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Optical tuning of the scattering length of cold alkaline-earth-metal atoms

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It is possible to tune the scattering length for the collision of ultracold $^1S_0$ ground-state alkaline-earth-metal atoms using an optical Feshbach resonance. This is achieved with a laser far detuned from an excited molecular level near the frequency of the atomic intercombination $^1S_0$-$^3P_1$ transition. Simple resonant-scattering theory, illustrated by the example of ^{40}Ca, allows an estimate of the magnitude of the effect. Unlike alkali metal species, large changes of the scattering length are possible while atom loss remains small, because of the very narrow linewidth of the molecular photoassociation transition. This raises prospects for control of atomic interactions for a system without magnetically tunable Feshbach resonance levels.

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In recent years the ability to change the interaction between ultracold colliding atoms has opened the way for unique and exciting experiments with ultracold atomic gases. The observation of a Bose-Einstein condensate (BEC) in atomic cesium [1] would have been impossible without the ability to change the interaction from being attractive to being repulsive. More impressively, time-varying interactions have allowed the creation of condensates of two-atom molecules starting from an atomic Bose condensate [2,3]. Most recently, the observation of the condensation of pairs of fermionic [4] atoms has started investigations into the so-called BEC-BCS crossover [5], where BCS is the abbreviation for the Bardeen-Cooper-Schrieffer phase transition in a fermionic gas [6].

The key to these developments has been the ability to change the interaction between atoms by a magnetically tuned Feshbach resonance [7]. Theoretical discussion of the properties of these resonances can be found in Refs. [8–11]. The interaction between the atoms at ultracold temperature can be characterized by a single parameter, the scattering length [12,13], which can be controlled in sign and magnitude using these resonances.

Another way to change the scattering length of two colliding atoms is to optically couple the ground scattering state with an excited bound state [14]. These optical Feshbach resonances are theoretically analyzed in Refs. [15,16] and implemented experimentally in Refs. [17,18]. The recent experiment of Theis *et al.* [18] with ^{87}Rb atoms showed, however, that a significant change of the scattering length is accompanied with substantial loss of atoms. The same is true if a two-color Raman process is used [19].

In this paper we discuss the optical tuning of scattering lengths in ultracold alkaline-earth-metal atom vapors. To do so we will assume that the laser is far detuned from excited molecular states near the intercombination transition, $^1S_0$-$^3P_1$, as recently analyzed in Ref. [20]. We show that significant changes of the scattering strength can be achieved without the excessive atom loss that plagues experiments with alkali-metal gases [18]. Prospects for an optically tuned scattering length in ultracold alkaline-earth vapors seem to be particularly attractive, since magnetically tuned Feshbach resonances do not occur between the isotopes of ground-state $^1S_0$ alkaline-earth-metal atoms with zero nuclear spin. Several alkaline-earth-metal atoms also have isotopes with nonzero half-integer nuclear spin. Optical methods could be used to tune their scattering lengths, although we will not consider these specifically in this paper. Optical Feshbach control can be also applied to other atomic systems having a similar electronic structure. The recent Bose-Einstein condensation of ytterbium [21] makes this system especially interesting.

The theoretical description of optical Feshbach resonances and the closely related photoassociation (PA) process is well established [14–16]. The elastic- and inelastic-scattering rates due to a single photoassociation resonance level depends on (1) the natural linewidth $\Gamma_{e,\mathrm{nat}} \approx 2\Gamma_A$ of the excited molecular level e, (2) the stimulated width $\Gamma_{eg}(\varepsilon_r, I)$ that couples the excited level to the s-wave collision of the ground state g at relative kinetic energy ε_r, and (3) the detuning $\Delta - \Delta_e$ from optical resonance. Here, following the notation of Ref. [20] for PA near the $^1S_0$-$^3P_1$ intercombination line of a group II atomic species, Γ_A is the natural decay width of the atomic transition, $\Delta = \hbar\omega - E_A$, $\Delta_e = E_e - E_A$, where E_e is the energy of an isolated excited molecular bound level, E_A is the energy of the ^{3}P$_1$ atom, and ω is the frequency of the light driving the transition. The stimulated width is

$$\Gamma_{eg}(\varepsilon_r, I) = 2\pi |\langle e|V_{\mathrm{las}}|g\rangle|^2 = \Gamma_A \frac{3}{4\pi} \frac{I\lambda_A^3}{c} f_{\mathrm{rot}} f_{\mathrm{FC}}, \qquad (1)$$

where V_{las} is the optical coupling proportional to the laser intensity I, λ_A is the wavelength of the atomic transition, c is the speed of light, f_{rot} is a dimensionless rotational line strength factor of order unity, and f_{FC} is the Franck-Condon factor per unit energy for the free-bound PA transition

$$f_{\mathrm{FC}} = \left| \int_0^\infty F_e(R) F_g(\varepsilon_r, R) dR \right|^2. \qquad (2)$$

Here, F_e is the unit normalized excited-state wave vibrational function and $F_g(\varepsilon_r, R)$ is the energy normalized ground-state scattering wave function. The low-energy s-wave form of the latter is $(2\mu/\pi\hbar^2 k_r)^{1/2} \sin[k_r(R - a_{\mathrm{bg}})]$ at large R, where μ is reduced mass of the atom pair, $\hbar$ is Planck's constant divided

by 2π, $k_r=\sqrt{2\mu\varepsilon_r}/\hbar$, and $a_{\rm bg}$ is the ground-state s-wave scattering length in the absence of light. It should be noted that the details of the molecule structure are hidden in $\Gamma_{eg}(\varepsilon_r,I)$, Δ_e, and $a_{\rm bg}$.

The rate constant for inelastic collisions that lead to atom loss is typically large when the detuning from molecular resonance is small. Consequently, we will only consider the case of unsaturated transitions at large detuning, defined by the condition

$$|\Delta-\Delta_e| \gg \Gamma_{e,\rm nat}+\Gamma_{eg}(\varepsilon_r,I). \tag{3}$$

We also require that $|\Delta-\Delta_e|$ be much larger than other contributions to the width of the photoassociation line such as the thermal width, Doppler width [20], light-induced shift [16,22], and the mean-field shift in the case of BEC [23].

The theoretical description can be framed using the definition of a complex scattering length $\mathcal{A}$ based on the elastic-scattering S-matrix element as $k_r\to 0$ [15],

$$S_{gg}=\exp(-2i\mathcal{A}k_r). \tag{4}$$

The length $\mathcal{A}$ is complex and in the presence of light can be written as

$$\mathcal{A}(\Delta,I)=a_{\rm bg}+a_{\rm opt}(\Delta,I)-ib_{\rm opt}(\Delta,I), \tag{5}$$

where the dependence on Δ and I are made explicit. The optically induced $a_{\rm opt}(\Delta,I)$ and $b_{\rm opt}(\Delta,I)$ vanish for $I=0$ and are linear in I for the limit in Eq. (3). The length $a_{\rm scat}(\Delta,I)=a_{\rm bg}+a_{\rm opt}(\Delta,I)$ is interpreted as the usual scattering length, and $b_{\rm opt}$ is related to the atom loss rate coefficient $K(\Delta,I)$ determined from the S matrix,

$$\lim_{k_r\to 0} K(\Delta,I)=\lim_{k_r\to 0}\frac{\pi\hbar}{\mu k_r}(1-|S_{gg}|^2)=\frac{4\pi\hbar}{\mu}b_{\rm opt}(\Delta,I). \tag{6}$$

The real and imaginary parts of $\mathcal{A}$ are directly related to the mean-field energy and the lifetime of a Bose-Einstein condensate. For the case of a condensate at density n, the requirement $|a_{\rm scat}|\gg b_{\rm opt}$ ensures that the mean-field energy per atom pair $4\pi\hbar^2 a_{\rm scat}n/\mu$ is large compared to the decay width $\hbar Kn=4\pi\hbar^2 b_{\rm opt}n/\mu$. The time scale for decay is $(Kn)^{-1}$ for a condensate and $(2Kn)^{-1}$ for a noncondensed thermal gas [24]. In the noncondensed thermal gas $\dot{n}=-2Kn^2$ if other loss processes are neglected.

Given the large detuning condition of Eq. (3), the expressions in Refs. [15,16] reduce to

$$a_{\rm opt}(\Delta,I)=\frac{1}{2k_r}\frac{\Gamma_{eg}(\varepsilon_r,I)}{\Delta-\Delta_e}=a_{\rm bg}\frac{\delta_{eg}(I)}{\Delta-\Delta_e}, \tag{7}$$

$$a_{\rm scat}(\Delta,I)=a_{\rm bg}\left(1+\frac{\delta_{eg}(I)}{\Delta-\Delta_e}\right), \tag{8}$$

$$b_{\rm opt}(\Delta,I)=\frac{1}{2}a_{\rm opt}(\Delta,I)\frac{\Gamma_{e,\rm nat}}{\Delta-\Delta_e}, \tag{9}$$

where $a_{\rm bg}$ is the background scattering length defined previously, and

$$\delta_{eg}(I)=\frac{\Gamma_{eg}(\varepsilon_r,I)}{2k_r a_{\rm bg}}. \tag{10}$$

Since the threshold properties of low-energy scattering ensure that $\Gamma_{eg}(\varepsilon_r,I)\propto k_r$ as $\varepsilon_r\to 0$, we see that $\delta_{eg}(I)$, $a_{\rm opt}(\Delta,I)$, and $b_{\rm opt}(\Delta,I)$ are independent of collision energy for $\varepsilon_r\to 0$. Equation (8) shows that the change in scattering length for an optically induced Feshbach resonance has the same form as that for a magnetically tunable Feshbach resonance when the width $\delta_{eg}(I)$ is used. With our definitions, $\Delta-\Delta_e>0$ corresponds to blue detuning and a positive change in scattering length.

For optical Feshbach resonances it is also convenient to express the detuning dependence in terms of the natural linewidth, namely

$$a_{\rm opt}(\Delta,I)=l_{\rm opt}(I)\frac{\Gamma_{e,\rm nat}}{\Delta-\Delta_e}, \tag{11}$$

$$b_{\rm opt}(\Delta,I)=\frac{1}{2}l_{\rm opt}(I)\left(\frac{\Gamma_{e,\rm nat}}{\Delta-\Delta_e}\right)^2, \tag{12}$$

where the "optical length" is defined as

$$l_{\rm opt}(I)=\frac{\Gamma_{eg}(\varepsilon_r,I)}{2k_r\Gamma_{e,\rm nat}}=a_{\rm bg}\frac{\delta_{eg}(I)}{\Gamma_{e,\rm nat}}. \tag{13}$$

This length depends on the molecular physics parameters of the ground and excited states but is independent of collision energy in the low-energy threshold regime and is proportional to the laser intensity I, given our large detuning assumption. The optical length is the same as the radius introduced in Eq. (12) of Ref. [15].

In order to make useful changes in the scattering length, the change has to be large while the losses remain small. The former criterion requires that $|a_{\rm opt}|\gg|a_{\rm bg}|$, whereas the latter requires that $|a_{\rm opt}|\gg b_{\rm opt}$. Equation (7) shows that the first criterion is satisfied as long as $|\Delta-\Delta_e|\ll\delta_{eg}$, whereas Eq. (9) shows that the second is satisfied if $|\Delta-\Delta_e|\gg\Gamma_{e,\rm nat}$. The condition in Eq. (3) requires a more stringent condition on the detuning, which we can state in terms of $l_{\rm opt}$ by combining Eqs. (3) and (13): $|\Delta-\Delta_e|\gg\Gamma_{e,\rm nat}(1+2k_r l_{\rm opt})$, where we may take k_r typical of a collision energy in the system. Combining these criteria, they may be stated either in terms of the detuning,

$$\delta_{eg}\gg|\Delta-\Delta_e|\gg(1+2k_r l_{\rm opt})\Gamma_{e,\rm nat}, \tag{14}$$

or the length parameters,

$$\frac{l_{\rm opt}}{1+2k_r l_{\rm opt}}\gg a_{\rm opt}(\Delta,I)\gg a_{\rm bg}. \tag{15}$$

In general it will be difficult to satisfy these criteria for the case of strongly allowed molecular transitions with large $\Gamma_{e,\rm nat}$ since they typically have a relatively small $l_{\rm opt}$ at the large detunings that are necessary. However, using the example of Ca atoms, we now will show that these criteria can be satisfied by an intercombination line transition, for which the needed large detuning can be achieved close enough to atomic resonance that the Franck-Condon factor is large enough that $l_{\rm opt}$ is not too small.

Experimental demonstration of the optical tuning of the

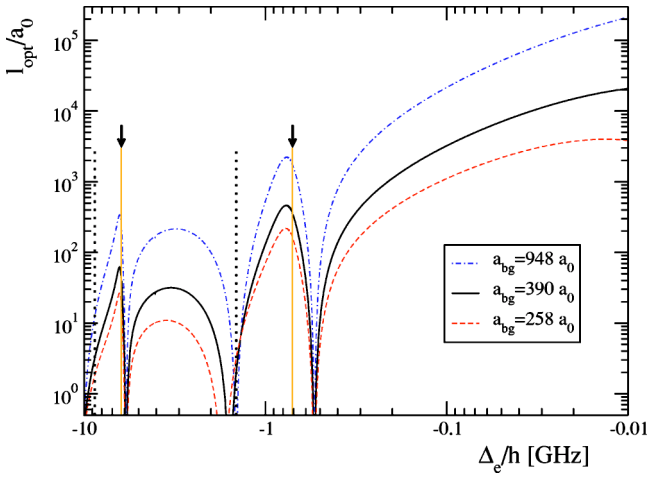

FIG. 1. (Color online) The optical length $l_{\rm opt}$ calculated for rovibrational states of the 0_u^+ band of Ca_2 as a function of their line position (binding energy) Δ_e and background scattering length $a_{\rm bg}$ of the ground-state potential. The laser intensity is 1 W/cm^2. The short range of the 0_u^+ potential is varied to change Δ_e. The arrows show the position of the last two unperturbed 1_u levels, which are held fixed in the calculation. The vertical dotted lines mark the edges of the energy ranges ("bins") within which one and only one level of 0_u^+ symmetry will lie, given some 0_u^+ potential curve (the first "bin" starts at $\Delta_e=0$). The actual 0_u^+ and 1_u line positions are not known and will need to be determined experimentally.

^{87}Rb scattering length was presented by Theis *et al.* [18]. Measurements were done with a moderate laser intensity of about 500 W/cm^2. The authors observed a tuning range of the scattering length of about $200a_0$ accompanied by a trap loss coefficient as large as 2×10^{-10} cm^3/s (a_0 =0.052 917 72 nm). The optical length for this strongly allowed $^{87}Rb_2$ transition is $l_{\rm opt}\approx100a_0$, which is relatively small and comparable to $a_{\rm bg}=103a_0$. Therefore, a significant change of the scattering length, i.e., $a_{\rm opt}\sim a_{\rm bg}$, can only be induced close to resonance and is accompanied by a large trap loss.

We have calculated properties of optical Feshbach resonances for calcium near the intercombination line. The molecular structure and transition dipole moments are evaluated as in Ref. [20]. The molecular structure is insufficiently known to quantitatively predict the absolute positions of the excited bound vibrational levels. It is necessary to measure these positions experimentally. Moreover, the background scattering length of the ground state is not precisely known but is believed to be positive and on the order of a few hundred a_0 [25]. Nevertheless, we can map out the values of $l_{\rm opt}$, $a_{\rm opt}$, and other Feshbach properties as a function of the background scattering length, binding energy, and laser detuning and intensity.

Figure 1 shows $l_{\rm opt}$ as a function of both background scattering length $a_{\rm bg}$ and Δ_e (the positive binding energy relative to $^3P_1+{}^1S_0$ atoms is $-\Delta_e$). Details of the calculation of the stimulated width $\Gamma_{eg}(\varepsilon_r)$, necessary for the evaluation of $l_{\rm opt}$, are described in the figure caption and in Ref. [20]. Figure 1 shows several maxima and minima in $l_{\rm opt}$. The optical length at the maxima ranges between $10a_0$ and 10^5a_0. The interference minima to the right of the arrows are due to the mixing of 0_u^+ and 1_u bound states. The third minimum is due to vanishing overlap between excited 0_u^+ and ground-state wave functions. The nature and properties of these features are discussed in detail in Ref. [20].

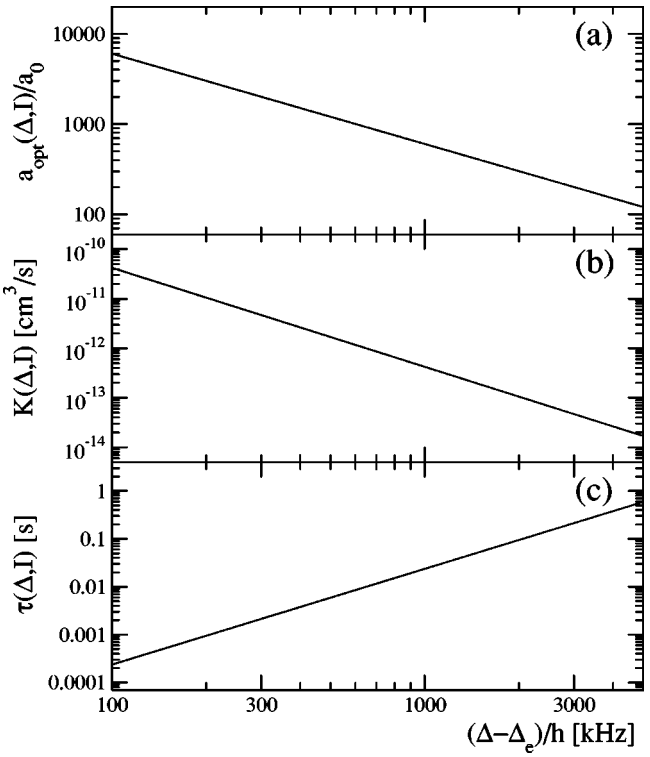

FIG. 2. (a) The optically induced scattering length $a_{\rm opt}(\Delta,I)$, (b) the optically induced trap loss rate $K(\Delta,I)$, and (c) the time scale $\tau(\Delta,I)=[K(\Delta,I)n]^{-1}$ are shown as a function of the detuning $(\Delta-\Delta_e)/\hbar$. The figure also applies if the sign of $(\Delta-\Delta_e)/\hbar$ is reversed, in which case $a_{\rm opt}(\Delta,I)$ also changes sign. Results were obtained for $a_{\rm bg}=389.8$, $\Delta_e/h=-150$ MHz, $I=500$ W/cm^2, $\Gamma_{e,\rm nat}=0.663$ kHz, $l_{\rm opt}=0.9\times10^6a_0$, and $n=10^{14}$ atom/cm^3. For collision energy $\varepsilon_r/k_B=1$ nK the stimulated width $\Gamma_{eg}(\varepsilon_r)/h=18.3$ kHz and $k_r=1.52\times10^{-5}a_0^{-1}$.

The figure also shows that the envelope of $l_{\rm opt}$ (i.e., ignoring oscillations) increases when $|\Delta_e|$ decreases or $a_{\rm bg}$ increases. In fact, for a laser intensity of 1 W/cm^2 and binding energies on the order of 1 GHz the optical length can be bigger than 10^3a_0, while it is 0.5×10^6a_0 for $\Delta_e\approx-1$ MHz and $a_{\rm bg}\approx1000a_0$.

In order to provide a specific example of $a_{\rm opt}(\Delta,I)$ and $b_{\rm opt}(\Delta,I)$, we assume a bound state with $-\Delta_e/h=150$ MHz and $a_{\rm bg}=389.8a_0$. (This optical resonance corresponds to line number 1 of the 0_u^+ band as defined in Ref. [20].) For this case $l_{\rm opt}=0.9\times10^6a_0$ at a laser intensity of 500 W/cm^2. This is the same laser intensity as that used in Ref. [18], but $l_{\rm opt}$ is four orders of magnitude larger than that for Ref. [18].

Figures 2(a) and 2(b) show the optically induced scattering length $a_{\rm opt}(\Delta,I)$ and loss rate coefficient $K(\Delta,I)$ as a function of blue detuning $\Delta-\Delta_e$ for the parameters defined above. The laser detunings shown in the figure are orders of magnitude larger than the natural linewidth of 0.663 kHz. For these parameters the stimulated linewidth is 18.2 kHz at a collision energy of 1 nK, for which $2k_rl_{\rm opt}=27$. The re-

quirement that $|\Delta-\Delta_e|/h \gg (1+2k_r l_{\rm opt})\Gamma_{e,\rm nat}/h = 19$ kHz is easily satisfied. However, for collision energies on the order of 1 μK, $\Gamma_{e,\rm nat}(1+2k_r l_{\rm opt})$ is of the same order as the frequency range in Fig. 2 and our assumptions are broken. Consequently, for these collision energies we need a detuning $\Delta-\Delta_e$ that is larger than 5 MHz.

In the figure both $a_{\rm opt}$ and $K(\Delta,I)$ decrease with increasing detuning. The optically induced scattering length is $\approx 1200a_0$ for $(\Delta-\Delta_e)/h = 500$ kHz, while simultaneously the trap loss rate is relatively small with $K(\Delta,I) = 1.7 \times 10^{-12}$ cm^3/s. This loss rate coefficient is two orders of magnitude less than in the case of rubidium. The time-scale parameter $(Kn)^{-1} \approx 6$ ms, assuming an initial atom density $n = 10^{14}$ atom/cm^3.

Equations (11) and (12) apply to red as well as blue detunings so that negative $\Delta-\Delta_e$ gives a negative $a_{\rm opt}(\Delta,I)$. Using the parameters in Fig. 2, it should be possible to tune the scattering length $a_{\rm scat}$ from $\approx -800a_0$ to zero to $\approx +400a_0$ while the loss rate remains below 1.7×10^{-12} cm^3/s.

The essential molecular physics that sets the magnitude of $l_{\rm opt}$ depends on the molecular Franck-Condon factor in Eqs. (1) and (2). The transition dipole moment cancels in the definition of $l_{\rm opt}$ in Eq. (13) due to the relation $\Gamma_{e,\rm nat} \approx 2\Gamma_A$. However, the small natural linewidth of the $^1S_0 - {}^3P_1$ transition for alkaline-earth-metal atoms has an important role to play, since much smaller detuning from atomic resonance can be used than in the case of alkali-metal atoms. Both numerical and analytic calculations, similar to those used in the Appendix of Ref. [16], show that the magnitude of the Franck-Condon factor (ignoring an oscillating phase factor) increases as the binding energy of the excited level decreases. To operate at sufficiently large detuning to satisfy Eqs. (14) and (15) requires a quite large binding energy for strongly allowed transitions, i.e, many GHz to more than a THz. On the other hand, binding energies in the MHz range can be used in the case of weak intercombination line transitions. Consequently, we find that optical lengths can be orders of magnitude larger for weak intercombination lines than allowed transitions, since the Franck-Condon factors can be intrinsically much larger once the necessary conditions are satisfied for changing scattering length without major losses.

In summary, we have shown that molecular energy levels close to the $^1S_0 + {}^3P_1$ dissociation limit of alkaline-earth-metal atoms provide optical Feshbach resonance states that allow for a significant change of scattering length even for moderate laser intensities and laser frequencies far detuned from optical resonance, with a relatively small trap loss rate coefficient. A small loss rate coefficient leads to longer observation times. Although we have used calcium as an example system, we expect our conclusions to remain valid for other alkaline-earth-metal atoms as well as atoms with similar electronic structure, such as ytterbium [21]. Optical Feshbach resonances seem to be a promising tool that will allow a tunable interaction strength in atomic systems which do not have magnetic Feshbach resonances.

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