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A unitary quantum gas in a harmonic trap: exact mapping to free space zero energy eigenstates and application to the three-body problem

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For a gas of particles interacting with a zero range potential of infinite scattering length, we show that the N -body eigenstates in an isotropic harmonic trap can be exactly expressed in terms of the zero energy untrapped eigenstates. This reduces the trapped case to the free space one. As first applications of this mapping, we calculate moments of the trapping potential energy, and the exact spectrum and eigenstates for three trapped identical particles.

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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 infinite scattering length [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]. This makes the unitary Fermi gas the most fundamental of all the quantum gases, and its understanding is crucial for several many-body systems, including neutron stars [11]. In contrast, the trapped unitary Bose gas can form Efimov-like states [13, 14] which are not universal. It also supports universal states, as shown explicitly for three particles [15]. These universal states have not been observed yet, which makes the unitary Bose gas a very open subject.

Very few N -body analytical results have been obtained for the trapped unitary quantum gas. Recently an exact scaling solution was found in a time dependent isotropic harmonic trap [16]. Here we derive another remarkable property of the universal states of fermions or bosons in an isotropic harmonic trap: there exists an exact mapping between universal N -body eigenstates in the trap and zero-energy N -body eigenstates in free space. We present first applications of this mapping: exact expressions for the universal eigenstates of the 3-body problem for bosons (generalizing to a non-zero angular momentum the calculation of [15]) and for identical fermions in a trap; mean value and variance of the trapping potential energy of a unitary quantum gas.

Assuming that the effective range and the true range of the interaction potential are negligible as compared to the de Broglie wavelength of the N particles of the gas, we replace the interaction potential by the Bethe-Peierls contact conditions: there exists a function A such that

$$\psi(\mathbf{r}_1, \dots, \mathbf{r}_N) = \left(\frac{1}{r_{ij}} - \frac{1}{a} \right) A(\mathbf{R}_{ij}, \{\mathbf{r}_k, k \neq i, j\}) + O(r_{ij}) \quad (1)$$

in the limit $r_{ij} \rightarrow 0$ taken for fixed positions of the other

particles 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 many-body wavefunction ψ obeys Schrödinger's equation $H\psi = E\psi$ with

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

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

Consider a zero energy eigenstate of N particles in free space, that is a wavefunction ψ^0 such that $\sum_i \Delta_{\mathbf{r}_i} \psi^0 = 0$ and the contact conditions are satisfied. Since both the free space Hamiltonian and the contact conditions introduce no privileged length scale at zero energy, we take ψ^0 as being invariant under a spatial rescaling [17]:

$$\psi^0(\lambda \mathbf{r}_1, \dots, \lambda \mathbf{r}_N) = \lambda^\nu \psi^0(\mathbf{r}_1, \dots, \mathbf{r}_N). \quad (3)$$

By deriving this relation with respect to λ for $\lambda = 1$:

$$\sum_{i=1}^N \mathbf{r}_i \cdot \partial_{\mathbf{r}_i} \psi^0(\mathbf{r}_1, \dots, \mathbf{r}_N) = \nu \psi^0(\mathbf{r}_1, \dots, \mathbf{r}_N). \quad (4)$$

We now multiply the free space solution by a Gaussian:

$$\psi(\mathbf{r}_1, \dots, \mathbf{r}_N) = e^{-\sum_i r_i^2 m \omega / (2\hbar)} \psi^0(\mathbf{r}_1, \dots, \mathbf{r}_N). \quad (5)$$

This wavefunction satisfies the contact conditions in the unitary limit (since $r_i^2 + r_j^2 = 2R_{ij}^2 + r_{ij}^2/2$, the Gaussian factor varies quadratically with r_{ij}). By direct insertion in Schrödinger's equation, one concludes that ψ is an eigenstate of the trapped gas with energy [18]:

$$E = \left(\nu + \frac{3N}{2} \right) \hbar \omega. \quad (6)$$

We will now obtain all the *other* eigenstates in the trap. To this end, we use the coordinates: $\mathbf{C} = \sum_i \mathbf{r}_i / N$ the position of the center of mass (CM);

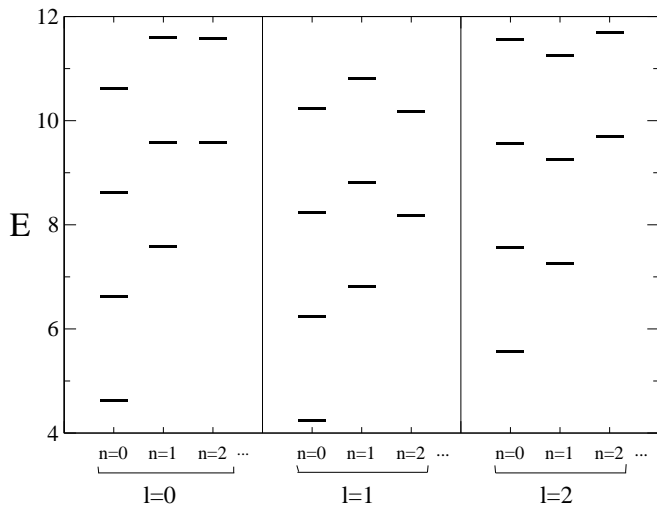


FIG. 1: The universal spectrum of the trapped unitary gas is formed of ladders with energy steps $2\hbar\omega$: $E_{\nu,q} = (\nu + 3N/2 + 2q)\hbar\omega$. The values of ν are known for $N = 3$ particles, which gives the above spectrum for 3 trapped fermions (in units of $\hbar\omega$). l is the total angular momentum of the system.

$R = \sqrt{\sum_i (\mathbf{r}_i - \mathbf{C})^2}$ the hyperradius; and $\mathbf{\Omega} = ((\mathbf{r}_1 - \mathbf{C})/R, \dots, (\mathbf{r}_N - \mathbf{C})/R)$ the hyperangles. The free space zero energy states then take the form:

$$\psi_{\nu_i}^0(R, \mathbf{\Omega}) = R^{\nu_i} \phi_{\nu_i}(\mathbf{\Omega}). \quad (7)$$

Applying the previous mapping (5) gives the following eigenstates of the trapped gas:

$$\psi_{\nu_i,0}(R, \mathbf{\Omega}, \mathbf{C}) = e^{-(NC^2 + R^2)m\omega/2\hbar} R^{\nu_i} \phi_{\nu_i}(\mathbf{\Omega}). \quad (8)$$

Since the CM is separable in this problem, we can restrict to the states where the CM is in its ground state. We define the following raising and lowering operators:

$$\mathcal{L}_{\pm} = \pm \left(\frac{3N-3}{2} + R \cdot \partial_R \right) + \frac{H}{\hbar\omega} - \frac{3}{2} - \frac{m\omega}{\hbar} R^2. \quad (9)$$

Consider an eigenstate ψ of the trapped gas, with energy E . Then one can show that $\mathcal{L}_{\pm}\psi$ satisfy the contact conditions, and $H(\mathcal{L}_{\pm}\psi) = (E \pm 2\hbar\omega)\mathcal{L}_{\pm}\psi$. Therefore, the spectrum is formed of semi-infinite ladders, each ladder having energy steps exactly equal to $2\hbar\omega$ [19]. For an example, see Fig.1. This property is a consequence of the scaling solution for the trapped unitary quantum gas [16] and of the subsequent embedding of the Hamiltonian H in a $SO(2,1)$ algebra [20].

Each of the eigenstates $\psi_{\nu_i,0}$ that we have obtained by the previous mapping is actually at the bottom of a ladder. Indeed, expression (8) implies that $\mathcal{L}_-(\psi_{\nu_i,0}) = 0$. One can even show that we have obtained *all* the states which are at the bottom of a ladder [21]. All the universal eigenstates of the trapped gas (with the CM in the ground state) can therefore be obtained from the

free space, zero energy, scale invariant states by multiplication by a Gaussian (5) and repeated action of the operator \mathcal{L}_+ . The resulting spectrum is:

$$E_{\nu_i,q} = \left(\nu_i + \frac{3N}{2} + 2q \right) \hbar\omega \quad (10)$$

with q non-negative integer, and the wavefunctions:

$$\begin{aligned} \psi_{\nu_i,q}(R, \mathbf{\Omega}, \mathbf{C}) &= e^{-R^2 m\omega/2\hbar} R^{\nu_i} L_q^{(\nu_i + \frac{3N-5}{2})} \left(R^2 \frac{m\omega}{\hbar} \right) \\ &\times \phi_{\nu_i}(\mathbf{\Omega}) e^{-NC^2 m\omega/2\hbar} \end{aligned} \quad (11)$$

where $L_q^{(\cdot)}$ is the generalized Laguerre polynomial of degree q .

We have thus separated the hyperradius R and the hyperangles $\mathbf{\Omega}$. The hyperangular wavefunctions $\phi_{\nu_i}(\mathbf{\Omega})$ and the exponents ν_i are not known exactly for $N \geq 4$. However, we obtained the hyperradial wavefunction, i.e. the R dependent part of the many-body wavefunction.

As a first application of this result, one can compute the probability distribution of the trapping potential energy $E_{\text{pot}} = m\omega^2 \sum_i r_i^2/2$. At zero temperature the moments as a function of the ground state energy E_0 are:

$$\langle (E_{\text{pot}})^n \rangle = E_0(E_0 + \hbar\omega) \dots (E_0 + (n-1)\hbar\omega) / 2^n. \quad (12)$$

At finite temperature T , the first moment is given by the virial theorem, $\langle E_{\text{pot}} \rangle = \langle H \rangle/2$. For the second moment, a simple expression can also be obtained [22]:

$$\langle (E_{\text{pot}})^2 \rangle = \left[\langle H^2 \rangle + \langle H \rangle \coth \left(\frac{\hbar\omega}{k_B T} \right) \right] / 4. \quad (13)$$

We now turn to the three-body problem, and first consider 3 fermions (particles 1 and 2 with spin \uparrow and 3 with spin \downarrow). Analytical solutions were found in free space by Efimov [13, 23]. In what follows $s \equiv \nu + 2$ and l is the total angular momentum of the 3 particles. For each l , the allowed values of s form an infinite sequence $(s_{l,n})_{n \geq 0}$, which is the set of solutions of a transcendental equation [24]. This equation is readily solved numerically (Fig.2a). Our mapping then gives the spectrum in a trap (Fig.1). Note that the hyperangular wavefunctions $\phi_{\nu}(\mathbf{\Omega})$ are also known [25]. Thus (11) gives the analytical expressions of the 3-body wavefunctions in a trap.

It appears clearly on Fig.2a that $s_{l,n}$ gets close to an integer value $\bar{s}_{l,n}$ as soon as l or n increases, with

$$\bar{s}_{l,n} = l + 1 + 2n \text{ for } l \geq 1, \text{ and } \bar{s}_{l=0,n} = 3 + 2n. \quad (14)$$

To check this analytically, the transcendental equation is not useful. We rather use the fact that $(s_{l,n})$ is the set of solutions to the problem [23]:

$$-\varphi''(\alpha) + \frac{l(l+1)}{\cos^2 \alpha} \varphi(\alpha) = s^2 \varphi(\alpha) \quad (15)$$

$$\varphi(\pi/2) = 0 \quad (16)$$

$$\varphi'(0) - (-1)^l \frac{4}{\sqrt{3}} \varphi(\pi/3) = 0. \quad (17)$$

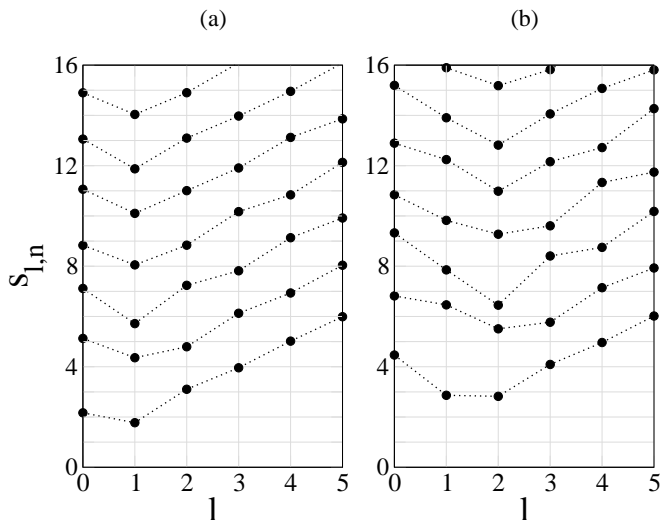


FIG. 2: The exponents $s_{l,n} = \nu_{l,n} - 2$ for (a) 3 identical fermions and (b) 3 bosons, obtained by numerical solution of a transcendental equation. Each exponent generates a ladder in the spectrum. Note that the ground state has an angular momentum $l = 1$ for fermions and $l = 2$ for bosons.

Using semi-classical WKB techniques, we obtained [26]:

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

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

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

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

What happens for three bosons? The results are similar, except that the boundary condition (17) on φ is changed to $\varphi'(0) + (-1)^l \frac{8}{\sqrt{3}} \varphi(\pi/3) = 0$. Now, there exists an *imaginary* solution $s_{l=0,n=0}$. This gives rise to non-universal states, such as the free-space Efimov bound states [13]. However, all the other solutions are real (Fig.2b). In free space, they do not give rise to bound states, and thus they were of little interest for nuclear physics. But in a trap, each real $s_{l,n}$ generates a ladder of universal bosonic states. The lowest universal state energy is $E_0 \simeq 5.32 \hbar\omega$. This is above the non-interacting ground-state, contrarily to the fermionic case.

We now check that the Efimov effect is absent for 3 fermions. This is important to know: 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 (15,16,17). Let us assume that $s^2 \leq l(l+1)$, and that (15,16) 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 (17). We rewrite

(15) 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 $s_{n=0,l=0} \simeq i \times 1.00624$.

We did not yet obtain all the universal three-body states [27]. Indeed, all the above states satisfy the contact condition (1) with a *non-zero* function A . There are also wavefunctions of the unitary gas which *vanish* when two particles are at the same point; these are also eigenstates of the ideal gas. An example in free space is:

$$\psi^0(\mathbf{r}_1, \dots, \mathbf{r}_N) = \prod_{1 \leq n < m \leq N} [(x_n + iy_n) - (x_m + iy_m)]$$

for fermions, and the square of this expression for bosons. Applying the mapping (5) then gives the Laughlin state of the Fractional Quantum Hall Effect for fermions and bosons [28]. In the limit of high energies $E \gg \hbar\omega$ for fixed N , there are actually many of these $A \equiv 0$ states: their density of states (DOS) is almost as high as the DOS of the ideal gas:

$$\frac{\rho_{A \equiv 0}(E)}{\rho_{\text{ideal}}(E)} \underset{E \rightarrow \infty}{=} 1 - O\left(\left(\frac{\hbar\omega}{E}\right)^2\right). \quad (21)$$

In contrast, the DOS of the $A \neq 0$ states for $N = 3$ is

$$\frac{\rho_{A \neq 0}(E)}{\rho_{\text{ideal}}(E)} \underset{E \rightarrow \infty}{=} O\left(\left(\frac{\hbar\omega}{E}\right)^3\right). \quad (22)$$

Equation (22) is a consequence of (14). We found (21) by applying the rank theorem to the operator $\psi(\mathbf{r}_1, \dots, \mathbf{r}_N) \mapsto (\psi(\mathbf{r}_1, \mathbf{r}_1, \mathbf{r}_3, \dots, \mathbf{r}_N), \psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_1, \dots, \mathbf{r}_N), \dots, \psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_{N-1}, \mathbf{r}_{N-1}))$ which associates, to each ideal gas state of energy E , $N(N-1)/2$ functions of $N-1$ variables, and whose kernel is the space of $A \equiv 0$ states of energy E [29].

Finally, we comment on the lifetime of the 3-body universal states found here in the trap. The 3-body recombination process to a deeply bound molecular state clearly depends on the details of the interaction potential, and cannot be obtained exactly from the zero-range model. However, it is argued in [30] that the loss rate is proportional to the probability of finding three particles within a volume of radius on the order of the range b of the interaction potential, times $\hbar/m b^2$. For a universal 3-body state in the trap with an exponent s , this gives

$$\Gamma_{\text{loss}} = K \omega \left(b^2 \frac{m \omega}{\hbar} \right)^s \quad (23)$$

with K a dimensionless quantity depending on short-range details of the interaction. Since $s > 0$ for all universal states (see Fig. 2), their rescaled lifetime $\omega/\Gamma_{\text{loss}}$ tends to infinity when the rescaled range $b\sqrt{m\omega}/\hbar$ tends to zero.

Therefore, the loss rate is small not only for fermions, but also for universal bosonic states. The Pauli principle is thus not a necessary condition for a reduced loss rate. Experiments with bosonic gases at a Feshbach resonance suffer from high loss rates [31, 32, 33, 34]. This indicates that they populate non-universal states.

In summary, we have shown an exact relation between the many-body wavefunctions of the unitary trapped gas and the solutions in free space at zero energy. For three particles, the free space problem is known, which leads to a complete analytical solution of the problem in a trap. We also proved the absence of Efimov phenomenon for 3 identical fermions. Finally we showed that universal states are stable with respect to three-body losses for *both* 3 fermions and 3 bosons. This long lifetime, as well as our result for 3-body spectra and wavefunctions, could be checked experimentally by trapping 3 bosons or 3 fermions at a site of a deep optical lattice [35, 36].

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[18] This shows that one has to exclude the states with a complex ν from the model, such as the Efimov states, if one wishes to preserve its hermiticity. Extra contact conditions are required to deal with Efimov states [13].
[19] Why *semi*-infinite? If the repeated action of \mathcal{L}_- would never lead to zero, the spectrum of H would not be bounded from below. This would violate the hermiticity of the Hamiltonian, since the virial theorem for the harmonical trapped unitary quantum gas (derived by F. Chevy, private communication) implies $E \geq 0$.
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[22] We used the fact the Laguerre polynomials obey: $(q+1)L_{q+1}^{(\alpha)}(x) - (2q+1+\alpha-x)L_q^{(\alpha)}(x) + (q+\alpha)L_{q-1}^{(\alpha)}(x) = 0$
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[24] If one sets $(x)_n \equiv x(x+1)\dots(x+n-1)$, s obeys

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

where $-$ is for fermions, $+$ is for bosons. The integer solutions must be eliminated ($l=0, s=2$ for fermions; $l=0, s=4$ and $l=1, s=3$ for bosons).

[25] The hyperangular three-body wavefunctions are:

$$\phi_\nu(\mathbf{\Omega}) = \begin{cases} (1 - P_{12}) \chi(\mathbf{\Omega}) & \text{for fermions} \\ (1 + P_{12} + P_{23}) \chi(\mathbf{\Omega}) & \text{for bosons} \end{cases}$$

where $\chi(\mathbf{\Omega}) = \varphi(\alpha)(\sin 2\alpha)^{-1} Y_l^m(\boldsymbol{\rho}/\rho)$, P_{ij} transposes particles i and j , $\boldsymbol{\rho} = (\mathbf{r}_1 + \mathbf{r}_3 - 2\mathbf{r}_2)/\sqrt{3}$, $\alpha = \arctan(r_{13}/\rho)$, and

$$\varphi(\alpha) = \text{Im} \left[i^l \sum_{k=0}^l \frac{(-l)_k (l+1)_k}{k! 2^k} (1+i \tan \alpha)^k \frac{(1-s)_l}{(1-s)_k} e^{is(\frac{\pi}{2}-\alpha)} \right].$$

[26] For (18) we used $\partial_{s^2} \varphi'(0) = \int_0^{\pi/2} \varphi^2(\alpha)$ where φ solves (15,16) with the normalization $\varphi(0) = 1$.
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