Broad Feshbach resonance in the 6Li-40K mixture

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A decade of experiments with degenerate fermionic quantum gases has delivered major scientific advances as well as a whole new class of quantum many-body systems [1–3]. Feshbach resonances [4] played a central role in this development, as they offer exceptional control over the interatomic interactions at low temperatures [5]. In gases with the appropriate spin mixture, the sign and magnitude of the $s$-wave scattering length $a$ can be tuned to any positive or negative value by choosing the proper magnetic field in the vicinity of a resonance. In the case of fermionic atoms, the role of Feshbach resonances is especially remarkable because Pauli exclusion dramatically suppresses three-body losses to deeply bound molecular states [6,7]. The tunability has been used with great success in two-component Fermi gases of $^6$Li and of $^{40}$K to study and control pairing mechanisms, both of the Cooper type on the attractive side of the resonance ($a < 0$) [8] and of the molecular type on the repulsive side ($a > 0$) [9]. In particular, the universal crossover from the superfluidity of a molecular Bose-Einstein condensate (BEC) towards the Bardeen, Cooper, Schrieffer (BCS) limit received a lot of attention [10]. Essential for these studies is the availability of sufficiently broad Feshbach resonances in the $^6$Li and $^{40}$K homonuclear gases.

Recently, the study of heteronuclear fermionic mixtures has strongly gained in interest due to its additional mass imbalance. Theoretical studies on these mixtures include, e.g., superfluidity [11], phase separation [12], crystalline phases [13], exotic pairing mechanisms [14], and long-lived trimers [15]. Many of these studies require the mixture to be strongly interacting and in the universal limit; i.e., the scattering length should be very large and the only parameter that determines the two-body interaction. Recently, the first mass-imbalanced ultracold fermionic mixture has been realized, namely, a mixture of the only stable fermionic alkaline species $^6$Li and $^{40}$K [16]. The basic interaction properties of the $^6$Li/$^{40}$K system were established in experiments by the Innsbruck group [17], in which the loss features of 13 Feshbach resonances were observed and assigned. The first $^6$Li$^{40}$K molecules were recently reported from Munich [18]. Despite this experimental progress, a sufficiently broad Feshbach resonance to use the $^6$Li/$^{40}$K system for universal studies has not been reported so far.

In this Letter, we identify and characterize the optimal Feshbach resonance of the $^6$Li/$^{40}$K mixture. We develop a generic model to estimate the positions and widths of all available $s$-wave Feshbach resonances in quantum gases. By applying this model to the two-component $^6$Li/$^{40}$K mixtures stable against spin exchange, we select the optimal resonance compromising between resonance width and convenience for detection. We present the first measurement of a resonance width in the $^6$Li/$^{40}$K mixture by measuring the asymmetric line shape (Fano profile) of the interspecies elastic cross section near the Feshbach resonance. We measure the rate of distillation of $^6$Li atoms from a potassium-rich $^6$Li/$^{40}$K mixture confined in an optical dipole trap. The measured resonance width is shown to be promising for reaching the universal regime in the $^6$Li/$^{40}$K mixture.

In search of broad and accessible Feshbach resonances, we extend the asymptotic bound-state model (ABM) [17] to include the description of resonance widths. We start from the two-body Hamiltonian for the relative motion

$$\mathcal{H} = p^2/2\mu + \mathcal{V} + \mathcal{H}^{\text{int}} = \mathcal{H}^{\text{rel}} + \mathcal{H}^{\text{int}},$$

containing the relative kinetic energy with $\mu$ the reduced mass, the electron-spin-dependent central interatomic interaction $\mathcal{V}$, and the internal energy $\mathcal{H}^{\text{int}}$ of the two atoms. Here we restrict $\mathcal{H}^{\text{int}}$ to the hyperfine and Zeeman terms and consider $s$-wave interactions only.
Instead of solving coupled radial Schrödinger equations, the ABM approach relies on the knowledge of the binding energies of the highest bound states in the two-body system. This is sufficient to determine the scattering properties and, in particular, the position of Feshbach resonances. For $^6\text{Li}/^{40}\text{K}$ only the least bound levels of $\mathcal{H}^{\text{rel}}$ are relevant and can be obtained using the eigenvalues $E_S$ of the least bound states in the electron-spin singlet ($S = 0$) and triplet ($S = 1$) potentials as free parameters; here we adapt $E_0$ and $E_1$ from Ref. [17].

The mixture is prepared in one of the two-body hyperfine eigenstates of $\mathcal{H}^{\text{int}}$ at magnetic field $B$, referred to as the $P$ channel or open channel, denoted via the $B = 0$ hyperfine quantum numbers as $|f, m_f\rangle_\alpha \otimes |f, m_f\rangle_\beta$. The corresponding energy of two free atoms at rest defines a $B$-dependent reference value representing the threshold between the scattering states ($E > 0$) and the bound states ($E < 0$) of $\mathcal{H}$. We define $\mathcal{H}$ relative to this threshold energy. A basis for the spin properties is defined via the quantum numbers $S$, its projection $M_S$, and the nuclear-spin projections $\mu_\alpha$ and $\mu_\beta$, while requiring that the total projection $M_S + \mu_\alpha + \mu_\beta = m_f + m_f = M_F$ is fixed. By diagonalizing $\mathcal{H}$ starting from this “singlet-triplet” basis we find the bound-state energies, and the Feshbach resonances are localized at the magnetic fields where they intersect with the energy of the threshold.

Threshold effects cause the approximately linear magnetic field dependence of the bound-state energies to change to quadratic behavior close to the field of resonance [3,5]. This provides information about the width of a Feshbach resonance. The ABM, as discussed thus far, does not show these threshold effects, which is not surprising because the threshold is not explicitly built into the theory; it is merely added as a reference value for comparison with the ABM eigenvalues.

However, the ABM contains all ingredients to also obtain the resonance width. The Hamiltonian (1) describes all two-body bound states, belonging to both open and closed channels. The width depends on the coupling between the open channel and the various closed channels, which is determined after two basis transformations to identify the open channel and the resonant closed channel respectively. First, we separate the open channel, defined above, from all other channels: the closed channels $Q$ [19]. This is realized with a basis transformation from the singlet-triplet basis to the $|f, m_f\rangle_\alpha \otimes |f, m_f\rangle_\beta$ basis. In this basis we identify the open channel, namely, the hyperfine state in which the system is experimentally prepared. We refer to this diagonal subspace as $\mathcal{H}_{pp}$, a single matrix element that we identify with the (bare) open-channel bound-state energy $E_p = -\hbar^2 k_p^2/2\mu$. Second, we perform a basis transformation that diagonalizes the closed-channel subspace $\mathcal{H}_{QQ}$, leaving the open-channel $\mathcal{H}_{pp}$ unaffected. The $\mathcal{H}_{QQ}$ matrix contains the closed-channel bound-state energies $E_Q$ disregarding the coupling to $\mathcal{H}_{pp}$. This transformation allows us to identify the resonant closed channel. The coupling between the open and the resonant closed channel is referred to as $\mathcal{H}_{PQ}$ and is a measure for the resonance width.

To obtain the magnetic field width of the resonance from $\mathcal{H}_{PQ}$, we use Feshbach’s resonance theory [20,21]: a closed-channel bound state acquires a finite width $\Gamma$ and its energy undergoes a shift $\Delta_{\text{res}}$. If the binding energy of a certain $Q$-channel bound state $|\phi_Q\rangle$ is sufficiently close to the threshold, we can effectively consider a two-channel problem where the complex energy shift is given by $\Gamma$.

\[
A(E) = \Delta_{\text{res}}(E) - \frac{i}{2} \Gamma(E) = \frac{\mu}{\hbar^2} \frac{-iA}{\kappa_p(k - i\kappa_p)}, \tag{2}
\]

where $A = |\langle \phi_p | \mathcal{H}_{PQ} | \phi_Q \rangle|^2$ is the coupling strength to the $P$-channel bound state $|\phi_p\rangle$. For $k \rightarrow 0$, the expression $\Gamma = \hbar^2 k/\mu R^\ast$ defines the characteristic length $R^\ast = \hbar^2/(2\mu a_{bg} \mu_{rel} \Delta_{\text{res}})$ of the resonance [22], where $\mu_{rel} = \frac{\delta E_Q}{\delta B_{B0}}$ is the magnetic moment of the bare $Q$ channel relative to the open-channel threshold. The binding energy $E = \hbar^2 k^2/2\mu$ of the dressed bound state is obtained by solving the pole equation of the scattering matrix, given by $E - E_Q - A(E) = 0$, assuming that near threshold the bare bound state can be approximated by $E_Q = \mu_{rel}(B - B_0) - \Delta_{\text{res}}$. Close to threshold, we obtain for the dressed bound-state energy $E = -2|\epsilon_p|^{3/2} |\mu_{rel}(B - B_0)/A|^2$, thus retrieving the characteristic quadratic dependence of the molecular state on the magnetic field. Using the dispersive formula for the field dependence of the scattering length near a Feshbach resonance, $a(B) = a_{bg}[1 - \Delta B/(B - B_0)]$, we obtain an expression for the magnetic

![FIG. 1. ABM calculated widths of all s-wave Feshbach resonances in stable two-component $^6\text{Li}/^{40}\text{K}$ mixtures below 500 G. The lines are a guide to the eye. The point at $M_p = -5$ corresponds to the $[1/2, -1/2]_{1\text{h}} - [9/2, -9/2]_h$ mixture. All other mixtures contain the $^6\text{Li}$ ground state $[1/2, +1/2]_{1\text{h}}$. The width measurement reported in this work. The mixtures with $-M_p = 5, 4, 3, 2$ (gray squares) were studied in Ref. [17]. The resonance used in Ref. [18] is indicated with an arrow.](image-url)
The off-resonance scattering is described by the background scattering length $a_{bg} = a_{bg}^0 + a^p$, where $a_{bg}^0 = r_0$ and $a^p = \kappa_p^{-1}$. Here $r_0 = (\mu C_6/8\hbar^3)^{1/4} \approx 41\alpha_0$ is the interspecies van der Waals range, with $C_6$ the van der Waals coefficient and $\alpha_0$ the Bohr radius.

The results for all $s$-wave resonances in two-component $^6\text{Li}/^4\text{K}$ mixtures stable against spin exchange below 500 G are shown in Fig. 1. The widest resonances for the $^6\text{Li}/^4\text{K}$ mixture are found to be of the order of 1 G. From these results, the optimal resonance is selected to be in the $M_F = 5$ manifold, $|1/2, +1/2\rangle_{\text{Li}} \otimes |9/2, +9/2\rangle_{\text{K}}$ with the predicted position of $B_0 = 114.7$ G as obtained with the ABM parameters $E_{0,1}$ from Ref. [17]. The predicted width is $\Delta B = 0.9$ G. This value is known to slightly underestimate the actual width [23,25]. The resonance in the $M_F = 3$ manifold, $|1/2, +1/2\rangle_{\text{Li}} \otimes |9/2, +5/2\rangle_{\text{K}}$, is predicted to be the broadest, 20% wider than the $M_F = 5$ resonance. However, because the $|9/2, +9/2\rangle_{\text{K}}$ state has an optical cycling transition, facilitating detection in high magnetic field, the $M_F = 5$ resonance is favorable for experimental use. Therefore, this resonance offers the best compromise between resonance width and an experimentally favorable internal state.

Our procedure to create an ultracold mixture of $^6\text{Li}$ and $^{40}\text{K}$ is described in detail elsewhere [26,27]. Here we briefly summarize the procedure. We perform forced evaporative cooling on both species in an optically plugged magnetic quadrupole trap [28]. A small amount of spin-polarized $^6\text{Li}$ in the $|3/2, +3/2\rangle_{\text{Li}}$ hyperfine state is sympathetically cooled by rethermalization with a three-component mixture of $^{40}\text{K}$ in the hyperfine states $|9/2, +5/2\rangle_{\text{K}}, |9/2, +7/2\rangle_{\text{K}}$, and $|9/2, +9/2\rangle_{\text{K}}$. The interspecies singlet and triplet scattering lengths are nearly identical [17]; therefore, spin-exchange losses in collisions of $|3/2, +3/2\rangle_{\text{Li}}$ with $|9/2, +5/2\rangle_{\text{K}}$ or $|9/2, +7/2\rangle_{\text{K}}$ are suppressed. This allows us to achieve efficient sympathetic cooling of the lithium down to $T \approx 10 \mu$K with $10^5$ atoms for both $^6\text{Li}$ and $^{40}\text{K}$. For the Feshbach resonance width measurement, we transfer the mixture into an optical dipole trap with a well depth of $U_0 = 360 \mu$K for $^{40}\text{K}$ ($U_0 = 160 \mu$K for $^6\text{Li}$) serving as an optical tweezer. The sample is transported over 22 cm to a quartz cell extending from the main vacuum chamber by moving a lens mounted on a precision linear air-bearing translation stage. In the quartz cell, we can apply homogeneous fields (<10 ppm/mm) of up to 500 G. For the Feshbach resonance width measurement, we prepare a $|1/2, +1/2\rangle_{\text{Li}} - |9/2, +9/2\rangle_{\text{K}}$ mixture consisting of $4 \times 10^3\ ^6\text{Li}$ and $2 \times 10^4\ ^{40}\text{K}$ atoms at temperature $T = 21(2) \mu$K.

To observe the resonance, we first ramp the field up to ~107 G where any remaining potassium spin impurities are selectively removed by resonant light pulses. The Fano profile of the resonance is observed by measuring the distillation rate of the Li from the potassium-rich Li-K mixture in the optical trap as a function of magnetic field. To initiate this process, we decrease the depth of the dipole trap in 10 ms to $U/U_0 = 0.15$. Aside from a small spilling loss of the $^6\text{Li}$, this decompresses the mixture with a factor $(U/U_0)^{3/4} \approx 0.24$ in the adiabatic limit and reduces the temperature accordingly by a factor $(U/U_0)^{1/2} \approx 0.39$. The truncation parameter for evaporation, $\eta = U/k_B T$, drops for both species by the same amount. After decompression, the central density of the potassium is $n_{\text{K}} = 2 \times 10^{11}$ cm$^{-3}$ ($n_{\text{Li}} = 9 \times 10^9$ cm$^{-3}$ for Li) and the temperature of the mixture is $T = 9(1) \mu$K. As the truncation parameter of the lithium ($\eta_{\text{Li}} = 2.7$) is much smaller than that of potassium ($\eta_{\text{K}} = 6.2$), the Li preferentially evaporates at a rate proportional to the interspecies elastic cross section. As the lithium is the minority component, this distillation process proceeds at an approximately constant rate. We have verified that a pure lithium cloud experiences no rethermalization by itself. The final trap depth $U$ was determined from the total laser power and the measured trap frequency for the potassium, $\omega_r/2\pi = 1.775(6)$ kHz. In Fig. 2, we plot the atom number after various holding times and as a function of magnetic field. We analyze our data by modeling the distillation rate. Before decompression ($\eta_{\text{Li}} = 7$), we observe a loss of 30% for 1 s holding time on resonance. As the decompression reduces the density by a factor of 4, the three-body losses can be neglected in the decompressed trap. The distillation of the lithium as a function of time $t$ is de-
scribed by \( N(t) = N_0 e^{-t/\tau_{\text{vac}}} e^{-t/\tau_{\text{bg}}}, \) where \( N_0 = 3 \times 10^3 \) is the initial number of lithium atoms, \( \tau_{\text{bg}} = 25 \) s the vacuum limited lifetime, and \( \tau_{\text{bg}}^{-1} \approx n_K (\sigma(k)h/k/\mu) e^{-n_K} \) the thermally averaged evaporation rate. Here is

\[
\sigma(k) = 4\pi \frac{a^2(k)}{1 + k^2a^2(k)}
\]  

the elastic cross section with

\[
a(k) = a_{\text{bg}} + \frac{a_{\text{bg}} \mu_{\text{rel}} \Delta B}{\hbar^2 k^2/2\mu - \mu_{\text{rel}} (B - B_0)}
\]

the “Doppler shifted” scattering length, with \( a_{\text{bg}} = 56.6a_0 \) at the resonance position \( B_0, \) and \( \mu_{\text{rel}} = 1.57\mu_B. \)

The solid lines in Fig. 2 show the best simultaneous fit of the thermally averaged Eq. (4) to the four subfigures, accounting for 25% variation in \( N_0 \) from one day to the next. The best fit is obtained for \( B_0 = 114.47(5) \) G and \( \Delta B = 1.5(5) \) G \( (R^* = 100 \) nm\), where \( B_0 \) is mostly determined by the data of Fig. 2(a) and \( \Delta B \) by those of Fig. 2(d). Uncertainties in \( T \) and \( n_K \) can result in broadening of the loss features, but the difference in asymmetries between Figs. 2(a)–2(d) can only originate from the asymmetry of the elastic cross section around the resonance. The zero crossing of \( a(k) \), prominently visible in systems with a resonantly enhanced \( a_{\text{bg}} \) like \(^6\text{Li} \) [29] and \(^{40}\text{K} \) [30], remains within the noise of our distillation measurements because in the \(^6\text{Li}^{40}\text{K}\) system \( a_{\text{bg}} \) is nonresonant \( (\sigma_{\text{bg}} = 1 \times 10^{-12} \text{ cm}^{-2}). \)

The investigated resonance offers good perspectives for reaching the universal regime, for which the Fermi energy and magnetic field have to obey: \( E_F, \mu_{\text{rel}} |B - B_0| \ll \Gamma/2, \) where \( E_F = \hbar^2 k_F^2/2\mu \) is the characteristic relative energy of a colliding pair of atoms at their Fermi energy. The former condition corresponds to the condition for a broad resonance, \( k_F R^* \ll 1, \) and is satisfied for Fermi energies \( E_F \ll 5 \) \( \mu \)K. The latter condition corresponds to the condition for strong interaction, \( k_F a \gg 1, \) and is satisfied for \( |B - B_0| \ll 43 \) mG at \( E_F = 5 \) \( \mu \)K.

In summary, we developed a model to estimate the positions and widths of all Feshbach resonances in an ultracold gas. We selected the optimal resonance in the \(^6\text{Li}^{40}\text{K}\) system to reach the strongly interacting regime. The experimentally observed width of this resonance, \( \Delta B = 1.5(5) \) G, is in good agreement with the theory and offers promising perspectives to study a strongly interacting mass-imbalanced Fermi gas in the universal regime using realistic experimental parameters.

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[23] We thank Professor E. Tiemann for sharing with us his coupled-channel result \( B_0 = 114.78 \) G, \( a_{\text{bg}} = 57.1a_0, \) \( \Delta B = 1.82 \) G, based on the potential of Ref. [24].
[25] For details, see T. G. Tieleke et al. (to be published).