# Inelastic losses in radio-frequency-dressed traps for ultracold atoms

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We calculate the rates of inelastic collisions for ultracold alkali-metal atoms in radio-frequency-dressed traps, using coupled-channel scattering calculations on accurate potential energy surfaces. We identify a radio-frequency-induced loss mechanism that does not exist in the absence of radio frequency (rf) radiation. This mechanism is not suppressed by a centrifugal barrier in the outgoing channel, and can be much faster than spin relaxation, which is centrifugally suppressed. We explore the dependence of the rf-induced loss rate on singlet and triplet scattering lengths, hyperfine splittings, and the strength of the rf field. We interpret the results in terms of an adiabatic model of the collision dynamics, and calculate the corresponding nonadiabatic couplings. The loss rate can vary by 10 orders of magnitude as a function of singlet and triplet scattering lengths. <sup>87</sup>Rb is a special case, where several factors combine to reduce rf-induced losses; as a result, they are slow compared to spin-relaxation losses. For most other alkali-metal pairs, rf-induced losses are expected to be much faster and may dominate.

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## I. INTRODUCTION

Radio-frequency-dressed traps [1,2] have been widely used [3] to confine ultracold atoms in complex geometries, including shells [4] and rings [5]. These geometries are valuable in many fields, including condensate splitting and atom interferometry [6] and the study of low-dimensional quantum systems [7]. The atoms are trapped using a combination of magnetic and radio frequency (rf) fields, and are confined in an adiabatic potential obtained by diagonalizing a simple Hamiltonian in a basis set of rf-dressed atomic states. Radio frequency dressing has also been used to form new structures in optical lattices [8,9].

There are various sources of losses of atoms from rf-dressed traps. The rf-dressed state that is adiabatically trapped is not the lowest that exists, and Burrows *et al.* [10] have considered one-body losses due to nonadiabatic transitions to lower states. Such losses may be made acceptably small by avoiding very low rf coupling strengths. However, the presence of rf radiation introduces additional loss mechanisms that are not present for atoms in a purely magnetic trap, due to rf-induced inelastic collisions.

Tscherbul *et al.* [11] have developed a coupled-channel theory of atomic collisions in rf fields and applied it to rf-induced resonances in <sup>87</sup>Rb. Hanna *et al.* [12] developed an approach based on multichannel quantum defect theory, and also explored rf-induced resonances in <sup>87</sup>Rb and <sup>6</sup>Li. However, Hanna *et al.* stated that calculations with their method were impractical close to atomic rf transitions, which is precisely the case that is required to investigate collisions of atoms in rf-dressed traps. Owens *et al.* [13] have shown that rf dressing can be used to create new Feshbach resonances at desired magnetic fields that are convenient for atomic cooling. These resonances may be valuable for molecule formation, particularly in heteronuclear systems.

Most experimental work with rf-dressed traps to date has used <sup>87</sup>Rb atoms. However, there is considerable interest in extending this to other atomic species. In this paper we use coupled-channel calculations to explore the rates of rf-induced inelastic collisions theoretically. We show that <sup>87</sup>Rb is a special case, where the losses induced by rf radiation are very small. Most other alkali-metal atoms may be expected to have much faster rf-induced collisional losses.

### **II. METHODS**

We use the convention that lower-case quantum numbers refer to individual atoms and upper-case quantum numbers refer to the colliding pair. In the absence of fields, each atom is described by its electron spin s = 1/2 and nuclear spin *i*, which couple to form a resultant *f*. In a magnetic field *B*, each state splits into components labeled by  $m_f = m_s + m_i$ , where each *m* is the projection of the corresponding quantity on the magnetic field axis *Z*. The Hamiltonian for each atom is

$$\hat{h} = \zeta \hat{i} \cdot \hat{s} + (g_S \hat{s}_z + g_i \hat{i}_z) \mu_{\rm B} B, \tag{1}$$

where  $\zeta$  is the hyperfine coupling constant and  $g_s$  and  $g_i$  are electron and nuclear spin g factors with the sign convention of Arimondo *et al.* [14]. At the low magnetic fields considered here, f is nearly conserved but  $m_s$  and  $m_i$  are not.

To incorporate the effects of rf radiation on a single atom, we use a basis set of photon-dressed functions in an uncoupled representation,  $|sm_s\rangle|im_i\rangle|NM_N\rangle$ , where N is the photon number with respect to the average photon number  $N_0$ . In the present work we focus on circularly polarized radiation, with either  $M_N = N$  (right-circularly polarized,  $\sigma_+$ ) or  $M_N = -N$ (left-circularly polarized,  $\sigma_-$ ). In the present work we consider  $\sigma_-$  polarization, with  $B(t) = B_{\rm rf}[\hat{e}_x \cos 2\pi vt - \hat{e}_y \sin 2\pi vt]$ , where  $\hat{e}_x$  and  $\hat{e}_y$  are unit vectors along the X and Y axes. The Hamiltonian of the rf field is

$$\hat{h}_{\rm rf} = h \nu (\hat{a}_{-}^{\dagger} \hat{a}_{-} - N_0),$$
 (2)

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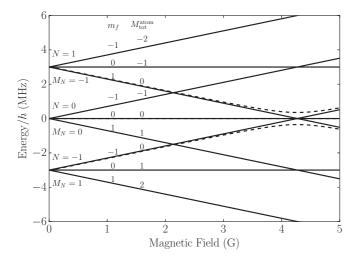


FIG. 1. rf-dressed atomic levels of f = 1 states of <sup>87</sup>Rb for frequency 3.0 MHz and photon numbers N = -1, 0, and 1, shown with respect to the energy of the f = 1,  $m_f = 0$  state for N = 0. Solid lines show levels for zero rf intensity and dashed curves show levels for  $B_{\rm rf} = 0.5$  G with  $M_{\rm tot}^{\rm atom} = 0$ . Atoms can be trapped at the minimum in the upper dashed curve.

where  $\hat{a}_{-}$  and  $\hat{a}_{-}^{\dagger}$  are photon annihilation and creation operators for  $\sigma_{-}$  photons. Its interaction with an atom is

$$\hat{h}_{\rm rf}^{\rm int} = \frac{\mu_{\rm B} B_{\rm rf}}{2\sqrt{N_0}} [(g_S \hat{s}_+ + g_i \hat{i}_+) \hat{a}_-^\dagger + (g_S \hat{s}_- + g_i \hat{i}_-) \hat{a}_-], \quad (3)$$

where  $B_{\rm rf}$  is the amplitude of the oscillating magnetic field,  $\hat{s}_+$ and  $\hat{s}_-$  are raising and lowering operators for the electron spin, and  $\hat{i}_+$  and  $\hat{i}_-$  are the corresponding operators for the nuclear spin. For  $\sigma_+$  polarization,  $\hat{a}_+$  replaces  $\hat{a}_-^{\dagger}$  and  $\hat{a}_+^{\dagger}$  replaces  $\hat{a}_$ in Eq. (3). For  $\sigma_X$  radiation with rf field  $B(t) = B_{\rm rf} \cos 2\pi \nu t$ , both  $\sigma_+$  and  $\sigma_-$  coupling terms are present, renormalized by 1/2 [15].

If couplings involving the photon annihilation and creation operators are neglected, states with different  $m_f$  values and different photon numbers N cross as a function of magnetic field. For example, for <sup>87</sup>Rb, with i = 3/2, and 3.0-MHz radiation, the  $(f, m_f, N) = (1, +1, 1), (1, 0, 0)$ , and (1, -1, -1)states all cross near B = 4.27 G, as shown in Fig. 1. If the radiation has  $\sigma_{-}$  polarization, these three states all have the same total projection quantum number  $M_{\rm tot}^{\rm atom}$ , and are coupled by the interaction (3), so the triple crossing becomes an avoided crossing; for  $B_{\rm rf} = 0.5$  G, the minimum separation between the states is  $h \times 0.35$  MHz. Ultracold atoms in the uppermost state can be trapped in the vicinity of the avoided crossing. These atoms are in a state whose character is principally (1,+1,1)on the low-field side of the crossing, but is (1, -1, -1) on the high-field side and a complicated mixture of all three states close to the crossing itself.

We carry out quantum scattering calculations of collisions between pairs of atoms in rf-dressed states. The Hamiltonian for the colliding pair is

$$\frac{\hbar^2}{2\mu} \left[ -R^{-1} \frac{d^2}{dR^2} R + \frac{\hat{L}^2}{R^2} \right] + \hat{V}(R) + \hat{h}_1 + \hat{h}_2 + \hat{h}_{\rm rf} + \hat{h}_{\rm rf,1}^{\rm int} + \hat{h}_{\rm rf,2}^{\rm int},$$
(4)

where  $\mu$  is the reduced mass,  $\hat{L}^2$  is the operator for the end-over-end angular momentum of the two atoms about one another, and  $\hat{V}(R)$  is the interaction operator,

$$\hat{V}(R) = \hat{V}^{c}(R) + \hat{V}^{d}(R).$$
 (5)

Here  $\hat{V}^{c}(R) = V_{0}(R)\hat{\mathcal{P}}^{(0)} + V_{1}(R)\hat{\mathcal{P}}^{(1)}$  is an isotropic potential operator that depends on the electronic potential energy curves  $V_{0}(R)$  and  $V_{1}(R)$  for the singlet and triplet electronic states and  $\hat{V}^{d}(R)$  is a relatively weak anisotropic operator that arises from the combination of spin dipolar coupling at long range and second-order spin-orbit coupling at short range. The singlet and triplet projectors  $\hat{\mathcal{P}}^{(0)}$  and  $\hat{\mathcal{P}}^{(1)}$  project onto subspaces with total electron spin quantum numbers 0 and 1, respectively. The potential curves for the singlet and triplet states are taken from Ref. [16] for Rb<sub>2</sub> and from Ref. [17] for K<sub>2</sub>.

The basis set of photon-dressed functions for a pair of atoms is

$$|s_1m_{s1}\rangle|i_1m_{i1}\rangle|s_2m_{s2}\rangle|i_2m_{i2}\rangle|LM_L\rangle|NM_N\rangle, \qquad (6)$$

where L is the angular momentum for relative motion and  $M_L$  is its projection onto Z. The basis set is symmetrized to take account of exchange symmetry. The matrix elements of the Hamiltonian in this basis set have been given in the appendix of Ref. [18], except for the rf terms, which involve raising and lowering operators with nonzero matrix elements,

$$\langle sm_s \pm 1 | \hat{s}_{\pm} | sm_s \rangle = [s(s+1) - m_s(m_s \pm 1)]^{\frac{1}{2}};$$
 (7)

$$\langle im_i \pm 1 | \hat{i}_{\pm} | im_i \rangle = [i(i+1) - m_i(m_i \pm 1)]^{\frac{1}{2}};$$
 (8)

and photon creation and annihilation operators with nonzero matrix elements,

$$\langle N + 1M_N \pm 1 | \hat{a}_{\pm}^{\dagger} | NM_N \rangle = (N_0 + N + 1)^{\frac{1}{2}};$$
 (9)

$$\langle N - 1M_N \mp 1 | \hat{a}_{\pm} | NM_N \rangle = (N_0 + N)^{\frac{1}{2}};$$
 (10)

$$\langle NM_N | \hat{a}_{\pm}^{\dagger} \hat{a}_{\pm} | NM_N \rangle = N_0 + N.$$
<sup>(11)</sup>

We assume  $N_0 \gg N$ , so that the matrix elements of  $\hat{a}_{\pm}^{\dagger}$  and  $\hat{a}_{\pm}$  cancel with the factor  $N_0^{1/2}$  in the denominator of Eq. (3).

The only conserved quantum numbers in a collision are parity  $(-1)^L$  and the total projection  $M_{\text{tot}} = M_F + M_L + M_N$ , where  $M_F = m_{f1} + m_{f2}$ . Our basis set includes all possible values of  $m_{s1}, m_{s2}, m_{i1}, m_{i2}$ , and  $M_L$ , for each value of L and  $M_N$  that give the required parity and  $M_{\text{tot}}$ . The values of L, N, and  $M_N$  are limited by  $L \leq L_{\text{max}}$ ,  $|N| \leq N_{\text{max}}$ , and  $|M_N| \leq N_{\text{max}}$ ; the values used for  $L_{\text{max}}$  and  $N_{\text{max}}$  will be described for each set of calculations.

Expanding the scattering wave function in the basis set described above produces a set of coupled equations in the interatomic distance coordinate *R*. The number of coupled equations varies from 30 to 208. These equations are solved using the MOLSCAT package [19]. In the present work we use the hybrid log-derivative propagator [20] to propagate the coupled equations from short range out to  $R_{max} = 15000$  bohr. MOLSCAT applies scattering boundary conditions to extract the scattering *S* matrix, and then obtains the complex energydependent scattering length  $a(E,B) = \alpha(E,B) - i\beta(E,B)$ 

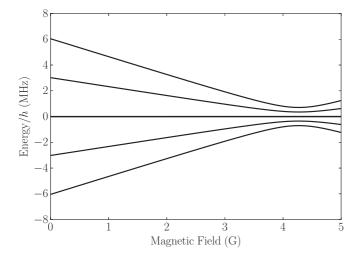


FIG. 2. The rf-dressed atomic thresholds of <sup>87</sup>Rb + <sup>87</sup>Rb for f = 1 and  $M_{\text{tot}} = 0$ . The corresponding thresholds of <sup>39</sup>K + <sup>39</sup>K are almost identical. The rf-induced collisions that cause trap loss are from the uppermost of these thresholds to all the lower ones. The thresholds are calculated for  $\nu = 3.0$  MHz and  $B_{\text{rf}} = 0.5$  G. Near zero magnetic field the thresholds can be labeled from top to bottom as  $M_F = -2, -1, 0, +1, +2$  with N = -2, -1, 0, +1, +2, respectively.

from the identity [21],

$$a(E,B) = \frac{1}{ik} \left( \frac{1 - S_{00}(E,B)}{1 + S_{00}(E,B)} \right),$$
(12)

where  $k^2 = 2\mu E/\hbar^2$  and  $S_{00}(E,B)$  is the diagonal S-matrix element in the incoming s-wave channel. This is constant as  $E \rightarrow 0$ , where it reduces to the usual zero-energy scattering length in the absence of inelastic collisions. For s-wave collisions (incoming L = 0), the rate coefficient for inelastic loss is [22]

$$k_2(E,B) = \frac{2hg_{\alpha}\beta(E,B)}{\mu[1+k^2|a(E,B)|^2+2k\beta(E,B)]},$$
 (13)

where  $g_{\alpha}$  is 2 for identical bosons and 1 for distinguishable particles. This is independent of energy in the limit  $E \rightarrow 0$ , but resonant peaks are moderated by the  $k^2 |a|^2$  term in the denominator at the collision energy of  $1 \,\mu \text{K} \times k_{\text{B}}$  used in the present calculations.

### **III. RESULTS**

In this section we present the results of coupled-channel scattering calculations for rf-dressed states of <sup>39</sup>K and <sup>87</sup>Rb in the vicinity of an rf-dressed trap. Since <sup>87</sup>Rb is a special case with highly atypical properties, we consider first the more typical case of <sup>39</sup>K, which (like <sup>87</sup>Rb) has nuclear spin i = 3/2 and a hyperfine ground state with f = 1.

To describe an rf-dressed trap for f = 1 atoms requires a minimum of three rf-free states with  $(f,m_f,N) = (1,+1,1)$ , (1,0,0), and (1,-1,-1), as shown in Fig. 1. To describe a *pair* of such states requires photon numbers N from -2 to 2. For rf field amplitude  $B_{\rm rf} = 0.5$  G, this produces atomic collision thresholds as shown for <sup>87</sup>Rb + <sup>87</sup>Rb in Fig. 2. The thresholds for <sup>39</sup>K + <sup>39</sup>K are almost identical. Pairs of atoms are trapped at the highest of the five thresholds shown, and can undergo

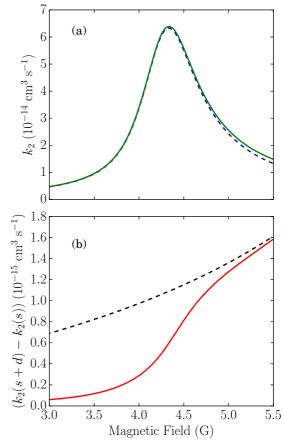


FIG. 3. (a) Rate coefficient for inelastic loss of adiabatically trapped <sup>39</sup>K + <sup>39</sup>K as a function of magnetic field with  $\nu = 3.0$  MHz and  $B_{\rm rf} = 0.5$  G, from calculations with  $L_{\rm max} = 2$  (solid, green) and  $L_{\rm max} = 0$  (dashed, blue). (b) Contribution from rf-modified spin-relaxation collisions, obtained from the difference between the  $L_{\rm max} = 0$  and  $L_{\rm max} = 2$  results (red, solid) compared with rf-free spin relaxation for  $(f, m_f) = (1, -1)$  atoms (black, dashed).

inelastic collisions to produce atoms at the lower thresholds. Such inelastic collisions release kinetic energy of at least  $h \times 0.25$  MHz  $\approx k_{\rm B} \times 12.5 \,\mu$ K, and the recoil will usually eject both collision partners from the trap.

# A. Inelastic collisions of rf-dressed <sup>39</sup>K

The inelastic collision rates for  ${}^{39}\text{K} + {}^{39}\text{K}$  at  $B_{\rm rf} = 0.5 \text{ G}$  are shown in Fig. 3(a), as a function of magnetic field across the trap. The solid line shows the inelastic rate from calculations with  $L_{\rm max} = 2$ , while the dashed line shows the rate from simplified (and computationally far cheaper) calculations with  $L_{\rm max} = 0$ . Both calculations use photon numbers  $-2 \le N \le 2$ , and adding additional values of N makes no further difference to the results.

The main source of inelasticity in <sup>39</sup>K + <sup>39</sup>K collision exists even for  $L_{\text{max}} = 0$ . It arises from collisions that conserve  $m_{f1} + m_{f2} + M_N$  and thus do not change  $M_L$ ; we refer to these are rf-induced collisions. Since L does not need to change, there is no centrifugal barrier in the outgoing channel and no centrifugal suppression of the inelastic rate. For  $B_{\text{rf}} = 0.5$  G, the loss rate peaks at  $k_2^{\text{max}} = 6.33 \times 10^{-14}$  cm<sup>3</sup> s<sup>-1</sup>

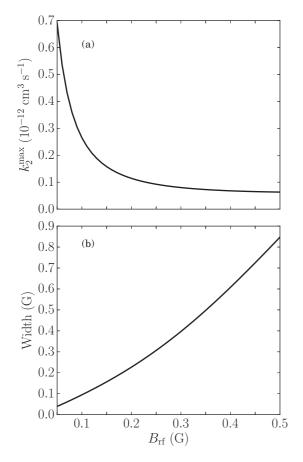


FIG. 4. Height and FWHM width of the peak in inelastic rate coefficient for  ${}^{39}\text{K} + {}^{39}\text{K}$ , as a function of rf amplitude  $B_{rf}$ .

 $(\beta = 0.015 \text{ bohr})$  near the trap center and dies off on either side. However, the peak is a strong function of  $B_{rf}$ . Figure 4 shows the height  $k_2^{max}$  and full width at half maximum (FWHM) of the peak as a function of  $B_{rf}$ , obtained from calculations with  $L_{max} = 0$ ; the peak width increases as  $B_{rf}$ increases, but the peak height decreases. The width increases faster than linearly with  $B_{rf}$ ; although the range of *B* across which the atomic states are strongly mixed by rf dressing is linear in  $B_{rf}$ , the kinetic energy released also depends on  $B_{rf}$ and this affects the inelastic cross sections in a complicated way. The peak cross section decreases as the kinetic energy release increases.

For <sup>39</sup>K + <sup>39</sup>K, the inelastic rates are fairly similar for  $L_{\text{max}} = 2$  and  $L_{\text{max}} = 0$ . The small difference arises because, even in the absence of rf radiation, atoms in  $f = 1, m_f < 1$  may undergo spin-relaxation collisions to produce atoms in lower magnetic sublevels. Such collisions are driven only by the weak anisotropic part of the interaction,  $V^d(R)$  in Eq. (5). Since they change  $M_F = m_{f1} + m_{f2}$ , and  $M_F + M_L$  must be conserved, they must also change  $M_L$ . For *s*-wave collisions, L is initially zero, so changing  $M_L$  requires a final state with L > 0, which must have  $L \ge 2$  to conserve parity. The rates of spin-relaxation collisions are therefore suppressed because the products are trapped inside an L = 2 centrifugal barrier, which has height  $k_B \times 1.5$  mK for <sup>39</sup>K + <sup>39</sup>K. Figure 3(b) shows the *difference* between the  $L_{\text{max}} = 2$  and  $L_{\text{max}} = 0$  results in Fig. 3(a) and compares it with the rate of spin-relaxation

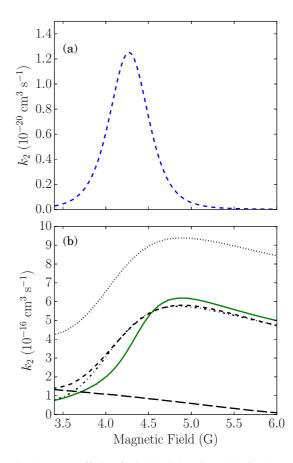


FIG. 5. Rate coefficient for inelastic loss for adiabatically trapped <sup>87</sup>Rb in f = 1 as a function of magnetic field with  $\nu = 3.0$  MHz and  $B_{\rm rf} = 0.5$  G. (a) Calculation using  $L_{\rm max} = 0$ . (b) Calculation including spin relaxation, using  $L_{\rm max} = 2$  (solid green line). Rate coefficients for rf-free spin relaxation are shown as dashed lines for (1,-1) + (1,-1), dashed-dotted lines for (1,-1) + (1,0), dotted lines for (1,0) + (1,0) and long dashed lines for (1,0) + (1,1).

collisions from an rf-free calculation for two atoms initially in the  $(f,m_f) = (1,-1)$  state. It may be seen that the difference approaches the rf-free spin-relaxation rate at high magnetic field, where the adiabatically trapped state is principally (1,-1). However, it decreases to zero at low magnetic field, where the trapped state is principally (1,1), which is the rf-free ground state and cannot undergo inelastic collisions. At the trap center the rf-modified spin-relaxation rate is about half its rf-free value.

## B. Inelastic collisions of rf-dressed <sup>87</sup>Rb

Figure 5 shows the calculated inelastic rate constant as a function of magnetic field for <sup>87</sup>Rb, for the same rf frequency and field strength as Fig. 3. Figures 5(a) and 5(b) show calculations with  $L_{max} = 0$  and 2, respectively. In this case the rate coefficient for rf-induced loss (with  $L_{max} = 0$ ) reaches a maximum of only  $k_2^{max} = 1.25 \times 10^{-20}$  cm<sup>3</sup>s<sup>-1</sup> ( $\beta = 6.47 \times 10^{-8}$  bohr) at B = 4.2713 G (the trap center). This is more than 6 orders of magnitude slower than for <sup>39</sup>K<sub>2</sub>, and 4 orders of magnitude lower than the rf-modified spin-relaxation rate at the trap center. Consequently Fig. 5(b) is totally dominated by spin relaxation. In this case, however,

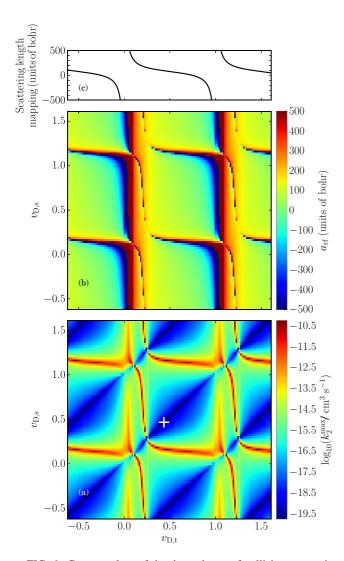


FIG. 6. Contour plots of the dependence of collision properties on the fractional part of  $v_D$  for the singlet and triplet states, for adiabatically trapped <sup>87</sup>Rb in f = 1 with v = 3.0 MHz and  $B_{rf} =$ 0.5 G. (a) Rate coefficient for rf-induced loss at the trap center  $k_2^{max}$ . (b) Real part of scattering length  $a_{rf}$ . (c) Mapping between  $v_D$  and the singlet and triplet scattering lengths for <sup>87</sup>Rb, according to Eq. (14).

the spin relaxation itself shows more complicated structure as a function of *B*; the dashed lines in Fig. 3(b) show the rf-free spin relaxation rates for (1,1) + (1,1), (1,1) + (1,0), (1,1) + (1,-1), and (1,0) + (1,-1) collisions. As for <sup>39</sup>K, the losses for rf-dressed states approach those for rf-free (1,1) + (1,1) at high magnetic field, but around the trap center there are also contributions from other components of the wave function of the rf-dressed atomic states.

The rf-induced loss rate depends strongly on the singlet and triplet scattering lengths  $a_s$  and  $a_t$ . In order to explore this, we have carried out  $L_{max} = 0$  calculations on a set of potentials modified at short range to allow adjustment of  $a_s$  and  $a_t$ . We retained the functional forms of the potential curves of Strauss *et al.* [16], but modified the short-range matching point  $R_{SR}$  to 3.5 Å for the singlet potential and to 5.6 Å for the triplet potential in order to provide sufficient flexibility to adjust the scattering lengths through a complete cycle. We then adjusted

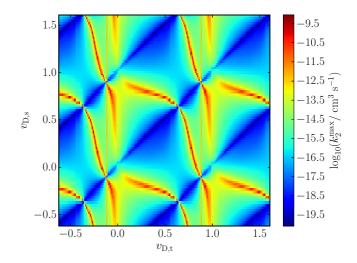


FIG. 7. Contour plot of the rate coefficient for rf-induced loss at the trap center, for adiabatically trapped f = 1 states of an artificial atom with a hyperfine splitting 0.7 times that of <sup>87</sup>Rb. All other quantities are the same as for Fig. 6.

the short-range power  $N_{\rm SR}$  to obtain modified potentials with different scattering lengths, maintaining continuity of the potential and its derivative at  $R_{\rm SR}$  as described in Ref. [23].

Contour plots of the resulting rf-induced peak loss rates  $k_2^{\text{max}}$ and the corresponding real part of the scattering length  $a_{\text{rf}}$  (for collisions of rf-dressed atoms) are shown in Fig. 6, calculated at the trap center for  $B_{\text{rf}} = 0.5$  G. Since the possible singlet and triplet scattering lengths range from  $-\infty$  to  $+\infty$ , the loss rate is displayed as a function of two phases, defined as the fractional parts of the quantum numbers at dissociation  $v_{\text{D,s}}$ and  $v_{\text{D,t}}$  for the singlet and triplet states. These each map onto the corresponding scattering length according to

$$a = \bar{a} \left[ 1 - \tan\left(v_{\rm D} + \frac{1}{2}\right) \pi \right],\tag{14}$$

where  $\bar{a} = 0.477988...(2\mu C_6/\hbar^2)^{-1/4}$  is the mean scattering length of Gribakin and Flambaum [24] and  $C_6$  is the leading long-range dispersion coefficient. For <sup>87</sup>Rb,  $\bar{a} = 78.95$  bohr. The mapping between scattering length and  $v_D$  is shown for <sup>87</sup>Rb in the top panel of Fig. 6.

Figure 6 shows that  $k_2^{\text{max}}$  varies by more than 10 orders of magnitude as a function of the singlet and triplet scattering lengths. Both  $k_2^{\text{max}}$  and  $a_{\text{rf}}$  depend only on the fractional parts of  $v_{\rm D}$  for the singlet and triplet states (and hence on  $a_{\rm s}$  and  $a_{\rm t}$ ), as indicated by the repeating patterns in Fig. 6. The most striking feature of Fig. 6(a) is a deep diagonal trough in the rf-induced loss rate when  $v_{D,s} \approx v_{D,t}$  ( $a_s \approx a_t$ ), with no corresponding feature in  $a_{\rm rf}$ . Superimposed on this are peaks in  $k_2^{\text{max}}$  and poles in the corresponding  $a_{\text{rf}}$ . These are of three different types. First, there are near-vertical bands near integer values of  $v_{D,t}$ , corresponding to  $|a_t| = \infty$ . These are entrance-channel resonances; they occur near integer values of  $v_{D,t}$  because the incoming channel is mostly triplet in character. Secondly, there is a Feshbach resonance due to a closed channel with excited hyperfine character (f = 2 here), which produces curving bands of peaks in  $k_2^{\text{max}}$  that cross the vertical bands near  $v_{D,s} = 0.1$ . Lastly, there is an additional Feshbach resonance that produces very narrow vertical bands

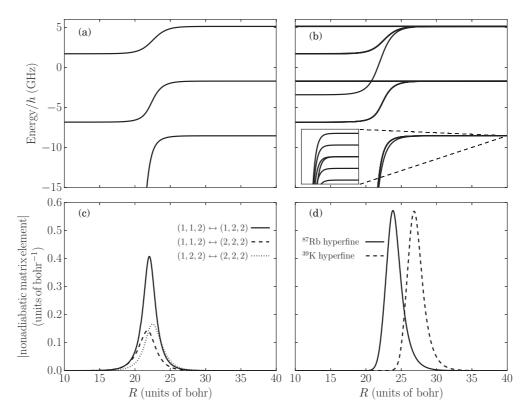


FIG. 8. Adiabats [eigenvalues of the Hamiltonian of Eq. (4) at fixed R] with respect to a pure triplet curve (a) for field-free collisions with  $(f_1, f_2, F = 2)$  and (b) for collisions of rf-dressed atoms with f = 1, at the trap center with rf field frequency 3 MHz and strength  $B_{\rm rf} = 0.5$  G, for  $M_{\rm tot} = 0$ . (c) Nonadiabatic matrix elements between (1,1,2), (1,2,2), and (2,2,2) in (a). (d) Nonadiabatic matrix element between the uppermost of the six  $(f_1, f_2, M_{\rm tot}) = (1,1,0)$  rf-dressed states and the next-highest state.

of peaks near  $v_{D,t} = 0.3$ ; these probably arise from pure triplet states that exist at the  $(f_1, f_2) = (1, 2)$  threshold in the absence of rf and magnetic fields.

To explore the dependence of the pattern on hyperfine splitting, we have repeated the calculations on a series of artificial systems with the <sup>87</sup>Rb hyperfine splitting reduced from its real value, using the same set of interaction potentials.

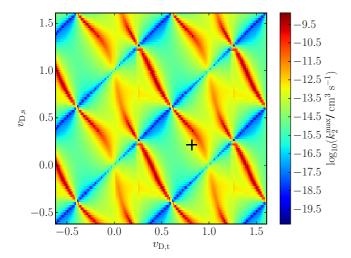


FIG. 9. Contour plot of the rate coefficient for rf-induced loss at the trap center, for adiabatically trapped f = 1 states of an artificial atom with the mass of <sup>87</sup>Rb with the hyperfine splitting of <sup>39</sup>K. All other quantities are the same as for Fig. 6.

The results with the hyperfine splitting at 70% of its real value are shown in Fig. 7. The general form of the contour plot is unchanged, with a deep trough around  $v_{D,s} \approx v_{D,t}$  ( $a_s \approx a_t$ ) and peaks around vertical bands at integer values of  $v_{D,t}$ . As expected, however, the Feshbach peaks have shifted. They now

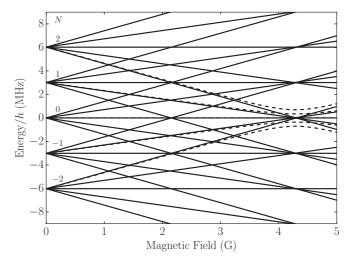


FIG. 10. rf-dressed atomic levels of f = 2 states of <sup>87</sup>Rb for frequency 3.0 MHz and photon numbers N = -2, -1, 0, 1, and 2, shown with respect to the energy of the f = 2,  $m_f = 0$  state for N = 0. Solid lines show levels for zero rf intensity and dashed lines show levels for  $B_{\rm rf} = 0.5$  G with  $M_{\rm tot} = 0$ . Atoms can be trapped at the minimum in the uppermost dashed curve.

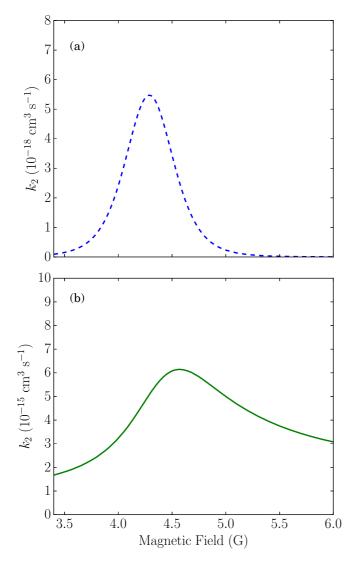


FIG. 11. Rate coefficient for inelastic loss of adiabatically trapped <sup>87</sup>Rb in f = 2 as a function of magnetic field with v = 3.0 MHz and  $B_{\rm rf} = 0.5$  G. (a) Calculation of rf-induced loss, using  $L_{\rm max} = 0$ . (b) Calculation including spin relaxation, using  $L_{\rm max} = 2$ .

display distinct *avoided* crossings with the vertical bands of peaks. For some values of the hyperfine splitting, the crossings are so strongly avoided that the vertical bands near integer  $v_{D,t}$  are barely identifiable.

The trough observed here for rf-induced inelastic collisions when  $a_s \approx a_t$  has a similar origin to that found for spinexchange collisions. Myatt *et al.* [25] measured a very low rf-free spin-exchange rate in dual Bose-Einstein condensates of <sup>87</sup>Rb in  $(f,m_f) = (1,-1)$  and (2,2) states. Julienne *et al.* [26] explained this using an adiabatic model of the collision dynamics [27] where the Hamiltonian of Eq. (4) (without rf) is diagonalized at each value of the interatomic distance *R*. For <sup>87</sup>Rb, the exchange splitting between the singlet and triplet curves is comparable to the hyperfine splitting around  $R_X = 22$  bohr. Inside this distance the adiabatic states are essentially pure singlet and triplet states, whereas outside it they are described by atomic quantum numbers  $(f,m_f)$ . Julienne *et al.* [26] considered scattering at zero magnetic

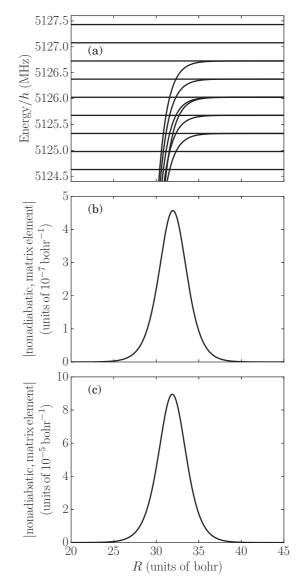


FIG. 12. (a) Adiabats [eigenvalues of the Hamiltonian of Eq. (4) at fixed *R*] for collisions of field-dressed <sup>87</sup>Rb atoms in f = 2 states, with respect to a pure triplet curve, for  $M_{\text{tot}} = 0$ . (b) Nonadiabatic matrix elements between the top two adiabatic states for <sup>87</sup>Rb. (c) Nonadiabatic matrix elements between the top two adiabatic states with the hyperfine splitting reduced to the value for <sup>39</sup>K.

field, with  $f_1$  and  $f_2$  coupled to give a resultant F. The resulting rf-free adiabats for F = 2 are shown in Fig. 8(a), with respect to the pure triplet interaction potential. The nonadiabatic matrix elements  $\langle i|d/dR|j\rangle$  between the states that are asymptotically  $(f_1, f_2, F) = (1, 1, 2)$ , (1, 2, 2), and (2, 2, 2) are shown in Fig. 8(c). The overall magnitude is usefully characterized by the integral,

$$D_{ij} = \int \left\langle i \left| \frac{d}{dR} \right| j \right\rangle dR, \qquad (15)$$

which is  $\pi/2$  for a complete avoided crossing, and 1.05, 0.55, and 0.49 for the three couplings in Fig. 8(c). The adiabats and nonadiabatic couplings are independent of the singlet and triplet scattering lengths. However, Julienne *et al.* [26] argued that, when  $a_s \approx a_t$ , the radial wave functions  $R^{-1}\chi_i(R)$  and

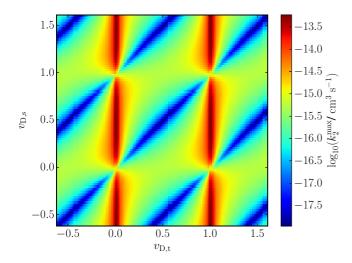


FIG. 13. Contour plot of the rate coefficient for rf-induced loss at the trap center, for adiabatically trapped f = 2 states of <sup>87</sup>Rb. All other quantities are the same as for Fig. 6.

 $R^{-1}\chi_j(R)$  in the incoming (1,2,2) and inelastic outgoing (1,1,2) channels are in phase around  $R_X$ . This minimizes the matrix element that controls inelastic scattering,

$$-\frac{\hbar^2}{2\mu}\int \chi_i(R)^* \left\langle i \left| \frac{d}{dR} \right| j \right\rangle \frac{d}{dR} \chi_j(R) \, dR.$$
 (16)

Figures 8(a) and 8(c) may be compared with the adiabats for collisions of rf-dressed <sup>87</sup>Rb atoms in f = 1 states at the trap center (4.27 G), which are shown in Fig. 8(b), and the nonadiabatic matrix element from the uppermost of the six  $(f_1, f_2, M_{tot}) = (1, 1, 0)$  states to the next-highest state, which are shown in Fig. 8(d). The nonadiabatic matrix element again peaks around 22 bohr for <sup>87</sup>Rb; the mechanism is similar to that for spin exchange, and the overall inelastic coupling is smallest when  $a_s \approx a_t$ , producing the diagonal troughs seen in Figs. 6 and 7.

The actual singlet and triplet scattering lengths for <sup>87</sup>Rb are indicated by a cross on Fig. 6(a). This shows that <sup>87</sup>Rb is special in two different ways. Not only are its singlet and triplet scattering lengths quite similar, but their actual values correspond to  $v_D \approx 0.5$  and lie well away from the peaks due to Feshbach resonances. The value of  $k_2^{\text{max}}$  at the deepest point in the trough in Fig. 6(a) is about  $k_2^{\text{max}} = 5.3 \times 10^{-21} \text{ cm}^3 \text{ s}^{-1}$ , which is not far from the value of  $1.25 \times 10^{-20} \text{ cm}^3 \text{ s}^{-1}$  obtained for <sup>87</sup>Rb on the potentials of Ref. [16].

Figure 9 shows a contour plot similar to Fig. 7 but with the hyperfine splitting of <sup>39</sup>K (462 MHz). The structure is similar, with a Feshbach resonance avoided crossing with vertical bands of peaks at integer  $v_{D,t}$ , though the resonances are distinctly wider than in Figs. 6(a) and 7. The actual scattering lengths of <sup>39</sup>K are shown as a black cross; the value of  $k_2^{max}$  at this point is  $5.3 \times 10^{-14}$  cm<sup>3</sup> s<sup>-1</sup>, which may be compared with  $k_2^{max} = 6.33 \times 10^{-14}$  cm<sup>3</sup> s<sup>-1</sup> from the calculation with the mass and interaction potentials for <sup>39</sup>K in Sec. III A.

#### C. Inelastic collisions of rf-dressed f = 2 states

A somewhat different case occurs for atoms in f = 2 states. Here there are 5 photon-dressed atomic states that cross as a

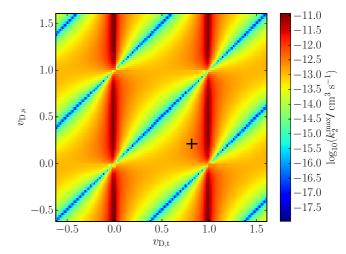


FIG. 14. Contour plot of the rate coefficient for rf-induced loss at the trap center, for adiabatically trapped f = 2 states of an artificial atom with the mass of <sup>87</sup>Rb but the hyperfine splitting of <sup>39</sup>K. All other quantities are the same as for Fig. 6.

function of magnetic field, as shown for <sup>87</sup>Rb in Fig. 10. It requires a minimum of five rf-free states (with photon numbers N from -2 to 2) to describe a single trapped atom, and describing two such atoms requires photon numbers from -4to 4. The coupled-channel calculation is thus computationally considerably more expensive. Nevertheless, the principles are exactly the same and rate coefficients for inelastic loss can again be obtained from  $\beta$ , the imaginary part of the complex scattering length, for atoms initially at the highest rf-dressed threshold.

Figure 11 shows the rate coefficient for inelastic loss for <sup>87</sup>Rb in f = 2, as a function of magnetic field near the trap center. As before, Fig. 11(a) shows the rf-induced loss, from a calculation with  $L_{\text{max}} = 0$ , while Fig. 11(b) shows the loss including spin relaxation, from a calculation with  $L_{\text{max}} = 2$ . The rf-induced loss rate is about a factor of 400 larger than for <sup>87</sup>Rb in f = 1, but it is still much lower than the loss rate due to spin relaxation. Once again this illustrates the special properties of <sup>87</sup>Rb.

It is notable that the rf-induced loss rate for f = 2 is far lower than the rf-free spin-exchange rates for (2,0) + (2,0)and (2,1) + (2,-1) collisions, which are  $1.73 \times 10^{-13}$  and  $1.25 \times 10^{-13}$  cm<sup>3</sup> s<sup>-1</sup>, respectively. This is true even though the wave function for the rf-dressed atomic state includes substantial amounts of (2,0) and (2,1) near the trap center. It may be again rationalized by considering adiabatic curves obtained by diagonalizing the Hamiltonian of Eq. (4) at each value of the interatomic distance R. For rf-free collisions of two f = 2 atoms, there are contributions from F = 0, 2,and 4. The inelasticity is dominated by F = 2, for which the adiabats and nonadiabatic matrix elements were shown in Figs. 8(a) and 8(c). Figure 12(a) shows the adiabats for collisions of rf-dressed <sup>87</sup>Rb atoms in f = 2 states at the trap center, and Fig. 12(b) shows the corresponding nonadiabatic matrix elements between the uppermost and next-highest state. The nonadiabatic coupling is quite different from the previous cases: There is no feature around 22 bohr, and

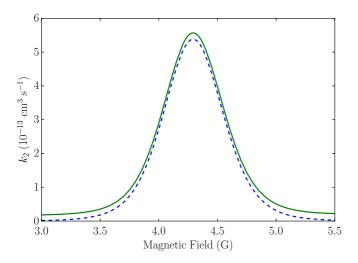


FIG. 15. Rate coefficient for inelastic loss of adiabatically trapped <sup>39</sup>K in f = 2 as a function of magnetic field with v = 3.0 MHz and  $B_{\rm rf} = 0.5$  G. Results are shown including spin relaxation, using  $L_{\rm max} = 2$  (solid, green) and for rf-induced loss alone, using  $L_{\rm max} = 0$  (dashed, blue).

instead the matrix element peaks around 32 bohr, where the difference between the singlet and triplet curves is comparable with the splittings  $\Delta_{\rm rf}$  due to rf dressing. The coupling is far weaker than in the cases shown in Fig. 8. The integral  $D_{ij}$  over the nonadiabatic coupling is only  $1.96 \times 10^{-6}$ , as compared to  $\pi/2$  for a completed avoided crossing.

We have also investigated the dependence of  $k_2^{\text{max}}$  for the f = 2 states of <sup>87</sup>Rb<sub>2</sub> on the singlet and triplet scattering lengths. The resulting contour plot is shown in Fig. 13. It has a considerably simpler structure than Figs. 6, 7, and 9, because the atoms are both in their upper hyperfine state and there are no closed channels that can cause Feshbach resonances. The only features are a diagonal trough for  $v_{D,s} \approx v_{D,t}$  ( $a_s \approx a_t$ ) and a near-vertical band of maxima where  $v_{D,t}$  is close to an integer. These have the same causes as discussed for f = 1 above.

For atoms trapped in their upper hyperfine state, with no Feshbach resonances, the dependence of  $k_2^{\text{max}}$  on  $a_s$  and  $a_t$ may be expected to resemble Fig. 13 qualitatively for all atoms. However, there is a strong overall dependence on the hyperfine coupling constant. To illustrate this, we have repeated the calculations shown in Fig. 13 with the hyperfine coupling constant set to the value for <sup>39</sup>K but the reduced mass retained at the value for <sup>87</sup>Rb. The results are shown in Fig. 14. It may be seen that the general structure of peaks and troughs is unchanged, but the peaks are about a factor of 200 higher for the smaller hyperfine splitting of  $^{39}$ K (462 MHz) than for that of <sup>87</sup>Rb (6,834 MHz). This effect may also be traced to the effects of nonadiabatic transitions. The adiabats for <sup>39</sup>K are similar to those shown for <sup>87</sup>Rb in Fig. 12(a). However, the nonadiabatic matrix element, shown in Fig. 12(c), is a factor of 200 larger than for <sup>87</sup>Rb, with integral  $D_{ij} = 3.8 \times 10^{-4}$ . The nonadiabatic matrix element reflects the amount of singlet character in the wave function of the rf-dressed atomic pair at long range; this in turn depends on the degree of mixing of f = 1 and f = 2 states in the magnetic field, which increases as the hyperfine splitting decreases.

The specific case of <sup>39</sup>K in rf-dressed f = 2 states is of interest. Figure 15 shows  $k_2$  as a function of magnetic field from calculations with  $L_{max} = 0$  and 2, using the potentials of Ref. [17]. It may be seen that, as for <sup>39</sup>K in f = 1, the rf-induced loss dominates the loss due to rf-modified spin relaxation. The rate coefficient peaks at  $k_2^{max} = 5.38 \times 10^{-13}$  cm<sup>3</sup> s<sup>-1</sup>. The rf-induced loss is about 5 orders of magnitude faster than for <sup>87</sup>Rb, and again more typical. The value is comparable to the one from Fig. 14 at the values of  $v_{D,s}$  and  $v_{D,t}$  for <sup>39</sup>K, shown with a black cross, which is  $k_2^{max} = 2.34 \times 10^{-13}$  cm<sup>3</sup> s<sup>-1</sup>. The difference between these two values arises because the calculations in Fig. 14 used the reduced mass and interaction potentials for <sup>87</sup>Rb rather than <sup>39</sup>K.

An atom for which f = 2 is not the highest state, such as <sup>85</sup>Rb, may be expected to show more complex behavior than Fig. 13, with Feshbach resonances reappearing at some values of  $v_{D,s}$  and  $v_{D,t}$  ( $a_s$  and  $a_t$ ). We will investigate this in future work.

#### **IV. CONCLUSIONS**

Cold atoms in radio-frequency-dressed traps may undergo inelastic collisions by mechanisms that do not occur in the absence of an rf field. These collisions may lead to trap loss. We have investigated inelastic losses for alkali-metal atoms in rf-dressed traps, using coupled-channel scattering calculations on accurate potential energy surfaces. We have explored the dependence of the loss rates on singlet and triplet scattering lengths, hyperfine splittings, and the strength of the rf field.

There are two components of the inelastic loss. One is due to spin-relaxation collisions, driven by the dipolar interaction between the electron spins of the two atoms. This component exists even in the absence of rf dressing, but is generally fairly small, both because the dipolar interaction is weak and because there is a centrifugal barrier in the outgoing channel. It is modified near the trap center because the rf-dressed states are mixtures of different spin states, and drops to zero on the low-field side of the trap, where the adiabatically trapped state correlates with the lowest state in the magnetic field. The second component, which we refer to as rf-induced loss, is potentially stronger; the inelastic collisions are driven by the difference between the singlet and triplet interaction potentials, and there is no centrifugal barrier in the outgoing channel.

For <sup>87</sup>Rb in f = 1 states, the calculated rate coefficient for rf-induced loss is very small. We obtain  $k_2^{\text{max}} = 1.25 \times 10^{-20} \text{ cm}^3 \text{ s}^{-1}$  at the trap center for an rf field strength  $B_{\text{rf}} = 0.5$  G. This is much smaller than the rf-modified spin-relaxation loss rate coefficient for <sup>87</sup>Rb.

We have explored the dependence of the rf-induced loss rate on the singlet and triplet scattering lengths  $a_s$  and  $a_t$ , and find that it can change by 10 orders of magnitude as the scattering lengths are varied. It is generally small when  $a_s \approx a_t$ , but may be enhanced by resonances of two different types. <sup>87</sup>Rb is a very special case: Not only is  $a_s$  very similar to  $a_t$ , but their actual values are such that there is no enhancement by either type of resonance. Other alkali-metal atoms will generally have much larger rf-induced loss rates. For <sup>39</sup>K, which is a more typical case, we obtain  $k_2^{\text{max}} = 6.33 \times 10^{-14} \text{ cm}^3 \text{ s}^{-1}$  for  $B_{\text{rf}} = 0.5 \text{ G}$ . This is much larger than the rf-modified spin-relaxation loss rate, and 6 orders of magnitude larger than for <sup>87</sup>Rb. The rf-induced loss rate at the trap center increases at lower rf field strengths.

We have also investigated rf-induced loss for alkali-metal atoms in their upper hyperfine states, f = 2 for <sup>87</sup>Rb and <sup>39</sup>K. These losses are also small when  $a_s \approx a_t$ . In this case there are no Feshbach resonances, but the loss rates may still be enhanced by entrance-channel effects when  $|a_t|$  is large. The rf-induced loss rates also depend strongly on the atomic hyperfine splitting, increasing as the hyperfine splitting

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decreases because of mixing of atomic f states by the magnetic field.

## ACKNOWLEDGMENTS

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same definition of  $B_{\rm rf}$  as here for  $\sigma_X$  but a different normalization for  $\sigma_+$  and  $\sigma_-$ . To match the present definition, the values of  $B_{\rm rf}$  given in Ref. [13] must be divided by  $\sqrt{2}$  for  $\sigma_+$  and  $\sigma_$ polarization. Note that Hanna *et al.* [12] use spin raising and lowering operators normalized by  $1/\sqrt{2}$  with respect to ours.

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