Efimov Effect for Three Interacting Bosonic Dipoles

Yujun Wang, J. P. D'Incao, and Chris H. Greene

Department of Physics and JILA, University of Colorado, Boulder, Colorado 80309-0440, USA

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Three oriented bosonic dipoles are treated by using the hyperspherical adiabatic representation, providing numerical evidence that the Efimov effect persists near a two-dipole resonance and in a system where angular momentum is not conserved. Our results further show that the Efimov features in scattering observables become universal, with a known three-body parameter; i.e., the resonance energies depend only on the two-body physics, which also has implications for the universal spectrum of the four-dipole problem. Moreover, the Efimov states should be long-lived, which is favorable for their creation and manipulation in ultracold dipolar gases. Finally, deeply bound two-dipole states are shown to be relatively stable against collisions with a third dipole, owing to the emergence of a repulsive interaction originating in the angular momentum nonconservation for this system.

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The recent advances in producing ultracold dipolar gases have sparked a great deal of interest in the novel phases that could be experimentally accessible [1]. Two key ingredients are the long-range and anisotropic nature of the dipolar interaction, which can be manipulated by applying an external electric field. This reorients current research scenarios in ultracold gases and opens up the possibility of intriguing phenomena across a broad range of different fields, from condensed matter physics to ultracold chemistry. Recent experiments [2] have been able to create a gas of ground-state dipolar molecules and observe the electric field and geometry dependence of chemical reactions [3]. Nevertheless, a number of interesting effects can be expected when the external field is tuned near a dipole-dipole resonance (i.e., zero-energy dipolar bound state); this causes the interaction to vary from strongly repulsive to strongly attractive, in close analogy to the control through magnetic Feshbach resonances [4].

For nonreactive ground-state dipolar molecules [5], inelastic three-dipole scattering will be the main loss mechanism, and these will determine the stability of the dipolar gas. A recent paper by Ticknor and Rittenhouse [6] predicts in fact that three-body recombination will be extremely important for bosonic dipolar gases. Three-body recombination in this context, $D + D + D \rightarrow D_2 + D$, involves three free dipoles colliding to form a dipolar dimer releasing enough kinetic energy to make the collision partners escape from typical traps. As Ref. [6] points out, in the strongly interacting regime universal aspects related to the Efimov physics tend to dictate the collisional aspects of such processes. Nevertheless, the persistence of the Efimov effect for long-range, anisotropic, dipolar interactions remains an open question. The Efimov effect [7] has proven to have a profound impact in both nuclear and atomic matter [8,9]. In systems with short-range isotropic interactions, the Efimov effect manifests when the two-body scattering length a_s is much greater than the range of the interactions r_0, through a series of three-body bound states with energies given by $E_{n+1}/E_n = e^{-2\pi/s_0}$ ($n = 0, 1, 2, \ldots$), where the universal constant $s_0 = 1.006\,24$ for identical bosons. Note that low-lying energies, however, are not universal and typically depend on the details of the interactions. In ultracold gases, the Efimov effect is explored near a Feshbach resonance through its impact on scattering processes [10].

In this Letter, we show that the Efimov effect persists for dipolar systems and, moreover, that the dipolar interaction is extremely beneficial for the study of Efimov states. In particular, we find that the positions of the Efimov resonances (e.g., in energy, in a_s, etc.), as well as other scattering properties, are universally determined by the two-dipole physics alone. Moreover, as the strength of the dipolar interaction increases, Efimov states tend to be increasingly long-lived. This scenario, introduced by the dipolar interaction, makes dipolar gases ideal systems for the creation and manipulation of Efimov states. Following the method introduced in Ref. [11], we have also derived the scaling laws for three-body recombination. Finally, we show the existence of an effective repulsive long-range interaction between a dipolar dimer and a free dipole, which can prevent the decay of such dimers.

The hyperspherical adiabatic representation [12] transforms the three-body Schrödinger equation into coupled hyperradial equations, given (in a.u.) by

$$\left[-\frac{1}{2\mu}\frac{d^2}{dR^2} + U_\nu(R) - E\right]F_\nu(R) - \frac{1}{2\mu}\sum_{\nu'}\left[2P_{\nu\nu'}(R)\frac{d}{dR} + Q_{\nu\nu'}(R)\right]F_{\nu'}(R) = 0, \quad (1)$$

where the hyperradius R describes the overall size of the system and ν represents all quantum numbers that label each channel. In the above equation, $\mu = m/\sqrt{3}$ is the three-body reduced mass, E is the total energy, and F_ν is the hyperradial wave function in channel ν. $P_{\nu\nu'}$ and $Q_{\nu\nu'}$ are nonadiabatic couplings that drive inelastic transitions, while the $U_\nu(R)$ are effective potentials that support bound and quasibound states of the system.

The most stringent challenge in this approach is the numerical solution of the hyperangular adiabatic eigenvalue equation at fixed values of R in order to determine the potentials $U_\nu(R)$ and channel eigenfunctions $\Phi_\nu(R;\Omega)$:

$$\left[\frac{\hat{\Lambda}^2(\Omega)+15/4}{2\mu R^2}+\hat{V}(R,\Omega)-U_\nu(R)\right]\Phi_\nu(R;\Omega)=0. \quad (2)$$

Here Ω represents the set of all hyperangles describing the system's internal motion, Λ^2 is the grand angular momentum operator [12], and $\hat{V}=v(\vec{r}_{12})+v(\vec{r}_{31})+v(\vec{r}_{23})$ is the pairwise sum of two-body interactions, given by

$$v(\vec{r})=V_0\mathrm{sech}(r/r_0)^2+\frac{2d_\ell}{m}\frac{1-3(\hat{z}\cdot\hat{r})^2}{r^3}f(r). \quad (3)$$

The first term above is an isotropic short-range contribution, and the second term is the anisotropic dipole-dipole interaction [with a short-range cutoff $f(r)$] between dipoles aligned in the $\hat{z}$ direction with the dipole length defined as $d_\ell = md_m^2/2$, where d_m is the electric dipole moment. We emphasize that although our model assumes point dipoles it is also applied to ground-state dipolar molecules, where all the details of its complicated structure are encapsulated in the short-range behavior of the interactions. Moreover, since the dipoles are free to interact in any geometry, the solutions we obtain from Eq. (2) already include both attractive and repulsive aspects of the dipolar anisotropic interaction. To test whether any property of interest is universal with respect to the three-body short-range physics, we have performed calculations for different values of d_ℓ as well as for different isotropic short-range potentials.

The major difficulty introduced by the dipolar interaction is that the three-body total angular momentum J is not conserved. To calculate $U_\nu(R)$, we expand Φ as

$$\Phi_\nu^{\Pi,M}(R,\Omega)=\sum_{J,K}\phi_\nu^{JK}(R;\theta,\varphi)D_{KM}^J(\alpha,\beta,\gamma), \quad (4)$$

where D_{KM}^J are the Wigner D functions, α, β, and γ are the Euler angles, and θ and φ are the Smith-Whitten hyperangles [13]. Here M is the space-fixed frame projection of the total angular momentum J, K is the quantum number for its body-fixed frame projection, and Π is the total parity. Finally, the body frame components ϕ_ν^{JK} at fixed R are numerically solved by expanding the θ and φ dependences in a B-spline basis.

Here, we study the three-dipole problem for $M^\Pi = 0^+$, which includes the $J^\Pi = 0^+$ symmetry where the Efimov effect occurs for nondipolar systems. Evidently, for $d_\ell \ll r_0$ the Efimov effect might be expected to remain unchanged. However, for $d_\ell > r_0$ the coupling among different J's might possibly compromise its persistence. In order to investigate the Efimov effect for dipoles, we tune $d_\ell > r_0$ in Eq. (3) to get a two-dipole zero-energy bound state, where $|a_s| \gg r_0$ [14]. Figure 1 summarizes our findings and sketches the three-body energy spectrum obtained. Figure 1(a) shows the adiabatic potentials U_ν for $d_\ell/r_0 = 38.11$ and $|a_s| \to \infty$, showing the overall topology of the potentials, including a family of channels converging to deeply bound dipolar dimers and channels describing the collision of three free dipoles. For each dipolar dimer channel there exists an infinity of channels converging to that same threshold due to the coupling of all different J's [we have truncated the J expansion (4) at $J_{\max} = 14$].

The inset in Fig. 1(a), however, shows the evidence of our central result. It confirms the existence of the universal Efimov potential

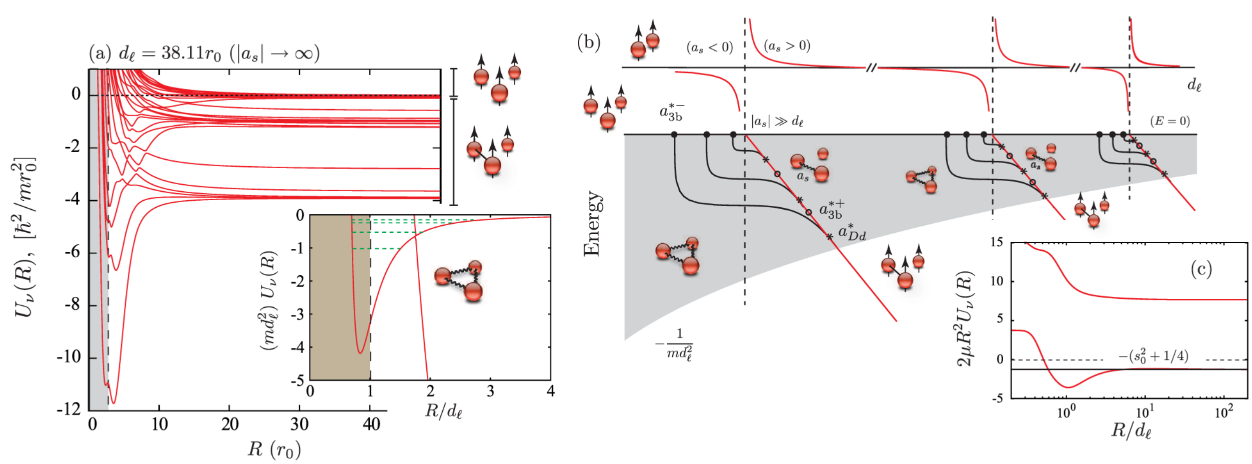

FIG. 1 (color online). (a) A typical set of adiabatic hyperspherical potentials $U_\nu(R)$ for three dipoles that exhibit the Efimov hyperradial potential curve ($d_\ell/r_0 = 38.11$ and $|a_s| \to \infty$). Inset: Rescaled adiabatic potentials showing the Efimov potential (the dashed lines are illustrations of the Efimov states in that potential, not to scale). (b) Schematic representation for the d_ℓ dependence of a_s (upper part) and the Efimov spectrum (lower part) for dipolar systems (see the text). (c) The Efimov potential signature at the first pole of a_s ($d_\ell/r_0 = 4.86$). The horizontal solid line shows the Efimov behavior given by Eq. (5) (see the text).

$$U_\nu(R) \simeq -\frac{s_0^2 + 1/4}{2\mu R^2}, \quad (5)$$

which supports the usual infinity of three-body Efimov states, illustrated schematically in the figure as horizontal dashed lines. Our numerical explorations suggest that, in the strong dipole limit where $d_\ell \gg r_0$, the rescaled potential in the inset in Fig. 1(a) is universal; i.e., the rescaled potentials for different values of d_ℓ or for different strengths of the isotropic interaction coincide almost perfectly. Figure 1(b) shows schematically the three-body energy spectrum versus dipole length. As $d_\ell > r_0$ increases, new dipolar dimers are created and so are new families of Efimov states. The binding energy of the lowest Efimov state scales in proportion to $1/md_\ell^2$, based on our adiabatic potential in the inset in Fig. 1(a) as well as Table I. Figure 1(c) gives further evidence for the long-range universal Efimov potential when $|a_s| \to \infty$. We checked that adiabatic corrections to the Efimov potential are negligible.

The existence of the Efimov effect for three dipoles might have been expected as a consequence of the s-wave dominance of the two-body physics near the pole of a_s [6]. Nevertheless, the Efimov effect for dipoles has a striking difference from the usual Efimov effect. As shown in the inset in Fig. 1(a) [see also Fig. 1(c)], the Efimov potential extends *only* from values of $R > d_\ell$, while for $R < d_\ell$ the dipolar interaction causes the Efimov channel to be repulsive. This critically affects the universal properties associated with the dipolar Efimov effect. Since the Efimov states are well separated from the short-range region (at $R \approx r_0$) by the repulsive barrier at $R < d_\ell$, properties of Efimov states are expected to be *fully* universal; i.e., they will depend on the two-dipole physics alone, namely, a_s and d_ℓ. This implies that, in contrast to the usual Efimov effect, the three-body phase (or parameter) [9,11] is now universal and one can derive the energies of the Efimov states (resonances) for both $a_s > 0$ and $a_s < 0$ ($|a_s| > d_\ell$). Moreover, the barrier for $R < d_\ell$ also suppresses decay of the Efimov states, and, therefore, the Efimov states for large values of d_ℓ are likely to be more long-lived than in the nondipolar scenarios.

To quantify the three-body parameter for dipolar interactions, we calculate the position and the width of the lowest Efimov resonance when $|a_s| \to \infty$. To handle the sharp crossings between the Efimov channel and other deeply bound channels [see Fig. 1(a) and inset], we solve Eq. (1) by the slow variable discretization method [15] and extract the position and width of the Efimov resonances. In Table I, we list the ground Efimov state energies E_0 and the widths Γ for a few values of d_ℓ. As we have expected, the positions of the Efimov resonances in Table I exhibit a universal trend. For the widths of these resonances, however, we do not observe nor expect a purely universal behavior, since they encapsulate the decay to deeply bound states at smaller distances. Nevertheless, for increasing d_ℓ, the resonance width is suppressed as $1/d_\ell^2$, indicating increased lifetimes of the Efimov states. The universal three-body parameter $\kappa_* = \sqrt{mE_0}$ [9] is then estimated to be $0.17/d_\ell$ in the limit of $d_\ell \gg r_0$. This knowledge of κ_* [9] then allows us to determine the universal formulas that predict some important three-body scattering observables

$$K_3^{(a_s>0)} \approx \frac{67.1}{e^{2\eta}}\left\{\sin^2\left[s_0 \ln\left(\frac{a_s}{d_\ell}\right) + 2.5\right] + \sinh^2\eta\right\}\frac{a_s^4}{m}, \quad (6)$$

$$K_3^{(a_s<0)} \approx \frac{4590\sinh(2\eta)}{\sin^2[s_0\ln(\frac{|a_s|}{d_\ell}) + 0.92] + \sinh^2\eta}\frac{a_s^4}{m}, \quad (7)$$

$$a_{Dd}^{(a_s>0)} \approx \left(1.46 + 2.15\cot\left[s_0\ln\left(\frac{a_s}{d_\ell}\right) + 0.86 + i\eta\right]\right)a_s, \quad (8)$$

$$V_{\rm rel}^{(a_s>0)} \approx \frac{20.3\sinh(2\eta)}{\sin^2[s_0\ln(\frac{a_s}{d_\ell}) + 0.86] + \sinh^2\eta}\frac{a_s}{m}. \quad (9)$$

Here K_3 is the rate coefficient for three-body recombination into weakly ($a_s > 0$) and deeply ($a_s < 0$) bound dipolar dimers. a_{Dd} is the dipole (D) plus dipolar dimer (d) scattering length, and $V_{\rm rel}$ is the corresponding relaxation rate for such inelastic collision processes, $D_2^* + D \to D_2 + D$. η is related to the probability of decay to deeply bound channels [9]. Equations (6)–(9) now predict the positions of the main features of such rates that characterize the Efimov physics. For instance, the minima in K_3 [Eq. (6)] should occur for values of a_s given by $a_{3b}^{*+} = 1.8e^{n\pi/s_0}d_\ell$ ($n = 0, 1, 2, \ldots$). The ratio a_{3b}^{*-}/d_ℓ determines the position of the Efimov resonances for K_3 ($a_s < 0$) [Eq. (7)], while a_{Dd}^*/d_ℓ determines the position of dipole plus dipolar dimer resonances [Eqs. (8) and (9)]. The second part of Table I lists these properties in terms of ratios for all processes (we have dropped the factor $e^{n\pi/s_0}$ for simplicity). The universality on the three-dipole problem also has key implications for its four-body analog. In particular, the positions of the four-dipole features [16] can be obtained from our results in Table I.

Our numerical results show that the attractive R^{-2} Efimov potential is absent when $|a_s| \lesssim d_\ell$. Nevertheless, the adiabatic potentials are still universal. As shown in Fig. 2(a), the diabatic potentials show universal scaling with d_ℓ. Figure 2(a) shows the lowest three-body continuum channel, and the lowest dipole plus dipolar dimer channel associated with the most weakly bound dimer whose binding energy is proportional to $1/md_\ell^2$. For this

TABLE I. The positions and the widths of the lowest Efimov state for different values of d_ℓ and the universal ratios for the positions of the Efimov features in three-dipole scattering observables.

$\lvert a_s\rvert \to \infty$	d_ℓ (r_0)	$md_\ell^2E_0$	$md_\ell^2\Gamma$
	14.534	3.06×10^{-2}	5.2×10^{-3}
	25.498	3.03×10^{-2}	6.6×10^{-3}
	38.110	2.95×10^{-2}	3.2×10^{-3}
	$a_{3b}^{*-}/d_\ell \approx -8.1$	$a_{3b}^{*+}/d_\ell \approx 1.8$	$a_{Dd}^{*}/d_\ell \approx 8.6$

case, recombination to such dimer states proceeds through an inelastic transition near $R \approx d_\ell$, leading to the $K_3 \propto d_\ell^4$ scaling for recombination, consistent with Ref. [6]. Since the dipole plus dipolar dimer channel is repulsive for $R < d_\ell$, we expect that recombination to more deeply bound states will be substantially less important since the pathway to this final state would require tunneling through to small $R < d_\ell$.

The behavior of the dipole plus dipolar dimer channels when the dimer is deeply bound also shows results interesting for dipole and dipolar dimer mixtures. These channels should be asymptotically described by

$$W_\nu(R) \simeq_{R \gg r_0} E_d + \frac{l_{Dd}(l_{Dd}+1)}{2\mu R^2}, \tag{10}$$

where E_d is the dimer energy and l_{Dd} represents its average or effective orbital angular momentum relative to the free particle. For three particles with isotropic short-range interactions, l_{Dd} obeys the usual rules of addition of angular momentum. For instance, if the two-body state is an s-wave state, $l_{Dd} = J$. For dipolar states, however, our results reveal that is no longer true, and we rationalize it by the fact that the two-body state is *not* a pure angular momentum eigenstate. In fact, our numerical calculations show that l_{Dd} becomes d_ℓ-dependent. Figure 2(b) shows that l_{Dd} increases with d_ℓ in the same trend as the expectation value of the angular momentum $\langle \vec{j}^2 \rangle$ for the dipolar dimer and the expectation value of the total (three-body) angular momentum $\langle \vec{J}^2 \rangle$. However, the d_ℓ dependence of l_{Dd} is not universal, as it varies with the short-range physics. Nevertheless, the nonzero l_{Dd} provides an average centrifugal barrier that suppresses the dipole plus dipole-dimer relaxation, $V_{\rm rel} \propto k_{Dd}^{2l_{Dd}} r_0^{2l_{Dd}+1}$ [11], where $k_{Dd} \ll r_0^{-1}$ is the relative wave number. This suppression opens up the

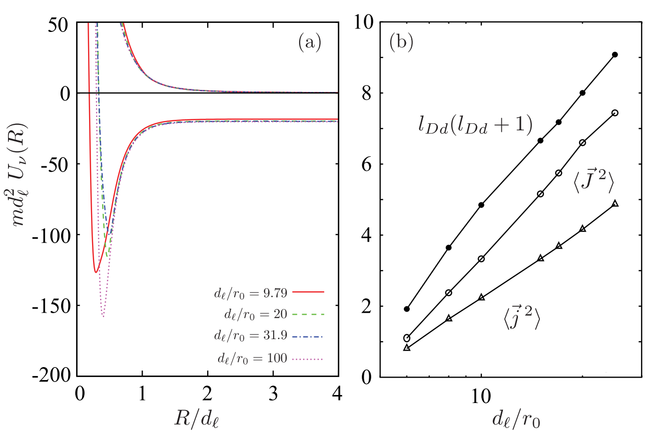

FIG. 2 (color online). (a) The diabatized hyperspherical potentials for the most weakly bound dipole plus dipolar dimer channel with different values of d_ℓ and $|a_s| \leq r_0$. (b) The d_ℓ dependence of the asymptotic angular momentum l_{Dd} and the expectation value of the angular momentum $\langle \vec{j}^2 \rangle$ for a deeply bound dipolar dimer and the total angular momentum $\langle \vec{J}^2 \rangle$.

possibility of creating stable mixtures of dipoles and two-dipole molecules. Furthermore, with the tunability of the barrier that can be achieved via field control of d_ℓ, the interaction between a dipole and a two-dipole molecule can be controlled, providing an innovation for studies in ultracold quantum gases at both the few-body and many-body levels.

In summary, we have characterized the Efimov effect for three bosonic dipoles. A key conclusion is that long-range, anisotropic dipolar interactions are predicted to make the Efimov physics more universal than in the traditional systems where this effect has been studied and observed. Efimov resonances with dipolar interactions are also predicted to be long-lived, which should aid their experimental observation and manipulation. The dipolar interactions introduce a tunable effective repulsion between a dipole and a deeply bound dipolar dimer, which can be used to control the collisions between the molecules and also to stabilize the ultracold quantum gas of dipolar dimers.

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