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► **To cite this version:**

Chao Gao, Shimpei Endo, Yvan Castin. The third virial coefficient of a two-component unitary Fermi gas across an Efimov-effect threshold. EPL - Europhysics Letters, 2015, 109, pp.16003. 10.1209/0295-5075/109/16003 . hal-01078973v2

**HAL Id: hal-01078973**

**<https://hal.science/hal-01078973v2>**

Submitted on 15 Jan 2015 (v2), last revised 10 Apr 2015 (v3)

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

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PACS 67.85.d – Ultracold gases, trapped gases.

**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  $\alpha$  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  $\alpha$  across  $\alpha_c$  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  $\lambda/a$  [3] or  $a/\lambda$  [4], where  $\lambda$  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  $\alpha$  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  $\Omega$ , this would imply a singular derivative of  $\Omega$  as a function of  $\alpha$ , 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  $T$ ,  $\beta = 1/(k_B T)$ ,  $\mu_i$  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  $\omega$  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  $\Omega$  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]<sup>1</sup>

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

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  $\Lambda_l$ , 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

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

<sup>1</sup>There exists a less explicit hypergeometric expression for  $\Lambda_l$  [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]<sup>2</sup>:

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

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  $\alpha$  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  $\alpha$ , 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  $\alpha$ . 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]:

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

<sup>2</sup>Actually 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.

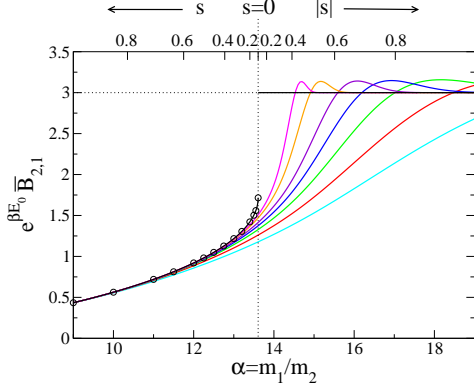


Fig. 1: Reduced third cluster coefficient  $e^{\beta E_0} \bar{B}_{2,1}$  of a trapped two-component three-dimensional unitary Fermi gas in the zero trapping frequency limit, as a function of the mass ratio  $\alpha = m_1/m_2$  of the two species (lower  $x$ -axis) or of the root  $s = u_{1,0}$  of  $\Lambda_1$  (upper  $x$ -axis), for various values of the three-body parameter  $R_t$ , and hence of the global energy scale  $E_{\text{glob}}$  of Eqs.(13,24). Here  $E_0$  is the ground free-space three-body energy, a smooth function of  $\alpha$ : 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),  $3 \times 10^2$  (red),  $10^3$  (green),  $3 \times 10^3$  (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  $\alpha$ , an increasing function of  $\beta E_{\text{glob}}$  (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  $\alpha_c$  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  $E_{\text{glob}}$  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  $\Gamma$  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  $\omega$ , 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 defect<sup>3</sup>:

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

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  $\epsilon$  and of  $|s|$ .

<sup>3</sup>This 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  $\beta E_{\text{glob}}$ , 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  $\alpha_c^\mp$  at non-zero  $R_t$ . When  $R_t \rightarrow 0$  ( $E_{\text{glob}} \rightarrow +\infty$ ) there is agreement at  $\alpha_c$ , 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)<sup>4</sup>:

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

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  $\alpha$  at  $\alpha_c^-$ . 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  $\alpha$  is close enough to  $\alpha_c$ . 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

<sup>4</sup>One 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 core<sup>5</sup>:

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

(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]<sup>6</sup>:

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

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  $E_{\text{glob}}$  to  $\alpha < \alpha_c$ <sup>7</sup>:

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

where the first factor is a smooth function of  $\alpha$ , 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  $R_t \approx b$ <sup>8</sup>:

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

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-

<sup>5</sup>If 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  $a_{\text{eff}}$  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.

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

<sup>7</sup>On 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  $f(z) = \Gamma(z-s)\Gamma(1+z-s)/[\Gamma(z+s)\Gamma(1+z+s)]$ .

<sup>8</sup>In peculiar cases, known as three-body resonances, see [18, 35],  $R_t/b$  can be arbitrarily large and  $\beta E_{\text{glob}}$  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]<sup>9</sup>:

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

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  $\alpha$  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  $\beta E_{\text{glob}}$  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  $\alpha$  at  $\alpha_c$  at fixed  $\beta E_{\text{glob}}$ , 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  $\epsilon$  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 constant<sup>10</sup>. Since  $s^2$  is a smooth function of  $\alpha$  across  $\alpha_c$ , so is  $\bar{B}_{2,1}$ .

<sup>9</sup>The 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.

<sup>10</sup>Exchange 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

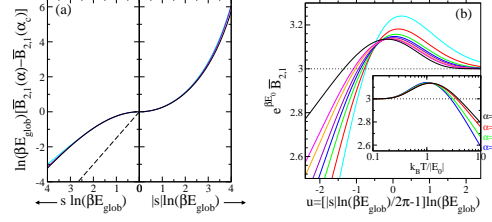


Fig. 2: Scaling-law analysis of Fig.1 for  $\alpha$  close to  $\alpha_c$  in the limit  $\beta E_{\text{glob}} \rightarrow +\infty$ . (a) For a fixed  $t \equiv s \ln(\beta E_{\text{glob}})$ : the data approach the law (33) (black solid line), provided that  $|t| < 2\pi$  on the side  $\alpha > \alpha_c$ . 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  $\beta E_{\text{glob}}$  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  $\alpha_c$  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  $\alpha_c$ : 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  $\beta E_{\text{glob}}$  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  $\alpha$  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  $\alpha_c$ . 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  $\lambda_t$  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 atoms<sup>11</sup>. As a consequence, for a given finite  $\lambda_t/R_t$  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  $^{40}\text{K}$ .

**Acknowledgments.** — S.E. thanks JSPS for support.

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<sup>11</sup>For  $s < 1/2$  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  $R_t \approx b$ .