2 \right) F \quad (4)$$

where s is any of the $u_{l,n}$, $M = 2m_1 + m_2$ is the mass of two particles of species 1 and one particle of species 2, and the hyperradius R is the corresponding mass-weighted root-mean-square deviation of the positions of the three particles from their center of mass. Solving Eq.(4) with the usual boundary conditions that $F(R)$ vanishes at zero and infinity gives

$$E = (s + 1 + 2q)\hbar\omega, \quad \forall q \in \mathbb{N} \quad (5)$$

¹There exists a less explicit hypergeometric expression for Λ_l [22].

The semi-infinite ladder structure of this spectrum, with equidistance $2\hbar\omega$, reflects the existence of an undamped breathing mode of the trapped non-Efimovian unitary gas [23] related to its $SO(2,1)$ dynamical symmetry [24].

Finally $B_{2,1}$ is the $\omega \rightarrow 0$ limit of a series [7, 12]²:

$$B_{2,1} = \lim_{\omega \rightarrow 0} \sum_{(l,n,q) \in \mathbb{N}^3} (2l+1) \left[e^{-(u_{l,n}+1+2q)\beta\hbar\omega} - e^{-(v_{l,n}+1+2q)\beta\hbar\omega} \right] \quad (6)$$

with $v_{l,n} = l + 2n + 1$ the positive poles of $\Lambda_l(s)$ [21]. The summation over q can be done, and even over n by inverse application of the residue theorem [12]:

$$B_{2,1} = - \sum_{l \in \mathbb{N}} \left(l + \frac{1}{2} \right) \int_0^{+\infty} \frac{dS}{\pi} \ln \frac{\Lambda_l(iS)}{\cos \nu} \quad (7)$$

As shown in Fig. 1, the result agrees with the numerical evaluation of the series by [16]. The analytics however directly allows to see why $B_{2,1}$ has an infinite derivative with respect to α at $\alpha = \alpha_c^-$: it suffices to isolate the contribution of the channel $(l,n) = (1,0)$ in Eq.(6), the only one where $u_{l,n}$ vanishes at $\alpha = \alpha_c$, by the splitting

$$B_{2,1} = B_{2,1}^{(1,0)} + B_{2,1}^{\neq(1,0)} \quad (8)$$

All the other channels have $u_{l,n} > 1$ over the figure range and give a smooth contribution to $B_{2,1}$. On the contrary

$$\begin{aligned} B_{2,1}^{(1,0)} &= \lim_{\omega \rightarrow 0} 3 \sum_{q \in \mathbb{N}} \left[e^{-(u_{1,0}+1+2q)\beta\hbar\omega} - e^{-(v_{1,0}+1+2q)\beta\hbar\omega} \right] \\ &= -\frac{3}{2} (u_{1,0} - v_{1,0}) \end{aligned} \quad (9)$$

and $u_{1,0}$, a decreasing function of α , vanishes as $(\alpha_c - \alpha)^{1/2}$ since $\Lambda_1(s)$ is even, so that $\frac{d}{d\alpha} B_{2,1}$ diverges as $(\alpha_c - \alpha)^{-1/2}$.

Case $\alpha > \alpha_c$: Efimov zero-range model. – We now assume that the mass ratio obeys $\alpha_c < \alpha < 75.99449\dots$ [25], so that the Efimov effect takes place in the sector $l = 1$ only. The function $\Lambda_{l=1}$ has a pair of complex conjugate purely imaginary roots $\pm s$ and we set

$$u_{1,0} = s = i|s| \quad (10)$$

$|s|$ vanishes as $(\alpha - \alpha_c)^{1/2}$ and increases with α . The $1/R^2$ potential in Schrödinger's equation (4) for $F(R)$ becomes attractive, which leads to a “fall to the center” [26] and to an unphysical continuous spectrum of bound states, forcing to modify the boundary condition at $R = 0$ [27]:

$$F(R) \underset{R \rightarrow 0}{=} (R/R_t)^{i|s|} - (R/R_t)^{-i|s|} + O(R^2) \quad (11)$$

²Actually one calculates the difference between partition functions of unitary and non-interacting problems; still this directly gives $B_{2,1}$ of the unitary gas since $B_{2,1}$ is zero for the ideal gases; the contributions of the Laughlinian states (whose wavefunction vanishes when two particles are at the same point) cancel out in the difference; the $v_{l,n}$ appear via the non-Laughlinian spectrum of the non-interacting three-body problem. Similarly, the contributions of the unphysical root $s = 2$ in the sector $l = 0$, which exists in both the unitary and non-interacting cases, automatically cancel out.

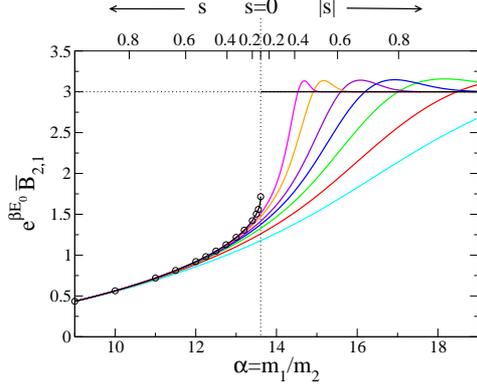


Fig. 1: Reduced third cluster coefficient $e^{\beta E_0} \bar{B}_{2,1}$ of a trapped two-component three-dimensional unitary Fermi gas in the zero trapping frequency limit, as a function of the mass ratio $\alpha = m_1/m_2$ of the two species (lower x -axis) or of the root $s = u_{1,0}$ of Λ_1 (upper x -axis), for various values of the three-body parameter R_t , and hence of the global energy scale E_{glob} of Eqs.(13,24). Here E_0 is the ground free-space three-body energy, a smooth function of α : for $\alpha \leq \alpha_c$, $E_0 = 0$; for $\alpha > \alpha_c$, $E_0 = -E_{\text{glob}} \exp(-2\pi/|s|)$ is the ground trimer energy and the factor $\exp(\beta E_0)$ ensures that the plotted quantity remains bounded. Curves from bottom to top for $\alpha \lesssim 15$: $\beta E_{\text{glob}} = 10^2$ (cyan), 3×10^2 (red), 10^3 (green), 3×10^3 (blue), 10^4 (violet), 10^5 (orange), 10^6 (magenta). The curves cross, which shows that $e^{\beta E_0} \bar{B}_{2,1}$ is not, at all fixed α , an increasing function of βE_{glob} (see inset in Fig. 2). Discontinuous black solid line: limit $\beta E_{\text{glob}} \rightarrow +\infty$, corresponding for $\alpha \leq \alpha_c$ to the genuine 0-parameter zero-range model studied numerically in [16] (black circles), and being, for $\alpha > \alpha_c$, identically equal to 3, the ground-trimer contribution. Vertical dotted line: critical mass ratio α_c where the Efimov effect sets in.

To make evident that the third cluster coefficient now depends on *one* parameter, this length R_t called three-body parameter, we write it as $\bar{B}_{2,1}$, that is with *one* overlining bar. In free space, Eq.(11) leads to a discrete infinite number of Efimov trimer states, with a purely geometric spectrum extending from $-\infty$ to 0. In any physical system, however, the interaction is not strictly zero range and the spectrum must be bounded from below [11]. One may expect that finite range effects then spoil the geometric nature of the spectrum for the more deeply bound trimers. However, for a narrow Feshbach resonance [21, 28], for momentum-space cut-off models of a Feshbach resonance [29, 30], and for the three-body hard core model [13], the spectrum is almost entirely geometric, at least when $|s|$ is not too large ($|s| \lesssim 1$), and becomes entirely geometric when $\alpha \rightarrow \alpha_c^+$, since the typical particle wavenumber times the interaction range tends to zero [21]. In what follows, we assume the bounded from below geometric free space spectrum:

$$\epsilon_q(0^+) \equiv \lim_{\omega \rightarrow 0} \epsilon_q(\omega) = -E_{\text{glob}} e^{-2\pi(1+q)/|s|}, \quad \forall q \in \mathbb{N} \quad (12)$$

The global energy scale E_{glob} can be calculated from a microscopic model for the interaction, as it was done in the

above mentioned models. Here we take it as a parameter that solution of Eq.(4) with $\omega = 0$ and with the boundary condition (11) relates to R_t as

$$E_{\text{glob}} = \frac{2\hbar^2}{MR_t^2} e^{[\ln \Gamma(1+s) - \ln \Gamma(1-s)]/s} \quad (13)$$

with $\ln \Gamma$ the usual branch of the Γ function logarithm.

The contribution to $\bar{B}_{2,1}$ of the channels $(l, n) \neq (1, 0)$ is unchanged since no Efimov effect occurs in these channels:

$$\bar{B}_{2,1}^{\neq(1,0)} = B_{2,1}^{\neq(1,0)} \quad (14)$$

We calculate it as in [12], using Eq.(7) as it is for $l \neq 1$, while substituting $\Lambda_l(iS)$ with $\frac{S^2+v_{1,0}^2}{S^2+u_{1,0}^2} \Lambda_l(iS)$ for $l = 1$. In the Efimovian channel $(l, n) = (1, 0)$, the spectrum is no longer given by Eq.(5), but by the solution of the transcendental equation deduced from [31] and rewritten as in [12, 32] to match Eq.(12) in free space:

$$\text{Im} \ln \Gamma\left(\frac{1+s-\epsilon_q/(\hbar\omega)}{2}\right) + \frac{|s|}{2} \ln\left(\frac{2\hbar\omega}{E_{\text{glob}}}\right) + (q+1)\pi = 0 \quad (15)$$

so that the first identity in Eq.(9) is replaced by

$$\bar{B}_{2,1}^{(1,0)} = \lim_{\omega \rightarrow 0} 3 \sum_{q \in \mathbb{N}} \left[e^{-\beta \epsilon_q(\omega)} - e^{-(v_{1,0}+1+2q)\beta \hbar\omega} \right] \quad (16)$$

For a small enough non-zero ω , two classes emerge in the three-body spectrum: (i) negative eigenenergies, that are the equivalent of free space trimer energies, and (ii) positive eigenenergies, that are the equivalent of the free space continuum. The second class is a harmonic spectrum except for an energy dependent ‘‘quantum defect’’ $\Delta(\epsilon)$ [32]

$$\frac{\epsilon_q(\omega)}{\hbar\omega} \Big|_{q \rightarrow +\infty} = 2q + \Delta(\epsilon_q(\omega)) + O(1/q) \quad (17)$$

where $q\omega$ is \approx fixed. By the reasoning of [12], we get

$$\bar{B}_{2,1}^{(1,0)} = 3 \sum_{q \in \mathbb{N}} [e^{-\beta \epsilon_q(0^+)} - 1] - \frac{3}{2} \int_0^{+\infty} d\epsilon \beta [\Delta(\epsilon) - (1+v_{1,0})] e^{-\beta \epsilon} \quad (18)$$

We obtained a new expression of the quantum defect³:

$$\Delta(\epsilon) = 2 + \frac{2}{\pi} \text{atan} \frac{\tan(\frac{|s|x}{2})}{\text{th}(\frac{|s|x}{2\pi})} + 2 \left\lfloor \frac{|s|x}{2\pi} \right\rfloor \quad (19)$$

where $x = \ln(\epsilon/E_{\text{glob}})$. The nearest-integer function in the last term exactly compensates the jumps of the atan function when $\tan(|s|x/2)$ diverges, so as to render $\Delta(\epsilon)$ a smooth function of ϵ and of $|s|$.

³This expression and the one (C6) of [32] are equal, since their difference is a continuous function of x that vanishes at zero and has an identically zero derivative.

The corresponding values of $\bar{B}_{2,1}$ for $\alpha > \alpha_c$ are shown in Fig.1, after multiplication by a factor $e^{\beta E_0}$, where $E_0 = \epsilon_{q=0}(0^+)$ is the ground trimer energy, so as to absorb its contribution that becomes rapidly dominant and divergent for $k_B T < |E_0|$ [33]. The result depends on βE_{glob} , a parameter that must be $\gg 1$: our theory, being zero range, requires that R_t , of order of the interaction range or effective range, as in the three-body hard core and narrow Feshbach resonance models respectively, is \ll the thermal de Broglie wavelength $\lambda_t = [2\pi\hbar^2/(Mk_B T)]^{1/2}$. Clearly, there is a discrepancy of $B_{2,1}(\alpha)$ and $\bar{B}_{2,1}(\alpha)$ at α_c^\mp at non-zero R_t . When $R_t \rightarrow 0$ ($E_{\text{glob}} \rightarrow +\infty$) there is agreement at α_c , as seen by first taking the $s \rightarrow 0$ limit in Eq.(19),

$$\Delta(\epsilon) \xrightarrow{\alpha \rightarrow \alpha_c^+} \Delta_0(\epsilon) = 2 + \frac{2}{\pi} \operatorname{atan} \frac{\ln(\epsilon/E_{\text{glob}})}{\pi} \quad (20)$$

then taking the $R_t \rightarrow 0$ limit in Eq.(18)⁴:

$$\begin{aligned} \bar{B}_{2,1}^{(1,0)}(\alpha_c^+) &= -\frac{3}{2} \int_0^{+\infty} d\epsilon \beta [\Delta_0(\epsilon) - (1 + v_{1,0})] e^{-\beta \epsilon} \\ &= \frac{3}{2} v_{1,0} - \frac{3}{\ln(\beta E_{\text{glob}})} + O\left(\frac{1}{\ln(\beta E_{\text{glob}})}\right)^2 \end{aligned} \quad (21)$$

successfully collated with the $u_{1,0} \rightarrow 0$ value of Eq.(9). The key point however is that this $R_t \rightarrow 0$ limit is in practice inaccessible, due to the very slow logarithmic convergence. We expect this problem to extend to $\alpha < \alpha_c$, which makes the strictly zero-range calculation of [16] not fully realistic. There also remains the puzzle of the diverging derivative of $B_{2,1}(\alpha)$ with respect to α at α_c^- . Both issues are solved in the next section.

Case $\alpha < \alpha_c$ revised: 1-parameter zero-range model. – We now see that a three-body parameter R_t must be introduced for $\alpha < \alpha_c$, i.e. even in the absence of Efimov effect, when α is close enough to α_c . The root $s = u_{1,0} > 0$ then vanishes as $(\alpha_c - \alpha)^{1/2}$ and the centrifugal barrier in the hyperradial equation (4) weakens, so that the function $F(R)$, the eigenenergies E and the third cluster coefficient become increasingly sensitive to short distance physics of the interaction [30, 34].

Assume that three-body physics inside the interaction range is described by an extra term $V(R)F$ compared to Eq.(4), e.g. a three-body hard core of radius b . Knowing that the relevant eigenenergies E are at most a few $k_B T$, and that $b \ll \lambda_t$, we can make the following reasonings.

(i) at $R \ll \lambda_t$, one can obtain the behavior of $F(R)$ by a zero-energy calculation (neglecting the EF term) in free space (since the harmonic oscillator length is $\gg \lambda_t$). Due to $b \ll \lambda_t$ there exists a range $b \ll R \ll \lambda_t$ where one can also neglect $V(R)$. Then $F(R)$ is a superposition of the two particular solutions R^s and R^{-s} , with relative amplitudes fixed by a length R_t that depends on microscopic

⁴One takes $\beta\epsilon$ as integration variable and one expands the integrand in powers of $1/\ln(\beta E_{\text{glob}})$.

details of $V(R)$, e.g. $R_t = b$ for the three-body hard core⁵:

$$F(R) \underset{b \ll R \ll \lambda_t}{\simeq} (R/R_t)^s - (R/R_t)^{-s} \quad (22)$$

(ii) one can approach the same range $b \ll R \ll \lambda_t$ from large distances. The trapping potential and the EF term must now be kept, and $F(R)$ is the unique solution (up to normalisation) of Eq.(4) that does not diverge at infinity, a Whittaker function of R^2 divided by R [19]. Then at $R \ll \lambda_t$, $F(R)$ is also found to be a linear superposition of R^s and R^{-s} , as it must be, but with coefficients $A_\pm(E)$ that are known functions of E . Matching with Eq.(22) gives an implicit equation for E , as if Eq.(4) was subjected to the modified boundary condition at $R = 0$ [18, 35]⁶:

$$F(R) \underset{R \rightarrow 0}{=} (R/R_t)^s - (R/R_t)^{-s} + O(R^{2-s}) \quad (23)$$

The third term in Eq.(23), coming from a property of the Whittaker function, is negligible as compared to the first one, and this model makes sense, for $s < 1$ i.e. $\alpha > 8.6185\dots$ Remarkably this reproduces the Efimov zero-range model (11) if one formally replaces s by $i|s|$. Then it is natural to extend the definition of E_{glob} to $\alpha < \alpha_c$ ⁷:

$$E_{\text{glob}} \underset{0 < s < 1}{=} \left(\frac{\Gamma(1+s)}{\Gamma(1-s)} \right)^{1/s} \frac{2\hbar^2}{MR_t^2} \quad (24)$$

where the first factor is a smooth function of α , as its series expansion involves only even powers of s .

The more common boundary condition $F(R=0) = 0$, that led to the spectrum (5), is usually justified as follows: at $R \approx \lambda_t$, the R^{-s} term in (22) is negligible as compared to the R^s term in the zero-range limit $b \ll \lambda_t$, that is $\beta E_{\text{glob}} \gg 1$ as one expects $R_t \approx b$ ⁸:

$$\frac{(\lambda_t/R_t)^{-s}}{(\lambda_t/R_t)^s} \approx (\beta E_{\text{glob}})^{-s} \ll 1 \quad (25)$$

However this condition becomes more and more difficult to satisfy when $\alpha \rightarrow \alpha_c^-$, and it will be violated when

$$s \lesssim \frac{1}{\ln(\beta E_{\text{glob}})} \quad (26)$$

This forces us to recalculate the third cluster coefficient with the boundary condition (23). From the implicit equa-

⁵If one sets $F(R) = R^{-s}\phi(r = R^{2s})$ then $F'' + F'/R - s^2 F/R^2 = 4s^2 R^{3s-2}\phi''(r)$ so that $R_t^{2s} = a_{\text{eff}}$, where a_{eff} is the s -wave scattering “length” of a particle of mass M on the potential $v(r) = V(r^{1/(2s)})r^{-2+1/s}/(4s^2)$. We suppose here that $a_{\text{eff}} > 0$, e.g. because $V(R)$ is non-negative.

⁶For $s = 0$ this becomes $F(R) \underset{R \rightarrow 0}{=} \ln(R/R_t) + O(R^2 \ln R)$.

⁷On a narrow resonance of Feshbach length R_* one gets from [21] $(\frac{m_r R_*^2}{2\hbar^2} E_{\text{glob}})^s = \frac{1-s}{1+s} \frac{\Gamma(1+2s)}{\Gamma(1-2s)} f(v_{1,0}) \prod_{n \in \mathbb{N}^*} \frac{f(v_{1,n})}{f(u_{1,n})}$ with $f(z) = \Gamma(z-s)\Gamma(1+z-s)/[\Gamma(z+s)\Gamma(1+z+s)]$.

⁸In peculiar cases, known as three-body resonances, see [18, 35], R_t/b can be arbitrarily large and βE_{glob} can remain finite in the zero-range limit. This is improbable here as there is already a two-body resonance.

tion for the energy spectrum $(\epsilon_q(\omega))_{q \in \mathbb{N}}$ [19]⁹:

$$\frac{\Gamma\left(\frac{1+s-E/\hbar\omega}{2}\right)}{\Gamma\left(\frac{1-s-E/\hbar\omega}{2}\right)} = \left(\frac{E_{\text{glob}}}{2\hbar\omega}\right)^s \quad (27)$$

we recalculate the quantum defect as in [32], using the Euler reflection and Stirling formulas:

$$\Delta(\epsilon) = 2 + \frac{2}{\pi} \operatorname{atan} \frac{\operatorname{th}\left[\frac{s}{2} \ln(\epsilon/E_{\text{glob}})\right]}{\tan\left(\frac{s}{2}\pi\right)} \quad (28)$$

When $R_t \rightarrow 0$, $\beta E_{\text{glob}} \rightarrow +\infty$ and this reproduces the value $1+s$ of the quantum defect in Eq.(5). Eq.(28) only revises the contribution of the channel $(1,0)$, since the other channels have $u_{i,n} > 1$ for the values of α in Fig. 1:

$$\bar{B}_{2,1}^{(1,0)} \underset{0 < s < 1}{=} -\frac{3}{2} \int_0^{+\infty} d\epsilon \beta [\Delta(\epsilon) - (1 + v_{1,0})] e^{-\beta\epsilon} \quad (29)$$

In Fig. 1 we plot for $\alpha < \alpha_c$ the corresponding values of $\bar{B}_{2,1}$, for the same values of the parameter βE_{glob} as in the part $\alpha > \alpha_c$ of the figure, leading to an apparently smooth connection at $\alpha = \alpha_c$. The continuity of the connection could be expected from the fact that (i) the formal change $s \rightarrow i|s|$ in Eq.(28) reproduces the value (19) of the quantum defect on the side $\alpha > \alpha_c$ apart from the nearest-integer function which is irrelevant when $|s| \rightarrow 0$, and (ii) the Efimovian trimer spectrum has a vanishing contribution to $\bar{B}_{2,1}$ when $\alpha \rightarrow \alpha_c^+$.

Indeed $\bar{B}_{2,1}^{(1,0)}(\alpha)$ (and $\bar{B}_{2,1}(\alpha)$) are smooth functions of α at α_c at fixed βE_{glob} , since $\Delta(\epsilon)$ is an even function of s and its series expansion only has even powers of s :

$$\Delta(\epsilon) \underset{s \rightarrow 0}{=} \Delta_0(\epsilon) - \frac{x}{6} s^2 + \frac{x^3 - \pi^2 x}{360} s^4 + O(s^6) \quad (30)$$

where $\Delta_0(\epsilon)$ is given by Eq.(20), $x = \ln(\epsilon/E_{\text{glob}})$, and s can be real or purely imaginary. Insertion in Eq.(29) leads to converging integrals over ϵ and to an expansion of $\bar{B}_{2,1}^{(1,0)}$ with only even powers of s :

$$\bar{B}_{2,1}^{(1,0)}(\alpha) - \bar{B}_{2,1}^{(1,0)}(\alpha_c) \underset{s \rightarrow 0}{=} -\frac{A}{4} s^2 - \frac{A(\pi^2 - 2A^2) - 4\zeta(3)}{480} s^4 + O(s^6) \quad (31)$$

where $A = \ln(e^\gamma \beta E_{\text{glob}})$ and $\gamma \simeq 0.577$ is Euler's constant¹⁰. Since s^2 is a smooth function of α across α_c , so is $\bar{B}_{2,1}$.

⁹The ground state solution of this equation must be omitted, because it connects when $\omega \rightarrow 0$ to a bound state of energy $-E_{\text{glob}}$ and spatial extension $\approx R_t$, which cannot be faithfully described by our zero-range model when $R_t \approx b$ (i.e. in the absence of three-body resonance) and indeed does not exist in the three-body hard-core or in the narrow Feshbach resonance model [21]. This is equivalent to the assumption in [16] of the absence of non-universal trimer states.

¹⁰Exchange of Taylor expansion and integration is justified by the theorem of derivation under the integral, where x is the integration variable. For $\alpha < \alpha_c$, one sets $u(x, s) = \operatorname{th}(sx/2)/s$ and $v(x, s) = \tan(s\pi/2)/s$ and one fixes some $\eta \in]0, 1[$. Then there exist positive

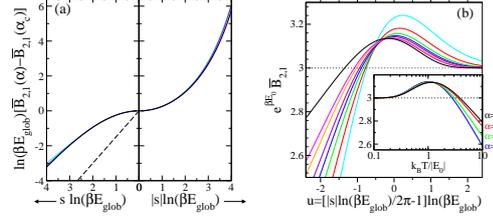


Fig. 2: Scaling-law analysis of Fig.1 for α close to α_c in the limit $\beta E_{\text{glob}} \rightarrow +\infty$. (a) For a fixed $t \equiv s \ln(\beta E_{\text{glob}})$: the data approach the law (33) (black solid line), provided that $|t| < 2\pi$ on the side $\alpha > \alpha_c$. Curves from top to bottom: $\beta E_{\text{glob}} = 10^2$ (cyan), 10^4 (violet). Dashed line: 0-parameter theory prediction $-3t/2$. (b) On the side $\alpha > \alpha_c$, for a fixed $u \equiv [|t|/(2\pi) - 1] \ln(\beta E_{\text{glob}})$: the data approach the law (34) (black solid line), which reproduces the peaked structure seen in Fig.1. From bottom to top for $u < -0.6$: values of βE_{glob} listed in the caption of Fig.1, with the same order and colors. Inset: from Eqs.(9,18,19), Eq.(34) taken with $u = \ln(\beta|E_0|)$ also gives the limit of $e^{\beta E_0} \bar{B}_{2,1}$ for $\alpha \rightarrow \alpha_c^+$ at fixed $k_B T/|E_0|$.

Eq.(31), combined with $\Lambda_1(s) = 0$, predicts how the first order derivative at α_c diverges when $\beta E_{\text{glob}} \rightarrow +\infty$:

$$\frac{d}{d\alpha} \bar{B}_{2,1}(\alpha_c) \underset{\beta E_{\text{glob}} \rightarrow +\infty}{\sim} C \ln(\beta E_{\text{glob}}) \quad \text{with } C \simeq 0.0478243 \quad (32)$$

It also suggests an interesting scaling law close to α_c : keeping in the coefficients of the powers of s in (31) only the leading terms in $\ln(\beta E_{\text{glob}})$, one uncovers, after multiplication of (31) by $\ln(\beta E_{\text{glob}})$, the following law when βE_{glob} tends to infinity at fixed $t \equiv s \ln(\beta E_{\text{glob}})$:

$$[\bar{B}_{2,1}(\alpha) - \bar{B}_{2,1}(\alpha_c)] \ln(\beta E_{\text{glob}}) \underset{\beta E_{\text{glob}} \rightarrow +\infty}{\overset{t \text{ fixed}}{\sim}} 3 - \frac{3t/2}{\operatorname{th}(t/2)} \quad (33)$$

with no constraint on the side $\alpha < \alpha_c$, and with the constraint that $|t| < 2\pi$ on the side $\alpha > \alpha_c$ due to the occurrence of a pole at $t = 2\pi i$ in the quantum defect contribution and to a divergence of the ground trimer contribution for $|t| > 2\pi$. Eq.(33) is obtained by neglecting $\ln(\beta\epsilon)$ as compared to $\ln(\beta E_{\text{glob}})$ in (19,28), as $\beta\epsilon$ is typically unity in the integrals (18,29). In Fig. 2a we replot the data of Fig.1 after rescaling as in Eq.(33): the results are indeed almost aligned on a single scaling curve given by Eq.(33), the better the larger $\ln(\beta E_{\text{glob}})$ is. The 0-parameter zero-range theory prediction $-3t/2$, see dashed line, is only asymptotically equivalent to the correct law at $t \rightarrow +\infty$.

numbers $(A_n, B_n)_{n \in \mathbb{N}}$ and $C > 0$ such that $\forall (x, s) \in \mathbb{R} \times [0, \eta]$, $\forall n \in \mathbb{N}$: $|\partial_s^n u(x, s)| \leq A_n |x|^{n+1}$, $|\partial_s^n v(x, s)| \leq B_n$, $u(x, s)^2 + v(x, s)^2 \geq C$. For $\alpha > \alpha_c$ one sets $u(x, |s|) = [\pi \sin(|s|x) - x \sinh(\pi|s|)]/|s|^2$ and $v(x, |s|) = [\cosh(\pi|s|) - \cos(|s|x)]/|s|^2$ and one fixes some $\eta > 0$. Then there exist positive numbers $(A_n, B_n, C_n, D_n)_{n \in \mathbb{N}}$ and $G > 0$ such that $\forall (x, |s|) \in \mathbb{R} \times [0, \eta]$, $\forall n \in \mathbb{N}$: $|\partial_{|s|}^n u(x, |s|)| \leq A_n |x| + B_n |x|^{n+2}$, $|\partial_{|s|}^n v(x, |s|)| \leq C_n + D_n |x|^{2+n}$, $|v(x, |s|)| \geq G$. The u and v functions appear in $\partial_s \Delta(\epsilon)$ as $(v \partial_s u - u \partial_s v)/(u^2 + v^2)$ for $\alpha < \alpha_c$, and in $\partial_{|s|} \Delta(\epsilon)$ as u/v for $\alpha > \alpha_c$. Then $|\partial_s^n \Delta|$ and $|\partial_{|s|}^n \Delta|$ are polynomially bounded in $|x|$ uniformly in s or $|s| \forall n \in \mathbb{N}^*$.

The scaling law fully justifies the intuitive condition (26): the crossover from the 0- to the 1-parameter zero-range regime indeed occurs for $s \approx 1/\ln(\beta E_{\text{glob}})$.

What happens on the side $\alpha > \alpha_c$ close to $|t| = 2\pi$? For $|t|$ fixed to a value $> 2\pi$, the ground-trimer contribution $3e^{-\beta E_0}$, where $E_0 = \epsilon_0(0^+)$, rapidly diverges when $\beta E_{\text{glob}} \rightarrow +\infty$ and dominates all other contributions, so that the reduced cluster coefficient $e^{\beta E_0} \bar{B}_{2,1}$ of Fig. 1 tends to three. However, before that, the reduced cluster coefficient exhibits as a function of α an interesting structure in Fig. 1, a sharp rise with a maximum, that corresponds to a neighbourhood of $|t| = 2\pi$ with a width $1/\ln(\beta E_{\text{glob}})$. This is revealed by the affine change of variable $u \equiv [|t|/(2\pi) - 1](\ln \beta E_{\text{glob}})$. When $\beta E_{\text{glob}} \rightarrow +\infty$ for fixed u , $\beta E_0 \rightarrow -e^u$, the ground-trimer contribution remains finite and, from dominated convergence theorem,

$$e^{\beta E_0} \bar{B}_{2,1} \underset{\beta E_{\text{glob}} \rightarrow +\infty}{\overset{u \text{ fixed}}{\longrightarrow}} e^{-e^u} \left[B_{2,1}(\alpha_c) + 3 \left(e^{e^u} - \frac{1}{2} \right) + \frac{3}{\pi} \int_0^{+\infty} d\epsilon \beta e^{-\beta \epsilon} \operatorname{atan} \frac{u - \ln \beta \epsilon}{\pi} \right] \quad (34)$$

where $B_{2,1}(\alpha_c) \simeq 1.7153$ [16] is the prediction of the 0-parameter zero-range theory at α_c . As shown in Fig. 2b, the rescaled data of Fig. 1 nicely converge to this law.

Conclusion. — As compared to the usual zero-range theory we have found corrections of order $1/\ln(\lambda_t/R_t)$ to the third virial coefficient of a two-component unitary Fermi gas, close to and below the threshold for the Efimov effect, at a distance $\alpha_c - \alpha$ scaling as $1/[\ln(\lambda_t/R_t)]^2$, where R_t is a three-body parameter and λ_t a thermal de Broglie wavelength; these $1/\ln(\lambda_t/R_t)$ corrections arise from short-range three-body correlations, that is from triplets of close atoms¹¹. As a consequence, for a given finite λ_t/R_t as in all realistic systems, the third virial coefficient reconnects smoothly to its values deduced from the Efimov zero-range model above the threshold, precluding the unphysical first-order phase transition predicted by zero-range theory. Our predictions may be tested by measuring the equation of state of mixtures of fermionic cold atoms with a mass ratio $\alpha \simeq 13.6$, such as $^3\text{He}^*$ and ^{40}K .

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¹¹For $s < 1/2$ they dominate over more usual (here neglected) energy corrections, due to the effect of a finite range b of the two-body interaction at the level of short-range two-body correlations (only involving pairs of close atoms), that vanish linearly in b [36]. From Eq.(29) for $R_t/\lambda_t \rightarrow 0$, $\bar{B}_{2,1} - B_{2,1} \sim -\frac{3}{\pi} \Gamma(s+1) \sin(s\pi)/(\beta E_{\text{glob}})^s$ then indeed vanishes more slowly than \bar{b} , assuming that $R_t \approx b$.