Universal Three-Body Physics for Fermionic Dipoles

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

Department of Physics and JILA, University of Colorado, Boulder, Colorado, 80309-0440, USA
(Received 30 June 2011; published 29 November 2011)

Our present study of the universal physics for three oriented fermionic dipoles in the hyperspherical adiabatic representation predicts a single long-lived three-dipole state, which exists in only one three-body symmetry and forms near a two-dipole resonance. Our analysis reveals the spatial configuration of the universal state and the scaling of its binding energy and lifetime with the strength of the dipolar interaction. In addition, three-body recombination of fermionic dipoles is found to be important even at ultracold energies. An additional finding is that an effective long-range repulsion arises between a dipole and a dipolar dimer that is tunable via dipolar interactions.

The recent advances in producing ground-state ultracold dipolar molecules [1] have sparked great interest in the novel phases that could be experimentally accessible [2]. With the ability to control the dipolar interaction by an external electric field [3], studies of dipolar molecules could stimulate the discovery of intriguing phenomena across a broad range of disciplines, from condensed matter physics to ultracold chemistry. In particular, the effects of the long-range anisotropic dipolar interaction on ultracold physics have already been studied for three bosonic dipoles [4,5]. A recent development has shown [5] that the Efimov effect [6] is more favorable for three bosonic dipoles, although the dipolar interaction has ingredients that could conceivably have destroyed it.

Stimulated by their ability to mimic a variety of exotic physical systems from superfluids to neutron stars, quantum degenerate Fermi gases with nondipolar interactions have been studied extensively in recent years [7]. In contrast to bosonic gases, whose lifetimes are mainly determined by three-body recombination [8], fermionic gases exhibit extraordinary stability against three-body inelastic collisions, except when the two-body interaction is tuned near a p-wave resonance [9,10]. Moreover, three-body physics for identical fermions is expected to be nonuniversal, i.e., short-range-dependent [9,11]. Consequently, three-body physics for identical fermions has, to some extent, been regarded as less exciting and/or difficult to observe. Nevertheless, the influence of dipolar interactions on the universal behavior of bosons triggers new interest in the study of universality for fermionic dipoles, and it is becoming increasingly important to understand such physics in order to guide ongoing experiments on ground-state fermionic dipolar molecules [3].

In this Letter, the behavior of three identical fermionic dipoles is demonstrated to be universal, thus differing fundamentally from the nondipolar cases. In particular, near a dipole-dipole resonance (i.e., where the two-dipole binding energy $E_{2d} \to 0$), a single long-lived, universal three-dipole state is formed. Its size and lifetime both

grow with stronger dipolar interactions. The stability of the fermionic dipolar gases is assessed through numerical calculations of the rate coefficient K_3 for three-dipole recombination, $D + D + D \to D_2 + D$, which is the dominant expected loss mechanism for nonreactive ground-state dipolar molecules [12]. In fact, we have found that K_3 grows rapidly with the strength of the dipolar interactions and it is strongly enhanced near a dipole-dipole resonance. This study also shows evidence for a long-range, dipolar interaction-dependent repulsion that suppresses $D_2 + D$ relaxation collisions when D_2 is deeply bound.

Consider the three-dipole Schrödinger equation in hyperspherical coordinates (in atomic units):

$$\left(-\frac{1}{2\mu} \frac{\partial^2}{\partial R^2} + H_{\mathrm{ad}} \right)\psi = E\psi, \tag{1}$$

where R is the hyperradius, $\psi = R^{5/2}\Psi$ is the scaled three-body wave function, and $\mu = m/\sqrt{3}$ is the three-body reduced mass for identical particles with mass m. The adiabatic H_{ad} is

$$H_{\mathrm{ad}} = \frac{\Lambda^2(\Omega)}{2\mu R^2} + \frac{15}{8\mu R^2} + V, \tag{2}$$

where Λ^2 is the usual grand angular momentum operator [13] and Ω are the hyperangles representing positions of the three particles at fixed hyperradius R. The potential energy $V = v(\vec{r}_{12}) + v(\vec{r}_{23}) + v(\vec{r}_{23})$ is a pairwise sum of two-dipole interactions:

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

The sech^2 term is isotropic and short-range and it encapsulates the complicated interactions between two polar molecules. The second term, with a short-range cutoff $f(r)$, is the interaction between two dipoles aligned in the $\hat{z}$ direction. The dipole length is defined in terms of the

electric dipole moment d_m as $d_\ell = md_m^2/2$. The universality of our calculations is tested by varying both d_ℓ and V_0.

Equation (1) can be routinely solved, either using the adiabatic representation [13] or else through slow variable discretization (SVD) [14]. Our study shows that it is advantageous to use the adiabatic scheme to treat the asymptotic behavior of three dipoles in scattering calculations, while SVD efficiently handles sharp avoided crossings at small distances. In both cases, the biggest challenge is to solve the adiabatic eigenvalue equation

$$H_{\rm ad}\Phi_\nu^{\Pi,M}(R;\Omega) = U_\nu(R)\Phi_\nu^{\Pi,M}(R;\Omega), \qquad (4)$$

where $U_\nu(R)$ is the adiabatic potential for channel ν, M is the space-fixed frame projection of the total angular momentum J, Π is the total parity, and $\Phi_\nu^{\Pi,M}(R;\Omega)$ is the corresponding eigenfunction. For interacting oriented dipoles, the major difficulty in solving Eq. (4) is that the total orbital angular momentum J is not conserved. The method of Ref. [5] is implemented to solve Eq. (4). Briefly, $\Phi_\nu^{\Pi,M}$ is expanded in terms of the Wigner D functions [see Eq. (4) in Ref. [5]], truncated at $J_{\rm max} = 13$ for the convergence of the three-body observables to the accuracy shown in this Letter.

The nature of three-dipole states near dipole-dipole resonances emerges from study of the adiabatic potentials for $M^\Pi = 0^+$. Note that the even and the odd J values decouple in this symmetry. This symmetry with only odd J is of particular interest because it includes the $J^\Pi = 1^+$, the least-repulsive partial wave for three noninteracting identical fermions [15]. One would also expect the binding of three dipoles is most likely to occur at $m_{2d} = 0$ dipole-dipole resonance, where m_{2d} is the projection of two-dipole angular momentum along the field direction. However, $m_{2d} = 0$ is not allowed for $M^\Pi = 0^+$ symmetry,
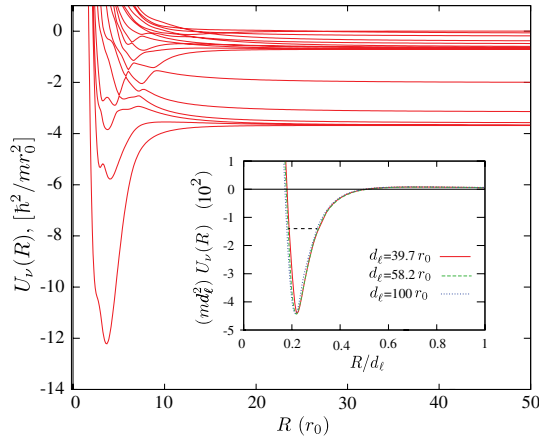

FIG. 1 (color online). A typical set of adiabatic hyperspherical potentials $U_\nu(R)$ for three fermionic dipoles with $d_\ell/r0 = 58.2$ and $E_{2d} \to 0$. The inset shows rescaled, diabatized potentials exhibiting universal behavior for a few values of d_ℓ at a dipole-dipole resonance. The horizontal dashed line in the diabatic potential wells indicates the position of the universal three-dipole states.

so the three-dipole system is considered instead near the $m_{2d} = 1$ resonances. Figure 1 shows the typical behavior of the adiabatic potentials. Asymptotically, the three-body continuum potentials behave in the same manner as the nondipolar interaction case, but, for dipole plus dipolar dimer channels, each threshold has a family of potential curves whose centrifugal barriers carry different effective angular momenta due to the J coupling.

Regardless of the complicated topology of the adiabatic potentials shown in Fig. 1, near a dipole-dipole resonance, it is possible to trace a diabatic potential well in the channel closest to the three-body continuum. It cuts through multiple sharp avoided crossings with deeply bound channels, as is visible in the inset of Fig. 1. Remarkably, all these potentials for different d_ℓ and different short-range potentials fall on top of each other after a proper scaling, thus providing a strong evidence of universal behavior. Our calculations also show that the WKB phase for these potentials at zero three-body energy approaches 1.1π in the limit $d_\ell \gg r_0$. This implies that, although there may be a great number of deeply bound nonuniversal three-dipole states, there is always only one universal quasibound three-dipole state near a $m_{2d} = 1$ resonance. A key implication of the scaling of the universal potentials is that the hyperradius of the repulsive barrier increases with d_ℓ, which suppresses decay of the three-dipole state and increases its lifetime as the dipolar interaction is increased. To quantify the energies of the universal states, we have solved Eq. (1) by using SVD. The energy E_{3d} and the width Γ of the three-body states are revealed by adding complex absorbing potentials in the lower decaying channels.

The universal trend in the energy E_{3d} shown in Table I confirms the universality expected from the universal potentials in the strong dipolar regime, but the width Γ exhibits less universal behavior, presumably due to the nonuniversal couplings to deeply bound channels. Nevertheless, the $1/d_\ell^2$ suppression in the width implies an increased lifetime of the universal three-dipole states as d_ℓ increases. Our numerical study also shows that the universal three-dipole states slowly become unbound or deeply bound as the system shifts away from a dipole-dipole resonance. In a broad region near a dipole-dipole

TABLE I. The upper rows: the energies E_{3d} and the widths Γ of the universal three-dipole states for different values of d_ℓ. The bottom row: the angle Θ between the three-dipole triangle and field direction, the long and short bond lengths b_l and b_s, and the smaller bond angle Δ from the most probable configuration of the three-dipole states.

$E_{2d} \to 0$	$d_\ell \ (r_0)$	$md_\ell^2 E_{3d}$	$md_\ell^2\Gamma$
	39.7	171	42
	58.2	135	43
	100	139	17
$\Theta \approx 16°$	$b_l \approx 0.26d_\ell$	$b_s \approx 0.14d_\ell$	$\Delta \approx 15°$

resonance, the properties of the three-dipole states are essentially unchanged.

Importantly, the interactions of the aligned dipoles break the overall rotational symmetry, reflecting that the three-dipole states have a preferential orientation in space. The geometry of these universal states can be analyzed by calculating the spatial distribution of the dipoles using the three-body wave functions. Specifically, the probability density for finding a dipole at $\vec{r}$ is

$$\rho(\vec{r}) = \frac{1}{3} \langle \Psi | \sum_i \delta(\vec{r} - \vec{r}_i) | \Psi \rangle, \qquad (5)$$

where $\delta(\vec{r})$ is the Dirac delta function and $\vec{r}_i$ is the position vector for the ith dipole. Figure 2 shows the isosurfaces of $\rho(\vec{r})$. The three-dipole states have a strongly preferential spatial configuration, as indicated by the triangle in the lower part of the figure. The isosurfaces can be viewed as the revolution of the triangle along the field axis. It is also interesting to note that the configuration of the three-dipole states is universal; only their overall size scales linearly with d_ℓ.

The configuration of a three-dipole state shown in Fig. 2 can be understood in terms of the anisotropic nature of the dipolar interactions and the symmetry of the state. The three dipoles tend to align in a line where the dipolar interactions in Eq. (3) are the most attractive, but this is forbidden by the odd partial wave symmetry. The state therefore has the configuration of an obtuse, isosceles triangle making a small angle with the field direction. The lower part of Table I lists the angle between the plane of the triangle and the field direction, the short and long
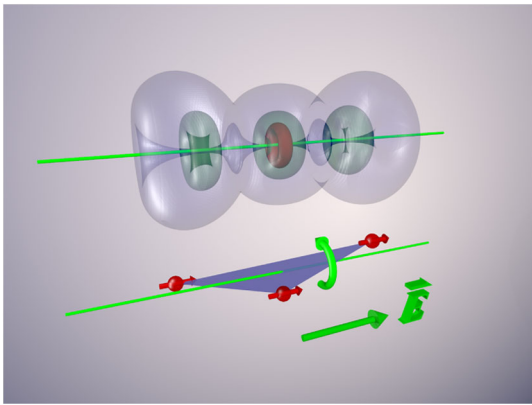

FIG. 2 (color online). The upper part: the isosurfaces of the one-dipole probability density $\rho(\vec{r})$ for the universal three-dipole states, centered in the space-fixed center-of-mass frame. By normalizing the peak density to be unity, the density of the following surfaces—the innermost one (red), three middle ones (green), and the outermost one (light blue)—are 0.8, 0.3, and 0.015, respectively. This crankshaft-resembling structure is a figure of rotation about the field axis. The lower part: the most probable orientation and geometry of the triangle formed by three dipoles. The axes (green) show the direction of the external electric field.

bond lengths, and the smaller bond angle determined from the most probable and also the dominant configuration of the three-dipole states.

The possibility of universal three-dipole states for other symmetries has been explored, in particular, the three-dipole system for $M^\Pi = 0^-$ symmetry with odd J's, which includes the less-repulsive partial wave contribution $J^\Pi = 1^-$ [15]. However, no universal three-dipole states have been found near both $m_{2d} = 0$ and $m_{2d} = 1$ dipole-dipole resonances. The situation is similar for $M^\Pi = 1^-$ and 1^+ symmetries, where the adiabatic potentials are found to be more repulsive. Based on these numerical calculations and the fact that, for higher M's and near higher m_{2d}'s resonances, three dipoles have larger centrifugal energy and therefore the potentials are expected to be more repulsive, we conclude that the $M^\Pi = 0^+$ three-dipole states presented above are the only class of universal states for identical fermions.

The universal three-dipole states affect scattering processes. As d_ℓ increases, a resonance in three-dipole recombination is expected whenever a three-dipole state passes through the three-body breakup threshold before a new two-dipole state becomes bound. To determine the stability of nonreactive fermionic dipolar gases, however, it is more important to know the general scaling of three-dipole recombination with d_ℓ and the behavior near a dipole-dipole resonance. The threshold behavior of the recombination rate K_3 for three fermionic dipoles can be obtained from a Wigner law analysis [15] of the $M^\Pi = 0^+$, J-odd low-energy-dominant contribution, giving

$$K_3 = \frac{C_3}{\mu} k^4, \qquad (6)$$

where $k = \sqrt{2\mu E}$ is the three-body wave number.

For short-range, nondipolar interactions, the coefficient C_3 in recombination rate is expected to scale with the scattering volume [9,10] and the effective range [10]. For dipolar interactions, however, the scattering physics is fundamentally different even in the two-body level [16]. In particular, we have numerically identified a distinct low-energy expansion of the p-wave phase shift δ for two fermionic dipoles. The real part of δ can be expanded as

$$\mathrm{Re}\,[\delta(k_2)] \approx -ak_2 - bk_2^2 - Vk_2^3 \qquad (k_2 \to 0), \qquad (7)$$

where k_2 is the relative two-dipole wave number. This expansion has a linear term in k_2, implying a nonvanishing scattering length a [16], as expected for r^{-3} interaction, and also a quadratic dependence on k_2, both of which are absent for nondipolar interactions. But, similar to the nondipolar interaction case, the scattering volume V goes through a pole across a dipole-dipole resonance.

Our scaling laws for three-dipole recombination are based on a calculation of the three-dipole scattering matrix using the eigenchannel R-matrix propagation method [17].
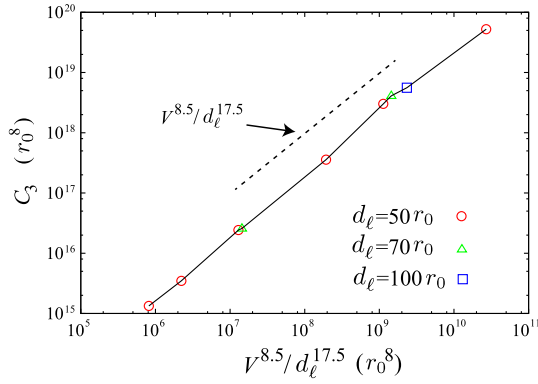
FIG. 3 (color online).   The dependence of the recombination scaling coefficient C_3 on the two-body scattering volume V and the dipole length d_ℓ near a dipole-dipole resonance. The lines connecting the numerical points just guide the eye.

First, the SVD solution of Eq. (1) obtains the R-matrix out to a distance that includes all the sharp avoided crossings. The R-matrix is then propagated farther in the adiabatic representation [13] in the asymptotic region until K_3 is fully converged. K_3 has been calculated for $V > 0$ near a dipole-dipole resonance, where the dipolar dimer is weakly bound. At ultracold energies, our calculation shows that only the lowest three-body continuum channel is important for recombination, and K_3 is dominated by recombination into the weakly bound dipole plus dipolar dimer channel, having the lowest effective angular momentum barrier asymptotically. Figure 3 shows the scaling coefficient C_3 near $m_{2d} = 1$ dipole-dipole resonances for a few d_l with different short-range interactions. The dipole-dipole resonances with higher m_{2d} are not of current interest because of their extremely narrow widths [16]. Dimensional analysis has suggested, and our numerical results in Fig. 3 confirm, that a universal scaling of C_3 exists,

$$C_3 = \lambda V^{17/2} d_\ell^{-35/2}, \qquad (8)$$

where dimensionless $\lambda \approx 2 \times 10^9$. This scaling is stronger with V than for nondipolar interactions [9,10]. Although Eq. (8) also seems to imply a strong suppression of three-dipole recombination with d_ℓ, instead, a general scaling of $C_3 \propto d_\ell^8$ is expected away from a dipole-dipole resonance, due to the d_ℓ^3 scaling of the background value of V [18]. This rapid growth of C_3 with d_ℓ may be unfortunate for experiments that require stable fermionic dipolar gas in three dimensions, since three-dipole recombination can be dramatic even in the ultracold threshold regime ($kd_\ell \ll 1$). On the other hand, scenarios exist where three-body recombination has a positive role, as a means to produce weakly bound dipolar dimers that are stable against collision with a free dipole, in close analogy to the technique used in ultracold spin-mixed fermions with nondipolar interactions [19].

Finally, consider the behavior of deeply bound dipole plus dipolar dimer channels and their impact on the stability of a mixed gas containing both dipoles and dipolar dimers. Similar to the bosonic dipole case [5], these channels have a centrifugal barrier characterized by a noninteger effective angular momentum quantum number, and it grows with increasing d_ℓ. Although our numerical study shows that this d_ℓ dependence is nonuniversal, the effective angular momentum barrier can nevertheless "protect" a mixture of dipoles and dipolar dimers from collisional decay and it may provide an alternative way to tune interactions in a mixed-species gas.

In summary, a class of universal physics has been identified for three fermionic dipoles. For scattering volumes near a dipole-dipole resonance, one universal three-dipole state exists at an energy near the three-dipole breakup threshold. This state has a universal geometry and orientation in the external field, with a variable size dependent on d_ℓ. Moreover, its long lifetime can be beneficial for experimental observation and manipulation. Our study also shows a universal trend of the three-dipole recombination rate, which increases rapidly near each dipole-dipole resonance and grows rapidly with stronger dipolar interactions. And, the effective repulsion between a dipole and a dipolar dimer can be tuned to control collisions in mixed quantum gases.

[1] K.-K. Ni *et al.*, Science **322**, 231 (2008); S. Ospelkaus *et al.*, Phys. Rev. Lett. **104**, 030402 (2010); J. G. Danzl *et al.*, Nature Phys. **6**, 265 (2010).
[2] M. A. Baranov, Phys. Rep. **464**, 71 (2008); L. D. Carr *et al.*, New J. Phys. **11**, 055049 (2009).
[3] S. Ospelkaus *et al.*, Science **327**, 853 (2010); K.-K. Ni *et al.*, Nature (London) **464**, 1324 (2010).
[4] C. Ticknor and S. T. Rittenhouse, Phys. Rev. Lett. **105**, 013201 (2010).
[5] Y. Wang, J. P. D'Incao, and C. H. Greene, Phys. Rev. Lett. **106**, 233201 (2011).
[6] V. Efimov, Sov. J. Nucl. Phys. **12**, 589 (1971); **29**, 546 (1979); Nucl. Phys. **A210**, 157 (1973).
[7] S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **80**, 1215 (2008).
[8] B. D. Esry, C. H. Greene, and J. P. Burke, Phys. Rev. Lett. **83**, 1751 (1999).
[9] H. Suno, B. D. Esry, and C. H. Greene, Phys. Rev. Lett. **90**, 053202 (2003).
[10] M. Jona-Lasinio, L. Pricoupenko, and Y. Castin, Phys. Rev. A **77**, 043611 (2008).
[11] J. P. D'Incao, B. D. Esry, and C. H. Greene, Phys. Rev. A **77**, 052709 (2008).
[12] P. S. Zuchowski and J. M. Hutson, Phys. Rev. A **81**, 060703(R) (2010).
[13] H. Suno *et al.*, Phys. Rev. A **65**, 042725 (2002).

[14] O. I. Tolstikhin, S. Watanabe, and M. Matsuzawa, J. Phys. B **29**, L389 (1996).

[15] B. D. Esry, C. H. Greene, and H. Suno, Phys. Rev. A **65**, 010705(R) (2001).

[16] J. L. Bohn, M. Cavagnero, and C. Ticknor, New J. Phys. **11**, 055039 (2009).

[17] M. Aymar, C. H. Greene, and E. Luc-Koenig, Rev. Mod. Phys. **68**, 1015 (1996).

[18] Y. Wang and C. H. Greene (unpublished).

[19] M. W. Zwierlein *et al.*, Phys. Rev. Lett. **91**, 250401 (2003); S. Jochim *et al.*, *ibid.* **91**, 240402 (2003).