

# Universal Trimers from Three-Body Interactions in One-Dimensional Lattices

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We investigate the formation of trimers in an infinite one-dimensional lattice model with single-particle hopping  $t$  and hard-core two-body  $U$  and three-body  $V$  interactions of relevance to Rydberg atoms and polar molecules. For sufficiently attractive  $U \leq -2t$  and positive  $V > 0$  a large trimer is stabilized, which persists as  $V \rightarrow \infty$ , while both attractive  $U \leq 0$  and  $V \leq 0$  bind a small trimer. Surprisingly, the excited state above this small trimer is also bound and has a large extent; its behavior as  $V \rightarrow -\infty$  resembles that of the large ground-state trimer.

*Introduction.*—Few-body physics forms the basis of our understanding of the microscopic building units of the universe [1]. It contributes to a plethora of fundamental phenomena, including Efimov’s universality [2], quantum impurities in cold gases [3, 4], quasiparticles [5, 6] and quasiparticle pairing [7–9] in nanoscale systems, the fractional quantum Hall effect [10], nuclear systems [11] and neutrons [12].

A principal problem in this field is one of particles in a central potential, and the ensuing binding of bound states. One intriguing effect prevalent in continuum systems is the formation of shallow bound states, which extend beyond the range of the potential. Such a feeble bound state can be the lowest-energy state of the system, such as one formed in a delta-function potential in lower dimensions, or an excited state, such as Feshbach molecules [13] and halo states [14]. Lattice systems with local two-body interactions do not host shallow excited bound states [15, 16]. It is therefore important to determine whether conditions exist under which shallow excited bound states can form in lattice systems in presence of higher-body interactions, *e.g.* three-body interactions.

In this work, we demonstrate that lattice systems with purely local nearest-neighbor two- and three-body interactions host bound states that extend well beyond the range of the binding forces, giving way to an emergent universality in one dimension [17–19] distinct from Efimov’s universality. Namely, we demonstrate that a combination of two-site  $U$  and three-site  $V$  interactions stabilize universal large three-body bound states, which are either the ground state (for  $V > 0$ ) or the first excited state (for  $V < 0$ ) of the system. Tuning the strengths of interactions allows control over the size of the bound states, providing access to the crossover between universal and non-universal few-body physics in experiments.

*Model.*—We consider a minimal one-dimensional model of structureless fermions (*e.g.* spinless electrons) or hard-core bosons with nearest-neighbor (NN) hopping,

and two- and three-body interactions

$$\hat{\mathcal{H}} = -t \sum_i (\hat{c}_i^\dagger \hat{c}_{i+1} + \hat{c}_{i+1}^\dagger \hat{c}_i) + U \sum_i \hat{n}_i \hat{n}_{i+1} + V \sum_i \hat{n}_i \hat{n}_{i+1} \hat{n}_{i+2}, \quad (1)$$

where  $t$  is the hopping amplitude,  $U$  is the NN two-body interaction and  $V$  is the NN three-body interaction,  $i$  is the site index,  $\hat{c}^\dagger$  ( $\hat{c}$ ) is the particle creation (annihilation) operator, and  $\hat{n}$  is the particle number operator. This model in the NN approximation serves to provide insight into the physics of the dominant three-body interactions in a wide range of experiments.

*Dimers.*—A nonzero value of  $|U| > 2t$  is required to bind a dimer state, so as to compensate for the kinetic energy lost in binding [15, 20].

*Trimers.*—We study three-particle states in the infinite chain by solving the equation of motion for the Green’s function  $\hat{G}(\omega) = (\omega + i\eta - \hat{\mathcal{H}})^{-1}$ . We derive an exact hierarchy of equations of motion for three-particle propagators  $G(m_1, m_2; n_1, n_2; K, \omega) = \langle K, m_1, m_2 | \hat{G}(\omega) | K, n_1, n_2 \rangle$  defined for states  $|K, n_1, n_2\rangle = \frac{1}{\sqrt{N}} \sum_i e^{iKR_i} \hat{c}_{i-n_1}^\dagger \hat{c}_i^\dagger \hat{c}_{i+n_2}^\dagger |0\rangle$  [20]. A stable attractively (repulsively) bound trimer (also known as trion) corresponds to the appearance of a discrete pole in the Green’s function below (above) the continuum of scattering states.

*Trimer stability diagram.*—To identify stable trimers we search for discrete peaks outside of the three-particle continuum. This consists of scattering states of three free particles,  $1 + 1 + 1$ , and those of a dimer and a free particle,  $2 + 1$ . In the current work, we discuss trimers formed below the continuum ( $U/t < 0$ ), *i.e.* attractively bound trimers.

In Figure 1, we plot the stability diagram for bound states with total quasimomentum  $K = k_1 + k_2 + k_3 = 0$ . The solid blue line identifies the stability behavior of attractive trimers. To characterize different regimes of physical behavior, we compute the average size of the trimer  $\langle M \rangle$ , where  $M = n_1 + n_2$  is the distance between the two outer particles in a given configuration of the

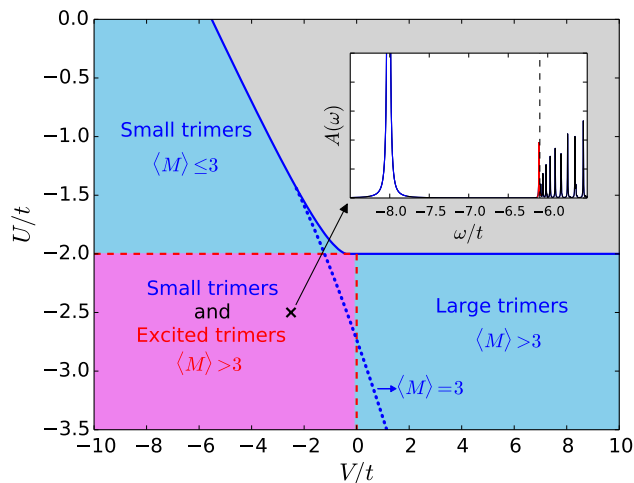


FIG. 1. (color online) Trimer stability diagram at  $K = 0$  as a function of  $V$  and  $U$  in units of  $t$ . The grey area indicates the continuum. The solid blue line identifies the boundary of the stability region of attractively bound states, while dashed red lines identify regions where an excited-state (ES) trimer co-exists with the ground-state (GS) trimer. The crossover from small ( $\langle M \rangle \leq 3$ ) to large ( $\langle M \rangle > 3$ ) GS trimers is indicated by the dotted blue line. In the inset, we show the spectral function  $A(\omega) = -\frac{1}{\pi} \text{Im} G(1, 1; 1, 1; 0, \omega)$  for the parameter values indicated by the cross:  $V = -2.5t$ ,  $U = -2.5t$ , demonstrating the appearance of the GS (blue) and ES (red) trimer peaks below the edge of the continuum (dashed line).

trimer.

First consider the upper-left quadrant of the diagram ( $V \leq 0$ ,  $U \geq -2t$ ). For  $U = 0$ , a bound trimer (blue region of Figure 1) appears for  $V \lesssim -5.5t$  with particles tightly bound in the trimer state  $\langle M \rangle \leq 3$  as expected of the short-range three-body attraction. Increasingly attractive  $U$  values lead to more tightly bound trimers and naturally lowers the  $V$  needed for binding.

Now consider the lower-right quadrant ( $U \leq -2t$ ,  $V \geq 0$ ). Surprisingly, for sufficiently attractive  $U \leq -2t$ , trimers are always stable regardless of the magnitude of the repulsive  $V$ . This behavior persists for extremely large  $V$  (not shown). The large  $V$  effectively pushes the particles in the trimer apart as it becomes energetically costly to occupy three consecutive sites, but fails to completely break down the trimer. These exotic large trimers with  $\langle M \rangle > 3$  are bound by non-perturbative higher-order interactions.

We now discuss the lower-left quadrant of Figure 1, ( $U \leq -2t$ ,  $V \leq 0$ ). As expected, these strongly attractive  $U$  and  $V$  bind a small trimer. Interestingly, however, a second bound state appears below the continuum, see also the inset of Figure 1. These feebly bound excited-state (ES) trimers are extended ( $\langle M \rangle > 3$ ) similar to the ground-state (GS) trimers at large repulsive  $V$ .

The large trimer states extend beyond the scale of a

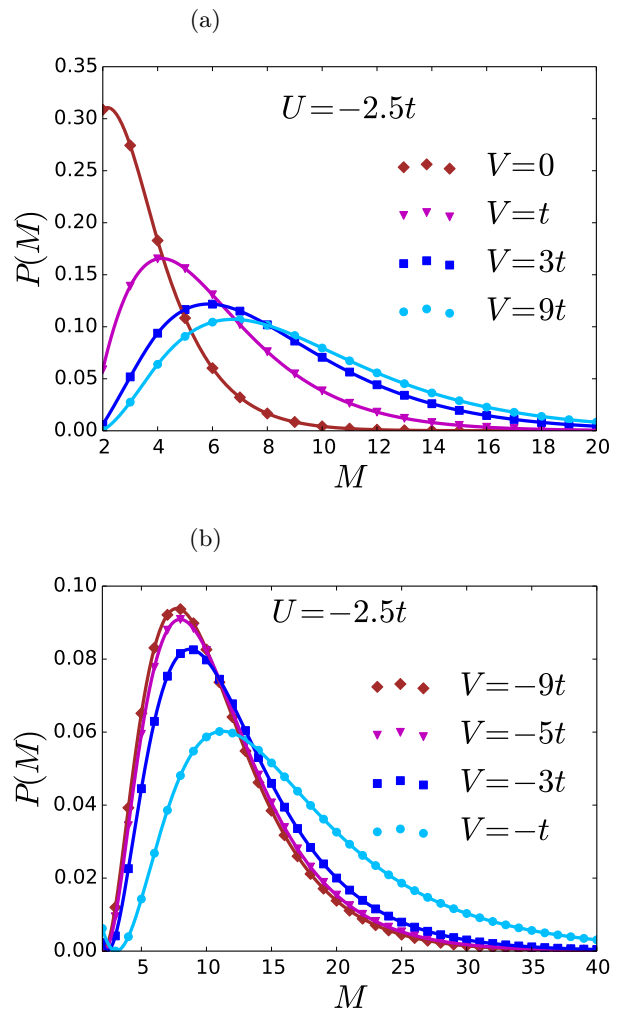


FIG. 2. (color online) Analysis of the size of trimers: The probability  $P(M) = \sum_{n_1+n_2=M} |\langle 0, n_1, n_2 | 0, \alpha_T \rangle|^2$  for the two outer particles in a trimer to be  $M = n_1 + n_2$  sites apart at  $U = -2.5t$  and various values of  $V$  for the (a) ground-state (GS) trimers (lower-right quadrant of Figure 1) and (b) excited-state (ES) trimers (lower-left quadrant of Figure 1). The two trimers exhibit qualitatively similar behavior with increasing  $V$  (compare lines of the same colors in (a) and (b)). Further analysis of the  $M = 8$  component of the GS trimer is presented in Figure 5.

single lattice spacing, demonstrating the possibility of an emergent long-wavelength continuum description and universal low-energy physics, see discussion below.

We note in passing that, for  $K = 0$ , only small, and no large, repulsively bound trimers appear above the continuum (not shown).

*Trimer structure.*—To shed light on the mechanism behind the formation of trimers and their structure, we analyze the probability density

$$P(M) = \sum_{n_1+n_2=M} |\langle 0, n_1, n_2 | 0, \alpha_T \rangle|^2 \quad (2)$$

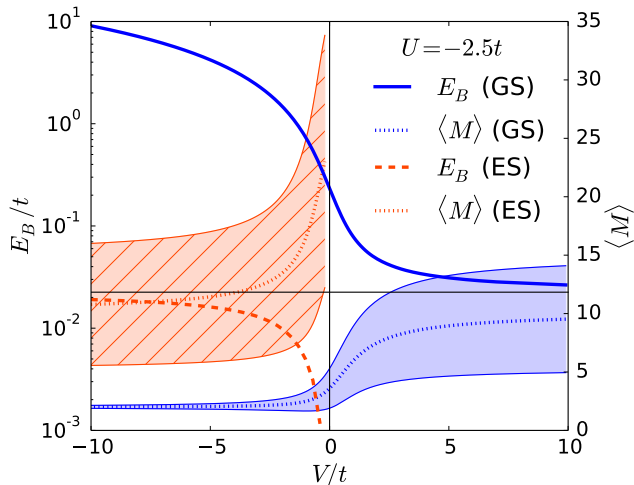


FIG. 3. (color online) Binding of ground-state (GS) (blue) and excited-state (ES) (salmon) trimers for  $U = -2.5t$  at  $K = 0$  as a function of  $V$ . We plot the binding energy  $E_B$  (solid and dashed lines) and the average trimer size  $\langle M \rangle$  (dotted lines) with  $\langle M \rangle \pm \sigma$  (boundary of the shaded regions), where  $\sigma$  is the standard deviation of  $P(M)$ .  $E_B$  approaches the horizontal black line in the asymptotic limit  $V \rightarrow -\infty(\infty)$  for the ES (GS) trimer.

of the trimer eigenstates  $|0, \alpha_T\rangle$  at quasimomentum  $K = 0$ .

We study  $P(M)$  as a function of  $V$  for a fixed  $U = -2.5t$  in Figure 2 for (a) the GS trimers and (b) the ES trimers.

The size of the GS trimer evolves with  $V$  from small ( $\langle M \rangle \approx 3$ ) to large ( $\langle M \rangle > 3$ ) (Figure 2(a)), see also the dotted line in Figure 1. This crossover behavior is characterized by a shift in the maximum of  $P(M)$  to larger values. In comparison, the ES trimer is much more extended, however its spread also grows with  $V$  (Figure 2(b)). That these bound states extend over several lattice sites is an indication of universality in the sense that the binding energy depends only on the two-body  $a_2$  and three-body  $a_3$  scattering lengths [17].

To corroborate this picture, we study the binding energy  $E_B$  of the trimer bound states. In Figure 3, we plot  $E_B$  along with  $\langle M \rangle$  and its spread for the GS (blue) and ES (salmon) trimers as a function of  $V$  for an exemplary  $U = -2.5t$  at  $K = 0$ . As expected, for  $V < 0$ ,  $E_B$  (solid line) of the GS trimer grows with  $|V|$ , saturating at the smallest possible size of  $M = 2$  with essentially no spread. For repulsive  $V > 0$ , the binding energy decreases, asymptotically approaching  $E_B \approx 0.0225t$  (horizontal solid line), and both  $\langle M \rangle$  and its spread increase, saturating at  $\langle M \rangle \approx 10.14$ . Intriguingly, we find the same asymptotic behavior for the ES trimer as  $V \rightarrow -\infty$  (we have verified this numerically).

We can understand this behavior as follows. In

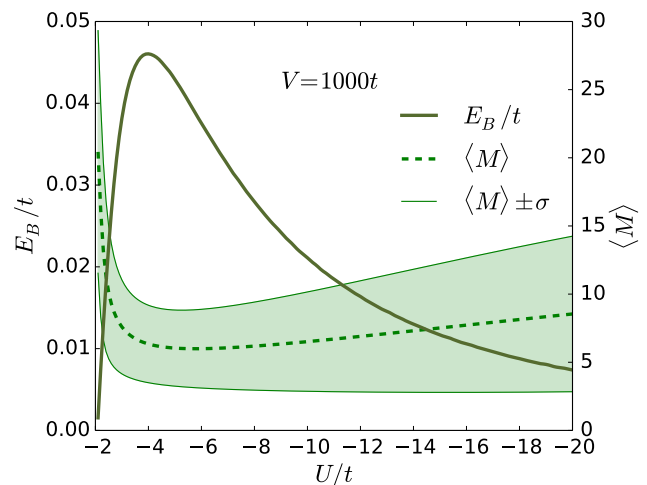


FIG. 4. (color online) Binding mechanism of the large GS trimer for  $V = 1000t$  at  $K = 0$  as a function of  $U$ . We plot the binding energy  $E_B$  (solid green line), the average trimer size  $\langle M \rangle$  (dashed green line), and  $\langle M \rangle \pm \sigma$  (boundary of shaded regions), where  $\sigma$  is the standard deviation of  $P(M)$ . The shaded region shows the spread of  $P(M)$  about the average  $\langle M \rangle$ .

the limit  $V \rightarrow -\infty$ , the ground-state trimer  $|\Psi_{\text{GS}}\rangle$  asymptotically approaches the state with the smallest possible size and no spread, *i.e.*  $|K, 1, 1\rangle$ . The ES trimer must be orthogonal to the GS trimer, and in this limit we find  $\langle \Psi_{\text{ES}} | \Psi_{\text{GS}} \rangle \rightarrow \langle \Psi_{\text{ES}} | K, 1, 1 \rangle = 0$ . On the other hand, in the limit  $V \rightarrow \infty$ , the NN configuration  $|K, 1, 1\rangle$  in the trimer wavefunction is energetically forbidden. This reflects in the relation  $\langle \Psi_{\text{GS}} | K, 1, 1 \rangle = 0$ . The problem of finding the Hamiltonian spectrum requires diagonalizing the Hamiltonian operator whose structure then takes the same exact form in these two asymptotic limits, explaining the resemblance between the asymptotic forms of the ES and GS trimers.

The asymptotic saturation of  $E_B$  and  $\langle M \rangle$  of the GS and ES trimers is yet another indication of universal behavior, which we now discuss. We find that the large GS and ES trimers asymptotically behave as  $E_B \rightarrow E_0(U) \exp(\gamma(U)t/V)$ , where  $E_0(-2.5t) \approx 0.0225t$  and  $\gamma(-2.5t) \approx 0.5\pi$  [21]. In the long-wavelength limit, the trimer's binding energy depends only on  $a_3$ ,  $E_B = 1/ma_3^2$ . Identifying  $m^{-1} = 2ta^2$ , we find, for  $U = -2.5t$ ,  $a_3 \approx \sqrt{\frac{2}{0.0225}} a \exp\left(-\frac{1}{2}\gamma(-2.5t)\frac{t}{V}\right)$ . This exponential dependence of  $a_3$  on  $1/V$  (or equivalently, the inverse logarithmic dependence of  $V$  on  $a_3$ , *i.e.*  $V \propto -1/\ln(a_3\Lambda)$ , where  $\Lambda \sim a^{-1}$  is the momentum cutoff) is a signature of three-body universality in one dimension [17–19].

*Binding mechanism of large trimers.*—We now turn to the binding mechanism of the large GS trimers, which are stable despite the strong three-body repulsion.

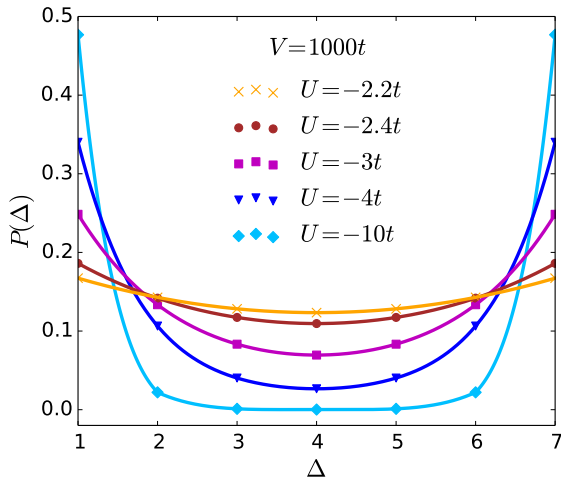


FIG. 5. (color online) Analysis of the internal structure of the large GS trimer through the probability  $P(\Delta) = \frac{|\langle 0, \Delta, M - \Delta | 0, \alpha_T \rangle|^2}{P(M)}$  to find the central particle  $\Delta$  sites apart from the outermost left particle for the  $M = 8$  component of the trimer wavefunction for  $V = 1000t$  at  $K = 0$  and for different values of  $U$ .

In Figure 4 we analyze  $E_B$  along with the corresponding  $\langle M \rangle$  of the GS trimer for  $V = 1000t$  at  $K = 0$  as a function of  $U$ . As expected  $E_B$  increases with increasingly attractive  $U$ , but only up to  $U \sim -3.9t$ . At this  $U$ ,  $E_B$  develops a maximum followed by a rapid decrease. This striking behavior accompanies an opposite trend in  $\langle M \rangle$  which has a minimum roughly coinciding with the maximum in  $E_B$ .

To explain this maximum in the binding energy as a function of  $U$ , we consider the probability density

$$P(\Delta) = \frac{|\langle 0, \Delta, M - \Delta | 0, \alpha_T \rangle|^2}{P(M)} \quad (3)$$

to find the central particle at a distance  $\Delta$  from the outer left particle in the trimer for a given  $M$  component of the wavefunction. In Figure 5, we plot  $P(\Delta)$  for the  $M = 8$  component of the GS trimer wavefunction at a fixed  $V = 1000t$  for different values of  $U$ . Simple perturbative arguments suggest that binding should be facilitated by the formation of configurations with NN particles  $\Delta = 1, 7$  as a result of the attractive NN two-body interaction. Surprisingly, for small  $|U|$  the central particle is only slightly more likely to be NN to either outer one and has a large probability to be anywhere in between. This is an example of the rare occurrence where a perturbatively small term has a large effect on the behavior of the system. A larger attractive  $U$  naturally favors NN configurations with  $\Delta = 1, 7$ .

With this insight in hand we can qualitatively explain the behaviour in Figure 4. Larger attractive  $U$  forces the central particle closer to either of the two outer particles. For moderate  $U > -3.9t$  in Figure 4 this

favors a smaller trimer, as intuitively expected. Larger  $U < -3.9t$ , however, forces the trimer into configurations with two NN particles and the third further apart (e.g.  $U = -10t$  result in Figure 4) accompanied by an increase in  $\langle M \rangle$ . This trimer configuration is a weakly bound state of a strongly bound dimer and a particle. Remarkably,  $\langle M \rangle \pm \sigma$  (shaded region of Figure 4), where  $\sigma$  is the standard deviation of  $P(M)$ , shows larger spread for more attractive  $U$  corroborating this picture of a dimer and a loosely bound third particle.

These results point to a non-perturbative binding mechanism: The large trimers are bound by higher-order interactions that mediate long-range binding yet avoid the forbidden  $M = 2$  configuration. Furthermore, this pattern of decrease in  $E_B$  for large trimers composed of NN pairs and a loosely bound particle indicates that configurations with the central particle ‘free’ in between the outer two play a crucial role in binding. There, the central particle mediates a three-body force through pairwise interactions with the outer two. This is most efficient in configurations with the central particle close to both the outer two, a situation favorable in smaller trimers formed for modest  $U$ . Larger  $U$  forces the central particle closer to one of the outer two, ultimately weakening the binding to the other one, which leads to a larger trimer with a  $2 + 1$ -like structure.

*Concluding remarks.*—We studied the interplay of two- and three-body interactions in a minimal one-dimensional lattice model. We constructed three-body bound-state stability diagram identifying regions in parameter space of attractively bound trimers. Trimers form even in the limit of infinite three-body repulsion. An ES bound trimer appears for attractive  $V$  and persists as  $V \rightarrow -\infty$ , where it develops asymptotic behavior similar to that of the GS trimer as  $V \rightarrow \infty$ .

These large trimers are bound by non-perturbative long-range forces mediated by short-range interactions, which favor large configurations with the central particle free in between the outer two. They extend over several lattice spacings pointing to an emergent long-wavelength universality, and are thus of great interest to efforts targeting the creation of large coherent quantum objects with non-trivial internal structure.

Our analysis applies to few-body bound states realized, for example, with polar molecules in optical lattices [22] or Rydberg atoms in tweezers [23], and to systems with three-site blockade ( $V \rightarrow \infty$  limit), such as Coulomb blockaded Rydberg gases [24] and quantum dots [25]. Other potential experimental systems with few-body interactions include trapped ultracold gases [26–28], ultracold atoms in optical lattices [29–33], Rydberg excitations in cold gases [34–39], Rydberg slow light polaritons [40–43], ion traps [44], optics coupled-cavity arrays [45], and circuit QED systems [46], where many of the ideas we discuss and others [47] can be investigated. We note that our method allows the simulation of

spectroscopy in the frequency domain (inset of Figure 1) and can be extended to analyze the time-resolved response in one and higher dimensions.

Note that our results imply universality for fermionic trimers in one dimension. An interesting question arises whether statistics play a role in universality in one dimension when the equivalence between hard-core bosons and spinless fermions [48] breaks down, *e.g.* for soft-core interactions. Another emergent line of inquiry is whether the universal correspondence between GS and ES complexes persists for larger number of particles.

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