Emergent four-body parameter in universal two-species bosonic systems

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Abstract
The description of unitary few-boson systems is conceptually simple: only one parameter – the three-body binding energy – is required to predict the binding energies of clusters with an arbitrary number of bosons. Whether this correlation between the three- and many-boson systems still holds for two species of bosons for which only the inter-species interaction is resonant depends on how many particles of each species are in the system. For few-body clusters with species $A$ and $B$ and a resonant $AB$ interaction, it is known that the emergent $AAB$ and $ABB$ three-body scales are correlated to the ground-state binding energies of the $AAAB$ and $ABBB$ systems, respectively. We find that this link between three and four bodies is broken for the $AABB$ tetramer whose binding energy is neither constrained by the $AAB$ nor by the $ABB$ trimer. From this de-correlation, we predict the existence of a scale unique to the $AABB$ tetramer. In our explanation of this phenomenon, we understand the $AABB$ and $AAAB/ABBB$ tetraters as representatives of two different universal classes of $N$-body systems with distinct renormalization-group and discrete-scaling properties.
1. Introduction

When a two-boson system is resonant, i.e., its scattering length is considerably larger than the interaction range, its behavior becomes independent of interaction details; in this sense, it is universal. Numerous instances of such systems are found in atomic, nuclear, and particle physics [6]. Resonant three-boson systems are even more intriguing as they display a characteristic geometric bound-state spectrum. This sequence of states was originally predicted by Efimov in the seventies [7] and observed experimentally decades later with $^{133}$Cs trimers [14]. The geometric factor between successive excited states in this spectrum is universal and equal to $(22.7)^2$, while the ground-state binding energy ($B_3$) remains sensitive to short-distance details of the interaction [3, 4] and becomes a parameter of the theory. If $B_3$ is known, the binding energies of larger clusters can be predicted. For the four-, five-, and six-boson systems at unitarity, the relations $B_4 \sim 4.7 B_3$, $B_5 \sim 10.1 B_3$, and $B_6 \sim 16.3 B_3$, respectively, were found numerically [19, 20, 21, 22].

The occurrence of the Efimov spectrum is not exclusive to systems composed of identical bosons. Three-body systems with two species $A$ and $B$, i.e., $AAB$ and $ABB$ (also referred to as Tango configurations [28]), in which the two identical particles are bosons, do have a geometric spectrum, too, even if only the $AB$ interaction is resonant. This was experimentally observed for the first time with $^{87}$Rb and $^{41}$K trimers [1]. If the masses of species $A$ and $B$ are equal, the geometric factor is $(1986.1)^2$ (see e.g. [15]). If the odd particle is lighter (heavier) than the other two this factor is reduced (increased). For $^6$Li and $^{133}$Cs, for example, the theoretical prediction of a factor of $(4.9)^2$ for the Li Cs Cs trimer spectrum has been confirmed experimentally [18].

At this point, it is natural to wonder what happens with larger clusters composed of two species $A$ and $B$. From the experience with bosonic systems, the naive expectation is that the ground-state energy of the two-species few-body clusters is proportional to that of the trimer. And indeed, this is the case for $AAAB$ clusters [27, 5] (or $ABBB$ clusters, depending on the statistics of species $A$ and $B$).

In this manuscript, we investigate the $AABB$ system, and find that its ground-state binding energy cannot be predicted solely from the $AAB$ or $ABB$ three-body parameters and a unitary $AB$ system. This behavior was already foreshadowed in the independent $AABB$ and $AAB/ABB$ limit cycles in the Born-Oppenheimer $m(A) \ll m(B)$ limit [17], and our study establishes...
this decorrelation between three and four-body systems for equal masses.

Furthermore, by treating the $ABBB$ and $AABB$ systems as representatives of generic classes of $N$-particle systems in which only a certain subset of pairs interacts resonantly with a contact $S$-wave potential (all the other two-body pairs are non-interacting), we gain a more general understanding of correlations amongst multi-species few-body clusters. Our description has the advantage of arranging the different two-species systems in two defined categories (which we call circle and dandelion) independently of their physical realizations. Based on numerical results, we conjecture that there is only one finite scale associated with each of these categories.

2. Theoretical framework:

We will first give a definition of the categories and later relate them to the specific two-species bosonic systems. We introduce the two classes (fig.1) for distinguishable particles (the nodes) in which only a specific subset of interactions is resonant (the dashed lines). In the first class – the $N$-circle – each of the $N$ nodes/particles interacts resonantly with exactly two neighbors. In the second class – the $N$-dandelion – a central particle interacts with all remaining $(N - 1)$ particles that do not interact amongst each other.

The quantum-mechanical nonrelativistic dynamics of these graphs obey the $N$-body Schrödinger equation

$$ (H_0 + V) |1, 2, \ldots, N\rangle = E_N |1, 2, \ldots, N\rangle , $$

with an equal-mass kinetic term $H_0$ acting on a state with energy $E_N$ (for bound state solutions, $-B_N := E_N < 0$). The shape of the graph is encoded in the potential $V$, which specifies the subset of all the $N(N - 1)/2$ interaction pairs $(i,j)$ that are resonant. In particular, the potentials defining the $N$-circle and $N$-dandelion are

$$ V^{N\text{-circle}} = \sum_{i=1}^{N} V(i, (i \mod N) + 1) , $$

$$ V^{N\text{-dandelion}} = \sum_{i=1}^{N-1} V(i, N) . $$

For the resonant interaction between equal-mass particles, we use a contact
Figure 1: Interaction graphs of two classes of $N$-body systems: the $N$-circle and the $N$-dandelion. Gray nodes represent particles and dashed lines/edges interactions between the connected particles.
potential regularized with a Gaussian cut-off function:

\[ V_2(\mathbf{r}; R_c) = C(R_c) \delta^{(3)}(\mathbf{r}; R_c), \]

\[ \delta^{(3)}(\mathbf{r}; R_c) = \frac{e^{-(r/R_c)^2}}{\pi^{3/2} R_c^3}, \]

which is the leading-order of an effective field theory for systems with large scattering length [12]. In order to prevent the three-body collapse (i.e. \( B_3 \to \infty \) when \( R_c \to 0 \) [24]), we introduce a zero-range three-body potential [3] adopting the regulator prescription from the pair interaction:

\[ V_3(\mathbf{r}_{123}; R_c) = D(R_c) \sum_{\text{cyc}} \delta^{(3)}(\mathbf{r}_{12}; R_c) \delta^{(3)}(\mathbf{r}_{23}; R_c). \]

Numerically, we realize the zero-range limit with \( R_c \in [0.01, 1] \) for dandelions and \( R_c \in [0.1, 10] \) for circles. At the lower end of these ranges the binding energies show relatively little dependence on \( R_c \). In order to approximate a zero-range interaction we choose the minimum value of the cut-off as to be much smaller than any other length scale in the systems we study (yet it cannot be reduced much further without impairing the numerical stability of the calculations). The two-body coupling strength \( C(R_c) \) was calibrated via the Numerov algorithm to approximate a unitary scattering length \( |1/a_0| < 10^{-5} \). In addition to \( \hbar = c = 1 \), we set \( m = 1 \). We chose a single three-body scale for the 3-circle and the 3-dandelion, namely the ground-state binding energy \( B_3 = 0.01 \) \( (1/a_0 \ll B_3 \ll m) \). Accordingly, we renormalized the strength of \( D(R_c) \) in both systems to reproduce this value of \( B_3 \). This results in two sets of three-body couplings \( D(R_c) \) representing a repulsive potential, where we note that setting the 3-circle energy to 0.01 demands a stronger repulsion than fixing the 3-dandelion’s ground state to 0.01.

The two interaction classes can be realized as two-species bosonic clusters in which only the inter-species interactions are resonant. Stated explicitly, the \( ABB \) and \( ABBB \) ground states are 3- and 4-dandelions, respectively, while the \( AABB \) cluster is a 4-circle (see fig. 1 and fig. 2). The 3-circle is
equivalent to the standard three-boson system at unitarity \(^1\) but it is no subsystem of the two-species clusters considered here. We advance this is why \(AABB\) exhibits its own characteristic four-body scale.

This equivalence is explained by noting that the ground state and the potential have the same symmetries, \(i.e.,\) cyclic permutations for the circle and permutations of the \((N - 1)\) non-interacting particles for the \(N\)-dandelion. This implies that these particles effectively behave as indistinguishable, though in principle not necessarily as bosons. Yet, the contact interactions (5) and (6) enforce bosonic behavior for the \(N = 3, 4\) circles and the \(N = 3, 4, 5\) dandelions. In the \(R_c \to 0\) limit, these interactions are only non-vanishing in relative \(S\)-wave configurations between interacting pairs, which requires them to behave as bosons. If the non-interacting pairs are antisymmetric, this will force the interacting pairs to be antisymmetric too \(^2\), resulting in a vanishing contribution from the contact-range interaction. As a consequence, provided

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\(^1\)In our notation, the 3-circle would be equivalent to the \(AAA\) system if same-species interactions were non-zero. If the latter were resonant too, the \(AAA\) (\(i.e.,\) 3-circle) system would exhibit the Efimov effect \(^7\). If we follow the convention used in this work of setting same-species interactions to zero, the 3-circle will be equivalent to an \(ABC\) system, with \(B, C\) representing different particle species (while the \(AAA\) system would be a free system). This system (\(i.e.,\) three distinguishable particles in the unitary limit) shows the same type of geometric Efimov spectrum as the standard three boson system \(^15\).

\(^2\)This follows from permutation algebra: labeling the particles according to species (\(A\) or \(B\) in fig. 2), any permutation involving \(AA\) or \(BB\) pairs must be expressed as the product of an odd number of permutations involving \(AB\) pairs. Sign consistency of permutations acting on the wave function thus requires the sign of \(AA/BB\) and \(AB\) exchanges to be the same.
that the interaction is of a contact-range type, all pairs behave symmetrically under pair permutations in the ground state. This is the reason why our calculations employ states with distinguishable particles. This choice allows us to avoid the explicit (and unnecessary) symmetrization of the numerical wave function, thus reducing the number of components to be computed. This in turn makes the computation of larger cut-off-radii ensembles feasible. However, we were careful to verify the equivalence numerically for selected three- and four-body cases.

All three- and four-body results obtained for this work employ the stochastic variational method [23] and were benchmarked for a sample set of three- and four-body predictions with the refined-resonating-group method [11]. Within this numerical framework, we calculate ground-state energies of three-, four-, and five-body representatives of the circle and dandelion. The convergence of these energies to a finite value indicates the renormalizability of the theory for the respective systems. The collapse of the ground states, \( B_N \to \infty \) for \( R_c \to 0 \), is, in turn, the signature of an emergent new scale.

3. Results:

We begin our analysis recovering the expected collapse associated with the original Efimov spectrum. Specifically, we demonstrate that in the absence of a three-body repulsion all considered systems collapse as \( B_N \propto 1/R_c^2 \) (see fig. 3). Then, we analyze the renormalizability of the \( N = 4, 5 \) dandelion and circle with a contact two-body resonant interaction and a contact three-body repulsion that stabilizes the respective trimers. In the large cut-off limit, we find the energy of these systems stable against variations of the cut-off and approximately \( B_4^{\text{dand}}/B_3^{\text{dand}} \approx 11 \) and \( B_4^{\text{circ}}/B_3^{\text{circ}} \approx 0.2 \) for the four-body dandelion and circle respectively, and \( B_5^{\text{dand}}/B_3^{\text{dand}} \approx 30 \) and \( B_5^{\text{circ}}/B_3^{\text{circ}} \approx 0.06 \) for the five-body dandelion and circle. The cut-off dependence of these ratios is shown in fig. 4 and fig. 5.

The 4- and 5-dandelion binding energies are large when compared to that of the 3-dandelion, but the reason why this is the case remains elusive. For circular systems, the absolute binding energy decreases with each additional

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3Specifically, we benchmarked the 3- and 4-circle systems at \( R_c = 0.25 \) and the 3- and 4-dandelions at \( R_c = 0.1 \). Furthermore, the 4-circle was tested for \( 0.17 < R_c < 2 \).
Figure 3: Cut-off dependence of ground-state binding energies ($B_N$) for trimer, tetramer, and pentamers with an interaction given by resonant two-body potentials which realize circular and dandelion systems. Results are obtained without a three-body counterterm. In showing $B_N R_c^2$, the divergent behavior of the binding energy is highlighted.

particle on the circle. Whether the binding energy of the circle converges to zero with the number of particles going to infinity remains an open question. Nevertheless, the circles are particle-stable because no $(N + 1)$-body circle can decay into an $N$-body circle. Although not obvious, we find the closest decay threshold to be the complete disintegration of the systems.

Next, we assess whether the three-body force that renormalizes the 3-dandelion suffices to renormalize the 4- and 5-circle too. The binding energy of the dandelion-regularized circle shows no sign of convergence to a particular value. However, its increase with the cut-off is less steep relative to the case without three-body repulsion (see fig. 5). The collapse was tested up to a cut-off of 100 (in units of mass), and although we cannot numerically exclude a stabilization at some even larger cut-off, we deem such behavior unlikely for two reasons: first, the extremely large binding of these systems
for the considered range of cut-offs suggests that any hypothetical finite limit has a highly unnatural energy which, \textit{a priori}, is not justified by any physical reason. Second, the fact that the circle is correctly renormalized via the repulsion set by the 3-circle means that it cannot be simultaneously renormalized by the repulsion that stabilizes the 3-dandelion. The discrete scaling factors of the 3-dandelion and 3-circle are \textit{de facto} different, being respectively 1986.1 and 22.7 for equal mass systems [15]. These results indicate that, in the unitary limit, the dandelion and circle categories represent two different types of universal behavior.

It is helpful to consider the consequences for two-species three-boson systems (either AAB or ABB) to which one additional boson is added. For an inter-species two-body potential at resonance, the AAB/ABB mixtures – the dandelions – exhibit bound states which are tied to those of the AAB/ABB three-boson spectrum. The AABB system, in contrast, is not renormalized by the same three-body repulsion. It obtains its renor-
Figure 5: Convergent behavior of the 3-, 4- and 5-dandelion ground-state binding energies with appropriately renormalized three-body repulsion (cf. fig. 3 for unrenormalized results).

The experimental verification of our theoretical results is complicated by
Figure 6: Divergent behavior of the 3-, 4- and 5-circle ground-state binding energies with a three-body repulsion inconsistently renormalized to a 3-dandelion (cf. fig. 5 for the results based on the properly running counter term).

the fact that most physical AABB systems have mass imbalances. The heteronuclear $^{85}$Rb-$^{87}$Rb system (both bosons), for which a Feshbach resonance has been observed [16], might be an exception. It is relatively close to the equal-mass limit and might enable (albeit experimentally challenging) a measurement of $B_{4}^{AABB}/B_{3}^{AAB}$ and $B_{4}^{AABB}/B_{3}^{AAB}$ ratios. To make a comparison we would need a second system with similar features, but no such system is known experimentally. Hence the identification of an independent four-body scale remains elusive. Yet, for multi-species systems with similar mass imbalances, such as $^{41}$K-$^{87}$Rb [126], $^{87}$Rb-$^{133}$Cs [13] and $^{23}$Na-$^{39}$K [10] (for which the mass imbalances are 0.47, 0.65, and 0.59, respectively), the comparison of their $B_{4}^{AABB}/B_{3}^{AAB}$ ratios might very well be meaningful. If these ratios are wildly different, it could represent an experimental verification of the existence of a four-body parameter in the AABB system. Another way to realize the equal-mass dandelion and circular systems is provided by Fes-
hbach resonances between atomic hyperfine levels. Our results could then be confirmed if besides $^{87}\text{Rb}$ \cite{24} a second atomic species could be tuned to such a resonance and that the trimer and tetramer energies within the respective condensates are experimentally accessible.

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