Ultracold atom-molecule collisions with fermionic atoms

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Elastic and inelastic properties of weakly bound *s*- and *p*-wave molecules of fermionic atoms that collide with a third atom are investigated. Analysis of calculated collisional properties of *s*-wave dimers of fermions in different spin states permit us to compare and highlight the physical mechanisms that determine the stability of *s*-wave and *p*-wave molecules. In contrast to *s*-wave molecules, the collisional properties of *p*-wave molecules are found to be largely insensitive to variations of the *p*-wave scattering length, and these collisions will usually result in short molecular lifetimes. We also discuss the importance of this result for both theories and experiments involving degenerate Fermi gases.

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I. INTRODUCTION

In the past decade, the advent of magnetic field control of interatomic interactions near a Feshbach resonance has rapidly sparked both experimental capabilities and theoretical understanding in the field of ultracold quantum gases. Using *s*-wave Feshbach resonances in an atomic Fermi gas with two different spin states [1], fundamental problems such as the crossover between Bose-Einstein condensation and the Bardeen-Cooper-Schrieffer-type superfluidity [2] have become accessible experimentally, allowing tests of fundamental theories and studies of novel phenomena (see [1], and references within). Recently, the observation of *p*-wave Feshbach resonances in spin-polarized Fermi gases [3] instigated theoretical studies that predicted a variety of novel many-body phenomena [4]. Moreover, the recent experimental observation of *p*-wave molecules [5] in a ^{40}K Fermi gas has provided a starting point for further investigations of novel many-body phenomena in the strongly interacting regime [4]. The experimental realization of the theoretical predictions will hinge on the lifetime and stability of *p*-wave molecules, since, e.g., the long lifetime predicted [6] and found [1,7] for *s*-wave molecules was one of the key ingredients that facilitated the observation of fermionic superfluid behavior in dilute gases. In Ref. [5], though, it was found that *p*-wave molecules are short lived, which limits the possible types of states that can be created for *p*-wave molecular condensates.

In this paper, we explore the physics of three-body collisions involving both *s*-wave and *p*-wave molecules with the goal of understanding what determines their different levels of stability. For both *s*- and *p*-wave cases, the dominant contribution to the inelastic atom-molecule rate coefficient at sufficiently low collision energies has *s*-wave character and therefore does not vanish, even at zero temperature. Such processes thus play an important role for atom-molecule mixtures near a *p*-wave Feshbach resonance. Our results indicate that many of the characteristics of *p*-wave $^{40}K_2$ molecules are likely to be shared by other atomic species. This expectation is based on the universal nature of our results that are discussed below. We have also found that, near a *p*-wave Feshbach resonance, *s*-wave atom-molecule collisions are likely to be insensitive to the presence of the Feshbach resonance, in contrast to the *s*-wave case. However, our results indicate that while inelastic *p*-wave atom-molecule collisions are suppressed, elastic *p*-wave atom-molecule collisions are enhanced near a *p*-wave resonance. We then briefly discuss the three-body parameters that might be important for understanding many-body aspects in degenerate Fermi gases with resonant *p*-wave interactions. The primary goal of the present study is to discuss calculations carried out for both *s*- and *p*-wave molecules that highlight the main mechanisms that cause their lifetimes to be so different.

Near a two-body Feshbach resonance, the physics that determines the collisional properties of *s*-wave molecules is closely related to what has been called Efimov physics [8,9]. Efimov physics occurs when the two-body *s*-wave scattering length, $a_s=-\lim_{k\to 0}\tan\delta_s/k$ with δ_s the phase shift and k the wave number, is abnormally large compared to the characteristic range r_0 of the interatomic interactions. For *s*-wave molecules composed of fermions in different spin states, say FF', Efimov physics predicts a universal repulsive effective interaction for $FF'+F$ collisions which is responsible for the $a_s^{-3.33}$ suppression of atomic and molecular losses [6,9]. For $FF'+F$ collisions, Efimov physics also predicts that the atom-molecule scattering length should be $a_{ad}\approx 1.2a_s$ [6], which ensures a strong atom-molecule interaction in the many-body quantum gas, and which provides efficient evaporative cooling near a Feshbach resonance. A positive a_{ad} can also protect the atom-molecule mixture against collapse.

However, as has been shown experimentally [5], near a *p*-wave Feshbach resonance the situation differs strikingly and *p*-wave molecules composed of spin-polarized fermions in a single internal substate, say FF, tend to have short lifetimes. Only recently has atom-molecule scattering for large *p*-wave scattering lengths, $a_p=\lim_{k\to 0}(-\tan\delta_p/k^3)^{1/3}$, been studied [10,11]. (Note that the *p*-wave scattering is sometimes characterized equivalently by the "*p*-wave scattering volume" $V_p\equiv a_p^3$ [10,12].) Three-body recombination of spin-stretched fermions received earlier attention [3,12] where it was shown that the recombination rate could be significant near a *p*-wave resonance despite the Fermi statistics suppression. More recently, the recombination channel in

the *FFF* system was studied using a zero-range *p*-wave pseudopotential interaction [13]. There, the existence of a large number of weakly bound three-body states analogous to the Efimov states for bosons [8] was proposed. In our calculations, we found similar three-body states at the simplest level of approximation of the hyperspherical adiabatic representation. They disappear, however, once nonadiabatic effects are included, which leads us to speculate that these nonadiabatic corrections might also eliminate the three-body states found in Ref. [13]. Moreover, it is not clear whether the energy dependence neglected in their *p*-wave pseudopotentials [14] affects the universality of the results predicted in Ref. [13]. Our results presented here do not suffer from such limitations because our two-body finite range model potential intrinsically includes such corrections.

In this paper we focus on atom-molecule scattering properties and find that both elastic and inelastic *s*-wave *FF*+*F* processes are largely and surprisingly insensitive to variations of a_p and potentially explain the loss rates observed in Ref. [5]. This result agrees with the qualitative arguments in Ref. [10]. We trace the insensitivity of the atom-molecule losses to the weakly attractive effective atom-molecule interaction and to the fact that the size of a *p*-wave molecule is mainly determined by r_0 and therefore does not change as a_p varies, in contrast to *s*-wave molecules whose size is directly related to a_s. Our results, therefore, indicate that the insensitivity to variations of a_p of both elastic and inelastic *FF*+*F* processes is likely to be a universal property of *p*-wave molecules. Based on these results we also speculate on which few-body parameters are important for many-body theories for spin-polarized Fermi gases.

II. THEORETICAL BACKGROUND

We have extracted the three-body elastic and inelastic collisional properties of *s*- and *p*-wave molecules from numerically converged solutions of the three-body Schrödinger equation carried out in the adiabatic hyperspherical representation [15], using model finite-range two-body interactions. This representation offers a simple, unifying picture from which we can quantitatively determine and then qualitatively interpret the origin of the significantly different collisional properties of *s*- and *p*-wave molecules. The use of finite-range two-body interactions allows us to study atom-dimer collisions including deeply bound decay channels in a more realistic fashion. If the three-body collision rates are truly universal, then any two-body interaction can be used that reproduces the two-body scattering length, leaving us free to choose an interaction that is convenient for the numerical calculation. Moreover, the use of a finite-range model ensures the proper energy dependence of the two-body scattering, often neglected in zero-range models, and which can be particularly important for *p*-wave interactions [14]. As we will show below, our finite-range model with multiple bound states confirms the universal predictions obtained using *s*-wave zero-range interactions [6,9] with the advantage that we can, in principle, more quantitatively estimate the limit of the validity of such predictions caused by the finite range of the two-body interactions.

In the adiabatic hyperspherical representation, the three-body system is described in terms of the hyperradius R, which gives the overall size of the system, and a set of five hyperangles [15], which mainly describe the interparticle correlations. In this representation the Schrödinger equation reduces to a system of coupled ordinary differential equations given (in atomic units) by

$$\left[-\frac{1}{2\mu}\frac{d^2}{dR^2}+W_\nu(R)\right]F_\nu(R)+\sum_{\nu'\neq\nu}V_{\nu\nu'}(R)F_{\nu'}(R)=EF_\nu(R), \tag{1}$$

where $\mu=m/\sqrt{3}$ is the three-body reduced mass for three identical particles (m being the atomic mass), E is the total energy, F_ν is the hyperradial wave function, and ν is a collective index that represents all quantum numbers necessary to label each channel. In the above expression, $V_{\nu\nu'}$ are the nonadiabatic couplings calculated in terms of the R derivative of the hyperangular solutions [15]. In Eq. (1), the nonadiabatic couplings $V_{\nu\nu'}$ drive transitions between different channels, represented by the effective potentials W_ν.

In our calculations we have used the two-body model interaction

$$v(r_{ij})=-D\ \mathrm{sech}^2(r_{ij}/r_0), \tag{2}$$

where r_{ij} is the interatomic separation. We have taken r_0 to be the van der Waals length [16] for the ^{40}K atoms, $r_0=\frac{1}{2}(mC_6)^{1/4}\approx 65$ a.u., and m to be the ^{40}K atomic mass. We varied a_s and a_p by changing the potential depth D around the vicinity of the value that produces a weakly bound state of *s*- and *p*-wave character, respectively. For *FFF'* systems we adjusted D to produce two deeply bound *FF'* molecules (one *s*-wave and one *p*-wave) in addition to the weakly bound *s*-wave molecule, and we neglected *FF* interactions. For *FFF* systems, we adjusted D to produce one deeply bound *p*-wave molecule and one weakly bound *p*-wave molecule. In a more realistic model for *p*-wave interactions near a Feshbach resonance, however, one needs to consider the magnetic dipole-dipole interaction which treats the resonance in terms of its angular momentum projection $m_p=0$ and $m_p=\pm 1$ [17]. Our model, which does not include dipole-dipole interactions, is applicable to $m_p=0$ and $|m_p|=1$ resonances individually and does not include coupling between $m_p=0$ and $|m_p|=1$ molecules.

At ultracold energies, the dominant contribution for both *F*+*FF* and *F*+*FF'* collisions comes from the relative *s* wave, which implies that the dominant three-body symmetry for *FFF'* is $J^\pi=0^+$ (J is the total orbital angular momentum and π is the total parity) while for *FFF* it is $J^\pi=1^-$. Figure 1 shows typical effective potentials W_ν for *FFF'* [Fig. 1(a)] and *FFF* systems [Fig. 1(b)] obtained for $a_s\approx 300$ and $a_p\approx 170$ a.u., respectively. For these scattering lengths, the binding energy for *s*-wave molecules, $E_b^s\approx 1/ma_s^2$, and *p*-wave molecules, $E_b^p\approx 2r_p/ma_p^3$ [18], are comparable, making it easier to contrast the two cases.

In Fig. 1 the series of effective potentials that converge to zero as $R\to\infty$ are three-body continuum channels representing collisions between three free atoms. Lower-lying potentials represent atom-molecule entrance or escape channels;

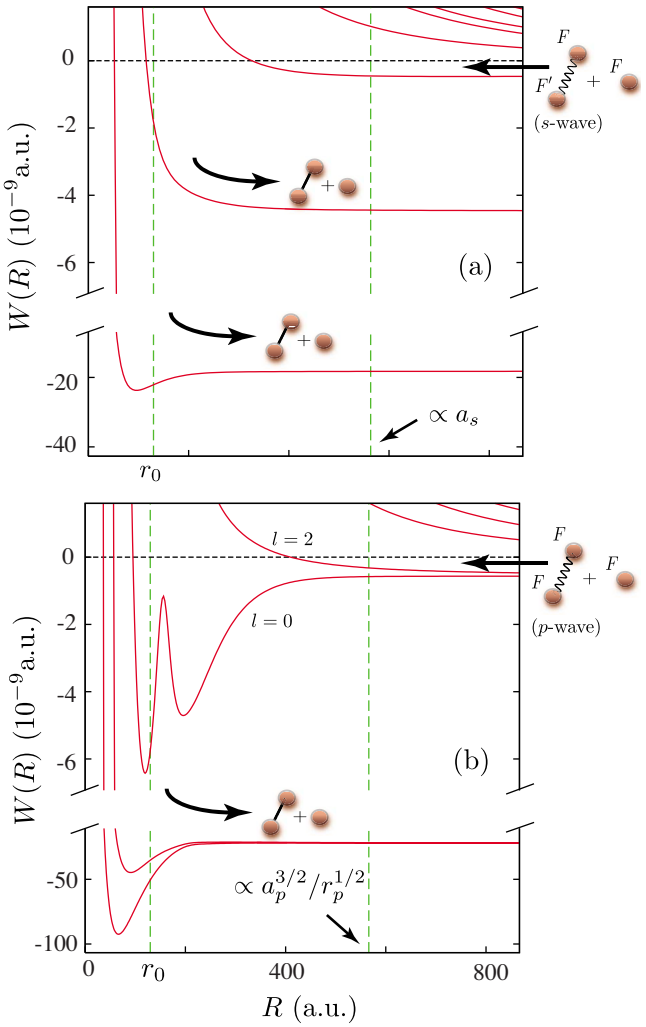

FIG. 1. (Color online) Three-body effective potentials for (a) $J^{\pi}=0^{+}$ FFF' fermionic systems with s-wave resonant interaction and for (b) $J^{\pi}=1^{-}$ FFF spin-polarized fermionic systems with p-wave resonant interactions. As is discussed in the text, these potentials illustrate the main mechanisms that produce different collisional behaviors of the s- and p-wave molecules presented here.

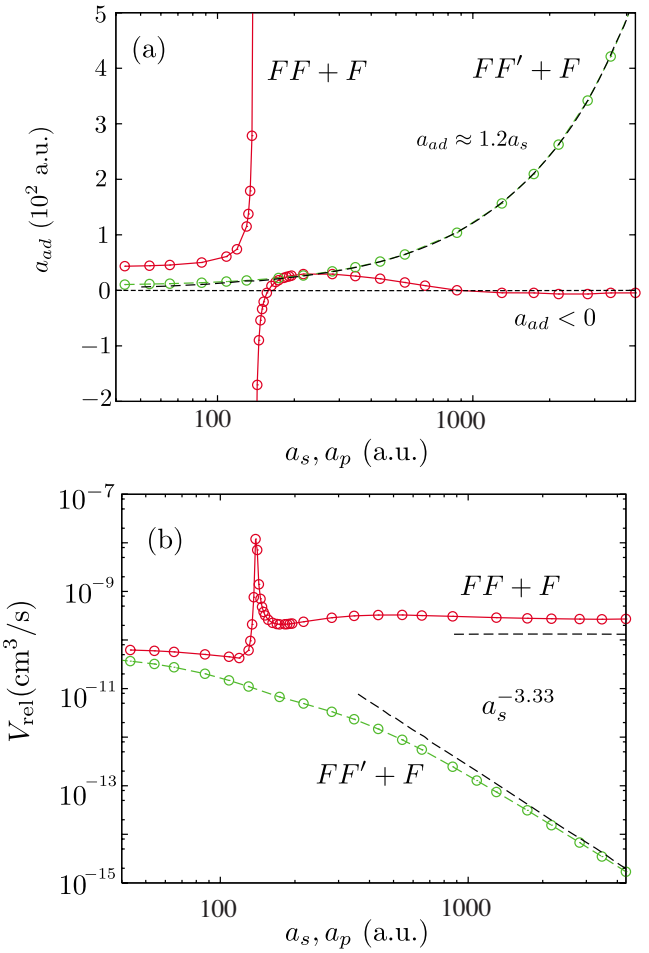

FIG. 2. (Color online) Numerical calculations for the (a) atom-molecule scattering length a_{ad} and (b) vibrational relaxation rate V_{rel} for $J^{\pi}=0^{+}$ $FF'+F$ (dash-circle line) and $J^{\pi}=1^{-}$ $FF+F$ (solid-circle line) collisions as a function of a_s and a_p, respectively. While for $FF'+F$ collisions a_{ad} and V_{rel} show a strong dependence on a_s, for $FF+F$ they are essentially insensitive to variations of a_p.

notice that there are two $FF+F$ channels in Fig. 1(b) converging to the p-wave FF molecule energy at large R due the possible $l=0$ and $l=2$ atom-molecule relative angular momenta allowed for $J^{\pi}=1^{-}$. In Fig. 1 we also sketch the elastic and inelastic pathways that are of interest here.

From the figure, we notice a fundamental difference between the initial $FF'+F$ and $FF+F$ collision channels. For $FF'+F$ collisions, the effective potential is repulsive (proportional to $1/R^2$ [9]) in the range $r_0 \ll R \ll a_s$, while the $l=0$ effective potential for $FF+F$ collisions is attractive in the analogous range $r_0 \ll R \ll a_p^{3/2}/r_p^{1/2}$ [the quantity $a_p^{3/2}/r_p^{1/2}$ can be understood from the length scale defined by the molecular binding energy $1/k_p=(mE_b^p)^{-1/2}$]. The presence of a repulsive barrier for $FF'+F$ collisions whose range scales with a_s suggests that a_{ad} should be proportional to a_s, in analogy to scattering from a hard sphere of radius a_s. The inelastic processes for this case, however, should be suppressed as a_s increases, since it becomes increasingly difficult for the system to tunnel to the region $R \approx r_0$ where the coupling to the deeper molecular states lies [we have verified this statement from our calculations of the nonadiabatic couplings in Eq. (1)]. In fact, in Ref. [9] it was demonstrated that the suppression of the inelastic losses scale with a as $a_s^{1-2p_0}=a_s^{-3.33}$, where p_0 is related with the strength of the repulsive potential barrier in the range $r_0 \ll R \ll a_s$. In contrast, the presence of an attractive potential for $FF+F$ collisions instead of a repulsive potential allows the atom and molecule to approach each other closely without any suppression of the inelastic transition probability. In addition, the absence of a repulsive barrier does not allow us to make an analogy to scattering from a hard sphere, which implies that a_{ad} is not necessarily a simple function proportional to a_p.

In Refs. [10,11], it has been speculated that there is one trimer state in this attractive potential that can cause resonant enhancement of the elastic and inelastic rates when varying a_p. As we show below, in our calculations (see Fig. 2) we do observe resonant effects for elastic and inelastic $FF+F$ collisions, and we do associate them with the formation of a trimer state as predicted in Refs. [10,11]. However, we be-

lieve such trimer states are likely to be nonuniversal in the sense that their energy as a function of a_p depends on the short-range physics not fully represented by the two-body parameters in Refs. [10,11]. Therefore, the resonant peaks in the elastic and inelastic rates will likely depend on a purely three-body nonuniversal parameter, similar to the problem with identical bosons where all three-body observables depend on a three-body parameter representing the short-range physics [8,9,19].

III. ELASTIC AND INELASTIC ATOM-MOLECULE COLLISIONS

We have verified the qualitative behavior described above for the elastic and inelastic rates by solving the Schrödinger equation (1) in coupled hyperradial form using an R-matrix approach [20]. We define the atom-molecule scattering length in terms of the real part of the complex phase shift obtained from the S-matrix element $[\exp(2i\delta_{ad})=S_{ad,ad}]$ associated with the atom-molecule channel,

$$a_{ad} = -\lim_{k_{ad}\to 0} \frac{\mathrm{Re}[\tan\,\delta_{ad}]}{k_{ad}}, \tag{3}$$

with $k_{ad}=[2\mu_{ad}(E+E_b)]^{1/2}$, where $\mu_{ad}=2m/3$ and E_b is the binding energy of the weakly bound dimer. For inelastic collisions, we define the vibrational relaxation rate V_{rel} as

$$V_{\mathrm{rel}} = \sum_f \frac{(2J+1)\pi}{\mu_{ad}k_{ad}}|S_{f\leftarrow i}|^2, \tag{4}$$

where i represents the initial collision channel (atom + weakly bound molecule), and f, all possible final collision channels (atom+deeply bound molecule). We have calculated a_{ad} and V_{rel} for values of a_s and a_p ranging from $r_0(\approx 65$ a.u.) up to approximately $70r_0$ at a collision energy of 1 nK, in order to satisfy the $k_{ad}\to 0$ limit in Eq. (3). The results are shown in Figs. 2(a) and 2(b).

For $FF'+F$ collisions, we have obtained both a_{ad} and V_{rel} in the $a_s \gg r_0$ regime that verifies the $a_{ad}\approx 1.2a_s$ universal prediction [6] and reproduces the strong $a_s^{-3.33}$ suppression of the inelastic rate [6,9]. This scenario is rather favorable for the realization of cold atom-molecule mixtures since it combines strong elastic rates with suppression of atomic and molecular losses.

On the other hand, $FF+F$ elastic and inelastic processes involving p-wave molecules are quite different. For smaller values of a_p, we observe a strong variation of both a_{ad} and V_{rel} (see Fig. 2) due to the presence of a trimer state [10,11] that becomes unbound as a_p increases. As we mentioned before, we do not expect the energy of such a trimer state, nor the value of a_p at which it appears, to be universal, since they both depend on the short-range physics. Consequently, the resonance position in Fig. 2 can change, and eventually disappear, for different choices of the two-body interaction. However, near a p-wave two-body Feshbach resonance, i.e., in the regime $a_p \gg r_0$, our results for a_{ad} and V_{rel} are insensitive to variations of a_p. We rationalize this result by recognizing that even though a_p changes substantially, the size of the weakly bound p-wave molecule is practically unchanged. We expect that this insensitivity of a_{ad} and V_{rel} to variations of a_p is universal but that their actual values will not be universal since the system must access small R where details of the two-body interactions become important. Further, it can be demonstrated by a simple WKB analysis [9] that the constant character of V_{rel} as a function of a_p is ensured provided the effective potential falls off faster than $1/R^2$. From our numerical calculations, for instance, we found that $a_{ad}<0$ in the regime $a_p \gg r_0$, in contrast to the $a_{ad}>0$ result of Refs. [10,11].

The consequences of the three-body physics discussed above for the lifetime and stability of spin-polarized fermionic mixtures of atoms and molecules are very different from the scenario found for a gas of fermions in two different spin states. The constant value of a_{ad} for $a_p \gg r_0$ means that atom-molecule collisions will not help much for evaporative cooling, unless a_{ad} is unnaturally large. More importantly, the insensitivity of V_{rel} to a_p implies that the molecular lifetimes do not change as we approach the point of divergence of a_p, in contrast to s-wave molecules whose lifetime increases near a zero-energy Fano-Feshbach resonance. These results are in agreement with recent experimental data for an atom-molecule gas mixture of ^{40}K atoms [5], where it was found that the lifetimes of both $m_p=0$ and $|m_p|=1$ molecules do not depend on the magnetic field and therefore on a_p. In Ref. [5], however, it was found that the molecules were shorter lived than one would expect based on the magnetic field independent two-body dipolar relaxation rates. More recently [21], loss rates substantially below those found in [5] were observed after the atoms had been removed from the trap, leaving only molecules. Therefore, since both dipolar relaxation and atom-molecule collisions yield molecular losses independent of the magnetic field, we believe that the shorter molecular lifetimes were due to vibrational relaxation as we have calculated here. Our prediction of approximately constant atom-molecule losses also demonstrates that even when atoms are prepared in their lowest hyperfine state, and therefore dipolar relaxation is energetically forbidden, a magnetic field independent molecular lifetime is likely to be found for other atomic species, but now limited by three-body loss processes. In the absence of atoms, molecule-molecule elastic and inelastic processes should also be important. We speculate that these are also likely to be insensitive to variations of a_p (see also Ref. [11]), based on the fact that the size of a p-wave molecule does not depend on a_p.

IV. FEW-BODY PARAMETERS FOR MANY-BODY THEORIES

The fact that a_{ad} does not seem to depend on a_p raises the question whether a_{ad} will be the important parameter for theories attempting to describe many-body aspects of atom-molecule mixtures in spin-polarized Fermi gases. A constant value of a_{ad} across a Feshbach resonance essentially means that the atom-molecule interaction does not "feel" the presence of the p-wave resonance. From this perspective, the atom-molecule interaction is not controllable, and the atom-molecule mixture cannot be claimed to be strongly interacting near the resonance. For this reason, we have also per-

formed some preliminary calculations to explore p-wave atom-molecule collisions. For $J^{\pi}=0^{+}$, 1^{+}, and 2^{+} (which are all the symmetries that allow p-wave collisions between an atom and a p-wave molecule), we have found that the three-body effective potentials are now repulsive in the range $r_0 \ll R \ll a_p^{3/2}/r_p^{1/2}$, instead of attractive as found for $J^{\pi}=1^{-}$. The presence of such a repulsive barrier suppresses inelastic p-wave atom-molecule collisions [9], making these collisions less important than s-wave collisions in determining the lifetime of p-wave molecules. On the other hand, the repulsive barrier indicates that the p-wave atom-molecule scattering length a_{ad}^{p}, should be proportional to $a_p^{3/2}/r_p^{1/2}$, again in analogy to scattering from a hard sphere. Therefore, it is likely that a_{ad}^{p} will be an important parameter for many-body theories of atom-molecule mixtures near a p-wave resonance, since a_{ad}^{p} is a controllable parameter. Experimentally, however, p-wave atom-molecule interactions will be comparably difficult to control as p-wave atom-atom interactions because of the suppression of the energy dependent elastic cross sections. Certainly, it will be necessary to explore in depth the importance of a_{ad}^{p}, but this discussion is outside the scope of this paper.

V. SUMMARY

In this paper, we have determined the atom-molecule scattering length a_{ad}, and vibrational relaxation rate V_{rel} for collisions involving s- and p-wave molecules of fermionic atoms as a function of a_s and a_p, which can be controlled with two-body Feshbach resonances. We have determined a_{ad} and V_{rel} for s-wave molecules of fermionic atoms in different spin states, verifying previously derived results. We could thus identify the mechanisms that control the collisional properties of p-wave molecules. For spin-polarized systems, we have found that both a_{ad} and V_{rel} are insensitive to variations of the two-body p-wave scattering length a_p for $a_p \gg r_0$, consistent with the recent experimental data in Ref. [5]. We expect the results for a_{ad} and V_{rel} to be universal with respect to their insensitivity to variations of a_p but their values can change for different atomic species. We also speculated that, due to the constant character of a_{ad}, the relevant parameter for many-body theories for a spin-polarized mixture of atoms and molecules is likely to be associated with p-wave collisions between a fermionic atom and a p-wave molecule. Our preliminary results indicate that the p-wave scattering length for such collisions, a_{ad}^{p}, is likely to be proportional to $a_p^{3/2}/r_p^{1/2}$.

Note that the very recent preprint by Jona-Lasinio *et al.* [10] argues that the threshold exponent for three-body recombination of spin-polarized fermions should be proportional to $K_3 \propto a_p^{15/2} r_p^{1/2}$ at large p-wave scattering lengths. This differs slightly from the prediction of Suno *et al.* [12] that $K_3 \propto a_p^{8}$. The derivation of Suno *et al.* was, in fact, based on dimensional analysis, starting from the assumption that a_p was the dominant length scale. In fact, it is now understood that a_p alone does not adequately describe the dominant length scale for two-body p-wave scattering, implying that a modification of the dimensional analysis prediction of Suno *et al.* should be expected. Investigation of this point will be relegated to future studies.

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