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Phys. Rev. Lett. **107**, 200402 — Published 11 November 2011

DOI: 10.1103/PhysRevLett.107.200402

Five- and Six-Body Resonances Tied to an Efimov Trimer

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We explore the properties of weakly bound bosonic states in the strongly interacting regime. Combining a correlated-Gaussian basis set expansion with a complex scaling method, we extract the energies and structural properties of bosonic cluster states with $N \leq 6$ for different two-body potentials. The identification of five- and six-body resonances attached to the first-excited Efimov trimer provides strong support to the premise of Efimov universality in bosonic systems. Our study also reveals a rich structure of bosonic cluster states. Besides the lowest cluster states that behave as bosonic droplets, we identify cluster states weakly bound to one or two atoms forming effective cluster-atom "dimers" and cluster-atom-atom "trimers." The experimental signatures of these cluster states are discussed.

Understanding the universal nature of low-energy few-body physics is a fundamental prerequisite for the development of effective many-body descriptions in the ultracold regime. In two-component Fermi gases, the characterization of two-body physics in terms of a single interaction parameter (the scattering length) is at the heart of our understanding of the BCS-BEC crossover. In bosonic systems, the underlying few-body physics is enriched by the Efimov effect [1, 2] which is currently a subject of intense experimental exploration in ultracold atoms [3–7]. Efimov physics leads to the formation of a series of weakly bound trimers that acquire peculiar properties such as a borromean nature and a discrete scale invariance [2]. While this complexity of three-boson systems has led to a deeper understanding of universal few-body physics, it poses an important question as to whether the low-energy behavior of larger bosonic systems can be understood and characterized within a simple universal framework.

The natural starting point for addressing this question is the exploration of Efimov and universal phenomena in increasingly larger systems. For $N > 3$ systems, a new concept of universality arises in which the low-energy physics is only characterized by the scattering length and Efimov's three-body parameter. In these systems, the exploration of universality in the low-energy regime is significantly more challenging because it requires the study of an unstable part of the spectrum, and therefore the analysis of resonances rather than bound states. Nevertheless, in the last few years, tremendous progress has been achieved in the understanding of universality in four-boson systems [8–12]. Despite these important advances, there still remain controversies regarding the scope of universality, the role of the four-body parameter, and nonuniversal corrections [13–15]. For $N > 4$ systems, the applicability of universal theory is even more debatable because of the lack of theoretical or experimental evidence of universal behavior. However, the natural continuation to the four-body predictions of Refs. [8, 9] would indicate that universality extends to larger clusters whose behavior follows the Efimov discrete scale invariance and is only controlled by two and three-body physics. Thus, for each Efimov state ($N = 3$), there would be a series of $N > 3$ cluster states (or resonances) associated to it, forming an *Efimov family*. A recent study [16] based on such a premise of universality has characterized some properties of the lowest weakly bound cluster states up to $N \leq 13$. While this study provides key predictions to be theoretically and experimentally explored, it leaves open questions such as the validity of the universality hypothesis and the existence of additional weakly bound cluster states.

In this article, we address these questions through the analysis of the structure of the strongly interacting few-boson spectra. Our main result is the identification of five- and six-boson resonances tied to the first excited-Efimov state (see Fig. 1). These resonant states represent small bosonic droplets and are in good qualitative agreement with the prediction of Ref. [16]. Such evidence of cluster states associated with excited-Efimov families provides important first indications of discrete-scale invariance in few-boson systems. Thus, our results provide much-needed support to the premise of Efimov universality in few-boson systems. We extend our analysis to the exploration of different types of cluster states formed in the lowest Efimov family, which is strongly modified by nonuniversal corrections. For a range of model potentials, we find that cluster states ($N = 3, ..., 6$) are likely to bind weakly to atoms forming effective cluster-atom "dimers" and cluster-atom-atom "trimers." We identify one of these cluster-atom-atom "trimers" as a resonance that appears energetically slightly below the lowest Efimov trimer; it can be qualitatively described as an Efimov trimer formed by an Efimov trimer and two atoms. This state is one of the simplest bizarre cluster structures mathematically proposed [17]; similar cluster-atom-atom structures are expected for larger systems. Our studies reveal an intricate structure of bosonic cluster states and provide estimates of the N-body resonant positions relevant to experiments.

Our starting point is the few-boson Hamiltonian,

$$\mathcal{H} = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i<j} V(r_{ij}), \tag{1}$$

where m is the mass of the bosons, and r_{ij} is the interparticle distance between particles i and j. The two-body model potential takes the form $V(r) = V_0(\exp[-r^2/(2r_0^2)] - \alpha\exp[-2r^2/r_0^2])$, where r_0 is the interaction range, and V_0 and α are tuned to change the shape and scattering length of the potential. For simplicity, we focus on the $a < 0$ region with no two-body bound state. To test the model dependence, we consider two qualitatively different potentials: purely attractive ($V_0 < 0$ and $\alpha \leq 1$) and attractive with repulsive core potentials ($V_0 < 0$ and $\alpha > 1$). While the studies considered $-10 < \alpha < 10$, most of the results will be presented for two cases: a purely attractive interaction V_a ($\alpha = 0$) and an attractive potential with a soft repulsive core V_r ($\alpha = 2$ and $V_0 < 0$). The range r_0 and the energy $E_{sr} \equiv \hbar^2/(mr_0^2)$ are the typical energy and length scales that characterize the interactions. The universal regime is characterized by energies $|E| \ll E_{sr}$ and length scales (characterizing scattering length and clusters sizes) of $\ell \gg r_0$.

To describe the bound states, we use a correlated-Gaussian (CG) basis set expansion combined with the stochastical variational method (SVM) [18] that has been very successful in describing ground and excited states of bosonic and fermionic systems with short-range interactions [9, 19]. In our implementation, the eigenstates of a system are expanded in the set of CG basis functions in which the center-of-mass coordinate has been removed and $L^\pi = 0^+$. Each basis function is a symmetrized product of Gaussian functions, each of which depends on one of the $N(N-1)/2$ interparticle distances and can be written as $\psi_\beta(\mathbf{x}) = \exp\left(-\sum_{ij} A^\beta_{i,j} \mathbf{x}_i \cdot \mathbf{x}_j/2\right)$, where $\mathbf{x} = \{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_{N-1}\}$ is a set of (relative) Jacobi coordinates, and the $A^\beta_{i,j}$ are a set of parameters that characterize the Gaussian function widths. The convergence of the results is carefully analyzed by increasing and reoptimizing the basis set. To explore the structure of the few-body states, we extract the pair-distribution function defined as $4\pi r^2 P_N(r) = \langle\Psi_N|\delta(r_{12} - r)|\Psi_N\rangle$, where r_{12} is the interparticle distance between particles 1 and 2, and $|\Psi_N\rangle$ is the fully symmetrized N-body wave function.

To study resonances, which have a finite lifetime associated to the decay onto lower energy states, we use the complex-scaling method (CSM) [20–22]. In the CSM, all coordinates are rotated as $\mathbf{r} \to \mathbf{r}e^{\imath\theta}$ by a transformation $U(\theta)$. The wave function of the resonance is square integrable in these rotated coordinates and can be expanded in the same square-integrable basis functions that describe bound states:

$$\Psi_\theta(\mathbf{x}) \equiv U(\theta)\Psi(\mathbf{x}) = \sum_i C_i(\theta)\psi_i(\mathbf{x}), \qquad (2)$$

where $\mathbf{x} = \{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_{N-1}\}$ is a set of (relative) Jacobi coordinates. The wave function $\Psi_\theta(\mathbf{x})$ is a solution of the rotated Hamiltonian $\mathcal{H}_\theta = U(\theta)\mathcal{H}U(\theta)^{-1}$ with complex energy $E_\theta = E_R - \mathrm{i}\Gamma/2$, where Γ is associated with the width of the resonance.

Universal Droplets.– The analysis of the five and six-body spectra in an energy window close to the first excited Efimov trimer allow us to approach the universal regime. Figure 1 summarizes the energies of these cluster states for $N = 3, ..., 6$. The results are presented as a function of the relevant universal parameters: $1/\kappa a$ and E/E_3^u, where $\kappa = \sqrt{m|E_3^u|/\hbar^2}$ is the three-body parameter, and E_N^u is the energy of the N-body cluster at unitarity ($a = \infty$). The five- and six-body results are obtained from an analysis of reso-

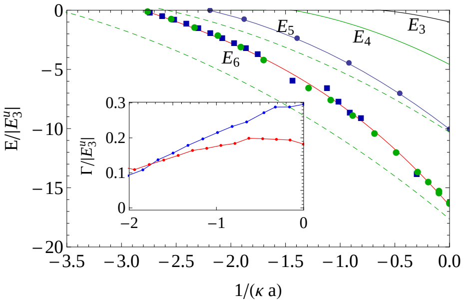

FIG. 1: (color online). Energies of the lowest universal cluster state as a function of inverse scattering length. From top to bottom, the solid curves represent the $N = 3, 4, 5, 6$ energies, respectively. The energies for $N = 3$ and $N = 4$ were obtained in previous studies [9]. Note that, in this figure, the energy of the second $N = 4$ state would lie almost on top of the trimer energy. The $N = 5$ solid curve and symbols correspond to predictions from an excited resonance for V_r and V_a, respectively. The circles and squares are the $N = 6$ predictions for V_r and V_a, respectively, and the solid curve is a guide to the eye. Dashed curves correspond to the $N = 5, 6$ predictions from Ref. [16]. Inset: Width of the five-body resonances for V_r (red) and V_a (blue).

nances attached to the first-excited Efimov family. These resonances are observed for both the V_a and V_r potentials. At unitarity, we obtain $E_5^u \approx 10.1(1)E_3^u$ [23], in close agreement of Ref. [16] predictions of $E_5^u \approx 10.4(2)E_3^u$. For $N = 6$, we find that $E_6^u \approx 16.3(2)E_3^u$, which is slightly smaller in magnitude than the predictions from Ref. [16] of $E_6^u \approx 18.4(2)E_3^u$. Interestingly, the energies of the universal states at unitarity scale roughly with the number of trimer configurations the cluster contains, i.e., 1, 4, 10, 20 for $N = 3$, 4, 5, and 6, respectively. To further verify the model independence of the predictions, we analyze the pair distribution function at unitarity (see Fig. 2). The good agreement between three different predictions of P_5 and P_6 illustrates the universality of such few-body resonances.

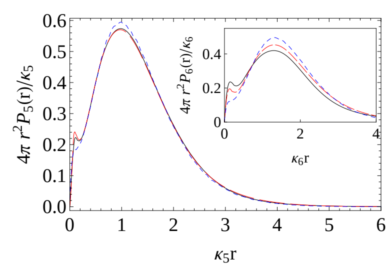

FIG. 2: (color online). Pair distribution function of the universal five-body (main figure) and six-body (inset) states. Here $\kappa_N = \sqrt{m|E_N^u|/\hbar^2}$, where E_N^u is the binding energy of the N-body droplet at unitarity. Solid and long-dashed curves are the prediction from the V_a and V_r potential, while the short-dashed curves are predictions from Ref. [16].

The widths of the four- and five-body resonances depend strongly on the open decay channels. In our calculations, resonances of the first-excited Efimov family can only decay into the lowest Efimov family, i.e., into decay channels that are not in the universal regime. Therefore, we expect the width of the resonance to be more sensitive to nonuniversal corrections. For example, our analysis of the first-excited four-body resonance leads to a $\Gamma^u_{4b} \approx 0.1E^u_3$, which is a factor of three larger than the predicted universal width [12] (similar deviations were reported in the four-body system). The width of the first-excited five-body resonance is presented in Fig. 1 for both V_a and V_r. The clear differences between the different Γ predictions illustrate the importance of the nonuniversal corrections for resonances belonging to the lowest-excited Efimov families. However, as in the four-body case, we expect that the width extracted from the first-excited five-body resonance provides a correct order of magnitude estimate of the widths in the universal limit. We also estimate $\Gamma^u_{6b} \sim 0.3E^u_3$.

The description of these five- and six-body resonances is challenging since it entails an exploration of an energy window that is orders of magnitude smaller than the lowest cluster-atom fragmentation threshold energy. To obtain an accurate representation of these resonances, we carry out a numerical procedure inspired by previous implementations of the SVM+CSM [21, 22]. In the six-body system, the large number of avoided crossings between the resonant state and other states makes it particularly challenging to quantitatively estimate the resonance energy. However, the main source of uncertainty in predicting the universal energies comes from the nonuniversal corrections in the first-excited Efimov family. Comparing with similar studies for $N = 4$, we estimate that the energies and positions of the resonances discussed below are within 10% of their corresponding universal values.

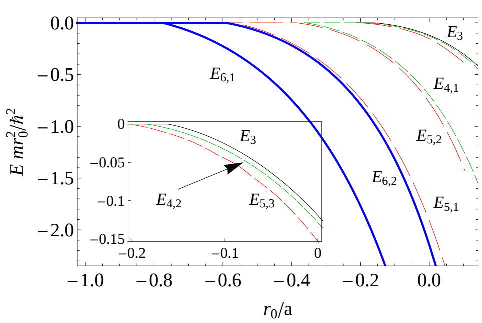

FIG. 3: (color online) Spectrum of the lowest Efimov family as a function scattering length for $3 \leq N \leq 6$. The thin solid curve corresponds to the trimer state energy, the short-dashed curves correspond to the four-body states, the long-dashed curves correspond to the five-body states, and the thick solid curves correspond to the six-body states. Inset: States formed below the trimer threshold.

Excited cluster states and nonuniversal corrections.– Next, we analyze the formation of bound states for $3 < N \leq 6$ in the lowest Efimov family. This study illustrates the structure of the spectrum in the strongly interacting regime by identifying other types of bound states. It also addresses the issue of nonuniversal corrections in the regime $|a| \gtrsim r_0$ that are particularly important for understanding ^{133}Cs and ^{7}Li Efimov experiments in which five- and six-body resonant phenomena are expected to occur at $|a| \lesssim 3r_{vdw}$, where r_{vdw} is the Van der Waals length. The general structure of the bosonic spectrum is shown in Fig. 3. These results correspond to the potential V_a. This structure, although it changes quantitatively, remains qualitatively the same for a range of model potentials. The lowest N-body state is analogous to the universal states shown in Fig. 1. However, the energy of the lowest N-body states grows very fast with the number of particles, implying that nonuniversal corrections increase with N (in agreement with Ref. [14]). For example, the energy per particle of the lowest trimer state of V_a at unitarity is $\sim 0.04E_{sr}$, while the energy per particle of the lowest six-body state at unitarity is $\sim 0.6E_{sr}$. The latter result implies that $E^u_6/E^u_3 \sim 30$, almost a factor of two larger than the universal predictions. The introduction of a repulsive three-body force, as proposed in Ref. [16], leads to a ratio of $E^u_6/E^u_3 \sim 18$, which is significantly closer to the universal predictions.

The increasing importance of nonuniversal corrections as N increases is also reflected in the pair distribution functions presented in Fig. 4. As N increases, the lowest cluster states become more localized in the nonuniversal region ($r \lesssim r_0$) and, therefore, become less universal. The single peak structure of the pair distribution indicates that these states are basically droplets that are mainly described by configurations in which all particles are at similar distances.

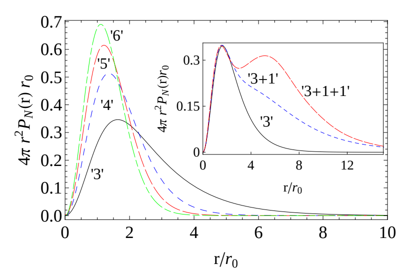

FIG. 4: (color online) Pair distribution functions of the lowest N-body cluster states ($N = 3, ..., 6$) at unitarity. Inset: Distribution functions for the trimer ('3'), the trimer-atom four-body state ('3+1'), and the trimer-atom-atom five-body state ('3+1+1').

The excited states (with energies $E_{4,2}$, $E_{5,2}$, and $E_{6,2}$) are much closer to the lowest fragmentation threshold and can be qualitatively described as cluster-atom "dimers" with one particle loosely bound to an $N - 1$ cluster state. This structure can also be identified in the pair correlations that coincide at small r with the $N - 1$ cluster pair correlation, but it has a longer tail that describes the cluster-atom correlation (cf. the inset in Fig. 4).

We also identify another five-body resonance, presented in Fig. 3 as $E_{5,3}$, that is a state energetically below the lowest trimer-atom-atom fragmentation threshold that can decay into the lowest tetramer-atom channel. The energy and the pair-distribution function show that the state is qualitatively described as a trimer weakly bound to two atoms, forming a trimer-atom-atom state. The energies at unitarity of such states are $1.3E_3^u$ (V_a) or $1.2E_3^u$ (V_r), i.e., slightly below the trimer and the second tetramer energies, suggesting that most of the contribution of the energy comes from the bonding of the trimer subcluster. Furthermore, the pair-distribution function shows two clear peaks that can be identified as coming from atom-atom correlations inside the trimer subcluster and atom-atom correlations between an atom inside the trimer and an atom outside the trimer.

These states can be experimentally observed in ultracold gases through the analysis of N-body recombination processes [24]. Current experiments have identified three- and four-body resonances through the observation of losses at the predicted resonance positions [3–7]. At low temperatures, the N-body resonant enhancement of losses occurs at the critical interaction strengths at which an N-body cluster becomes resonant with the free particle-scattering continuum. If the N-body clusters behave universally, the positions of the resonances are given by critical scattering lengths a_N^* that are only controlled by the three-body parameter; the ratio between any two a_N^* is a universal number. We estimate nonuniversal corrections to these scattering-length ratios by analyzing the lowest Efimov family. In a range of model interactions, we find that $0.45 \lesssim a_4^*/a_3^* \lesssim 0.47$ and $0.63 \lesssim a_5^*/a_4^* \lesssim 0.67$. The description of the six-body state is more challenging, and we estimate $a_6^*/a_5^* \sim 0.73 - 0.74$ in a reduced set of model potentials. The four-body predictions are relatively close to the universal prediction of $a_4^*/a_3^* \approx 0.43$, and their deviations are comparable to those observed in experiments (which also analyze the first Efimov family). The five- and six-body scattering-length ratios are in the same ballpark of Ref. [25] predictions ($a_5^*/a_4^* \approx 0.69$ and $a_6^*/a_5^* \approx 0.78$) and of Ref. [16] ($a_5^*/a_4^* \approx 0.6$ and $a_6^*/a_5^* \approx 0.7$) based on different model interactions. From the analysis of the five and six-body resonances in the first excited Efimov family, we estimate universal scattering-length ratios of $a_5^*/a_4^* \approx 0.66$, and $a_6^*/a_5^* \approx 0.78$.

In conclusion, we have investigated the existence of universal five- and six-body resonances. In experiments, these five- and six-body states should manifest as a loss peak at the critical scattering lengths that, for the Cs experiments at Innsbruck [3, 4], should occur approximately within $-290a_0 \lesssim a_5^* \lesssim -260a_0$ and $-230a_0 \lesssim a_6^* \lesssim -180a_0$. Future studies, with a more realistic description of the short-range physics, can further restrict these values. Our results provide support for the hypothesis of a universal regime in which bosonic systems are only controlled by two- and three-body physics. We extended the analysis to the lowest Efimov family and identified a rich structure of bound states and resonances in bosonic systems with large scattering lengths. While this structure is affected by important nonuniversal corrections, it can be still *interpreted* as emerging from a universal behavior. Therefore, part of this qualitative structure is expected to persist in the universal regime. In particular, we expect the persistence of universal trimer-atom-atom resonant states. A recent study [12] predicts a large atom-trimer scattering length, implying that, even in the universal regime, the trimer-atom-atom system fulfils Efimov conditions for the formation of weakly bound trimers. The emergence of a universal picture for bosons suggests a reinterpretation of previous studies on strongly interacting systems. For example, one can speculate that the similarities found in the formation of small ^{4}He and Tritium clusters [26] have their root in an underlying universal behavior that has Efimov physics at its root, but is modified by nonuniversal corrections.

Enlightening discussions with N. Baas, M. Berninger, D. Blume, J. P. D'Incao, F. Ferlaino, C. H. Greene, and D. A. Huse are acknowledged. This work was initiated at the INT-10-46W workshop and partially supported by NSF.

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