Unitary boson-boson and boson-fermion mixtures: third virial coefficient and three-body parameter on a narrow Feshbach resonance

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Received 29 July 2016 / Received in final form 27 September 2016
Published online 10 November 2016 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2016

Abstract. We give exact integral expressions of the third cluster or virial coefficients of binary mixtures of ideal Bose or Fermi gases, with interspecies interactions of zero range and infinite $s$-wave scattering length. In general the result depends on three-body parameters $R_t$ appearing in three-body contact conditions, because an Efimov effect is present or because the mixture is in a preefimovian regime with a mass ratio close to an Efimov-effect threshold. We give a new, exact integral expression of $R_t$ for the microscopic narrow Feshbach resonance model. A divergence of $R_t$ in the preefimovian regime at a scaling exponent $s = 1/2$ is predicted and physically discussed. The analytical results are applied to typical species used in cold atom experiments.

1 Introduction

The field of atomic quantum gases has been witnessing in the last decade the emergence of a new paradigm, the regime of resonant interactions, thanks to the possibility of controlling at will the $s$-wave scattering length $a$ via magnetic Feshbach resonances [1–4]. This leads to a rich interplay between strong few-body correlations and many-body physics that was scarcely studied before. At unitarity, where $a^{-1} = 0$ and the interaction is scale invariant, there are still some adjustable parameters, namely the quantum statistics and the mass ratio of the particles, that can deeply affect the many-body properties of the gas.

The experimental studies have concentrated up to now on the strongly interacting spin-1/2 Fermi gas, and in particular on the unitary Fermi gas. The gas equation of state was measured both in the superfluid and normal phases, and the coefficients of the cluster expansion of the pressure in powers of the low fugacity, not to be confused with the virial coefficients of the expansion in powers of the low density, have been extracted up to order four [5,6]. These coefficients constitute an intriguing bridge between few-body and many-body physics.

Although they have not been experimentally realised yet, less conventional phases with different manifestations of superfluidity have been proposed, that take advantage of a rich underlying few-body physics. With several component fermions, trimer or tetramer states can exist [7–10] and interact [11,12], which creates new channels competing with the usual BCS pairing and opening the door to new phases [13,14]. With resonantly interacting spinless bosons, $N$-body bound states can exist [15], leading to a liquid-gas transition in addition to the expected normal-superfluid transition [16,17].

In this paper, we present a general analytical calculation of the third cluster coefficient $b_3$ of a two-component gas at unitarity in the spirit of [18] with the harmonic regulator method of [19–22], building on the fact that the trapped three-body unitary problem is soluble [23,24] due to separability in hyperspherical coordinates [25]. As the particular case of unitary fermion-fermion mixture was already treated [26], we complete the study by including the unitary boson-boson and boson-fermion mixtures. We adhere here to the philosophy of zero-range models, replacing interparticle interaction potentials by contact conditions on the three-body wavefunction, namely: (i) two-body Wigner-Bethe-Peierls contact conditions, that are scale invariant at unitarity [27–29], and (ii) three-body contact conditions on the hyperradial wavefunction: (a) in general, these are also scale invariant (the hyperradial wavefunction vanishes as a power law); (b) if the Efimov effect [7–9] takes place however, they must involve a three-body length scale $R_t$, the so-called three-body parameter [7–9,30], and a lower cut-off must be introduced by hand in the geometric spectrum of trimers (to eliminate trimer states of binding energy $\approx \hbar^2/m_r R_t^2$ or larger, where $m_r$ is the two-species reduced mass, since they are in general inconsistent with the zero range model); (c) last,
if no Efimov effect is present, but the mass ratio is close enough to an Efimov-effect threshold, they must also involve a three-body parameter $R_t$, so that $b_3$ has a smooth variation as a function of the mass ratio across the threshold [26] (also removing by hand in this case the trimer state predicted by these modified contact conditions).

Two important issues must however be answered, before one proceeds with the calculation of $b_3$. The first issue is theoretical, it is a shortcoming of the zero-range models [31–34]. In $B - B$ boson-boson mixtures, this issue is worsened because two three-body parameters $R_t$ must be introduced, $R_t^{BB}$ and $R_t^{BB}$, so that one cannot even fully absorb $R_t$ in a rescaling of the temperature as done in reference [18].

The second issue is experimental: when the Efimov effect is present in current experiments, strong three-body losses take place even in the zero-range limit $k_F b \to 0$, where $k_F$ is a Fermi wavenumber and $b$ the interaction range, due to recombination into strongly bound dimers [35,36]. This is due to the fact that the probability that three atoms are within a radius $b$ vanishes too slowly, only as $b^2$, whereas the recombination rate in such a close-atom configuration is $\propto h^2/m_b b^2$ [37]. Up to now, this has restricted thermal equilibrium bosonic many-body studies to the strongly non-degenerate regime [38,39], where only loss rates, not virial coefficients, can be measured and compared to theory [38], and this has restricted quantum degenerate bosonic studies to a non-equilibrium regime [40–42].

Here we use as a microscopic model the (infinitely) narrow Feshbach resonance model [43], where at unitarity the effective range of two-body $s$-wave scattering is negative ($-2R_b$) and much larger in absolute value than the van der Waals length $b$ of the interaction. This solves the two aforementioned issues. It solves the theoretical issue because the zero-energy $E = 0$ three-body problem can be solved analytically and $R_t$ can be extracted [44–46]; we refine the theory by: (i) giving an integral expression of $R_t$ in terms of Efimov's transcendental function $\Lambda_l(s)$ (in Refs. [44,45], an infinite product representation in terms of the infinite-number roots of $\Lambda_l(s)$ was given; in Ref. [46] the given integro-differential expression is only an asymptotic expansion), (ii) by extending the zero-energy solution and the calculation of $R_t$ to the non-Efimovian case, for a mass ratio close to an Efimov-effect threshold. It also solves the experimental issue: choosing a narrow Feshbach resonance in the experiment is expected to reduce the efimovian three-body losses, now dominated by the probability of having an atom and a closed-channel molecule within a distance $b$ [47]1, where a loss event can take place with a rate $\propto h^2/m_b b^2$ [37]. If one considers the atom and the molecule as distinguishable non-interacting particles as in reference [47], the probability of finding them at distances $< b$ is $O(b^4)$ since their relative wavefunction is $O(1)$. One then predicts a $O(k_F b)$ three-body loss rate, that vanishes in the zero-range limit. It remains of course the magnetic field stabilisation challenge due to the narrowness of the resonance.

### 2 Third cluster coefficient in zero-range models

The cluster expansion for the total pressure $P$ of a mixture of two species at thermal equilibrium in a cubic box in the thermodynamic limit is defined as

$$\frac{P\lambda^3}{k_B T} = \sum_{(n_1,n_2)\in\mathbb{Z}^2} b_{n_1,n_2} s_1^{n_1} s_2^{n_2}$$

where the fugacities $s_i = \exp (\mu_i/k_B T)$ tend to zero at fixed temperature $T$, $\mu_i$ is the chemical potential of species $i$ and $\lambda = [2\pi h^2/(m_1,m_2,k_B T)]^{1/2}$ is the thermal de Broglie wavelength associated to the reduced mass $m_r = m_1 m_2 / (m_1 + m_2)$.

In what follows, we assume that there is no intraspecies interaction and that the interspecies interaction is in the unitary limit, that is with an infinite $s$-wave scattering length and a negligible range. The homogeneous gas cluster coefficients $b_{n_1,n_2}$ are related to the $\omega \to 0$ limit $B_{n_1,n_2}$ of the cluster coefficients of the gas in isotropic trapping potentials with the same trapping angular frequency $\omega$ for both species [48],

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

which is easier to calculate in the unitary limit as explained in the introduction. Due to rotational invariance, all the cluster coefficients, in particular the third order ones, can be written as sums over all angular momentum sectors contributions. Due to the absence of intraspecies interactions, $B_{3,0}$ and $B_{0,3}$ have ideal gas values. On the contrary, $B_{2,1}$ differs from the zero, ideal-gas value. It is the only nontrivial third order coefficient that we need to calculate since $B_{1,2}$ is obtained by exchanging the role of species 1 and 2. We write its decomposition over the angular momentum sectors as

$$B_{2,1} = \sum_{\ell \in \mathbb{N}} (2\ell + 1)\sigma_\ell.$$

We shall restrict to low particle wavenumbers, much smaller than $1/b$, where $b$ is now the interaction range or the effective range if it is larger, so that we can use the Wigner-Bethe-Peierls zero-range model, where the interspecies interactions are replaced by boundary conditions on the wavefunction. The resulting unitary three-body problem can be solved analytically in free space [7–9] and in isotropic harmonic traps [23,24]2. The three-body

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1 The probability of having three open-channel atoms within a distance $b$ with a relative angular momentum $\ell$ is $O(b^{\ell+4})$ for a narrow Feshbach resonance, see footnote 41 in reference [46].

2 The free space three-body problem can be solved analytically also for a finite scattering length [49].
partition functions in the trap and ultimately the coefficient $B_{2,1}$ can be calculated. The result applies in the temperature regime

$$k_B T \ll \frac{\hbar^2}{2m_b b^2}. \quad (5)$$

As we shall see, a central actor in our analytical expression is the Efimov transcendental function. It is an even function of a single variable $s$ that, in the angular momentum sector $\ell \in \mathbb{N}$ for the three-body 112 problem, takes the form\(^3\) [46]:

$$\bar{A}_\ell(s) \overset{\ell \text{ even}}{=} 1 - \frac{2\eta}{\sin 2\nu} \int_0^\nu d\theta P_\ell \left( \frac{\sin \theta}{\sin \nu} ; \frac{\cos(s\theta)}{\cos(s\pi/2)} \right) \quad (6)$$

$$\bar{A}_\ell(s) \overset{\ell \text{ odd}}{=} 1 + \frac{2\eta}{\sin 2\nu} \int_0^\nu d\theta P_\ell \left( \frac{\sin \theta}{\sin \nu} ; \frac{\sin(s\theta)}{\sin(s\pi/2)} \right) \quad (7)$$

with $P_\ell$ a Legendre polynomial,

$$\nu = \arcsin \frac{m_1}{m_1 + m_2} \quad (8)$$

the mass angle and $\eta = 1$ ($\eta = -1$) if the species 1 is bosonic (fermionic). An equivalent and useful writing can be obtained from the hypergeometric form of [50,51]:

$$\bar{A}_\ell(s) = 1 - \frac{\eta(- \sin \nu)^\ell}{2^{\ell+1} \cos \nu} \times \sum_{k \in \mathbb{N}} \frac{\Gamma(k + \ell + 1)}{\Gamma(k + \ell + \frac{3}{2})} \sin^{2k} \nu \frac{k!}{k!} \quad (9)$$

where $\Gamma$ is Euler’s Gamma function.

As we shall see, in the realm of zero-range models, the Wigner-Bethe-Peierls model is not the end of the story, as it only specifies two-body contact conditions. To select the appropriate zero-range model for the three-body problem, one must discuss the existence of a root of $A_\ell(s)$ over the interval $[0, \ell + 1]$. Over this interval, $A_\ell(s)$ is a smooth function of $s$ because the smallest positive pole of the terms of the series (9) is at $\ell + 1$. In the discussion, one can take advantage of a useful result: the function $s \mapsto A_\ell(s)$ is monotonically decreasing (increasing) over $[0, \ell + 1]$ when $\eta(-1)^\ell$ is positive (negative)\(^4\) and tends to $-\infty$ ($+\infty$) when $s \to \ell + 1$ + . As a consequence, it has either zero or one root in $[0, \ell + 1]$, depending on the sign of $A_\ell(0)$. We have at hand a second useful result: the function $S \mapsto A_\ell(iS)$ is monotonically increasing (decreasing) over $\mathbb{R}^+$ when $\eta(-1)^\ell$ is positive (negative)\(^5\) and tends exponentially rapidly to 1 at $+\infty$ according to equations (6), (7). Then one faces only one of the three possible cases listed below: for $\eta(-1)^\ell$ negative, only the first case is actually accessible since $\bar{A}_\ell(s)$ is then $>1$ over $[0, \ell + 1]$.

1. The plain nonfeminovan case: $\bar{A}_\ell(s)$ has only real roots, and the smallest positive root is $s_t > 1$. The hyperradial wavefunction $F(R)$ is subjected to the boundary condition\(^6\)

$$F(R) = O(R^{\ell}) \quad (10)$$

where the hyperradius $R$ of the 112 system is the corresponding mass-weighted root-mean-square deviation of the positions of the three particles from their center of mass. Then the contribution $\sigma_\ell$ of the angular momentum $\ell$ to $B_{2,1}$ as defined in equation (4) is given by [18,26]

$$\sigma_\ell = - \int_{\mathbb{R}^+} \frac{dS}{2\pi} \ln \bar{A}_\ell(iS). \quad (11)$$

2. The prefetcheminovan case: $\bar{A}_\ell(s)$ has only real roots, but the smallest positive root $s_t \in ]0, 1[$. In the channel associated to the root $s_t$, there is an enriched boundary condition [53–55], that must be used when $s_\ell$ is small enough [26]:

$$F(R) = (R/R_t)^{s_t} - (R/R_t)^{-s_t} + O(R^{2-s_t}) \quad (12)$$

where the length $R_t$ is a three-body parameter. This predicts in free space a 112 bound state of degeneracy $2\ell + 1$ and binding energy

$$E_{\text{glob}} = \frac{2\hbar^2}{(m_1 + m_2) R_t^2} \left( \frac{\Gamma(1 + s_t)}{\Gamma(1 - s_t)} \right)^{1/s_t} \quad (13)$$

that must be disregarded in the absence of three-body resonance. Then [26]

$$\sigma_\ell = - \int_{\mathbb{R}^+} \frac{dS}{2\pi} f_\ell(S) - \int_{\mathbb{R}^+} d\epsilon \Delta(\epsilon) e^{-\beta \epsilon} \quad (14)$$

with $\beta = 1/k_B T$,

$$\Delta(\epsilon) = \frac{1}{\pi} \tan \left( \frac{\epsilon}{\tan} \frac{\tan}{\sin} \right) \frac{\sin^2 \theta}{\sin^2 \theta + s_t^2} A_\ell(iS). \quad (15)$$

and the smooth real-valued function on the real axis:

$$f_\ell(S) \equiv \ln \left[ \frac{S^2 + 1}{S_t^2 + s_t^2} A_\ell(iS) \right]. \quad (16)$$

In this prefeminovan case, the enriched zero-range model has the same validity condition as in equation (5) under the generic assumption that $R_t$ and $\ell$ are of the same order of magnitude [26].

\(^3\) The Efimov function is here divided by $\cos \nu$ with respect to previous references, hence the bar in the notation $A_\ell(s)$.

\(^4\) Use equation (9) and the fact that $x \mapsto \Gamma(x + a) \Gamma(x - a)$ is positive and has a nonnegative logarithmic derivative $\sum_{n \in \mathbb{N}} (a + n)^{-x} x^{-x}$ over $[0, a]$ for $a > 0$, see Section 8.362(1) in reference [52].

\(^5\) $\forall a > 0$, the logarithmic derivative of $x \mapsto \Gamma(a + ix)$ over $\mathbb{R}$ is $\sum_{n \in \mathbb{N}} (a + n + a)^{-x}$, see Section 8.362(1) in reference [52].

\(^6\) More precisely, the three-body wavefunction is written in the form $\rho(r_1, r_2, r_3) = \phi(\Omega) F(R)/R^{\ell^2}$ where $\Omega$ is the set of hyperangles [7–9,25].

\(^7\) It shall not be used for $s_t > 1$ as the wavefunction is not square integrable in $R = 0$, $\int_0^{R_0} dR R R(F(R))^2 = +\infty$ for any finite $R_0$. 
3. The Efimovian case: $A_I(s)$ has real roots and a pair of purely imaginary roots $\pm s_\ell$ with $s_\ell = |s_\ell|$. In the Efimovian channel, one must use the boundary condition [7–9,30]

$$F(R) = (R/R_\ell)|^{i|s_\ell|} - (R/R_\ell)^{-i|s_\ell|} + O(R^2). \quad (17)$$

As $F(R)$ has an infinite number of zeroes when $R \to 0$, the model predicts in free space an infinite number of trimers states of energies $\epsilon_q$ and degeneracy $2\ell + 1$, forming a geometric sequence that we truncate by hand to make it consistent with the zero-range assumption:

$$\epsilon_q = -E_{\text{glob}}e^{-2\pi(1+q)/|s_\ell|}, \forall q \in \mathbb{N}. \quad (18)$$

The global energy scale is an analytic continuation of equation (13):

$$E_{\text{glob}} = \frac{2\hbar^2}{(2m_1 + m_2)R_\ell^2}e^{\text{Im} \ln \Gamma(1+s_\ell)-\text{Im} \ln \Gamma(1-s_\ell)]/s_\ell} \quad (19)$$

with $\ln \Gamma$ the usual branch of the $\Gamma$ function logarithm. In addition to the zero-range condition (5), one requires for the model to be valid that the ground trimmer is in the zero-range regime,

$$|\epsilon_0| \ll E_{\text{glob}} \quad (20)$$

that is $|s_\ell| \lesssim 1.5$. As $|s_\ell|$ is an increasing function of the mass ratio $m_1/m_2$, this puts an upper bound on $m_1/m_2$. Then [26]

$$\sigma_\ell = -\int_{\mathbb{R}^+} \frac{dS}{2\pi} f_I(S) - \int_{\mathbb{R}^+} \text{d} \epsilon \Delta(\epsilon) \beta e^{-\beta \epsilon} + \sum_{q \in \mathbb{N}} \left( e^{-\beta s_\ell} - 1 \right) \quad (21)$$

where $f_I(S)$ is still given by equation (16) and the new form of the function $\Delta$:

$$\Delta(\epsilon) = \frac{1}{\pi} \text{atan} \left( \frac{\epsilon}{2\pi} \right) + \left\lfloor \frac{|s_\ell|\epsilon}{2\pi} \right\rfloor \quad (22)$$

remains a smooth function of $x = \ln(\epsilon/E_{\text{glob}})$ thanks to the nearest-integer function in the last term.

The conditions on the mass ratio to have an Efimov effect are known. For $\eta = 1$ there is an Efimov effect in the sector $\ell = 0$ for all mass ratios, in the sector $\ell = 2$ for $m_1/m_2 > 38.6301\ldots$ in the sector $\ell = 4$ for $m_1/m_2 > 125.764\ldots$, etc. For $\eta = -1$ there is an Efimov effect in the sector $\ell = 1$ for $m_1/m_2 > 13.6069\ldots$ [57], in the sector $\ell = 3$ for $m_1/m_2 > 75.9944\ldots$ [58], etc. In Figure 1, corresponding to $\eta = 1$, we plot the imaginary part of $s_\ell$ as a function of the mass angle (with a comparison to its Taylor expansions at small and large mass ratio); we also plot the real and imaginary parts of $s_\ell$ close to the Efimov-effect threshold.

3 Three-body parameter for a narrow Feshbach resonance

For the narrow Feshbach resonance microscopic interaction model, we now show how to obtain a new analytical expression for the three-body parameter and we discuss the interval of mass ratio where the enriched preefimovian model shall be used instead of the plain nonefimovian one.

In (a) one uses the mass angle $\nu = \arcsin \frac{m_1 + m_2}{m_1 m_2} \in \left[ 0, \frac{\pi}{2} \right]$ as a parameter, to cover all mass ratios, and $\text{Im} s_\ell$ is divided by $\tan \nu$ to form a bounded quantity. Solid lines: from a numerical solution of the transcendental equation $A_I(s_\ell) = 0$. Dashed lines in (a): Taylor expansions for a low mass ratio $\nu \to 0^+$, $\text{Im} s_\ell/\tan \nu = \frac{1}{\sqrt{2}} \left[ 1 + \left( \frac{1 + \frac{m_1}{m_2}}{\frac{m_1}{m_2}} \right) \left( 1 - \cos 2\nu \right) + O(\nu^4) \right]$, and for a large mass ratio $\nu \to \frac{\pi}{2}$ as in [46], $\text{Im} s_\ell/\tan \nu = \Omega \left[ 1 + \frac{\nu}{\Omega} \left( 1 + \cos 2\nu \right) + O\left( \frac{\nu}{\Omega} \right) \right]$ where the constant $\Omega$ obeys $\Omega \exp \Omega = 1$. Vertical dotted lines in (a): the mass ratios $m_1/m_2 = 3$ and $3 + \sqrt{12}$ where $\cos 2\nu = \pm \frac{\nu}{2}$.
be obtained either using modified two-body contact conditions [43] or a two-channel model with separable potentials of range tending to zero [46,60–64]. In the sector of angular momentum $\ell$, both models lead for $1/\alpha = 0$ and at negative energy $E = -\hbar^2 q^2/2m_r$ in the center-of-mass frame to

$$
[q_{\ell\alpha}(k) + q_{\ell\alpha}^2(k)R_\alpha] \, d(k) = 
\eta \int_{R^+} \frac{dk^2}{\pi} \int_{-1}^{1} du \frac{P_r(u)k^2d(k')}{q^2 + k^2 + k'^2 + 2kk'u\sin\nu} \tag{23}
$$

with $P_r$ the Legendre polynomial of degree $\ell$, $q_{\ell\alpha}(k) \equiv |q + ik\cos\nu|$ and $R_\alpha > 0$ is the Feshbach length such that the 12 scattering amplitude at energy $E$ in the center-of-mass frame is $f_\alpha = -1/(iq + q^2R_\alpha)$. One has taken advantage of rotational invariance by the following ansatz for the unknown function:

$$
D(k) = Y_i^m(k)d(k) \tag{24}
$$

where $\hat{k} \equiv k/k$ is the direction of $k$ and $Y_i^m$ is a spherical harmonic. In the two-channel model (assuming for simplicity the absence of direct open channel interaction) $D(k)$ is the closed channel probability amplitude of having one particle of wavevector $k$ and one molecule of wavevector $-k$. In the model of [43] $D(k)$ is the Fourier transform of the regular part $A$ of the wavefunction, $D(k) = \int q^3 d\mathbf{x} e^{-i\mathbf{k} \cdot \mathbf{x}} A(\mathbf{x}) \tag{25}$ such that $\psi(r_1, r_2, r_3) \sim \frac{A(r_3 - R_\alpha)}{r_{12}}$ when the distance impurity-first identical particle $r_{12} \rightarrow 0$ at fixed positions $R_{12}$ of their center-of-mass and of the second identical particle. In the zero-range limit and in the angular momentum sector $\ell$, it is related to the hyperradial wavefunction $F(R)$ by

$$
A(\mathbf{x}) \propto Y_i^m(\hat{x})x^{-1} F \left( R = \frac{x\sin^{1/2}\nu}{1 + \sin\nu} \right). \tag{26}
$$

In the zero-energy limit $E = -\hbar^2/2m_r$, there is scale invariance of the integral operator in equation (25), which becomes a convolution product when one uses $X = \ln(kR_\alpha \cos\nu)$ as the new variable. Then one takes the Fourier transform of $d(k)k^2$ with respect to $X$ as the new unknown function; it obeys a solvable finite difference equation. Fourier transforming back and using the residue theorem, one can calculate analytically the $X \rightarrow -\infty$, that is the $k \rightarrow 0$ behavior of $d(k)$, allowing one to access the three-body parameter $R_\alpha$. This procedure was already implemented in references [44–46] in the Efimow case $s_i = 1/s_f$. We push it to subleading order for a validity condition for the zero-range model:

$$
d(k) \underset{k \to 0}{=} C(-s_i)(kR_\alpha \cos\nu)^{-s_i-2} \left[ 1 - \frac{kR_\alpha \cos\nu}{\Lambda_i(1-s_i)} \right]^{s_i+1} + C(s_i)(kR_\alpha \cos\nu)^{s_i+2} \left[ 1 - \frac{kR_\alpha \cos\nu}{\Lambda_i(1+s_i)} \right] + o(kR_\alpha)^{-1} \tag{27}
$$

with

$$
C(s) = \frac{\Gamma(-2s)}{\Gamma(1+2s)} \prod_{n \in \mathbb{N}} \frac{\Gamma(u_{\ell,n} - s)\Gamma(1 + u_{\ell,n} + s)}{\Gamma(v_{\ell,n} - s)\Gamma(1 + u_{\ell,n} + s)} \tag{28}
$$

where the $u_{\ell,n}$, $n \geq 1$, are the positive roots and $v_{\ell,n} = \ell + 1 + 2n$, $n \geq 0$, the positive poles of $\lambda_i(s)$ in ascending order. Using equations (17), (26) to obtain $A(x)$ in the zero-range model and Fourier transforming it as in equation (25) one gets

$$
\left( \frac{q_{\ell\alpha}R_\alpha}{2} \right)^{2s_i} = C(-s_i) C(s_i) \prod_{k=0}^{\ell} \frac{k - s_i}{k + s_i} \tag{29}
$$

where

$$
E_{\text{glob}} \equiv \frac{\hbar^2 q_{\ell\alpha}^2}{2m_r} \tag{30}
$$

is related to the three-body parameter by equation (19). This extends reference [46] to the case of two bosons and one impurity. Remarkably, we have found a new analytical form not requiring the computation of the roots $u_{\ell,n}$, $n \geq 1$, of the transcendental function $\lambda_i(s)$.

9 A better estimate of the remainder in equation (27) is $O(kR_\alpha)^n$ with $\alpha = \min(u_{\ell,1} - 2, 0)$ for $s_i \in \mathbb{R}^+$ and $\alpha = -s_i$ for $s_i \in [0, 1]$ (in which case $\ell \geq 1$).

10 One uses $\int_0^{+\infty} dx x^{s-1} J_{\ell+i}(x) \sim 2^{s-i} \frac{\Gamma(\ell+i+s)}{\Gamma(\ell+i)}$, where the Bessel function $J$ originates from the spherical harmonics expansion of a plane wave.

11 We use the identity $\frac{\Gamma(x+a)}{\Gamma(\ell+1+a)} \frac{\Gamma(x+1)}{\Gamma(\ell+1)} = \exp \left[ -i \pi \text{sgn}(a) \left( \ln \Gamma(x) - \ln \Gamma(x+1) \right) \right] \psi(z) = \frac{\sin z}{\pi} + \cos z \left( \frac{2\sin x}{\cos z} \right)$, which is clearly obeyed at $s = 0$, and its logarithmic derivative with respect to $s$ results from the formula Section 8.361(3) in reference [52].

12 For $s_i \in \mathbb{R}^+$, one takes the logarithm of equation (31) to express $q_{\ell\alpha}R_\alpha$ univocally in terms of the usual branch of the function $\ln \Gamma(z)$, and one may take the numerically more convenient form $2i \left[ \int_0^1 ds f(s) + i \int_{s_f} \frac{1}{1 - \frac{1}{\ln(s_f)}} \left| f(s + (s_f - s_i) - f(s - s_i) \right| \right]$ for the argument of the exponential function in equation (31).
The way of solving the zero-energy integral equation can be extended to the preefimovian regime \(0 < s_t < 1\). All the results (27)–(31) of the efimovian case directly extend to the preefimovian case. For \(0 < s_t < 1/2\) the right-hand side of equation (31) is positive. For \(1/2 < s_t < 1\) it is negative; this means that \(R_{s}^{2s_t}\) is negative, leading in equation (12) to a boundary condition \(F(R) = (R/R_{s})^{s_t} + (R/R_{s})^{-s_t} + O(R^{2 - s_t})\) not supporting any more a three-body bound state as discussed in reference [53].

Interestingly, at a mass ratio \(m_1/m_2\) such that \(s_t = \frac{1}{2}\), \(q_{glob}\) and \(1/R_s\) vanish as \(1 - 2s_t\) due to the first \(\Gamma\) factor in the denominator of equation (31) and to \(\Gamma(z) \sim 1/z\) for \(z \to 0\), suggesting a three-body resonance. If it was a veritable three-body resonance, however, one would believe in the boundary condition (12) at any energy scale much smaller than the interaction-range energy scale \(E\).

When \(s_t\) is very close to \(1/2\), \(k_BT\) becomes in practice \(\approx E_{glob}\), and one must return to the usual zero-range model (10), under the validity condition (5) written for \(b = R_s\). Equation (27) then indeed becomes

\[
k_BT \ll E_{glob}\tag{33}
\]

\(d(k)^{s_t=\frac{1}{2}}\) and \(k_BT\) in the sector \(1\) vanish as \(1 - 2s_t\) when \(s_t \to 1/2\), so \(k_{lim} cos \nu \approx q_{glob}\) and \(E_{lim} \approx E_{glob}\). This explains the absence of trimer state even for \(q_{glob}/R_s \ll 1\). One can thus calculate the 12 cluster coefficient on a narrow Feshbach resonance close to \(s_t = 1/2\) using the enriched zero-range model (12) only under the condition

\[
k_BT \ll E_{glob}\tag{34}
\]

which automatically includes the constraint obtained above close to \(s_t = 1/2\). The \(quantitatively\) determined temperature regimes where the usual zero-parameter zero-range model and the enriched one-parameter zero-range model can be used to calculate the third cluster coefficient for a mass ratio leading to \(s_t \in [0, 1/2]\) are represented in Figure 2, taking as an example the bosonic case \(\eta = +1\) in the sector \(\ell = 2\). They confirm the above \(qualitative\) analysis.

In Figure 3, we have plotted the three-body parameter \(R_{\ell}\), or more conveniently \(q_{glob}/R_s\), as a function of the mass ratio \(m_1/m_2\), in the bosonic case \(\eta = 1\), for \(\ell = 0\) at all mass angles and on a vicinity of the Efimov-effect threshold for \(\ell = 2\). On the efmovian side, we also compare \(E_{glob}\) to the values \(-\epsilon_q \exp[2\pi(q + 1)/|s_t|]\), for the first few trimer states \(q = 0, q = 1\), etc. of the narrow Feshbach resonance model, which at the level of accuracy of the zero-range theory coincide with \(E_{glob}\).

With our new expression (31), some explicit analytical results for the three-body parameter can be obtained in the limit of a heavy \(m_2/m_1 \gg 1\) or a light \(m_2/m_1 \ll 1\) impurity particle 2, in the case \(\eta = +1\) of bosonic particles 1
In the light impurity limit $\nu \to \frac{\pi}{2}^-$, the analytical expansion takes the form\textsuperscript{15}:

\[
\frac{q_{\text{glob}} R_\ell}{2} \propto \nu^{-\pi/4} \left[ 1 + \left( \frac{17}{27} - \frac{1}{9\pi^2} + \frac{19\pi}{72} \right) \sin^2 \nu + O(\sin^4 \nu) \right].
\]

The leading term in the right-hand side of equation (37) agrees with \textsuperscript{46}, the subleading one is new. The $\nu \to 0^+$ and $\nu \to \frac{\pi}{2}^-$ expansions are plotted as dashed lines in Figure 3a.

### 4 Application to concrete atomic mixtures

As an illustration of the analytical expressions obtained in this paper, we plot in Figure 4 the third harmonic ratio, Efimov exponent $B_\ell$, and $\nu$-dependent factor $\Omega_{\ell}$, as a function of temperature for realistic unitary boson-boson mixtures ($\eta = 1$), taking atomic species $^7$Li, $^{41}$K and $^{87}$Rb that have already been experimentally cooled to ultralow temperatures. We include the case of a unit mass ratio as it corresponds to the same atomic species taken in two different internal states. We recall that the homogeneous gas cluster coefficients are given by equation (3). To control the numerical truncation in the sum over $\nu$ in equation (4), we use the large-$\nu$ equivalent resulting from footnote 11 of \textsuperscript{18}:

\[
\sigma_\ell \sim -\frac{\eta(1)^f}{\pi \sin 2\nu} \Omega_{\ell} \left( \frac{1}{\sin \nu} \right).
\]

In the integral over $S$ under the exponential in equation (31), one must treat separately the contribution of $S = (1)$ and of $S \approx |s_0|$. The former contribution leads to $\ln(q_{\text{glob}} R_\ell)$ to a term linear in $\nu$ that exactly cancels the one originating from the logarithm of the $\Gamma$ factors in the prefactor of equation (31).

\textsuperscript{15} In the integral over $S$ under the exponential in equation (31), one must treat separately the contribution of $S = (1)$ and of $S \approx |s_0|$. The former contribution leads to $\ln(q_{\text{glob}} R_\ell)$ to a term linear in $\pi/2 - \nu$ that exactly cancels the one originating from the logarithm of the $\Gamma$ factors in the prefactor of equation (31).

\textsuperscript{16} From relation 8.723(2) of \textsuperscript{52} one further has $Q_{\ell}(1/\sin \nu) \sim (\pi/\ell)^{1/2} \tan^2(\nu/2) \sin(\nu/2)/\cos^{1/2} \nu$ for $\ell \to +\infty$ but keeping $Q_{\ell}$ renders the estimate much more precise at moderately high $\ell$, for small $\nu$. 

---

**Fig. 3.** Value of $q_{\text{glob}} R_\ell$, giving the global energy scale $E_{\text{glob}} = \hbar^2 q_{\text{glob}}^2/2m_{\ell}$ [or equivalently the three-body parameter $R_\ell$ according to Eqs. (13), (19)] for two identical bosons of species 1 and a particle of a different species 2 interacting with an infinite $s$-wave scattering length on a narrow Feshbach resonance, as a function of the mass ratio $m_1/m_2$ or the mass angle $\nu = \arcsin(m_1/m_2)$, in the angular momentum sector $\ell = 0$ for (a) and $\ell = 2$ for (b). Thick solid line: exact value equation (31), both for the preefimovian case restricted to $s_\ell \in [0, 1/2]$ [in (b) to the left of the vertical dotted line] and for the efimovian case $s_\ell \in [0, 1/2]$ [everywhere in (a) and to the right of the vertical dotted line in (b)]. Symbols and thin lines: value equation (31), both for the preefimovian case restricted to $s_\ell \in [0, 1/2]$ [in (b) to the left of the vertical dotted line] and for the efimovian case $s_\ell \in [0, 1/2]$. When $m_1/m_2 \to +\infty$ or $|s_\ell| \to 0$, where $\epsilon_\ell$ is the energy of the ground trimer state, $q \in N$, obtained numerically from equation (23) as 

\[
J_\ell \equiv \int_0^1 \frac{dt}{\sqrt{\nu}} \frac{\cos 2\nu \exp[2\pi(q + 1)/|s_\ell|]}{1 + \nu} = 0.505560 \ldots
\]

\[
J_2 \equiv \int_0^1 \frac{dt}{\sqrt{\nu}} \frac{\cos 2\nu \exp[2\pi(q + 1)/|s_\ell|]}{1 + \nu} = 0.194862 \ldots
\]
Table 1. For all possible combinations of the bosonic species $^7\text{Li}$, $^{41}\text{K}$ and $^{87}\text{Rb}$, physical quantities of the three-body 12 problem that are relevant for the associated third cluster coefficient $B_{2,1}$ (see text). The $X \times X'$ case, with unit mass ratio, corresponds to a given atomic isotope taken in two different internal states. The interaction between species 1 and 2 is described by the narrow Feshbach resonance model of Feshbach length $R_s$. The corresponding ground state trimer energy $\epsilon_0$ (when not too small to be obtained numerically from Eq. (23)) and the global energy scale $E_{\text{glob}}$, related to the three-body parameter by equation (19) are given in units of $\hbar^2/2m_s R_s^2$. For the considered mass ratios, the Efimov effect takes place in the sector $\ell = 0$ only, and $s_\ell > 1$ in all other sectors. The non-efimovian part $B_{2,1}^{\text{non-efim}}$ of $B_{2,1}$ is the sum of the first term in equation (21) for $\ell = 0$ and of all $\ell > 0$ contributions in equation (4), it is temperature and three-body-parameter independent.

| Species 1 | Species 2 | $m_1/m_2$ | Im $s_0$ | $-\epsilon_0$ | $-\epsilon_0 e^{2\pi s_0/|\epsilon_0|}$ | $E_{\text{glob}}$ | $B_{2,1}^{\text{non-efim}}$ |
|-----------|-----------|-----------|--------|-------------|---------------------------------|----------------|------------------|
| $^7\text{Li}$ | $^{87}\text{Rb}$ | 0.080728 | 0.055037 | – | – | 0.845022 | -0.13645 |
| $^7\text{Li}$ | $^{41}\text{K}$ | 0.17128 | 0.108458 | 6.12 $\times 10^{-26}$ | 0.884(1) | 0.884068 | -0.14692 |
| $^{41}\text{K}$ | $^{87}\text{Rb}$ | 0.47132 | 0.246214 | 9.13 $\times 10^{-12}$ | 1.104669 | 1.104669 | -0.17285 |
| $^X$ | $^X'$ | 1 | 0.413697 | 4.07 $\times 10^{-7}$ | 1.606453 | 1.606449 | -0.20539 |
| $^{87}\text{Rb}$ | $^{41}\text{K}$ | 2.12171 | 0.644404 | 1.55 $\times 10^{-4}$ | 2.663601 | 2.662428 | -0.25361 |
| $^{41}\text{K}$ | $^7\text{Li}$ | 5.8383 | 1.073851 | 1.50 $\times 10^{-2}$ | 5.221479 | 5.125277 | -0.31954 |
| $^{87}\text{Rb}$ | $^7\text{Li}$ | 12.3873 | 1.321051 | 1.29 $\times 10^{-1}$ | 8.038473 | 7.329207 | -0.20990 |

Fig. 4. Third harmonic-regulated cluster coefficient $B_{2,1}$ as a function of temperature, for unitary binary mixtures of typical bosonic atomic species $^7\text{Li}$, $^{41}\text{K}$ and $^{87}\text{Rb}$ in ultracold gas experiments. There is no intraspecies interaction. The interspecies interaction is treated in the zero-range model with scale invariant two-body and three-body contact conditions, except in the efimovian $\ell = 0$ sector where the three-body conditions involve a parameter $R_0$ as in equation (17), with a value obtained from the narrow Feshbach resonance model of Feshbach length $R_s$, see equations (19), (31). The zero-range model has an applicability limited to the low temperature regime (35), and to not-too-large atomic mass ratios so that the ground trimer remains in the zero-range limit. Here $m_r = \frac{m_1+m_2}{m_1+m_2}$ is the reduced mass of the two species, and $XXX'$ corresponds to a mixture of two different internal states of the same atomic isotope.

the crossover temperature $k_BT \approx |\epsilon_0|$ between the low-temperature trimer-dominated regime $B_{2,1} \sim \exp(\beta |\epsilon_0|)$ and the high-temperature strongly dissociated regime $B_{2,1} \approx \frac{2\pi}{\beta}\ln(\beta E_{\text{glob}})$, see [18] and our footnote 8.

5 Conclusion

We have considered thermal equilibrium binary mixtures of bosonic or fermionic particles with no intraspecies interactions, but with unitary interspecies interactions of infinite s-wave scattering length and of true and effective ranges much smaller than the thermal de Broglie wavelength, a situation that can be realised experimentally with ultracold atoms. The properties of the system crucially depend on the mass ratio of the two species.

Generalising previous results, we have obtained within the zero-range model analytical expressions for the third virial or cluster coefficients, involving integrals of the logarithm of Efimov transcendental functions. This was made possible by the scale invariance of the two-body Wigner-Bethe-Peierls contact conditions. In general, the result depends on three-body parameters $R_0$ appearing in three-body contact conditions, either because the Efimov effect takes place (a scaling exponent $s$ is purely imaginary), or because the system is in the precinfimovian regime (a scaling exponent $s$ is real and close to zero, because the mass ratio is close to an Efimov-effect threshold).

To predict the value of the three-body parameters, we have taken the microscopic model of an infinitely narrow Feshbach resonance of Feshbach length $R_s$, which is also expected to suppress three-body particle losses in an experiment. We have then obtained a new analytical expression for $R_0$, in the form of an integral involving again the logarithm of the Efimov transcendental function, both in the efimovian and in the precinfimovian regimes. It is found that $R_0$ diverges for $s = 1/2$, but that this is not a veritable three-body resonance, because the three-body contact conditions faithfully represent the true microscopic interaction only at energy scales much lower than $\hbar^2/m_r R_s^2$ (and than $\hbar^2/m_r R_s^2$, obviously), with $m_r$ the reduced mass of the two species. In particular, in the narrow Feshbach resonance model, there exists no trimer state in the precinfimovian regime, contrarily to the prediction of the zero-range model.

Finally, we have applied this analytical work to explicit calculations of the third cluster coefficients as functions of temperature for all binary combinations of three bosonic atomic species routinely used in cold atom experiments.

S.E. thanks JSPS for support.
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