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The unitary three-body problem in a trap

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We consider either 3 spinless bosons or 3 spin-1/2 fermions, interacting with a short range potential of infinite scattering length and trapped in an isotropic harmonic potential. In the zero-range limit, we obtain analytically the exact spectrum and eigenfunctions, and find that even the *bosonic* universal states have a vanishing collisional loss rate. For realistic values of the interaction range, the numerical solution of a finite range model shows that the coupling between universal and efimovian states remains weak, which confirms that the bosonic universal states are long-lived and observable.

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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, 2, 3]. The properties of this gas, including its superfluidity, are under active experimental investigation [4, 5, 6, 7, 8, 9, 10]. They have the remarkable feature of being universal, as was checked in particular for the zero temperature equation of state of the gas using a Monte Carlo method [11, 12]. In contrast, experiments with Bose gases at a Feshbach resonance suffer from high loss rates [13, 14, 15, 16], and even the existence of a unitary Bose gas phase is a very open subject [17].

In this context, fully understanding the few-body unitary problem is a crucial step. In free space, the unitary 3-boson problem has Efimov bound states [18]. In a trap, it has efimovian states [19, 20] but also universal states whose energy depends only on the trapping frequency [19]. Several experimental groups are currently trapping a few particles at a node of an optical lattice [21] and are controlling the interaction strength *via* a Feshbach resonance. Results have already been obtained for two particles per lattice node [22], a case that was solved analytically [23]. 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 [19] to a non-zero angular momentum) and for identical 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 calculations of [20].

Assuming that the effective range and the true range of the interaction potential are negligible as compared to the de Broglie wavelength of the 3 particles, we replace the interaction potential by the Bethe-Peierls contact conditions: there 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 $r_{ij} \rightarrow 0$ 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 distances r_{ij} are non zero, the 3-body wavefunction ψ obeys the non-interacting Schrödinger equation

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

where ω is the oscillation frequency and m the mass of a particle.

To solve this problem, we extend the approach of Efimov [18, 24] to the trapped case, and obtain the form

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

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 Q ensures the correct exchange symmetry of ψ : for spinless bosons, $Q = P_{13} + P_{23}$, where P_{ij} transposes particles i and j ; for spin 1/2 fermions, we assume a spin state $\uparrow\downarrow\uparrow$ so that $Q = -P_{13}$. The Jacobi coordinates are $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$ and $\boldsymbol{\rho} = (2\mathbf{r}_3 - \mathbf{r}_1 - \mathbf{r}_2)/\sqrt{3}$. For a given total internal angular momentum l of the system, the function $\varphi(\alpha)$, where $\alpha = \arctan(r/\rho)$ is a hyperrangle, 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 $\varphi(\alpha)$ [25], which leads to the transcendental equation for s [26]:

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

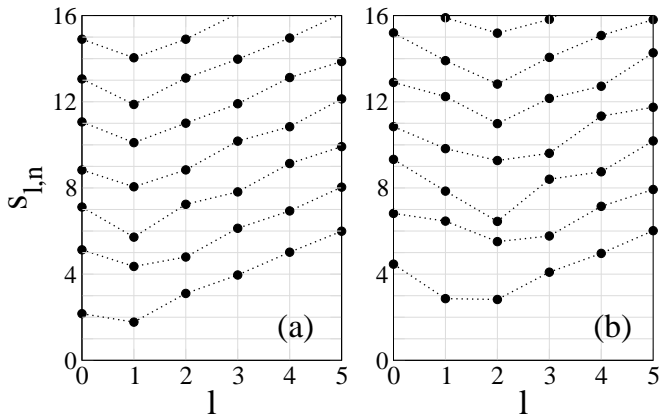


FIG. 1: The constants $s_{l,n}$ for (a) 3 identical fermions and (b) 3 bosons, obtained by numerical solution of the transcendental equation Eq.(7). We have not represented the $s_{l=0,n=0}$ solution for bosons, which is purely imaginary. According to Eq.(10), each real $s_{l,n}$ gives rise to a semi-infinite 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, $s_{l=0,n=0} \simeq i \times 1.00624 \equiv s_0$, the well known Efimov solution. Finally, the function $F(R)$, where the hyperradius is $R = (r^2 + \rho^2)^{1/2}$, solves the problem:

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

where $V(R) = \hbar^2 s^2 / (mR^2) + m\omega^2 R^2 / 4$, s being one of the $s_{l,n}$. This is the Schrödinger equation for a fictive particle of zero angular momentum and mass $m/2$ moving in two dimensions in the potential $V(R)$.

When $s^2 > 0$, the solution for F is

$$F(R) = e^{-R^2/4a_{\text{ho}}^2} R^s L_q^{(s)}(R^2/2a_{\text{ho}}^2) \quad (9)$$

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 [27] and the subsequent embedding of the Hamiltonian in a $SO(2,1)$ algebra [28].

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 [29] and has to be supplemented by a boundary condition for $R \rightarrow 0$:

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

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

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

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

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

We did not yet obtain all the 3-body eigenstates [30]. 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 for fermions and bosons [31]:

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

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

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

Eq.(16) is a consequence of Eq.(17). 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 [32].

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

We now prove that the Efimov effect is absent for 3 fermions. This fact is known but to our knowledge not demonstrated. This is important in practice: if Efimov states would exist, they could be populated in an experiment, thus destroying universality. 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 $Q(l, s^2) \equiv \varphi'(0) - (-1)^l \varphi(\pi/3)$ is non zero, which is incompatible with (6). We rewrite (4) as $\varphi''(\alpha) = U(\alpha)\varphi(\alpha)$, and take the normalization: $\varphi(0) = 1$. From $U(\alpha; l, s^2) = \frac{l(l+1)}{\cos^2 \alpha} - s^2 > 0$, it follows: $\varphi'(0) \leq 0$, 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 intermediary 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 $Q_2 \leq Q_1$. 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 [33]:

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

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

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

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

We now discuss the lifetime of the 3-body universal states found here in the trap, due to 3-body recombination to a deeply bound molecular state. We estimate the loss rate Γ_{loss} as the probability that 3 particles approach each other to distances of the order of the range σ of the interaction potential, times $\hbar/m\sigma^2$ [34]. Using the 3-body wavefunctions obtained above for the zero range model, this gives for a universal state with exponent s :

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

Since $s \geq 1.77$ for fermions and $s \geq 2.82$ for bosons (Fig. 1), the rescaled lifetime $\omega/\Gamma_{\text{loss}}$ of all the universal states tends to infinity when the rescaled range σ/a_{ho} tends to zero. Therefore, the loss rate vanishes in the zero range limit, not only for fermions, but also for universal bosonic states. The Pauli principle is thus not a necessary condition for a reduced loss rate.

What is the experimental relevance of our results? The unitary three-body problem in an isotropic harmonic trap

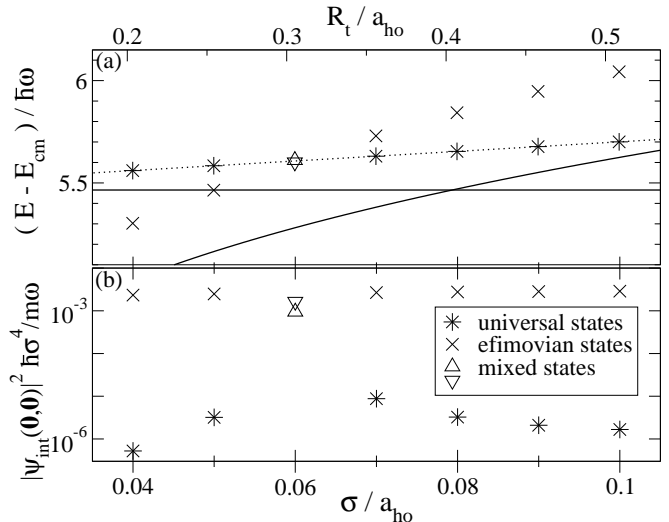


FIG. 2: Numerical solution of the separable potential model: (a) 3-body eigenenergies and (b) estimate of the 3-body loss rate in units of ω [34], as a function of the potential range σ (lower axis) and the 3-body parameter R_t (upper axis). (a) The lowest energy universal branch (stars) has a very weak avoided crossing with an efimovian branch (crosses). The analytical predictions of the zero-range model (solid lines) are in good agreement with the numerics; a linear extrapolation of the stars to $\sigma = 0$ (dotted line) matches the zero-range result. (b) The universal branch has a reduced loss rate except very close to the avoided crossing, where mixed states are formed (triangles).

may be realized by trapping 3 bosons or 3 fermions at a site of a deep optical lattice, and using a Feshbach resonance. A crucial condition is that the interaction potential range is much smaller than a_{ho} . For a broad Feshbach resonance with an effective range of the order of the Van der Waals range, we find that the potential range may be only one order of magnitude smaller than a_{ho} , for an usual lattice spacing of $\sim 0.5 \mu\text{m}$ and a lattice modulation depth of ~ 50 recoil energies. One may then fear that this experimental situation is not in the asymptotic regime of a zero range potential. 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); for a finite range, one expects a mixing between universal and efimovian states, leading to avoided crossings and a reduced lifetime for the universal states.

We therefore solve a finite interaction range model, the Gaussian separable potential of range σ [20], 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, as will be detailed elsewhere. 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 linear

extrapolation of the universal branch to the $\sigma = 0$ limit reproduces the analytical zero-range result at the 10^{-3} level. The zero-range prediction for the efimovian branch is also in acceptable agreement with the separable potential [35]. The avoided crossing between the two branches is hardly visible, which reveals that the coupling due to the finite range is weak. To estimate the 3-body loss rate, we calculate the quantity $|\psi_{\text{int}}(\mathbf{0}, \mathbf{0})|^2 \hbar \sigma^4 / m$, with $\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \psi_{\text{cm}}(\mathbf{C}) \psi_{\text{int}}(\mathbf{r}, \boldsymbol{\rho})$ and ψ_{int} normalized to unity [34]. Fig.2b shows that there is indeed a very long lifetime on the universal branch, as compared to the efimovian one, except very close to the avoided crossing.

Finally, we propose the following experimental sequence: 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 0.174..., a value dominated by the contribution (0.105...) of the lowest $l = 0$ universal state.

In summary, we have obtained the complete analytical solution of the unitary three-body problem in a trap. For bosons, there are both efimovian and universal states, while for fermions we proved that all states are universal. All universal states are stable in the zero-range limit with respect to three-body losses, not only for fermions, but also for bosons. From the numerical solution of a finite range model, we conclude that the bosonic universal states are indeed long-lived and observable in present experimental state of the art.

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[33] For (18) we used $\partial_{s^2} \varphi'(0) = \int_0^{\pi/2} \varphi^2(\alpha)$ where φ solves (4,5) with the normalization $\varphi(0) = 1$.
[34] This quantity is expected to be proportional to the true loss rate within a numerical factor depending on short-range details of the interaction. See also: D. S. Petrov, C. Salomon, and G. V. Shlyapnikov, *Phys. Rev. Lett.* **93**, 090404 (2004); E. Nielsen, H. Suno, and B. D. Esry, *Phys. Rev. A* **66**, 012705 (2002).
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