Dramatic Reductions in Inelastic Cross Sections for Ultracold Collisions near Feshbach Resonances

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We show that low-energy inelastic cross sections can decrease as well as increase in the vicinity of a zero-energy Feshbach resonance. When an external field is used to tune across such a resonance, the real and imaginary parts of the scattering length show asymmetric oscillations with both peaks and troughs. In favorable circumstances, the inelastic collision rate can be reduced to almost zero. This may be important for efforts to achieve evaporative and sympathetic cooling for molecules.

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Cold and ultracold molecules have fascinating properties that will find applications in many areas of physics, ranging from precision measurement to quantum computing [1]. Ultracold molecules offer new possibilities for quantum simulations and quantum control, while quantum gases of ultracold polar molecules are expected to exhibit a wide range of new quantum phases.

Cold and ultracold molecules must always be confined in traps, and trap losses are crucial. In particular, collisional stability is very important. Magnetic and electrostatic traps can trap molecules only when they are in low-field-seeking states, and such states are never the lowest in the applied field. Any inelastic collision that transfers internal energy into relative translational motion causes either heating or trap loss. It is thus very important to understand inelastic collisions and to find ways to minimize them. The purpose of the present Letter is to show that inelastic collision rates can sometimes be dramatically reduced by tuning close to a Feshbach resonance [2] with an applied electric or magnetic field.

It has been possible for about 5 years to create molecules in highly vibrationally excited states in ultracold atomic gases [3], both by photoassociation [4] and by magnetoassociation [5]. A major goal was achieved in 2008 when Ni *et al.* [6] succeeded in transfering KRb molecules formed by magnetoassociation at $T = 350$ nK into their ground rovibrational state by stimulated Raman adiabatic passage (STIRAP). Experiments on collisional trap loss are already under way [7]. Danzl *et al.* [8,9] and Lang *et al.* [10] have carried out analogous experiments on Cs_2 and triplet Rb_2, respectively. There have also been considerable successes in direct photoassociation to produce low-lying states [11–14].

Methods based on photoassociation and magnetoassociation are limited to molecules formed from atoms that can be laser cooled, such as the alkali metals. However, a wider range of molecules can be cooled directly from high temperature to the millikelvin regime, using methods such as buffer-gas cooling [15] and Stark deceleration [16]. Polar molecules such as ND_3 and OH can be held in electrostatic or alternating current traps [17,18], while paramagnetic molecules such as CaH, O_2, NH, and OH can be held in magnetic traps. However, at present the lowest temperatures that can be achieved in static traps are around 10 mK, and there are a variety of proposals for ways to cool the molecules further, including evaporative cooling, sympathetic cooling, and cavity-assisted cooling [19–21].

Magnetic fields have important effects on the interactions and collisions of paramagnetic molecules [22–24]. In a previous work [25], we explored the use of Feshbach resonances to *control* molecular collisions with applied fields. For the prototype system He + NH ($^3\Sigma^-$), we located magnetic fields at which bound states cross open-channel thresholds and then characterized the resulting low-energy Feshbach resonances as a function of magnetic field. For a resonance at which a bound state crosses the *lowest* open-channel threshold, the real scattering length a behaves in the same way as in the atomic case [26] and exhibits a pole as a function of magnetic field B. However, for resonances in which a state crosses a *higher* threshold, we observed quite different behavior. In this case, inelastic scattering can occur and the scattering length is complex. The complex scattering length $a(B) = \alpha(B) - i\beta(B)$ was found to follow the formula [25]

$$a(B) = a_{\rm bg} + \frac{a_{\rm res}}{2(B - B_{\rm res})/\Gamma_B^{\rm inel} + i}, \qquad (1)$$

where $a_{\rm bg}$ is a slowly varying background term and $B_{\rm res}$ and $\Gamma_B^{\rm inel}$ are the position and width of the resonance. The *resonant scattering length* $a_{\rm res}$ characterizes the strength of the resonance. The elastic and total inelastic cross sections are given approximately by

$$\sigma_{\rm el}(B) \approx 4\pi|a(B)|^2 \quad \text{and} \quad \sigma_{\rm inel}^{\rm tot}(B) \approx \frac{4\pi\beta(B)}{k_0}. \qquad (2)$$

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The inelastic scattering in He + NH is very weak except near resonance. Under these circumstances, $\sigma_{\rm el}(B)$ shows a symmetric oscillation at resonance and $\sigma_{\rm inel}^{\rm tot}(B)$ shows a simple peak [25]. This corresponds to a real value of $a_{\rm res}$. However, a more complete derivation [27] subsequently showed that, when the background scattering is significantly inelastic, it is possible for $a_{\rm res}$ to be complex. When this occurs, inelastic cross sections show troughs as well as peaks near resonance. This is potentially of great importance, since inelastic collisions generally provide trap loss mechanisms and since strong inelastic processes can prevent evaporative or sympathetic cooling.

In this Letter, we consider a more strongly coupled system, with significant inelastic scattering, in order to demonstrate the dramatic reductions in inelasticity that can occur near Feshbach resonances. The system we have chosen is ^{4}He + $^{16}O_2$ ($^3\Sigma_g^-$), for which a reliable potential energy surface has been calculated by Groenenboom and Struniewicz [28]. The $^{16}O_2$ molecule has a ground state with rotational quantum number $n = 1$ because the ^{16}O nucleus is a boson with nuclear spin $I = 0$. The bound-state Schrödinger equation for ^{4}He + $^{16}O_2$ is solved by propagating coupled differential equations using the BOUND package [29,30], as modified to handle magnetic fields [25]. The calculations are carried out in a completely decoupled basis set [23], $|nm_n\rangle|sm_s\rangle|Lm_L\rangle$, where $s = 1$ is the electron spin of O_2 and L is the end-over-end rotational angular momentum of He and the molecule. All of the m quantum numbers represent space-fixed projections on the axis defined by the magnetic field. The only good quantum numbers are the parity $(-1)^{n+L+1}$ and the total projection quantum number $M_{\rm tot} = m_n + m_s + m_L$. At energies above the lowest threshold, BOUND locates both physical quasibound states and artificial states that result from box quantizing the continuum for open channels. However, it is straightforward to identify the physical states by inspecting the dependence of the eigenvalues on the outer limit of the propagation.

Figure 1 shows the bound and quasibound states of the ^{4}He-$^{16}O_2$ complex near the $n = 1$ thresholds as a function of magnetic field B, with artificial levels removed, together with the thresholds for dissociation to form He + O_2. The thresholds are characterized at zero field by O_2 quantum numbers n, s, and j, with $s = 1$ and $j = 0, 1, 2$ for $n = 1$; each one splits into $2j + 1$ components labeled by m_j at nonzero magnetic field. He-O_2 is a weakly anisotropic system, so n and s remain nearly good quantum numbers and the levels of the complex are characterized by additional quantum numbers L and J, where the total angular momentum J is the resultant of j and L. At zero field, each (n, j, and L) level splits into $\min(2j + 1, 2L + 1)$ sublevels with different values of J. When a magnetic field is applied, each sublevel splits into $2J + 1$ components with different values of $M_{\rm tot}$. The J quantum number remains a useful label for magnetic fields up to about 1000 G, but above that, the levels of different J are strongly mixed. By about 5000 G, the levels have separated into groups that may be labeled with an approximate quantum number $\tilde{m}_j$ that takes values from $-j$ to $+j$.

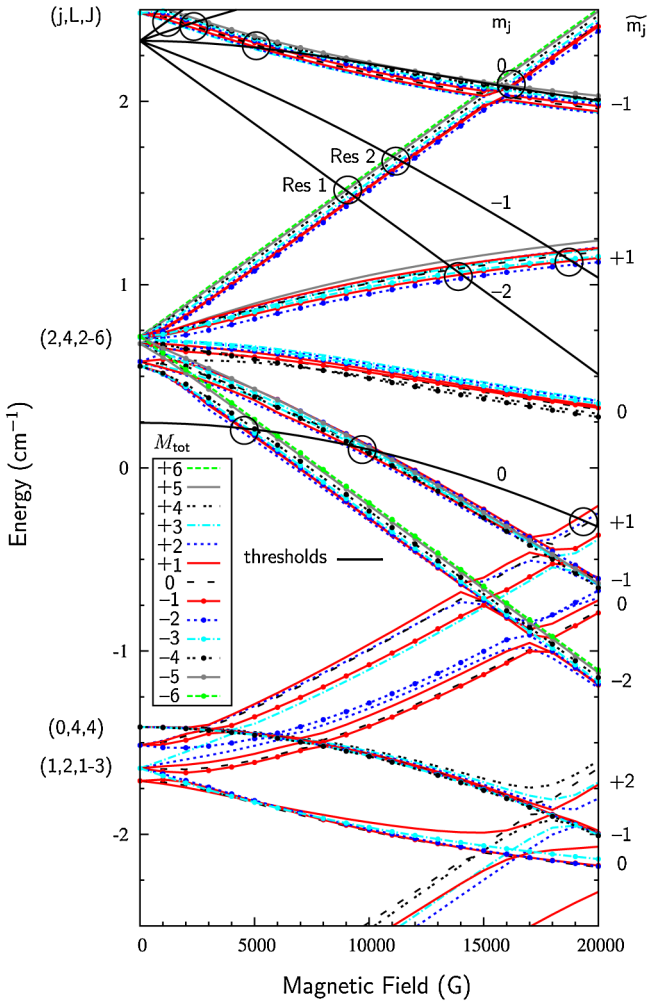

FIG. 1 (color online). The pattern of levels from bound-state calculations on ^{4}He-$^{16}O_2$ near the $n = 1$ thresholds, with artificial levels removed, as a function of magnetic field B. The calculations are for even parity, $M_{\rm tot} = -6$ to $+6$. The $^{16}O_2$ threshold energies are shown as solid black lines. The circles show crossings between bound states and thresholds with $m_j = M_{\rm tot}$ that produce zero-energy Feshbach resonances in s-wave scattering.

Crossings between quasibound states and thresholds will produce zero-energy Feshbach resonances in s-wave scattering if an $L = 0$ scattering channel is permitted by the constraints on parity and $M_{\rm tot}$. This occurs only for thresholds corresponding to $m_j = M_{\rm tot}$ as shown by the circles in Fig. 1. In the present work, we are particularly interested in resonances that occur at *excited* thresholds, where inelastic scattering may occur.

Once the crossing points have been located in Fig. 1, we carry out scattering calculations, holding the kinetic energy fixed at a small value while sweeping the magnetic field across the resonance. This is done using the MOLSCAT

package [31], as modified to handle collisions in magnetic fields [25].

Typical resonance profiles for $^4He + O_2$ are shown in Fig. 2 for the resonance labeled 1 in Fig. 1 at collision energies $E = 1\ \mu K$, 100 μK, and 10 mK. At all three energies, the total inelastic cross section (summed over outgoing partial waves L') drops by almost a factor of 1000 from its background value at a field just below B_{res}. At higher energies, the resonance is shifted slightly, but the resonant suppression is just as strong. The resonant contribution to the inelastic cross section follows the $E^{-1/2}$ Wigner threshold law [32] only at very low collision energies (below 100 μK). At higher energies, it actually decreases *faster* than predicted by the threshold law and the elastic cross section also decreases. The p-wave contribution to the inelastic cross section is nonresonant and increases approximately as $E^{+1/2}$ with energy while the s-wave contribution decreases. For the resonance in Fig. 2, its value is about 1 Å^2 at 10 mK so that p-wave scattering will dampen the suppression of inelastic scattering at temperatures above this.

The resonances for $He + O_2$ are quite wide, with $|\Gamma_B| =$ 250–500 G. The resonance in Fig. 2 provides substantial suppression of inelastic cross sections across a range of at least 100 G. This would be sufficient to provide a working energy range of about 10 mK for magnetically trapped states of a molecule in a $^3\Sigma$ electronic state. The broad resonances observed here contrast with those previously characterized for He-NH, which had $|\Gamma_B| < 10^{-2}$ G [25]. The difference arises in this case because the $n = 1$ closed channels involved for O_2 are directly coupled to the inelastic channel(s) by the potential anisotropy, whereas the $n = 0$ closed channels involved for NH were only indirectly coupled to the open channels. However, broad resonances are likely to be common in molecule-molecule systems and indeed in atom-molecule systems involving atoms heavier than He because the couplings due to potential anisotropy are much stronger in heavier systems [33,34].

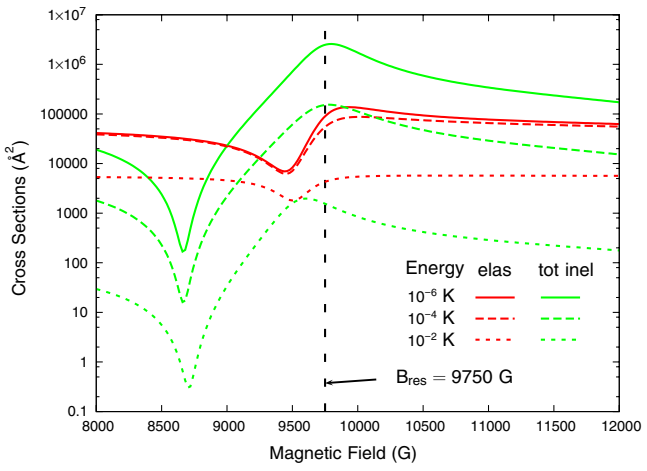

FIG. 2 (color online). Elastic (red) and total inelastic (green) cross sections for resonance 1 in $He + O_2$ as a function of magnetic field at collision energies of 10^{-6} K (solid lines), 10^{-4} K (dashed lines), and 10^{-2} K (dotted lines).

The asymmetric line shapes observed here are analogous to Fano line shapes [35] in bound-free absorption spectra. Fano considered the interference between the bound and continuum contributions to a transition matrix element near resonance. He showed that the bound-state contribution rises from zero to a peak at resonance while the continuum contribution drops from its background value to zero and changes sign at resonance. When there is only a single continuum channel, there is always a point near resonance where the bound and continuum contributions cancel completely. However, when there are N outgoing channels, there is one particular linear combination of them that is coupled to the bound state and $N - 1$ orthogonal linear combinations that are not [35]. The resonance suppresses inelastic scattering into the former but not into the latter, so the cross section does not drop to zero.

For low-energy resonant scattering in the presence of inelastic channels, the partial width for the incoming (elastic) channel is proportional to the incoming wave vector k_0, while the partial widths for the inelastic channels are essentially independent of k_0 [27]. At low energies, we may therefore consider the bound state to be coupled only to the outgoing (inelastic) channels and apply Fano theory directly to the inelastic cross sections.

Even for $^{16}O_2$ molecules at the $j = 2$, $m_j = -2$ threshold, which can relax only to form $j = 0$, $m_j = 0$, there are outgoing channels with several values of L'. For s-wave scattering ($L = 0$), L' must be at least Δm_j and must be even to conserve parity. The kinetic energy release of 1.9 K at $B = 9750$ G is above the centrifugal barrier for $L = 2$ (0.4 K) but below that for $L = 4$ (2.4 K). Because of this, the $L = 2$ channel dominates the inelastic scattering away from resonance *and* is the outgoing channel most strongly coupled to the bound state. The inelastic cross section therefore shows a deep minimum, though there is still a little background inelastic scattering that is not suppressed by the resonance.

The situation is somewhat different for resonances at the $j = 2$, $m_j = -1$ threshold, such as that shown in Fig. 3 (resonance 2 in Fig. 1). In this case, the resonance suppresses the total inelastic cross section by less than a factor of 10 from its background value. At 11660 G, the kinetic energy release is 0.55 K for relaxation to the $j = 2$, $m_j = -2$ (upper) threshold and 2.3 K for relaxation to the $j = 0$, $m_j = 0$ (lower) threshold. The $L = 2$ outgoing channels at both inelastic thresholds contribute significantly to the inelastic scattering far from resonance. However, the resonant bound state (with $m_j = +2$) is coupled much more strongly to $j = 0$, $m_j = 0$ channels than to $j = 2$, $m_j = -2$ channels. The resonance therefore suppresses inelastic scattering into the lower channel, but there is significant background inelastic scattering into the upper channel that is unaffected by the resonance.

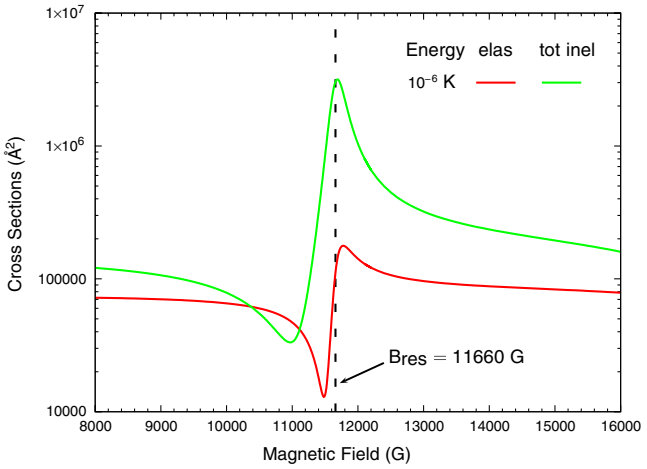

FIG. 3 (color online). Elastic (red) and total inelastic (green) cross sections for resonance 2 in $He + O_2$ as a function of magnetic field at collision energy 10^{-6} K.

The kinetic energy release needed to surmount centrifugal barriers depends on the reduced mass and will be smaller in heavier systems than for $He + O_2$, as will the temperature range in which *s*-wave scattering dominates. However, much lower temperatures are already being achieved in current experiments [6,9].

We conclude that inelastic cross sections may sometimes be reduced dramatically by tuning near a Feshbach resonance. This may be very important for attempts to produce ultracold molecules by evaporative or sympathetic cooling: applying a suitable bias field could suppress inelastic collisions near the bottom of a trap and allow cooling in cases where it would otherwise be prevented by inelastic losses. The reduction may occur for any atom or molecule in an internally excited state, but it is most dramatic when there is a single outgoing channel that dominates the inelastic scattering and is strongly coupled to the resonant channel. A common example of this will be systems in which all but one of the outgoing channels are suppressed by centrifugal barriers.

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