Feshbach resonances in an ultracold $^7\text{Li}^{133}\text{Cs}$ Bose-Bose mixture

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We present a study of interspecies Feshbach resonances in ultracold $^7\text{Li}^{133}\text{Cs}$ Bose-Bose mixtures. We locate ten interspecies resonances in three different spin-state combinations. By comparing to coupled-channel calculations, we assign six of the resonances to $s$-wave channels and the rest to $p$-wave channels. We use the $s$-wave resonances to refine the ground-state potentials of LiCs in the coupled-channel calculations and then obtain an accurate characterization of the scattering and bound-state properties of the mixtures. Our results will be useful for future experiments with ultracold $^7\text{Li}^{133}\text{Cs}$ mixtures.

I. INTRODUCTION

Feshbach resonances can be exploited to control the interactions of ultracold atoms, providing a versatile platform to explore few-body and many-body phenomena [1,2]. Notable examples include molecular Bose-Einstein condensates [3–5], Efimov states [6–9], polarons [10–13], and unitary quantum gases [14–17].

Feshbach resonances can also be used to produce Feshbach molecules [18–22]. These loosely bound molecules can be transferred efficiently into ground-state molecules via stimulated Raman adiabatic passage. The scheme was first demonstrated in KRb molecules by Ni et al. [23] and recently a dipolar quantum gas of KRb molecules was created by De Marco et al. [24]. The quantum gases of polar molecules provide unique opportunities to simulate many-body models with a strong anisotropic long-range interaction. Mixtures of Li and Cs have gained special interest, because fully polarized ground-state LiCs molecules possess a dipole moment almost ten times larger than KRb [25].

$^6\text{Li}$ and $^7\text{Li}$ are the stable isotopes of Li. The Feshbach resonances of $^6\text{Li}$ and $^{133}\text{Cs}$ have been studied in Refs. [26,27] and further analyzed in Ref. [28]. Recently, a few $^7\text{Li}^{133}\text{Cs}$ Feshbach resonances have been predicted based on a coupled-channel (CC) model using $^6\text{Li}^{133}\text{Cs}$ singlet and triplet potentials [29]. In this paper we report the observation of ten $^7\text{Li}^{133}\text{Cs}$ Feshbach resonances. These resonances are identified by enhanced trap losses of Li as the scanning magnetic field hits a resonance. Furthermore, we carry out full CC calculations to provide a characterization of the Li-Cs interactions.

We organize this article as follows. In Sec. II we describe the experimental setup and procedure for the trap-loss measurements. We also introduce a model to analyze finite-temperature atom-loss features. In Sec. III we show the results from our coupled-channel calculations. In Sec. IV we conclude with a discussion of the features of the Feshbach resonances and give an outlook on the future applications.

II. EXPERIMENT AND ANALYSIS

The experimental setup is based on the apparatus detailed in Ref. [30], which employs a lithium-ceium slow beam. The setup now includes two overlapping magneto-optical traps (MOTs) and two separated optical dipole traps, one MOT and one dipole trap for each species. The $^7\text{Li}$ MOT captures approximately $10^6$ Li atoms from the slow beam in 40 s, and the temperature of the Li atoms in the MOT is $\sim 0.4$ mK. For $^{133}\text{Cs}$, we use a dark-spot MOT [31] to suppress losses caused by light-assisted collisions [32]. The Cs MOT collects $10^6$ Cs atoms in a loading time of 2 s. Following a compression phase in the MOTs, the Cs atoms are further cooled down to 5 $\mu$K using gray molasses cooling [33].

To prepare ultracold $^7\text{Li}^{133}\text{Cs}$ mixtures for trap-loss measurements, we load the Li and Cs atoms into separated dipole traps (one for each species) first, then perform evaporation, and finally merge the two traps. The dipole traps are single-beam traps, created by independent 1064-nm laser sources. At this wavelength, the polarizability of Cs is approximately four times greater than that of Li. The two dipole beams cross at the center of the science cell with an angle of 7$^\circ$, as shown in Fig. 1. They are initially separated by a vertical distance of 300 $\mu$m. The distance is chosen such that the loading efficiencies of the two species are optimized. We use a high-power tightly focused ($P = 160$ W and $\omega_0 = 50$ $\mu$m) beam for Li and a low-power loosely focused ($P = 6$ W and $\omega_0 = 130$ $\mu$m) beam for Cs. The trap depths are estimated to be 2 mK for Li and 50 $\mu$K for Cs.

Independent evaporative cooling procedures are implemented for Li and Cs. Before evaporation, we apply a bias magnetic field of 819 G and a field gradient of...
The bias field enables efficient Li evaporation. To prepare Cs in the selected spin states for Feshbach spectroscopy, we use optical pumping to prepare Cs in the Cs states. We confirm that 85% of the Cs atoms are pumped to the designated state by the absorption images after Stern-Gerlach separations; nevertheless, only Cs atoms remain in the trap after the Cs evaporation. To prepare the Li spins, we pump the Li atoms to the \( F = 1 \) manifold and populate all three spin states. After the Li evaporation, most of the remaining atoms are in the Li state. The Li atoms in the Li state and the Li states are depleted because of the inelastic spin-changing collisions \(^{34,35}\). The collisions flip the spins of the colliding \( \text{Li}(a) \) and \( \text{Li}(c) \) atoms and put them in the \( \text{Li}(b) \) state. At \( B = 819 \) G, following each of the collisions, an excessive energy of \( K_B \times 1.4 \) mK is deposited to the atoms. The acquired kinetic energies allow them to escape from the trap. To check the Li spin purity, we perform Feshbach spectroscopy on the Li-only samples. In the scans, we find three resonant loss features (see red circles in Fig. 2); two are known resonances in the Li-Li channel \(^{36}\) and the one at 938 G is close to the Li-Li resonance \(^{37}\). From the profile, we estimate the spin purity of \( \text{Li}(b) \) to be ~90%.

The spin preparation of \( \text{Li}(a) \) and \( \text{Li}(c) \) is done through adiabatic rapid passage (ARP) from the Li state. During the ARP, we keep the bias magnetic field at 600 G. At this field, the transition frequencies of \( \text{Li}(b) \rightarrow \text{Li}(a) \) and \( \text{Li}(b) \rightarrow \text{Li}(c) \) differ by 37 MHz; thus, it is possible to achieve a selective transfer. We also take the Li-only Feshbach spectroscopy after the selective transfers (see Fig. 2). For the samples transferred to \( \text{Li}(a) \), one resonant feature is found at 738 G. The position agrees well with the previous observations for the \( \text{Li}(a)-\text{Li}(b) \) Fesh-
Feshbach resonance \[34, 36\]. We also found one resonant feature at 1036 G for the samples transferred to Li(|c⟩). The position is also in good agreement with the theoretical prediction for the Li(|c⟩)-Li(|c⟩) Feshbach resonance \[37\].

To perform interspecies Feshbach spectroscopy, we ramp the bias magnetic field to a desired value and measure the atom number of \(^7\)Li after a variable hold time, which is adjusted empirically to give the best signal-to-noise ratio. The remaining Li atoms are measured by standard absorption imaging at zero magnetic field. Near an interspecies Feshbach resonance, the Li samples experience enhanced trap losses through the three-body recombination processes, cross thermalization, and inelastic two-body collisions. A total of ten resonance features are located within the magnetic field range of 300–1065 G. These features do not exist when the Cs atoms are absent. They are fitted with Gaussian functions, from which the resonance positions \(B_0^{\text{expt}}\) and widths \(\delta_{\text{expt}}\) are determined. The results are summarized in Table I. We calibrate the magnetic field using the microwave transition between Cs\(|F = 3, m_F = 3\rangle\) and Cs\(|F = 4, m_F = 3\rangle\).

The resonant loss features, including the loss peak positions and widths, are temperature dependent. At a temperature of a few \(\mu\)K, thermal effects are usually negligible; the loss peaks shift from their zero-energy resonance positions by no more than 0.1 G. Since our measurements are taken at higher temperatures, \(T_{CS} = 60–100 \mu\)K, several thermal effects would need to be taken into account in order to achieve a precise determination of resonance position. First, all \(s\)-wave resonances observed in this work are closed-channel dominated resonances with \(s_{\text{res}} < 1\). In this case, the shift of pole position is approximately \(E/\delta\mu\). Here \(E\) represents the collision energy and is equal to \(k_B T\); \(\delta\mu\) is the difference between the magnetic moment of the separated atoms and the magnetic moment of the bare bound state. Since \(\delta\mu > 0\) for all the observed resonances, the resonance positions shift to higher fields at higher temperatures. Second, thermal averaging over a broad collision energy distribution will also shift the peaks. Finally, the intrinsic width of resonance increases as \(E^{1/2}\) for \(s\) waves and \(E^{3/2}\) for \(p\) waves \[38\]. Thermally broadened line shapes of different \(m_l\) components from a \(p\)-wave resonance can overlap strongly with one another, leading to an excessive error in the determination of the resonance position. Therefore, to avoid the errors, we perform the optimization of the Li-Cs potentials using only the six \(s\)-wave resonances. We note that the assignment of the resonances is done by comparing the measured resonance positions to the pole positions predicted by the CC calculations (see Sec. III).

Exploiting the analogy to optical Feshbach resonance and photoassociation \[39\], a similar theoretical model is developed to describe an \(s\)-wave Feshbach resonance with decay to loss channels (Appendix). The loss channels include, but are not limited to, cross thermalization and decay of quasi-molecules \[40, 41\]. Based on the model, we can derive a thermally averaged loss rate coefficient with chosen parameters and then integrate the rate equation for the Li number to generate an atom-loss line shape for fitting. The zero-energy resonance positions can be determined from the finite-temperature model fits. Figure 3 shows the fit for the \(s\)-wave resonance of the Li(|a⟩) + Cs(|a⟩) channel. The fitted resonance positions of all \(s\)-wave resonances are given in Table I.

III. THEORY

We take advantage of two open-source programs, BOUND \[42\] and MOLSCAT \[43\], to implement CC calculations for this work. The BOUND program solves the Schrödinger equation for the bound states and obtains the binding energies at a fixed value of magnetic field \[44\]. The MOLSCAT program carries out the scattering calculations for the scattering lengths \[45\]. Either BOUND or MOLSCAT can be used to locate Feshbach resonances. The calculations are done with a fully decoupled basis set \(|s_{Li}, m_{s,Li}|s_{Cs}, m_{s,Cs}|L, M_L\rangle\). Here \(s\) and \(i\) represent the electron and nuclear spins, respectively, and \(L\) is the relative angular momentum of the two atoms.

To use the programs for the \(^7\)Li-\(^{133}\)Cs mixtures, we construct the CC model based on the \(^6\)Li-\(^{133}\)Cs work \[27\]. First, we perform a mass-scaled version of the calculation and obtain resonance positions that are systematically higher (\(\sim 5\) G) than the observed values. We then add a small harmonic variation \(\alpha(R - R_e)^2\) to the inner wall of each potential in the region \(R < R_e\), where \(R_e\) is the

![FIG. 3. Li trap loss data from the aa channel near the s-wave resonance. The dashed line is a Gaussian fit to the data, and the loss peak position is located at 530.6 G. The solid line is another fit done with the procedure described in the Appendix. In the fitting procedure, the temperature \(T\), resonance position \(B_0\), decay rate \(\gamma\), and initial Li number \(N_{Li}(0)\) are the free parameters. The resonance position \(B_0 = 530.3\) G is found in the fit.](image-url)
TABLE I. Summary of the $^7\text{Li} - ^{133}\text{Cs}$ Feshbach resonances. The resonance positions $B_{0}^{\text{expt}}$ and widths $\delta^{\text{expt}}$ are determined by Gaussian fits to the atom-loss features. The errors in $B_{0}^{\text{expt}}$ and $\delta^{\text{expt}}$ come from the fits, representing a 95% confidence level. We also note that the field calibration and drift result in an error of 0.5 G. The $B_{0}^{\text{fit}}$ are the zero-energy resonance positions determined by the finite-temperature model fits. The theoretical values for resonance positions $B_{0}^{\text{CC}}$ and zero crossing $B_{0}^{\text{CC}}$ are obtained from the coupled-channel calculations with the refined $^7\text{Li} - ^{133}\text{Cs}$ potentials. The errors in $B_{0}^{\text{CC}}$ include the uncertainties from the fits, the field calibration and drift, and the thermal effects.

| Channel                  | $B_{0}^{\text{expt}}$ (G) | $\delta^{\text{expt}}$ (G) | $l$ | $B_{0}^{\text{fit}}$ | $B_{0}^{\text{CC}}$ (G) | $B_{0}^{\text{CC}}$ (G) | $B_{0}^{\text{CC}}$ (G) |
|--------------------------|-----------------------------|-----------------------------|-----|----------------------|------------------------|------------------------|------------------------|
| $^7\text{Li}[1, 1] + ^{133}\text{Cs}[3, 3]$ | 353.2(4)                   | 0.7(2)                      | 1   | 530.3               | 530.2(6)              | 534.5                  | 538.43                 |
| $^7\text{Li}[1, 1] + ^{133}\text{Cs}[3, 3]$ | 439.8(2)                   | 1.9(3)                      | 1   | 609.8               | 609.7(6)              | 620.1                  | 618.31                 |
| $^7\text{Li}[1, 1] + ^{133}\text{Cs}[3, 3]$ | 530.6(1)                   | 1.1(1)                      | 0   | 732.0               | 731.9(7)              | 736.8                  | 735.76                 |
| $^7\text{Li}[1, 0] + ^{133}\text{Cs}[3, 3]$ | 561.8(1)                   | 2.0(2)                      | 1   | 850.8               | 850.7(9)              | 858.1                  |                       |
| $^7\text{Li}[1, 0] + ^{133}\text{Cs}[3, 3]$ | 610.0(2)                   | 2.6(3)                      | 0   | 979.2               | 979.1(7)              | 980.9                  |                       |
| $^7\text{Li}[1, 0] + ^{133}\text{Cs}[3, 3]$ | 732.3(3)                   | 3.0(5)                      | 0   | 1106.6              | 1106.5(9)             | 1110.3                 |                       |
| $^7\text{Li}[1, -1] + ^{133}\text{Cs}[3, 3]$ | 631.8(2)                   | 1.8(3)                      | 1   | 850.6               | 850.7(9)              | 858.1                  |                       |
| $^7\text{Li}[1, -1] + ^{133}\text{Cs}[3, 3]$ | 717.4(2)                   | 3.5(4)                      | 0   | 979.2               | 979.1(7)              | 980.9                  |                       |
| $^7\text{Li}[1, -1] + ^{133}\text{Cs}[3, 3]$ | 779.7(2)                   | 1.4(2)                      | 0   | 1106.6              | 1106.5(9)             | 1110.3                 |                       |
| $^7\text{Li}[1, -1] + ^{133}\text{Cs}[3, 3]$ | 850.8(7)                   | 5.0(10)                     | 0   | 1283.6              | 1283.5(9)             | 1287.1                 |                       |

equilibrium internuclear distance, $\alpha$ is the adjustable parameter, and $i$ is the potential index. We assign $i = 1$ and 3 for the singlet and triplet potentials, respectively. The two parameters $a_1$ and $a_3$ are adjusted to make slight changes in the singlet and triplet scattering lengths $a_1$ and $a_3$, and the resulting field values of the resonances are used to fit the observed $B$ fields of the resonances.

We use the fitted resonance positions $B_{0}^{\text{fit}}$ from the finite-temperature model fits to optimize the $^7\text{Li} - ^{133}\text{Cs}$ potentials in the CC calculations. The optimization is implemented using BOUND, and the theoretical values of the resonance positions are given in Table I. All molecular states associated with the s-wave resonances have mixed singlet-triplet characters and zero orbital angular momentum projection along the internuclear axis; thus, the projection of the total angular momentum $m_F$ is the only good quantum number. The MOLSCAT program is used to calculate the scattering lengths for the three channels at different magnetic fields. The refined potentials of $^7\text{Li}^7\text{Cs}$s yield singlet scattering length $a_1 = 45.82(2) a_0$ and triplet scattering length $a_3 = 873.8(70) a_0$. These values can be compared with $a_1 = 45.47 a_0$ and $a_3 = 908.2 a_0$, reported in Ref. [29]. The large $a_3$ indicates the presence of a near-threshold triplet bound state.

The overlapping effect are really pronounced in the s-wave resonances. In each channel, there is a nearly linear increase of the background scattering length with $B$, associated with the presence of strong resonances located around 3000 G (see Fig. 4). The single pole approximation, i.e., $a(B) = a_{bg}[1 - \Delta/(B - B_0)]$, only becomes valid within a small field range near the resonances. To summarize the CC calculations, we plot the measured atom-loss features for the s-wave resonances with the scattering lengths and binding energies in Fig. 5. The calculated pole and zero crossing positions are given in Table I.

![Image](image_url)

FIG. 4. Theoretical values for scattering lengths of the $^7\text{Li}^7\text{Cs}$ (blue solid line), $^7\text{Li}^7\text{Cs}$ (green dotted line), and $^7\text{Li} - ^{133}\text{Cs}$ (red dashed line) channels. The resonances located at $B < 1000$ G are strongly influenced by strong Feshbach resonances near 3000 G, causing scenarios of overlapping Feshbach resonances.

IV. CONCLUSION AND DISCUSSION

We have conducted a detailed study on the $^7\text{Li} - ^{133}\text{Cs}$ Feshbach resonances. We used Feshbach spectroscopy to locate ten interspecies Feshbach resonances in three different scattering channels. We also carried out the coupled-channel calculations to provide precise characterization of the interaction parameters, such as scattering length and binding energy. From the results, we are able to identify two interesting field regimes for the mixtures. First, near $B = 885$ G, the $^7\text{Li}^7\text{Cs}$ mixture has moderate inter- and intraspecies interactions; the respective values of the scattering lengths are approximately 250$a_0$, 100$a_0$, and 400$a_0$ for the $^7\text{Li}^7\text{Cs}$, $^7\text{Cs}^7\text{Cs}$ and $^7\text{Li} - ^{133}\text{Cs}$ channels. These val-
FIG. 5. Feshbach spectroscopy and the coupled-channel calculations for the $s$-wave resonances. (a) Observed Li trap loss features in the Li$|a\rangle +$ Cs$|a\rangle$ (blue), Li$|b\rangle +$ Cs$|a\rangle$ (red), and Li$|c\rangle +$ Cs$|a\rangle$ (green) channels. The solid lines are the Gaussian fits to the atom-loss features. Also shown are the theoretical values of (b) scattering lengths and (c) binding energies.

Values can support fast thermalization and slow three-body recombinations. Thus, it may be possible to create a dual-species Bose-condensed system of Li$|b\rangle$ and Cs$|a\rangle$ near 885 G. Second, near the Li$|b\rangle +$ Cs$|a\rangle$ resonance at $B = 732$ G, the Cs$|a\rangle +$ Cs$|a\rangle$ scattering length is positive and large, $\sim 5000 a_0$, while the Li$|b\rangle +$ Li$|b\rangle$ scattering length is positive and small, $\sim 9 a_0$. In this regime, Bose-Einstein condensates of Li$|b\rangle$ can interact resonantly with strongly interacting Cs atoms.

Finally, radio-frequency spectroscopy of LiCs dimers in the future can provide accurate measurements on the dimer binding energies near a resonance. These measurements can set tighter constraints to the pole positions and hence lead to highly accurate scattering length data. In addition, the spectra can also be used to verify higher partial-wave ($l \geq 1$) models in coupled-channel calculations.

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Appendix

In the presence of the decay that leads to atom loss, the $S$-matrix element describing an $s$-wave scattering channel coupled to an isolated bound state near a threshold is

$$S(k) = \left\{ 1 - \frac{i \hbar \Gamma(k)}{E - E_{\text{res}} + i \frac{1}{2} \hbar (\gamma + \Gamma(k))} \right\} e^{2i \eta_{bg}}, \quad (A.1)$$

where $E_{\text{res}} = \delta \mu (B - B_0)$ is the energy of the resonance, $B_0$ is the resonance position at the scattering threshold ($E = 0$), and $\gamma$ is the rate of atom loss. The decay rate $\gamma$ includes all loss sources. In the case of magnetic Feshbach resonances, $\hbar \Gamma(k) = 2k a_{\text{bg}} \delta \mu \Delta$ is related to the width of the resonance. The phase shift $\eta_{bg}$ is associated with the background scattering length $a_{\text{bg}}$ as $\tan \eta_{bg} = -k a_{\text{bg}}$.

Taking the expression for $S(k)$, the inelastic cross section $\sigma_{\text{in}} = \pi |1 - |S(k)|^2/k^2|$ can be written as

$$\sigma_{\text{in}} = \frac{2\pi}{k} \frac{\gamma^2 l_{\text{eff}}}{(E - E_{\text{res}})^2 + \frac{\gamma^2}{4} \left(1 + 2k l_{\text{eff}}\right)^2}, \quad (A.2)$$

where $l_{\text{eff}} = a_{\text{bg}} \delta \mu \Delta / \hbar \gamma$ is a characteristic length associated with the coupling strength. Then the thermally averaged loss rate coefficient $\langle K \rangle_{\text{th}}$ is given by

$$\langle K \rangle_{\text{th}} = \sqrt{\frac{8}{\mu \pi}} \frac{1}{(k_\beta T)^{3/2}} \int dE \sigma(E) E e^{-E/k_\beta T}. \quad (A.3)$$

The final step to derive an atom-loss line shape is to assume a loss model. In our experiment, the temperature
of Cs is much higher than Li and the trap depth is much shallower ($\sim \frac{1}{2}$) for Li. Thus, the dominant loss of Li is heating from colliding with Cs. In this case, the loss rate equation for the Li number $N_{\text{Li}}$ is

$$\frac{dN_{\text{Li}}}{dt} = -\langle K \rangle N_{\text{Li}},$$

(A.4)

where $n_{\text{CS}} = \int n_{\text{CS}}(\vec{r}) n_{\text{Li}}(\vec{r}) d^3\vec{r}$ is the average Cs density. In our measurements, the number loss of Cs is less than 10%; thus, we assume the Cs density is constant in the rate equation. After integrating Eq. (A.4) over an interaction time, we obtain atom-loss line shapes that can fit the measurements. Here $T$, $B_0$, $\gamma$, and $N_{\text{Li}}(0)$ are the free parameters in the fits.

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