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

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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.

PACS. 67.85.-d Ultracold gases, trapped gases. – 21.45.-v Few-body systems

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, 2, 3, 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, 8, 9, 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, 20, 21, 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, 28, 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, 8, 9] takes place however, they must involve a three-body length scale R_t , the so-called three-body parameter [7, 8, 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 model, that cannot *per se* predict a value of b_3 when a three-body parameter comes into play, since the knowledge of R_t requires a microscopic model [31, 32, 33, 34]. In B – b boson-boson mixtures, this issue is worsened because *two* three-body parameters R_t must be introduced, R_t^{BBb} and R_t^{bbB} , so that one cannot even fully absorb R_t in a rescaling of the temperature as done in [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 $k_F b \rightarrow 0$, 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 $\propto \hbar^2/m_r b^2$ [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, 41, 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 ($-2R_*$) 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, 45, 46]; we refine the theory by (i) giving an integral expression of R_t in terms of Efimov's transcendental function $\bar{A}_\ell(s)$ (in [44, 45], an infinite product representation in terms of the infinite-number roots of $\bar{A}_\ell(s)$ was given; in [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 $\propto \hbar^2/m_r b^2$ [37]. If one considers the atom and the molecule as distinguishable non-interacting particles as in [47], the probability of finding them at distances $< b$ is $O(b^3)$ 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

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

where the fugacities $z_i = \exp(\mu_i/k_B T)$ tend to zero at fixed temperature T , μ_i is the chemical potential of species i and $\lambda_r = [2\pi\hbar^2/(m_r k_B T)]^{1/2}$ is the thermal de Broglie wavelength associated to the reduced mass

$$m_r = \frac{m_1 m_2}{m_1 + m_2} \quad (2)$$

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 $\omega \rightarrow 0$ limit B_{n_1, n_2} of the cluster coefficients of the gas in isotropic trapping potentials with the same trapping angular frequency ω for both species [48],

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

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

$$B_{2,1} = \sum_{\ell \in \mathbb{N}} (2\ell + 1) \sigma_\ell \quad (4)$$

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, 8, 9] and in isotropic harmonic traps [23, 24]². The three-body

¹ The probability of having three open-channel atoms within a distance b with a relative angular momentum ℓ is $O(b^{2\ell+4})$ for a narrow Feshbach resonance, see footnote 41 in [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

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

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 form³ [46]:

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

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

with P_ℓ 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]:

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

where Γ 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 $\bar{\Lambda}_\ell(s)$ over the interval $]0, \ell + 1[$. Over this interval, $\bar{\Lambda}_\ell(s)$ 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 first useful result: the function $s \mapsto \bar{\Lambda}_\ell(s)$ is monotonically decreasing (increasing) over $]0, \ell + 1[$ when $\eta(-1)^\ell$ is positive (negative)⁴ and tends to $-\infty$ ($+\infty$) when $s \rightarrow \ell + 1^-$. As a consequence, it has either zero or one root in $]0, \ell + 1[$, depending on the sign of $\bar{\Lambda}_\ell(0)$. We have at hand a second useful result: the function $S \mapsto \bar{\Lambda}_\ell(iS)$ 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 eqs. (6,7). Then one faces only one of the three possible

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

⁴ Use eq. (9) and the fact that $x \mapsto \Gamma(x+a)\Gamma(a-x)$ is positive and has a nonnegative logarithmic derivative $\sum_{n \in \mathbb{N}} \frac{2x}{(a+n)^2 - x^2}$ over $[0, a[\forall a > 0$, see §8.362(1) in [52].

⁵ $\forall a > 0$, the logarithmic derivative of $x \mapsto \Gamma(a+ix)\Gamma(a-ix)$ over \mathbb{R} is $\sum_{n \in \mathbb{N}} \frac{-2x}{(n+a)^2 + x^2}$, see §8.362(1) in [52].

cases listed below; for $\eta(-1)^\ell$ negative, only the first case is actually accessible since $\bar{\Lambda}_\ell(s)$ is then > 1 over $]0, \ell + 1[$.

1. *The plain nonefimovian case:* $\bar{\Lambda}_\ell(s)$ has only real roots, and the smallest positive root is $s_\ell > 1$. The hyper-radial wavefunction $F(R)$ is subjected to the boundary condition⁶

$$F(R) \underset{R \rightarrow 0}{=} O(R^{s_\ell}) \quad (10)$$

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 σ_ℓ of the angular momentum ℓ to $B_{2,1}$ as defined in eq. (4) is given by [18, 26]

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

2. *The preefimovian case:* $\bar{\Lambda}_\ell(s)$ has only real roots, but the smallest positive root $s_\ell \in]0, 1[$. In the channel associated to the root s_ℓ , there is an enriched boundary condition [53, 54, 55], that must be used when s_ℓ is small enough [26]⁷:

$$F(R) \underset{R \rightarrow 0}{=} (R/R_t)^{s_\ell} - (R/R_t)^{-s_\ell} + O(R^{2-s_\ell}) \quad (12)$$

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

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

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

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

with $\beta = 1/k_B T$,

$$\Delta(\epsilon) = \frac{1}{\pi} \operatorname{atan} \frac{\operatorname{th}[\frac{s_\ell}{2} \ln(\epsilon/E_{\text{glob}})]}{\tan(\frac{s_\ell}{2}\pi)} \quad (15)$$

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

$$f_\ell(S) \equiv \ln \left[\frac{S^2 + 1}{S^2 + s_\ell^2} \bar{\Lambda}_\ell(iS) \right] \quad (16)$$

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

⁶ More precisely, the three-body wavefunction is written in the form $\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \phi(\Omega)F(R)/R^2$ where Ω is the set of hyperangles [7, 8, 9, 25].

⁷ It shall not be used for $s_\ell > 1$ as the wavefunction is not square integrable in $R = 0$, $\int_0^{R_0} dR R |F(R)|^2 = +\infty$ for any finite R_0 .

3. *The Efimovian case:* $\bar{\Lambda}_\ell(s)$ has real roots and a pair of purely imaginary roots $\pm s_\ell$ with $s_\ell = i|s_\ell|$. In the Efimovian channel, one must use the boundary condition [7, 8, 9, 30]

$$F(R) \underset{R \rightarrow 0}{=} (R/R_t)^{i|s_\ell|} - (R/R_t)^{-i|s_\ell|} + O(R^2) \quad (17)$$

As $F(R)$ has an infinite number of zeroes when $R \rightarrow 0$, the model predicts in free space an infinite number of trimers states of energies ϵ_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 eq. (13):

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

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

$$\begin{aligned} \sigma_\ell = & - \int_{\mathbb{R}^+} \frac{dS}{2\pi} f_\ell(S) - \int_{\mathbb{R}^+} d\epsilon \Delta(\epsilon) \beta e^{-\beta\epsilon} \\ & + \sum_{q \in \mathbb{N}} (e^{-\beta\epsilon_q} - 1) \end{aligned} \quad (21)$$

where $f_\ell(S)$ is still given by eq. (16) and the new form of the function Δ ,⁸

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

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 $m_1/m_2 > 38.6301\dots$, in the sector $\ell = 4$ for $m_1/m_2 > 125.764\dots$, etc. For $\eta = -1$ there is an Efimov effect in the sector $\ell = 1$ for $m_1/m_2 > 13.6069\dots$ [57], in the sector $\ell = 3$ for $m_1/m_2 > 75.9944\dots$ [58], etc. In fig. 1, corresponding to $\eta = 1$, we plot the imaginary part of s_0 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_2 close to the Efimov-effect threshold.

⁸ One has also $\Delta(\epsilon) = \frac{|s_\ell|x}{2\pi} + \frac{1}{\pi} \operatorname{Im} \ln \left(1 - e^{-\pi|s_\ell|} e^{-i|s_\ell|x} \right)$ [56], which leads to $-\int_{\mathbb{R}^+} d\epsilon \Delta(\epsilon) \beta e^{-\beta\epsilon} = \frac{|s_\ell|}{\pi} \left\{ \frac{1}{2} \ln(e^\gamma \beta E_{\text{glob}}) - \sum_{n \in \mathbb{N}^*} e^{-n\pi|s_\ell|} \operatorname{Re}[\Gamma(-in|s_\ell|)(\beta E_{\text{glob}})^{in|s_\ell|}] \right\}$ as in [18], $\gamma = 0.577215\dots$ being Euler's constant.

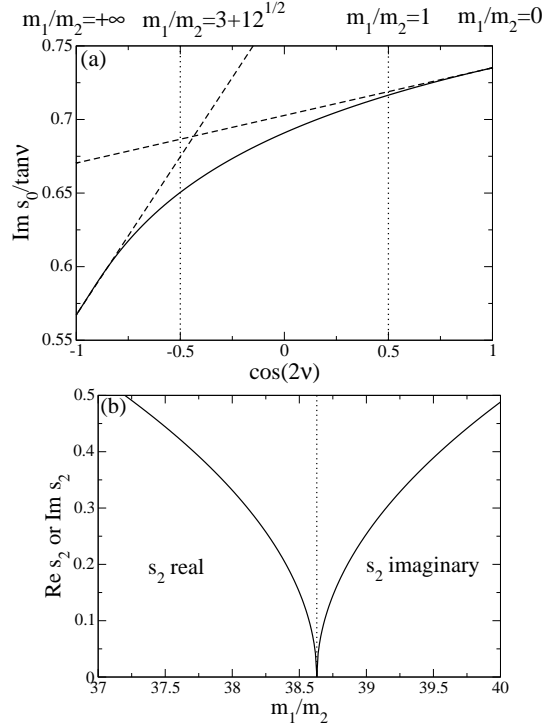


Fig. 1. Real or imaginary part of s_ℓ as a function of the mass ratio m_1/m_2 in the 112 problem for $\eta = 1$ (particles of species 1 are identical bosons) in angular momentum sector (a) $\ell = 0$ (s_0 is always purely imaginary), (b) $\ell = 2$ (s_2 switches from real to purely imaginary for $m_1/m_2 = 38.6301\dots$ at the vertical dotted line). In (a) one uses the mass angle $\nu = \arcsin \frac{m_1}{m_1+m_2} \in [0, \frac{\pi}{2}]$ as a parameter, to cover all mass ratios, and $\operatorname{Im} s_0$ is divided by $\tan \nu$ to form a bounded quantity. Solid lines: from a numerical solution of the transcendental equation $\bar{\Lambda}_\ell(s_\ell) = 0$. Dashed lines in (a): Taylor expansions for a low mass ratio $\nu \rightarrow 0^+$, $\operatorname{Im} s_0 / \tan \nu = \frac{4}{\pi\sqrt{3}} \left[1 + \left(\frac{1}{3\pi^2} - \frac{7}{90} \right) (1 - \cos 2\nu) + O(\nu^4) \right]$, and for a large mass ratio $\nu \rightarrow \frac{\pi}{2}^-$ as in [46], $\operatorname{Im} s_0 / \tan \nu = \Omega \left[1 + \frac{3+\Omega}{6(1+\Omega)} (1 + \cos 2\nu) \right] + O[(\frac{\pi}{2} - \nu)^4]$ where the constant Ω obeys $\Omega \exp \Omega = 1$. Vertical dotted lines in (a): the mass ratios $m_1/m_2 = 1$ and $3 + \sqrt{12}$ where $\cos 2\nu = \pm \frac{1}{2}$.

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.

The starting point is the equivalent of the Skorniakov–Ter-Martirosian integral equation [59] for the 112 three-body problem on a narrow Feshbach resonance. It can 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, 61, 62, 63, 64]. In the sector of angular momentum ℓ , both models lead for $1/a = 0$ and at negative energy $E = -\hbar^2 q^2 / 2m_r$ in the center-of-mass

frame to

$$[q_{\text{rel}}(k) + q_{\text{rel}}^2(k)R_*]d(k) = \eta \int_{\mathbb{R}^+} \frac{dk'}{\pi} \int_{-1}^1 du \frac{P_\ell(u)k'^2 d(k')}{q^2 + k^2 + k'^2 + 2kk'u \sin \nu} \quad (23)$$

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

$$D(\mathbf{k}) = Y_\ell^m(\hat{\mathbf{k}})d(k) \quad (24)$$

where $\hat{\mathbf{k}} \equiv \mathbf{k}/k$ is the direction of \mathbf{k} and Y_ℓ^m is a spherical harmonic. In the two-channel model (assuming for simplicity the absence of direct open channel interaction) $D(\mathbf{k})$ is the closed channel probability amplitude of having one particle of wavevector \mathbf{k} and one molecule of wavevector $-\mathbf{k}$. In the model of [43] $D(\mathbf{k})$ is the Fourier transform of the regular part $A(\mathbf{x})$ of the wavefunction,

$$D(\mathbf{k}) = \int d^3x e^{-i\mathbf{k}\cdot\mathbf{x}} A(\mathbf{x}) \quad (25)$$

such that $\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \sim \frac{A(\mathbf{r}_3 - \mathbf{R}_{12})}{r_{12}}$ when the distance impurity-first identical particle $r_{12} \rightarrow 0$ at fixed positions \mathbf{R}_{12} of their center-of-mass and \mathbf{r}_3 of the second identical particle. In the zero-range limit and in the angular momentum sector ℓ , it is related to the hyperradial wavefunction $F(R)$ by

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

In the zero-energy limit $E = 0^-$, there is scale invariance of the integral operator in eq. (23), which becomes a convolution product when one uses $X = \ln(kR_* \cos \nu)$ 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_t .

This procedure was already implemented in [44, 45, 46] in the Efimovian case $s_\ell = i|s_\ell|$. We push it to subleading order to obtain a validity condition for the zero-range model:

$$d(k) \underset{k \rightarrow 0}{=} C(-s_\ell)(kR_* \cos \nu)^{-s_\ell - 2} \left[1 - \frac{kR_* \cos \nu}{\Lambda_\ell(1 - s_\ell)} \right] + C(s_\ell)(kR_* \cos \nu)^{s_\ell - 2} \left[1 - \frac{kR_* \cos \nu}{\Lambda_\ell(1 + s_\ell)} \right] + o(kR_*)^{-1} \quad (27)$$

with⁹

$$C(s) = \Gamma(-2s) \frac{\Gamma(1 + v_{\ell,0} + s)}{\Gamma(v_{\ell,0} - s)} \times \prod_{n \in \mathbb{N}^*} \frac{\Gamma(u_{\ell,n} - s)\Gamma(1 + v_{\ell,n} + s)}{\Gamma(v_{\ell,n} - s)\Gamma(1 + u_{\ell,n} + s)} \quad (28)$$

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 $\Lambda_\ell(s)$ in ascending order. Using eqs. (17,26) to obtain $A(\mathbf{x})$ in the zero-range model and Fourier transforming it as in eq. (25) one gets¹⁰

$$\left(\frac{q_{\text{glob}}R_*}{2}\right)^{2s_\ell} = \frac{C(-s_\ell)}{C(s_\ell)} \prod_{k=0}^{\ell} \frac{k - s_\ell}{k + s_\ell} \quad (29)$$

where

$$E_{\text{glob}} \equiv \frac{\hbar^2 q_{\text{glob}}^2}{2m_r} \quad (30)$$

is related to the three-body parameter by eq. (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 $\Lambda_\ell(s)$:¹¹

$$\left(\frac{q_{\text{glob}}R_*}{2}\right)^{2s_\ell} = \frac{\Gamma(1 + 2s_\ell)\Gamma(v_{\ell,0} - s_\ell)\Gamma(2 - s_\ell)}{\Gamma(1 - 2s_\ell)\Gamma(v_{\ell,0} + s_\ell)\Gamma(2 + s_\ell)} \times \exp\left[-i \int_0^{+\infty} dS \frac{f_\ell(S - is_\ell) - f_\ell(S + is_\ell)}{\text{th}(\pi S)}\right] \quad (31)$$

where the function f_ℓ is given by eq. (16). This is as explicit as it can be since $\Lambda_\ell(s)$ is known explicitly thanks to eqs. (6,7)¹².

The way of solving the zero-energy integral equation can be extended to the preefimovian regime $0 < s_\ell < 1$.¹³

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

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

¹¹ We use the identity $\frac{\Gamma(u+s)\Gamma(u+1+s)\Gamma(v-s)\Gamma(v+1-s)}{\Gamma(u-s)\Gamma(u+1-s)\Gamma(v+s)\Gamma(v+1+s)} = \exp\left\{-i \int_{\mathbb{R}^+} \frac{dx}{\text{th} \pi x} [\ln \Psi(x - is) - \ln \Psi(x + is)]\right\}$ with $\Psi(z) = \frac{u^2+z^2}{v^2+z^2}$ and $u, v > 0$. It holds for all $s \in i\mathbb{R}^+$, and also for $0 < s < u, v$. It is clearly obeyed at $s = 0$, and its logarithmic derivative with respect to s results from the formula §8.361(3) in [52], $\frac{d}{dz} \ln \Gamma(z) = \ln z - \frac{1}{2z} - \int_{\mathbb{R}^+} \frac{2t dt}{(t^2+z^2)[\exp(2\pi t)-1]}$ with $\text{Re } z > 0$.

¹² For $s_\ell \in i\mathbb{R}^+$, one takes the logarithm of eq. (31) to express $q_{\text{glob}}R_*$ univocally in terms of the usual branch of the function $\ln \Gamma(z)$, and one may take the numerically more convenient form $2i \int_0^{|s_\ell|} dS f_\ell(S) + i \int_{\mathbb{R}^+} dS \left(1 - \frac{1}{\text{th}(\pi S)}\right) [f_\ell(S + |s_\ell|) - f_\ell(S - |s_\ell|)]$ for the argument of the exponential function in eq. (31).

¹³ The only subtle point is to shift the integration line defining the Fourier representation of $k^2 d(k)$ considered as a function of

All the results (27-31) of the efimovian case directly extend to the preefimovian case. For $0 < s_\ell < 1/2$ the right-hand side of eq. (31) is positive. For $1/2 < s_\ell < 1$ it is negative; this means that $R_t^{2s_\ell}$ is negative, leading in eq. (12) to a boundary condition $F(R) \underset{R \rightarrow 0}{=} (R/|R_t|)^{s_\ell} + (R/|R_t|)^{-s_\ell} + O(R^{2-s_\ell})$ not supporting any more a three-body bound state as discussed in [53].

Interestingly, at a mass ratio m_1/m_2 such that $s_\ell = \frac{1}{2}$, q_{glob} and $1/R_t$ vanish as $1 - 2s_\ell$ due to the first Γ factor in the denominator of eq. (31) and to $\Gamma(z) \sim 1/z$ for $z \rightarrow 0$, 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 $\hbar^2/(2m_t R_*^2)$; for $s_\ell = \frac{1}{2}$ small and negative, there would be a trimer state of binding energy E_{glob} . This is in contradiction with a numerical solution of eq. (23) for $\eta = -1$ [46] and for $\eta = 1$. To identify the correct energy scale E_{lim} below which the predictions of the enriched zero-range model (12) can be trusted, we require that for $k_{\text{lim}} \cos \nu \equiv (2m_r E_{\text{lim}})^{1/2}/\hbar$ the subleading term in eq. (27) is comparable to the leading term¹⁴:

$$k_{\text{lim}} R_* \cos \nu = |\bar{\Lambda}_\ell(1 - s_\ell)| \quad (32)$$

As $\bar{\Lambda}_\ell(s) \propto s - s_\ell$ close to its root s_ℓ , $\bar{\Lambda}_\ell(1 - s_\ell)$ vanishes as $1 - 2s_\ell$ when $s_\ell \rightarrow 1/2$, so $k_{\text{lim}} \cos \nu \simeq q_{\text{glob}}$ and $E_{\text{lim}} \simeq E_{\text{glob}}$. This explains the absence of trimer state even for $q_{\text{glob}} R_* \ll 1$. One can thus calculate the 112 cluster coefficient on a narrow Feshbach resonance close to $s_\ell = 1/2$ using the enriched zero-range model (12) only under the condition

$$k_B T \ll E_{\text{glob}} \quad (33)$$

When s_ℓ is very close to $1/2$, $k_B T$ becomes in practice $> E_{\text{glob}}$ and one must return to the usual zero-range model (10), under the validity condition (5) written for $b = R_*$. Eq. (27) then indeed becomes

$$d(k) \underset{k \rightarrow 0}{\stackrel{s_\ell = \frac{1}{2}}{=} (k R_* \cos \nu)^{-5/2} - (k R_* \cos \nu)^{-3/2} [\text{const} + \ln(k R_* \cos \nu)] + O[\ln(k R_* \cos \nu)(k R_* \cos \nu)^{-1/2}] \quad (34)$$

The leading term corresponds to the usual boundary condition (10), and the subleading one is negligible within logarithmic accuracy for $k R_* \cos \nu \ll 1$.

For s_ℓ significantly away from $1/2$ from below, or for s_ℓ purely imaginary, the enriched zero-range models (12,17) still predict the existence of a trimer state of binding energy E_{glob} , which is incorrect on a narrow Feshbach resonance. This means that these models are never correct at

X: rather than integrating over the line $\mathbb{R} + i0^+$ as in eq. (66) of [46], one must integrate over a line $\mathbb{R} + i\gamma$, $s_\ell < \gamma < 1 + \nu_{\ell,0}$, to pass in between the highest pole $i s_\ell$ of the Fourier transform originating from a root of $\bar{\Lambda}_\ell$ and the lowest pole $i(1 + \nu_{\ell,0})$ originating from a pole of $\bar{\Lambda}_\ell$.

¹⁴ The corresponding condition for $s_\ell \leftrightarrow -s_\ell$ involves $\bar{\Lambda}_\ell(1 + s_\ell)$ and is less stringent.

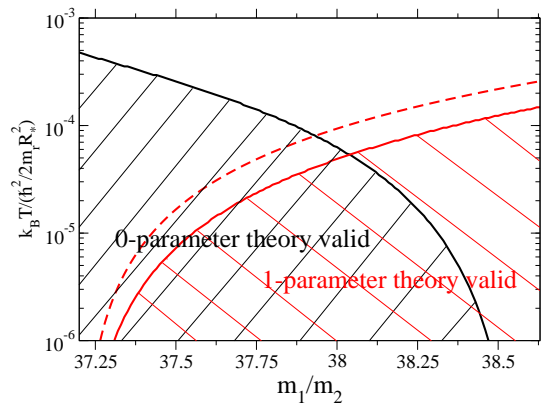


Fig. 2. For $\eta = +1$ in the $\ell = 2$ sector, validity zone in the plane (mass ratio, temperature) of the usual zero-parameter zero-range theory (black hatched) and of the enriched one-parameter zero-range theory (red hatched) for the calculation of the cluster coefficient $B_{2,1}$ at unitary on a narrow Feshbach resonance of Feshbach length R_* . Below the black solid line, the sum of the terms of degree $-s_2 - 1$ and $s_2 - 2$ in k is more than 3 times smaller than the term of degree $-s_2 - 2$ in eq. (27), for $k \cos \nu = (2m_r k_B T)^{1/2}/\hbar$. Below the red solid line, the sum of the terms of degree $-s_2 - 1$ and $s_2 - 1$ in k is more than 3 times smaller than the sum of the terms of degree $-s_2 - 2$ and $s_2 - 2$. Red dashed line: when $k_B T = E_{\text{glob}}$. At the borders of the mass interval, $s_2 = 1/2$ and $s_2 = 0$ respectively.

the energy scale E_{glob} . In the virial calculation, we thus take as their qualitative validity conditions

$$k_B T \ll E_{\text{glob}}, \frac{\hbar^2}{2m_r R_*^2} \quad (35)$$

which automatically includes the constraint obtained above close to $s_\ell = 1/2$. 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 $s_\ell \in [0, 1/2]$ are represented in fig. 2, taking as an example the bosonic case $\eta = +1$ in the sector $\ell = 2$. They confirm the above *qualitative* analysis.

In fig. 3, we have plotted the three-body parameter R_ℓ , or more conveniently $q_{\text{glob}} R_*$, 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 efimovian side, we also compare E_{glob} to the values $-\epsilon_q \exp[2\pi(q+1)/|s_\ell|]$, 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 sector $\ell = 0$. In the heavy impurity limit $\nu \rightarrow 0^+$,

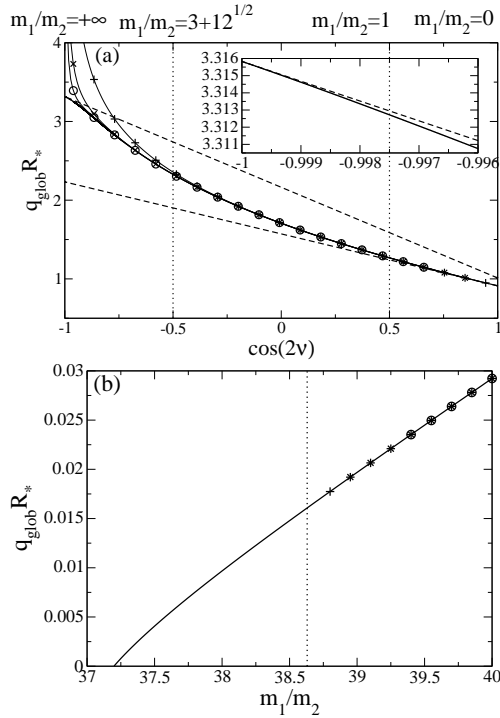


Fig. 3. Value of $q_{\text{glob}} R_*$ giving the global energy scale $E_{\text{glob}} = \hbar^2 q_{\text{glob}}^2 / 2m_r$ [or equivalently the three-body parameter R_t according to eqs. (13,19)] for two identical bosons of species 1 and a particle of a different species 2 interacting with an infinite s -wave scattering length on a narrow Feshbach resonance, as a function of the mass ratio m_1/m_2 or the mass angle $\nu = \arcsin \frac{m_1}{m_1+m_2}$, in the angular momentum sector $\ell = 0$ for (a) and $\ell = 2$ for (b). Thick solid line: exact value eq. (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 $s_\ell \in i\mathbb{R}^+$ [everywhere in (a) and to the right of the vertical dotted line in (b)]. Symbols and thin lines: in the efimovian case, from the estimates $E_{\text{glob}} \simeq -\epsilon_q \exp[2\pi(q+1)/|s_\ell|]$ (exact for $q \rightarrow +\infty$ or $|s_\ell| \rightarrow 0$), where ϵ_q is the energy of the q th trimer state, $q \in \mathbb{N}$, obtained numerically from eq. (23) when possible ($q = 0$: pluses, $q = 1$: crosses, $q = 2$: circles); when $m_1/m_2 \rightarrow +\infty$ the low lying part of the spectrum becomes hydrogenoid [46] (rather than geometric) and $(-2m_r \epsilon_q)^{1/2} R_* / \hbar \rightarrow +\infty$, hence the deviations from the thick solid line. In (a) the dashed oblique straight lines are the expansions (36) and (37), the latter being in reality useful over a very limited range, see magnification in the inset, and the vertical dotted lines are at the mass ratios $m_1/m_2 = 1$ and $3 + \sqrt{12}$ where $\cos 2\nu = \pm 1/2$. In (b) q_{glob} vanishes at the mass ratio such that $s_2 = 1/2$ but this is not a veritable three-body resonance (see text). The Feshbach length R_* is related to the two-body effective range by $r_e = -2R_*$ at unitarity.

we obtain the expansion

$$\frac{q_{\text{glob}} R_*}{2} \underset{\nu \rightarrow 0^+}{=} e^{-\pi/4} \left[1 + \left(\frac{17}{27} - \frac{1}{9\pi^2} + \frac{19\pi}{72} \right) \sin^2 \nu + O(\sin^4 \nu) \right] \quad (36)$$

In the light impurity limit $\nu \rightarrow \frac{\pi}{2}^-$, the analytical expansion takes the form¹⁵:

$$\frac{q_{\text{glob}} R_*}{2} \underset{\nu \rightarrow \frac{\pi}{2}^-}{=} e^{J_0} \left\{ 1 + \left[\frac{2\Omega J_2}{3(\Omega+1)} + \frac{1}{12\Omega^2} - \frac{2}{3\Omega} + \frac{1}{24(1+\Omega)} \right] \cos^2 \nu + O(\cos^3 \nu) \right\} \quad (37)$$

where we introduced $\Omega = 0.567143\dots$ solving $\Omega \exp \Omega = 1$ and the integrals

$$J_0 \equiv \int_0^1 d\tau \ln \frac{e^{\Omega\tau} + \tau - 1}{\tau} = 0.505560\dots \quad (38)$$

$$J_2 \equiv \int_0^1 d\tau \frac{\tau e^{\Omega\tau}}{e^{\Omega\tau} + \tau - 1} = 0.194862\dots \quad (39)$$

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

4 Application to concrete atomic mixtures

As an illustration of the analytical expressions obtained in this paper, we plot in fig. 4 the third harmonic-regulated cluster coefficient $B_{2,1}$ as a function of temperature for realistic unitary boson-boson mixtures ($\eta = 1$), taking atomic species ${}^7\text{Li}$, ${}^{41}\text{K}$ and ${}^{87}\text{Rb}$ 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 eq. (3). To control the numerical truncation in the sum over ℓ in eq. (4), we use the large- ℓ equivalent resulting from footnote 11 of [18]:

$$\sigma_\ell \underset{\ell \rightarrow +\infty}{\sim} \frac{\eta(-1)^\ell}{\pi \sin 2\nu} Q_\ell \left(\frac{1}{\sin \nu} \right) \quad (40)$$

where $Q_\ell(z) = \int_{-1}^1 \frac{du}{2} \frac{P_\ell(u)}{z-u}$ is a Legendre function of the second kind¹⁶. Relevant quantities, such as mass ratio, Efimov exponent s_0 , global energy scale E_{glob} and ground state trimer energy ϵ_0 , are given in the table. Comparing E_{glob} and $-\epsilon_0 e^{2\pi/|s_0|}$ indicates to which extent the ground trimer is in the zero-range regime, which is already marginally the case for the rubidium-lithium mixture. Knowing the value of ϵ_0 also gives the crossover temperature $k_B T \approx |\epsilon_0|$ between the low-temperature trimer-dominated regime $B_{2,1} \sim \exp(\beta|\epsilon_0|)$ and the high-temperature strongly dissociated regime $B_{2,1} \approx \frac{|s_0|}{2\pi} \ln(\beta E_{\text{glob}})$, see [18] and our footnote 8.

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

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

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 112 problem that are relevant for the associated third cluster coefficient $B_{2,1}$ (see text). The X – 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_* . The corresponding ground state trimer energy ϵ_0 [when not too small to be obtained numerically from eq. (23)] and the global energy scale E_{glob} related to the three-body parameter by eq. (19) are given in units of $\hbar^2/2m_r R_*^2$. 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 eq. (21) for $\ell = 0$ and of all $\ell > 0$ contributions in eq. (4), it is temperature and three-body-parameter independent.

species 1	species 2	m_1/m_2	$\text{Im } s_0$	$-\epsilon_0$	$-\epsilon_0 e^{2\pi/ s_0 }$	E_{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	6.12×10^{-26}	0.884(1)	0.884068	–0.14692
${}^{41}\text{K}$	${}^{87}\text{Rb}$	0.47132	0.246214	9.13×10^{-12}	1.104669	1.104669	–0.17285
X	X'	1	0.413697	4.07×10^{-7}	1.606453	1.606449	–0.20539
${}^{87}\text{Rb}$	${}^{41}\text{K}$	2.12171	0.644404	1.55×10^{-4}	2.663601	2.662428	–0.25361
${}^{41}\text{K}$	${}^7\text{Li}$	5.8383	1.073851	1.50×10^{-2}	5.221479	5.125277	–0.31954
${}^{87}\text{Rb}$	${}^7\text{Li}$	12.3873	1.521051	1.29×10^{-1}	8.038473	7.329207	–0.20990

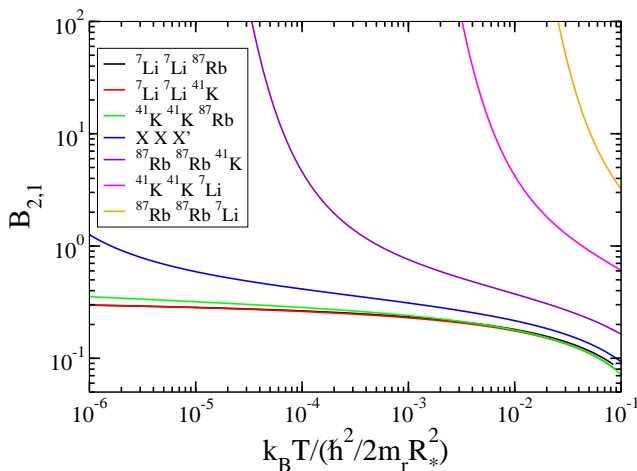


Fig. 4. Third harmonic-regulated cluster coefficient $B_{2,1}$ as a function of temperature, for unitary binary mixtures of typical bosonic atomic species ${}^7\text{Li}$, ${}^{41}\text{K}$ and ${}^{87}\text{Rb}$ in ultracold gas experiments. There is no intraspecies interaction. The interspecies interaction 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_t as in eq. (17), with a value obtained from the narrow Feshbach resonance model of Feshbach length R_* , see eqs. (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.

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_t 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 preefimovian 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_* , which is also expected to suppress three-body particle losses in an experiment. We have then obtained a new analytical expression for R_t , in the form of an integral involving again the logarithm of the Efimov transcendental function, both in the efimovian and in the preefimovian regimes. It is found that R_t 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 $\hbar^2/m_r R_t^2$ (and than $\hbar^2/m_r R_*^2$, 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 preefimovian 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.

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