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► **To cite this version:**

Felix Werner, Yvan Castin. The unitary three-body problem in a trap. *Physical Review Letters*, 2006, 97, pp.150401. hal-00007574v3

HAL Id: hal-00007574

<https://hal.science/hal-00007574v3>

Submitted on 13 Sep 2006

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The unitary three-body problem in a trap

Félix Werner and Yvan Castin

Laboratoire Kastler Brossel, École Normale Supérieure,
24 rue Lhomond, 75231 Paris Cedex 05, France

(Dated: September 13, 2006)

We consider either 3 spinless bosons or 3 equal mass spin-1/2 fermions, interacting *via* a short range potential of infinite scattering length and trapped in an isotropic harmonic potential. For a zero-range model, we obtain analytically the exact spectrum and eigenfunctions: for fermions all the states are universal; for bosons there is a coexistence of decoupled universal and efimovian states. All the universal states, even the *bosonic* ones, have a tiny 3-body loss rate. For a finite range model, we numerically find for bosons a coupling between zero angular momentum universal and efimovian states; the coupling is so weak that, for realistic values of the interaction range, these bosonic universal states remain long-lived and observable.

PACS numbers: 03.75.Ss, 05.30.Jp

With a Feshbach resonance, it is now possible to produce a stable quantum gas of fermionic atoms in the unitary limit, i.e. with an interaction of negligible range and scattering length $a = \infty$ [1]. The properties of this gas, including its superfluidity, are under active experimental investigation [2]. They have the remarkable feature of being universal, as was tested in particular for the zero temperature equation of state of the gas [3]. In contrast, experiments with Bose gases at a Feshbach resonance suffer from high loss rates [4, 5, 6], and even the existence of a unitary Bose gas phase is a very open subject [7].

In this context, fully understanding the few-body unitary problem is a crucial step. In free space, the unitary 3-boson problem has an infinite number of weakly bound states, the so-called Efimov states [8]. In a trap, it has efimovian states [9, 10] but also universal states whose energy depends only on the trapping frequency [9]. Several experimental groups are currently trapping a few particles at a node of an optical lattice [11] and are controlling the interaction strength *via* a Feshbach resonance. Results have already been obtained for two particles per lattice node [12], a case that was solved analytically [13]. Anticipating experiments with 3 atoms per node, we derive in this Letter exact expressions for *all* universal and efimovian eigenstates of the 3-body problem for bosons (generalizing [9] to a non-zero angular momentum) and for equal mass fermions in a trap. We also show the long lifetime of the universal states and their observability in a real experiment, extending to universal states the numerical study of [10].

If the effective range and the true range of the interaction potential are negligible as compared to the de Broglie wavelength of the 3 particles, the interaction potential can be replaced by the Bethe-Peierls contact conditions on the wavefunction ψ : it exists a function A such that

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \left(\frac{1}{r_{ij}} - \frac{1}{a} \right) A(\mathbf{R}_{ij}, \mathbf{r}_k) + O(r_{ij}) \quad (1)$$

in the limit $r_{ij} \equiv |\mathbf{r}_i - \mathbf{r}_j| \rightarrow 0$ taken for fixed positions

of the other particle k and of the center of mass \mathbf{R}_{ij} of i and j . In the unitary limit considered in this paper, $a = \infty$. When all the r_{ij} are non zero, the wavefunction ψ obeys the non-interacting Schrödinger equation

$$\sum_{i=1}^3 \left[-\frac{\hbar^2}{2m} \Delta_{\mathbf{r}_i} + \frac{1}{2} m \omega^2 r_i^2 \right] \psi = E \psi. \quad (2)$$

ω is the oscillation frequency and m the mass of an atom.

To solve this problem, we extend the approach of Efimov [8, 14] to the trapped case, and obtain the form

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \psi_{\text{cm}}(\mathbf{C}) F(R) \left(1 + \hat{Q} \right) \frac{1}{r\rho} \varphi(\alpha) Y_l^m(\boldsymbol{\rho}/\rho). \quad (3)$$

Since the center of mass is separable for a harmonic trapping, we have singled out the wavefunction $\psi_{\text{cm}}(\mathbf{C})$ of its stationary state of energy E_{cm} , with $\mathbf{C} = (\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3)/3$. The operator \hat{Q} ensures the correct exchange symmetry of ψ : for spinless bosons, $\hat{Q} = \hat{P}_{13} + \hat{P}_{23}$, where \hat{P}_{ij} transposes particles i and j ; for spin 1/2 fermions, we assume a spin state $\uparrow\downarrow\uparrow$ so that $\hat{Q} = -\hat{P}_{13}$. The Jacobi coordinates are $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$ and $\boldsymbol{\rho} = (2\mathbf{r}_3 - \mathbf{r}_1 - \mathbf{r}_2)/\sqrt{3}$. Y_l^m is a spherical harmonic, l being the total internal angular momentum of the system. The function $\varphi(\alpha)$, where $\alpha = \arctan(r/\rho)$, solves the eigenvalue problem

$$-\varphi''(\alpha) + \frac{l(l+1)}{\cos^2 \alpha} \varphi(\alpha) = s^2 \varphi(\alpha) \quad (4)$$

$$\varphi(\pi/2) = 0 \quad (5)$$

$$\varphi'(0) + \eta(-1)^l \frac{4}{\sqrt{3}} \varphi(\pi/3) = 0 \quad (6)$$

with $\eta = -1$ for fermions, $\eta = 2$ for bosons. An analytical expression can be obtained for $\varphi(\alpha)$ [15], which leads to the transcendental equation for s [16]:

$$\left[i^l \sum_{k=0}^l \frac{(-l)_k (l+1)_k}{k!} \frac{(1-s)_l}{(1-s)_k} \left(2^{-k} i^k (k-s) e^{is\frac{\pi}{2}} + \eta(-1)^l \frac{4}{\sqrt{3}} e^{i\frac{\pi}{6}(2k+s)} \right) \right] - [i \leftrightarrow -i] = 0, \quad (7)$$

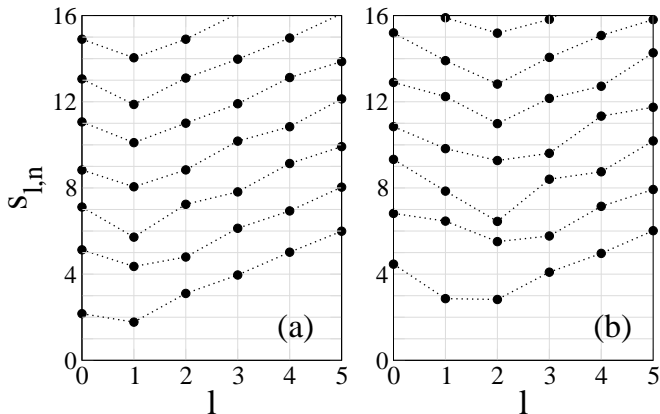


FIG. 1: The constants $s_{l,n}$ for (a) 3 equal mass fermions and (b) 3 bosons, obtained by numerical solution of the transcendental equation Eq.(7). We have not represented the $s_{l=0,n=0}$ solution for bosons, which is purely imaginary. According to Eq.(10), each real $s_{l,n}$ gives rise to a semi-infinite ladder of universal states. Note that the ground universal state has a total angular momentum $l = 1$ for fermions ($E \simeq 4.27\hbar\omega$) and $l = 2$ for bosons ($E \simeq 5.32\hbar\omega$).

with the notation $(x)_n \equiv x(x+1)\dots(x+n)$. This equation is readily solved numerically: for each l , the solutions form an infinite sequence $(s_{l,n})_{n \geq 0}$, see Fig.1. As we show below, all solutions are real, except for bosons in the $l = 0$ channel, where a single purely imaginary solution exists, $s_{l=0,n=0} \equiv s_0 \simeq i \times 1.00624$, the well known Efimov solution. Finally, the function $F(R)$, where the hyperradius is $R = \sqrt{(r^2 + \rho^2)}/2$, solves the problem:

$$\left[-\frac{\hbar^2}{2m} \left(\frac{d^2}{dR^2} + \frac{1}{R} \frac{d}{dR} \right) + U(R) \right] F(R) = (E - E_{\text{cm}})F(R) \quad (8)$$

where $U(R) = \hbar^2 s^2 / (2mR^2) + m\omega^2 R^2 / 2$, s being one of the $s_{l,n}$. This is the Schrödinger equation for a fictitious particle of zero angular momentum moving in two dimensions in the potential $U(R)$.

When $s^2 > 0$, one takes $s > 0$ and the solution is

$$F(R) = R^s e^{-R^2/2a_{\text{ho}}^2} L_q^{(s)}(R^2/a_{\text{ho}}^2) \quad (9)$$

where $a_{\text{ho}} = (\hbar/m\omega)^{1/2}$ is the harmonic oscillator length, $L_q^{(\cdot)}$ is the generalized Laguerre polynomial of degree q , q being an arbitrary non-negative integer. The resulting spectrum for the 3-body problem is

$$E = E_{\text{cm}} + (s_{l,n} + 1 + 2q)\hbar\omega. \quad (10)$$

The quantum number q leads to a semi-infinite ladder structure of the spectrum with a regular spacing $2\hbar\omega$. This is related to the existence of a scaling solution for the trapped unitary gas [17] and the subsequent embedding of the Hamiltonian in a $SO(2,1)$ algebra [18], leading to an exact mapping between trapped and free space universal states [19].

When $s^2 < 0$, as is the case in the $l = n = 0$ channel for bosons, the Schrödinger equation Eq.(8) does not define by itself an Hermitian problem and has to be supplemented by a boundary condition for $R \rightarrow 0$ [20, 21]:

$$F(R) \propto \text{Im} \left[\left(\frac{R}{R_t} \right)^{s_0} \right], \quad (11)$$

where R_t is an additional 3-body parameter. For the resulting efimovian states, the function F is given by

$$F(R) = R^{-1} W_{(E-E_{\text{cm}})/2\hbar\omega, s_0/2}(R^2/a_{\text{ho}}^2) \quad (12)$$

where W is a Whittaker function, and the energy solves:

$$\arg \Gamma \left[\frac{1 + s_0 - (E - E_{\text{cm}})/\hbar\omega}{2} \right] = -|s_0| \ln(R_t/a_{\text{ho}}) + \arg \Gamma(1 + s_0) \text{ mod } \pi. \quad (13)$$

We did not yet obtain all the 3-body eigenstates [22]. Indeed, all the above states satisfy the contact condition (1) with a *non-zero* function A . But there are wavefunctions of the unitary gas which *vanish* when two particles are at the same point; these are also eigenstates of the non-interacting case. An example is the Laughlin state of the Fractional Quantum Hall Effect [23]:

$$\psi = e^{-\sum_{i=1}^3 r_i^2/2a_{\text{ho}}^2} \prod_{1 \leq n < m \leq 3} [(x_n + iy_n) - (x_m + iy_m)]^{|\eta|}. \quad (14)$$

In the limit of high energies $E \gg \hbar\omega$, there are actually many of these $A \equiv 0$ states: their density of states (DOS) is almost as high as the DOS of the non-interacting case:

$$\frac{\rho_{A \equiv 0}(E)}{\rho_{\text{non-inter}}(E)} \underset{E \rightarrow \infty}{=} 1 - O\left(\left(\frac{\hbar\omega}{E}\right)^2\right). \quad (15)$$

In contrast, the DOS of the $A \neq 0$ states is only

$$\frac{\rho_{A \neq 0}(E)}{\rho_{\text{non-inter}}(E)} \underset{E \rightarrow \infty}{=} O\left(\left(\frac{\hbar\omega}{E}\right)^3\right). \quad (16)$$

Eq.(16) is a consequence of Eq.(17) given below. We found Eq.(15) by applying the rank theorem to the operator $\psi_0(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \mapsto (\psi_0(\mathbf{r}_1, \mathbf{r}_1, \mathbf{r}_3), \psi_0(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_1), \psi_0(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_2))$ which associates, to each non-interacting eigenstate ψ_0 of energy E , 3 functions of 2 atomic positions, and whose kernel is the space of $A \equiv 0$ states of energy E [24].

This completes our derivation of *all* eigenstates of the unitary 3-body problem in a trap. Three types of states are obtained in general: universal eigenstates common to the non-interacting case, universal interacting states, and efimovian states depending on a 3-body parameter.

We now prove that the Efimov effect is absent for 3 equal mass fermions. This fact is known but to our

knowledge not demonstrated. Numerically one can only check the absence of imaginary solution of the transcendental equation in some finite interval of s and l . Here we prove that for any l and any imaginary s , there is no solution to the problem (4,5,6). Let us assume that $s^2 \leq l(l+1)$, and that (4,5) are satisfied. We will show that the quantity $Q(l, s^2) \equiv \varphi'(0) - (-1)^l (4/\sqrt{3})\varphi(\pi/3)$ is non zero, which is incompatible with (6). We rewrite (4) as $\varphi''(\alpha) = u(\alpha)\varphi(\alpha)$. This is Newton's equation, α being the time and φ the position of a fictitious particle subject to an *expelling* harmonic force with time dependent spring constant $u(\alpha; l, s^2) = \frac{l(l+1)}{\cos^2 \alpha} - s^2 \geq 0$. Eq.(5) imposes that this particle reaches the origin at 'time' $\pi/2$. The particle then should not reach the origin earlier, otherwise the expelling force would prevent it from turning back to $\varphi = 0$. We thus can take the normalization $\varphi(0) = 1$, which implies $\varphi'(0) < 0$ and $\varphi(\alpha) > 0$ for $0 \leq \alpha < \pi/2$. Thus, $Q(l, s^2) < 0$ for l even. For l odd, one needs two intermediate results: (i) $Q(l=1, s^2=2) < 0$ (which we check by explicit calculation); (ii) if φ_1, φ_2 are two solutions with $u_2 \geq u_1$, then $\varphi_2 \leq \varphi_1$, and $Q_2 \leq Q_1$: because the spring constant for particle 2 is larger, particle 2 has to start faster and walk constantly ahead of particle 1 in the race towards the origin, to satisfy Eq.(5). Now the assumption $s^2 \leq l(l+1)$ implies $u(\alpha; l, s^2) \geq u(\alpha; l=1, s^2=2)$. One concludes that: $Q(l, s^2) \leq Q(l=1, s^2=2) < 0$. For bosons, we proved similarly that all the s^2 are positive, except for the well known $s_{n=0, l=0} \simeq i \times 1.00624$.

It appears clearly on Fig.1 that $s_{l,n}$ gets close to an integer value $\bar{s}_{l,n}$ as soon as l or n increases, with

$$\begin{aligned} \bar{s}_{l,n} &= l+1+2n & \text{for } l \geq |\eta| \\ \bar{s}_{l,n} &= 2n-l+(2\eta+11)/3 & \text{for } l < |\eta|. \end{aligned} \quad (17)$$

To check this analytically, the transcendental equation is not useful. We rather applied semi-classical WKB techniques to the problem (4,5,6), and obtained [25]:

$$s_{l,0} - \bar{s}_{l,0} \underset{l \rightarrow \infty}{\sim} \eta(-1)^{l+1} 2^{1-l} / \sqrt{3\pi l} \quad (18)$$

$$s_{l,n} - \bar{s}_{l,n} \underset{n \rightarrow \infty}{\sim} \eta \cos \left[\frac{\pi}{3}(l+1-n) \right] \frac{(-1)^{l+n+1} 4}{\pi \sqrt{3} n} \quad (19)$$

$$\max_n |s_{l,n} - \bar{s}_{l,n}| \underset{l \rightarrow \infty}{\sim} |\eta| \frac{4 A_{i_{\max}}}{3^{7/12} \pi^{1/2}} l^{-5/6} \quad (20)$$

with $A_{i_{\max}} \simeq 0.5357$ the maximum of the Airy function.

We now discuss the lifetime of the 3-body states found here in the trap, due to 3-body recombination to a deeply bound molecular state. The recombination rate is commonly estimated as $\Gamma_{\text{loss}} \propto P\hbar/(m\sigma^2)$, where σ is the range of the interaction potential, and P is the probability that $R < \sigma$ [26]. Evaluating P from the 3-body wavefunctions obtained above for the zero range model, this gives for E not much larger than $\hbar\omega$:

$$\Gamma_{\text{loss}}^{\text{univ}} \propto \omega \left(\frac{\sigma}{a_{\text{ho}}} \right)^{2s} \quad (21)$$

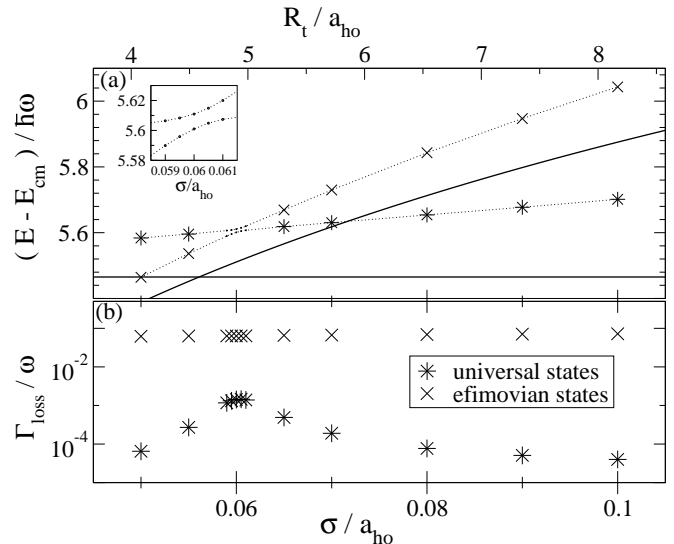


FIG. 2: Numerical solution of the separable potential model: (a) 3-body eigenenergies and (b) predicted 3-body loss rates (for the case of ^{133}Cs , see text), as a function of the potential range σ (lower axis) and the 3-body parameter R_t (upper axis) [27]. (a) The lowest energy universal branch (stars) and an efimovian branch (crosses) have a very weak avoided crossing (inset). The analytical predictions of the zero-range model (solid lines) are in good agreement with the numerics (except for the avoided crossing); a linear extrapolation of the stars to $\sigma = 0$ matches the zero-range result at the 10^{-3} level. (b) The universal states have a loss rate much smaller than ω .

for a universal state with exponent s , and $\Gamma_{\text{loss}}^{\text{efim}} \propto \omega$ for an efimovian state. Since $s \geq 1.77$ for fermions and $s \geq 2.82$ for bosons (Fig.1), Eq.(21) indicates that the lifetime of universal states is $\gg 1/\omega$ for $\sigma \ll a_{\text{ho}}$.

The existence of long-lived bosonic states is an unexpected feature that we now investigate in a more realistic way. The unitary three-body problem in an isotropic harmonic trap may be realized experimentally by trapping 3 atoms at a site of a deep optical lattice, and using a Feshbach resonance. For a broad Feshbach resonance, the effective range is of the order of the Van der Waals length, which is roughly one order of magnitude smaller than a_{ho} , for an usual lattice spacing of $\sim 0.5\mu\text{m}$ and a lattice depth of ~ 50 recoil energies. This experimental situation is not deeply in the asymptotic regime of a zero range potential. Moreover, in the zero range model, there are energy crossings between universal and efimovian states as a function of R_t/a_{ho} (see solid lines in Fig.2a); as we shall see, for a finite range, there is a coupling between $l=0$ universal and efimovian states, leading to avoided crossings [28], and to an additional contribution to the loss rate of $l=0$ universal states not included in Eq.(21).

We therefore solve a finite interaction range model, the

Gaussian separable potential of range σ [10], defined as

$$\langle \mathbf{r}_1, \mathbf{r}_2 | V | \mathbf{r}'_1, \mathbf{r}'_2 \rangle = -\frac{\hbar^2}{2\pi^{3/2}m\sigma^5} e^{-(r_{12}^2 + r_{12}'^2)/2\sigma^2} \delta(\mathbf{R}_{12} - \mathbf{R}'_{12}). \quad (22)$$

This leads to an integral equation that we solve numerically. In Fig.2a, we show two $l = 0$ energy branches as a function of σ , corresponding in the zero-range model to the lowest $l = 0$ universal state and to an efimovian branch. The smallness of the avoided crossing between the two branches shows that the coupling due to the finite range of the interaction is weak: the energy splitting at the avoided crossing is $\hbar\Omega \simeq 0.01\hbar\omega$, see inset of Fig.2a.

We now revisit the calculation of the 3-body loss rate for bosons, since Eq.(21) neglects the contamination of the universal state by the efimovian state. To account for the losses we add to the Hamiltonian H_{sep} of the separable potential model an antihermitian part leading to the effective Hamiltonian in second quantized form

$$H_{\text{eff}} = H_{\text{sep}} - iB_3 \frac{\hbar^2\sigma^4}{12m} \int [\psi^\dagger(\vec{r})]^3 [\psi(\vec{r})]^3 d\vec{r}, \quad (23)$$

where B_3 is a numerical factor, whose actual value depends on short-range atomic and molecular physics. Specializing to ^{133}Cs , we adjust the parameters of our model to $B_3 = 25$ and $\sigma = 6.5\text{nm}$ in order to reproduce the three-body loss rate measured in a non-condensed gas for several negative values of a in [5]. To obtain the loss rates shown in Fig.2b, we restricted H_{eff} to the two branches of Fig.2a: the eigenvalues of the resulting 2×2 matrix have complex parts $-i\hbar\Gamma_{\text{loss}}/2$. For the efimovian states, $\Gamma_{\text{loss}} \simeq 0.07\omega$. For the universal states Γ_{loss} is several orders of magnitude smaller; this remains true on the avoided crossing, because the coupling $\Omega/2$ of the universal state to the efimovian state is much smaller than the decay rate of the efimovian state [29].

Experimentally, if one starts with the non-interacting ground state, a superposition of 3-body unitary eigenstates can be prepared by switching suddenly the scattering length from zero to infinity. The Bohr frequencies in the subsequent evolution of an observable would give information on the 3-body spectrum. For bosons, there will be a finite fraction of the sites where the three atoms have a long lifetime. This fraction is equal to the probability of having populated a universal state, which we calculate to be $\simeq 0.174$, a value dominated by the contribution ($\simeq 0.105$) of the lowest $l = 0$ universal state.

In summary, we obtained the complete analytical solution of a zero-range unitary 3-body problem in a trap. For bosons, there are efimovian and universal states, while for equal mass fermions we proved that all states are universal. All universal states are stable in the zero-range limit with respect to 3-body losses, not only for fermions, but also for bosons. From the numerical solution of a finite range model, we find that, although the bosonic universal states of zero angular momentum

slightly mix with the efimovian states, their lifetime remains much larger than the oscillation period in the trap.

We thank L. Pricoupenko, D. Petrov, T. Köhler, A. Bulgac, D. Bauer for very useful discussions; T. Krämer *et al.* for their data. LKB is a Unité de Recherche de l'ENS et de l'Université Paris 6, associée au CNRS. Our research group is a member of IFRAF.

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