Feshbach resonances in 40K

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Chapter 2

Theoretical Background

In this chapter the theoretical concepts and notations used in this thesis are presented. This chapter gives an overview of scattering theory and Feshbach resonances and their description. We present the simplified model which was used to calculate the positions of Feshbach resonances in $^{40}\text{K}$. This chapter also presents the assumptions to analyse and model the behaviour of ultracold atoms in external potentials. We put emphasis on the peculiarities of $^{40}\text{K}$ and the nature of fermions.

Cold quantum gases have a density which is in general low enough to describe the interactions as two-body interactions. For low enough temperatures the description of scattering processes by $s$-wave interaction is sufficient. The field of cold atoms is very active and there are plenty of good textbooks and overview articles dealing with both the theoretical aspects and the experimental techniques involved, for example [Ing07, Met99, Ket99, Chi05].

2.1 Fermions

In the everyday world as we experience it, two identical particles are never truly indistinguishable. For example the movement and the trajectory of two billiard balls which look alike can be followed and backtracked either by eye or with the help of a fast camera. Additionally two otherwise identical billiard balls can be marked with different numbers and made distinguishable.

In quantum mechanics however, identical particles are truly indistinguishable. The particles can be specified by nothing more than a complete set of commuting observables. According to the Heisenberg uncertainty principle it is not possible to obtain an exact measurement of all the observables simultaneously. The particles cannot be labelled and followed individually as in classical mechanics. When measuring a two-particle system of indistinguishable particles in state $|k_a\rangle$ and state $|k_b\rangle$, where the $|k_i\rangle$ represent a collective index for the complete set of observables, all linear combinations of the two particles of the form

$$c_1 |k_a\rangle |k_b\rangle + c_2 |k_b\rangle |k_a\rangle$$

result in identical eigenvalues. The eigenvalues are degenerate with respect to the exchange of the two particles $|k_a\rangle$ and $|k_b\rangle$, so at this level of analysis the linear com-
bination to describe the pair is not uniquely defined yet. This exchange degeneracy is lifted by including the exchange of two particles with the permutation operator $P_{12}$ with

$$P_{12} |k_a⟩ |k_b⟩ = |k_b⟩ |k_a⟩ .$$

Its eigenvalues are +1 and -1, so the description of a two-body system is either symmetric or antisymmetric. It can be shown that in three dimensions the operator $P_{12}$ is a constant of motion, as it commutes with the Hamiltonian \[Sak94\]. Being a constant of motion also implies that the symmetric and the antisymmetric solutions cannot be converted into each other. Those two distinct solutions represent two distinct kinds of particles: bosons and fermions. Including the exchange of two particles, the non-degenerate solutions for the two-body wavefunction for two indistinguishable particles $a$ and $b$ at positions $r_1$ and $r_2$ in terms of the single-particle wavefunctions $ψ_i(r_i)$ are:

$$ψ_+(r_1, r_2) = C_N (ψ_a(r_1)ψ_b(r_2) + ψ_b(r_1)ψ_a(r_2))$$

$$ψ_−(r_1, r_2) = C_N (ψ_a(r_1)ψ_b(r_2) − ψ_b(r_1)ψ_a(r_2)),$$

(2.1)

with a normalizing factor $C_N$. Under exchange of the two particles the wavefunction is symmetric for the plus-sign and antisymmetric for the minus-sign. The symmetric wavefunction is applicable for bosons and the antisymmetric version describes fermions. From Eq. 2.1 the Pauli exclusion principle \[Pau25\] becomes clear: two identical fermions can neither occupy the same state $ψ_i$ nor the same position $r$. For $ψ_a = ψ_b$ the two-body wavefunction $ψ_−(r_1, r_2)$ vanishes, the same happens for $r_1 = r_2$. Particles with a half-integer spin, the fermions, obey Fermi-Dirac statistics \[Dir26, Fer26\], whereas particles with integer spin, the bosons, obey Bose-Einstein statistics \[Bos24, Ein25\]. For an ensemble of particles, the average number of particles $n_i$ per single particle state $ε_i$ is given by

$$\bar{n}_i^{BE} = \frac{1}{e^{(ε_i−µ)/kB T} − 1}$$

(2.2)

for bosons and

$$\bar{n}_i^{FD} = \frac{1}{e^{(ε_i−µ)/kB T} + 1}$$

(2.3)

for fermions. Here $µ$ is the chemical potential. The behaviour of fermions and bosons differs most strikingly at low temperatures. Bosons in a trapping potential as depicted in Fig. 2.1 collect in the ground state of the system and form a Bose-Einstein condensate (BEC), as has been demonstrated for the first time in 1995 by \[And95, Dav95a\]. Identical fermions on the other hand, fill up the states up to the Fermi-energy $E_F$ with one fermion occupying one state at a time. A Fermi degenerate gas of atoms has been realized for the first time in $^{40}$K in 1999 \[DeM99a\].

### 2.2 Two-body Hamiltonian

At the densities and temperatures relevant for experiments with ultracold atoms, most of the interactions can be characterized by two-body interactions. Two interacting atoms can be described by the two-body Hamiltonian as:

$$H = H_{rel} + H_{int}.$$  

(2.4)
2.2. TWO-BODY HAMILTONIAN

The behaviour of trapped fermions and bosons at zero temperature. Identical fermions fill the levels one by one up to the Fermi energy $E_F$, whereas bosons collect in the ground state to form a Bose-Einstein condensate.

with the Hamiltonian for the relative motion $H_{\text{rel}}$ of the two atoms and the Hamiltonian describing the internal energy of the two atoms $H_{\text{int}}$:

$$H_{\text{rel}} = \frac{p^2}{2m_r} + V,$$
$$H_{\text{int}} = H_{\text{hf},\alpha} + H_{\text{hf},\beta}$$

The operator $p^2/2m_r$ describes the relative kinetic energy of two atoms with reduced mass $m_r = m_1 m_2 / (m_1 + m_2)$ and the potential $V$ the effective interaction of the atoms. The internal Hamiltonian is presented in the following section.

2.2.1 INTERNAL HAMILTONIAN

The internal Hamiltonian for two alkali atoms in their electronic ground state is the sum of hyperfine interaction $H_{\text{hf}}$ and the Zeeman interaction $H_Z$ for each of the two atoms$^\dagger$ labelled $\alpha$ and $\beta$:

$$H_{\text{hf}} = H_{\text{hf}} + H_Z$$
$$= \frac{a_{\text{hf}}}{\hbar^2} i \cdot j + \frac{\mu_B}{\hbar} (g_J j + g_I i) \cdot B,$$

where $a_{\text{hf}}$ is the hyperfine constant for the fine structure level under consideration, $g_J$ the total Landé $g$-factor of the electron, $g_I$ the gyromagnetic factor of the nucleus, $\mu_B$ the Bohr magneton, $\hbar$ the reduced Planck constant $\hbar/2\pi$ and $B$ is the magnetic field. We use the convention $\mu_I = -g_I \mu_B I / \hbar$. The operators $i$ and $j$ are the nuclear spin and angular momentum operators with corresponding quantum numbers $m_i$ and $m_j$.$^\dagger$ $^{40}\text{K}$ has the electronic ground state $4^2S_{1/2}$, so $J$ equals to the spin operator $S$ and $S' = 1/2$.

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$^\dagger$Eq. 2.8 applies for the atoms in the ground state, for excited atoms see Appendix B

$^\dagger$To avoid confusion in this section, we label the operators $I$, $S$, $J$ and $F$ in capital letters when only one atom is concerned and for the coupled operators of the two atoms. For systems of two atoms, the individual operators and quantum numbers are labelled in lower case letters.
2. Theoretical Background

Theoretical Background

The nuclear spin of $^{40}$K is $I = 4$. The energy eigenvalues of the internal Hamiltonian of a $^{40}$K atom are shown in Fig. 2.2. The states are labelled with the low-field basis $|F, m_F\rangle$ quantum numbers, where $F = I + J$ and alphabetically with rising energy.

The hyperfine constant of $^{40}$K is $a_{hf} = h \times -285.7308(24)$ MHz, resulting in a hyperfine splitting $\Delta E_{hf} = h \times 1285.79$ MHz of the two hyperfine manifolds. Note that the hyperfine structure is inverted unlike in most other alkalis [Zac42]. In Appendix B the hyperfine structure of $^{40}$K is described in more detail and values for all relevant constants are given.

2.2.2 Hamiltonian for the relative motion

The effective interaction $V$ in the Hamiltonian of the relative motion in Eq. 2.5 can be expressed as the (central) Coulomb interaction $V_C(r)$ of the two atoms with internuclear distance $r$ and total spin $S = s_\alpha + s_\beta$.

$$V_C(r) = \sum_S |S\rangle V_S(r) \langle S| = \mathcal{P}_S V_s + \mathcal{P}_I V_t. \quad (2.11)$$

Depending on the coupling of the individual spins, the interaction potential $V_S(r)$ has for $s = 1/2$ atoms a singlet ($S=0$) or a triplet ($S=1$) character with the respective
singlet and triplet potentials \( V_s(r) \) and \( V_t(r) \). The operators \( \mathcal{P}_s \) and \( \mathcal{P}_t \) project out the singlet and triplet components of the wave function respectively. The interaction in Eq. 2.11 can then be rewritten into a sum of a direct \( V_D \) and an exchange interaction \( J(r) \) including the eigenvalues of \( \mathcal{P}_s \) and \( \mathcal{P}_t \):

\[
V^C(r) = V_D + J(r) s_\alpha \cdot s_\beta \tag{2.12}
\]

\[
= \frac{V_s(r) - 3V_t(r)}{4} + [V_t(r) - V_s(r)] s_\alpha \cdot s_\beta \tag{2.13}
\]

\[
= \frac{V_s(r) - 3V_t(r)}{4} + [V_t(r) - V_s(r)] \left( \frac{1}{2} S^2 - \frac{3}{4} \right) \tag{2.14}
\]

In the asymptote the direct interaction \( V_D \) corresponds to the van der Waals potential

\[
V_D = -\frac{C_6}{r^6} - \frac{C_8}{r^8} - \frac{C_{10}}{r^{10}} - \cdots \tag{2.15}
\]

\[
\approx -\frac{C_6}{r^6}, \tag{2.16}
\]

with the van der Waals range

\[
r_0 = \frac{1}{2} \left( \frac{2m_tr_0}{\hbar^2} \right)^{1/4} \tag{2.17}
\]

as the characteristic length of the potential \([\text{Gri93, Fla99}].\)

In the description of the two-body Hamiltonian in Eq. 2.4, we have not included dipole-dipole coupling. Neglecting dipole-dipole interaction, the two-body Hamiltonian can be separated into a radial and a spin part. The relative Hamiltonian \( H_{rel} \) acts only on the radial part of the atoms wavefunction and the internal Hamiltonian \( H_{int} \) acts only on the spin part.

### 2.3 Elastic collisions

The scattering of particles by a potential has been treated extensively in the literature (for example in \([\text{Sak94, CT77}]\)); here we present the main results important for the experiments with \(^{40}\text{K}\). The Pauli exclusion principle limits the types of two-body wavefunctions for fermions. When considering the scattering between two fermions the two-body wavefunction needs to be symmetrized properly. In systems of identical fermions s-wave collisions are forbidden due to the Pauli exclusion principle. To obtain the elastic scattering properties the time-independent radial wave equation needs to be solved for given values of \( l \) and \( s \) \([\text{Fli91}]\):

\[
ER_l(r) = \left[ \frac{\hbar^2}{2m_r} \left( \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{\hbar^2 l(l+1)}{2m_r r^2} + V_S(r) \right] R_l(r). \tag{2.18}
\]

For \( l = 0 \) the influence of the scattering potential on the scattered wavefunction in the asymptotic case \( (r \to \infty) \) can be expressed by the s-wave phase shift \( \eta_0 \). It is:

\[
a = -\lim_{k \to 0} \frac{\tan \eta_0}{k} \tag{2.19}
\]
The singlet \( V_s \) and triplet potentials \( V_t \) result in a singlet part \( a_s \) and a triplet part \( a_t \) of the \( s \)-wave scattering length \( a \).

The asymptotic solutions to Eq. 2.18 can be described as a partial wave expansion [Sak94]:

\[
\langle X | \Psi \rangle \xrightarrow{\text{large } r} \frac{1}{(2\pi)^{3/2}} \sum_l (2l + 1) \frac{P_l(\cos \theta)}{2ik} \left[ 1 + 2ikf_l(k) \frac{e^{ikr}}{r} - e^{-i(kr-l\pi)} \right],
\]

where \( P_l(\cos \theta) \) are Legendre polynomials for the scattering angle \( \theta \) and \( f_l(k) \) is the \( l \)th partial wave amplitude. The solution is expressed as a spherically incoming wave \( e^{-i(kr-l\pi)/r} \) and an outgoing spherical wave \( e^{ikr}/r \). The scattering event changes the coefficient of the outgoing wave. The partial wave amplitude is connected to a phase shift \( \eta_l \) [Sak94]:

\[
f_l(k) = \frac{1}{k \cot \eta_l - ik}.
\]

Collisions at low energies for partial waves with \( l > 0 \) are in general suppressed, because a centrifugal barrier forms a threshold with the effective potential

\[
V_{th}(l) = -\frac{C_6}{r^6} + \frac{\hbar^2}{2m_r} \frac{l(l+1)}{r^2}.
\]

The maximum threshold energy \( E_{th} \) can be approximated to

\[
E_{th}(l) = -\frac{C_6}{r_{\text{max}}^6} + \frac{\hbar^2}{2m_r} \frac{l(l+1)}{r_{\text{max}}^2}
\]

using the local maximum of the effective potential at

\[
r_{\text{max}}^4 = \frac{6C_6m_r}{\hbar^2l(l+1)}.
\]

In the case of \(^{40}\text{K} \) the threshold is 100\,\mu\text{K} for \( p \)-wave \( (l = 1) \) and 510\,\mu\text{K} for \( d \)-wave \( (l = 2) \) partial wave collisions. In the magneto-optical trap we have temperatures up to 190\,\mu\text{K}, in the magnetic trap and the optical trap they are in the range of a few 10\,\mu\text{K}. In the latter traps the main scattering channel will be \( s \)-wave.

## 2.4 Spin Exchange and \(^{40}\text{K} \)

Spin exchanging collisions are inelastic. Due to the Zeeman interaction (see Fig. 2.2) the different hyperfine states have different energies depending on the magnetic field. When spin exchange occurs, the energy difference of the total energy between final and initial states \( E_f - E_i \) can be negative or positive, leading to exothermic and endothermic collisions respectively. For a positive difference in energy, this is the activation energy
2.4. Spin Exchange and $^{40}$K

<table>
<thead>
<tr>
<th>Property</th>
<th>Symbol</th>
<th>Value</th>
<th>unit</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
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<td>$a_s$</td>
<td>104.41(9)</td>
<td>$a_0$</td>
<td>[Fal08]</td>
</tr>
<tr>
<td>triplet scattering length</td>
<td>$a_t$</td>
<td>169.67(24)</td>
<td>$a_0$</td>
<td>[Fal08]</td>
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<td>van der Waals range</td>
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<td>$a_0$</td>
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<tr>
<td>van der Waals coefficient</td>
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<td>3925.9</td>
<td>$E_Ha_0^6$</td>
<td>[Fal08]</td>
</tr>
<tr>
<td>van der Waals coefficient</td>
<td>$C_8$</td>
<td>$4.224 \times 10^5$</td>
<td>$E_Ha_0^8$</td>
<td>[Fal08]</td>
</tr>
<tr>
<td>van der Waals coefficient</td>
<td>$C_{10}$</td>
<td>$4.938 \times 10^7$</td>
<td>$E_Ha_{10}$</td>
<td>[Fal08]</td>
</tr>
</tbody>
</table>

Table 2.1: Scattering properties of $^{40}$K in units of the Bohr radius $a_0 = 5.2917720859 \times 10^{-11}$ m and the Hartree energy $E_H = 4.35974394 \times 10^{-18}$ J [NIST0].

$E_{act}$ needed to make spin exchanging collisions happen. In collisions described by the Hamiltonian in Eq. 2.4 the total spin $M_T = m_F + m'_F$ of two colliding atoms in the hyperfine states with quantum numbers $m_F$ and $m'_F$ is conserved. Furthermore in the case of fermions the two-body wave function obeys Fermi-Dirac statistics enforcing an antisymmetric total wavefunction for atoms in identical states. Therefore all spin exchanging s-wave collisions between atoms in the same hyperfine state $m_F = m'_F$ are forbidden. We only consider s-wave collisions between atoms in the electronic ground state $|2S_{1/2}\rangle$ of $^{40}$K in this section. Dipolar relaxation, where the atoms enter in a s-wave channel and leave in a d-wave channel, only plays a minor role (away from Feshbach resonances), as the temperature of the cold atoms is far below the d-wave threshold.

In the case of collisions between atoms in the two hyperfine manifolds $F = 9/2$ and $F = 7/2$, the collision is exothermic. The energy difference is of the order of the hyperfine splitting $\Delta E_{hf} = \hbar \times 1285.79$ MHz, corresponding to a temperature of 60 mK. This is much higher than all the trapping potentials employed in this experiment. Atoms in different hyperfine manifolds which undergo spin exchanging collisions will be lost from the trap. In our experiment spin exchange between atoms in the two hyperfine manifolds can play a role during a state preparation step, which will be described in detail in Sec. 4.2.

The case of collisions between $^{40}$K atoms within the lower hyperfine manifold ($F = 9/2$) needs to be considered for trapped cold clouds and when preparing atoms in specific binary mixtures to measure Feshbach resonances as will be described in Sec. 4.2. When considering binary state mixtures in the lower hyperfine manifold of $^{40}$K, there are several combinations of states which are stable or can be made stable against spin exchange. There are in general two possibilities for the final state combination when exchanging one quantum of angular momentum. For neighbouring states one of these combinations is excluded as it is identical to the initial states:

$$\ket{(m_F + 1), m_F} \rightarrow \ket{(m_F + 2), (m_F - 1)}$$ \hspace{1cm} (a)

$$\rightarrow \ket{(m_F), (m_F + 1)}.$$ \hspace{1cm} (b)

For states where $\Delta m_F = 2$, one combination is excluded due to the Pauli exclusion...
Figure 2.3: Activation temperature $T_{\text{act}}$ necessary for spin exchange between atoms in the lower hyperfine manifold, depending on the magnetic field $B$. The curves are for spin exchanging processes where one unit of angular momentum is exchanged. The solid lines show spin exchange between atoms in neighbouring states ($h + i$, ..., $b + c$). The dashed lines show the non-adjacent spin exchange channels which are present in the $f, g, h, i, j$ mixture. For the channels shown in red the reversed (exothermic) process is possible in the $f, g, h, i, j$ mixture. The inset shows the magnetic field range relevant for the state preparation described in Sec. 4.2.

Principle:

\[
\begin{align*}
|(m_F + 2), m_F \rangle & \rightarrow |(m_F + 3), (m_F - 1) \rangle \\
& \rightarrow |(m_F + 1), (m_F + 1) \rangle .
\end{align*}
\]

This can be understood as a time-reversed collision of identical fermions. In general the spin exchange channels for the exchange of one quantum of angular momentum are:

\[
\begin{align*}
|(m_F + i), m_F \rangle & \rightarrow |(m_F + i + 1), (m_F - 1) \rangle \\
& \rightarrow |(m_F + i - 1), (m_F + 1) \rangle .
\end{align*}
\]

The hyperfine structure of $^{40}\text{K}$ is inverted (see Fig. 2.2), so the energy of the state $|m_F + 1 \rangle$ is always higher than of the state $|m_F \rangle$. The channels labelled as (a) above are therefore endothermic channels, requiring activation energy $E_{\text{act}}$ to drive spin exchange. The channels labelled (b) above are exothermic, releasing energy when spin exchange takes place. The activation temperature

\[
T_{\text{act}} = E_{\text{act}}/k_B = (E_f - E_i)/k_B
\]

(2.25)
corresponds to the temperature at which the activation energy is provided by the thermal energy of the atom cloud. The difference in energy between final and initial states $E_f - E_i$ depends on the magnetic field and results in an activation temperature $T_{\text{act}}$ as shown in Fig. 2.3.
For binary mixtures consisting of neighbouring states or states with $\Delta m_F = 2$ it is always possible to stabilize the mixture by increasing the magnetic field or lowering the temperature of the cold atom cloud. The activation temperature necessary $T_{\text{act}}$ to drive spin exchange in mixtures of neighbouring states in the lower hyperfine manifold is shown as solid lines in Fig. 2.3. The activation temperature $T_{\text{act}}$ for states with $\Delta m_F = 2$ is even higher. As mixtures of neighbouring states and of states with $\Delta m_F = 2$ can be made stable, also mixtures of atoms in three adjacent states can be stabilized. The fact that $^{40}\text{K}$ is fermionic and has an inverted hyperfine structure allows for the realization of a multitude of stable state combinations, exceeding the possibilities in other alkalis.

### 2.4.1 Populated states in the magnetic trap

The cold atoms in the magnetic trap (and in the optical dipole trap) are in the states $f, g, h, i, j$ (labelled as in Fig. 2.2). The combination $|9/2 + 7/2\rangle (j + i)$ is stable against spin exchanging collisions as there is no other combination with $M_T = 8$. The binary mixture $|9/2 + 5/2\rangle (j + h)$ is stable against spin exchanging collisions as the only possible final state combination is excluded due to the Pauli exclusion principle\(^5\). The mixture $f, g, h, i, j$ has in total nine channels, where spin exchanging $s$-wave collisions can exchange one unit of angular momentum between two atoms. Of those nine channels six are endothermic, the three remaining channels are exothermic and correspond to the reversed processes of endothermic channels.

Of the six endothermic channels, five involve neighbouring states or states with $\Delta m_F = 2$. The dashed lines in Fig. 2.3 show the spin exchange channels present in the $f, g, h, i, j$ mixture for non-adjacent states. The red lines correspond to the reverse of the three exothermic spin exchanging channels possible for atoms in the mixture. The energy release from the exothermic spin exchanging processes leads to loss from the trap or – for low magnetic fields – a heating of the cold atom cloud.

### 2.4.2 Scattering rate for spin exchange

Apart from the existence of decay channels, in an experiment the actual loss rate and with that the stability of a mixture of two states is determined by the scattering rate. The two-body scattering rate $K_2$, depends on the density of the involved states, the spatial overlap of the states and the difference between singlet and triplet scattering length [Pet02]:

$$K_2 = 4\pi (a_s - a_t)^2 v_{\text{rel}}^2 \left| \langle F'_\alpha m'_{F,\alpha} F'_{\beta} m'_{F,\beta} | s_\alpha \cdot s_\beta | F_\alpha m_{F,\alpha} F_\beta m_{F,\beta} \rangle \right|^2,$$

(2.26)

where $|F'_\alpha m'_{F,\alpha} F'_{\beta} m'_{F,\beta}\rangle$ and $|F_\alpha m_{F,\alpha} F_\beta m_{F,\beta}\rangle$ denote the final and initial hyperfine states and $v'_{\text{rel}}$ is the relative velocity of the atoms in the final state. It is

$$v'_{\text{rel}} = \sqrt{\frac{2}{m_t} \left( E_{\text{kin}} + E^{\text{HF}}_\alpha + E^{\text{HF}}_\beta - E^{\text{HF'}}_\alpha - E^{\text{HF'}}_\beta \right)},$$

(2.27)

\(^5\)The same arguments hold for the combinations $|-9/2 + -7/2\rangle (a+b)$ and $|-9/2 + -5/2\rangle (a+c)$.
with the reduced mass \( m_r = (m_\alpha m_\beta)/(m_\alpha + m_\beta) \) and the kinetic energy \( E_{\text{kin}} \) of the initial states. The energies \( E_i^{\text{HF}} \) and \( E'_i^{\text{HF}} \) denote the hyperfine energies of the initial and final states. To calculate the spin exchange rate between atoms of the same atomic species, the hyperfine basis \( |F_\alpha m_{F,\alpha} F_\beta m_{F,\beta}\rangle \) is transformed to the total spin basis \( |S M_S I M_I\rangle \).

From the factor \((a_s - a_t)^2\) in Eq. 2.26 follows, that the two-body inelastic loss rate \( K_2 \) is expected to be low, when the singlet and triplet scattering lengths are similar. This effect can also be understood as an interference effect as has been shown for \(^{87}\text{Rb}\) \([\text{Kok97, Bur97}]\). In the group at JILA \([\text{DeM01}]\) an upper limit for the the non-resonant spin exchange rate in \(^{40}\text{K}\) was determined to be \( K_2 < 2 \times 10^{-14} \text{ cm}^3/\text{s} \). Compared to other alkali atoms where \( K_2 \approx 10^{-11} \text{ cm}^3/\text{s} \) \([\text{Pet02}]\), this is rather low.

### 2.5 Feshbach Resonances

So far we have covered the scattering properties for scattering from a central potential (Sec. 2.3). The potential determines the value of the scattering length \( a \) at low temperatures. A form of resonant scattering are Feshbach resonances; they are an important tool to control the interaction between ultracold atoms, as they allow to widely tune the scattering length of the atoms.

In the asymptotic case \((r \to \infty)\) the hyperfine energy of the two colliding atoms with distance \( r \) determines the total energy of the atom pair. The total energy of the unbound pair forms the so-called open channel, as \((s\text{-wave})\) collisions are always possible even when \( T \to 0 \). Feshbach resonances occur when in addition to the open channel there is also a two-body bound potential, a so-called closed channel, present. All scattering potentials which have a higher asymptotic energy than the open channel are referred to as closed channels (see Fig. 2.4). Due to resonant coupling to a bound state with binding energy \( E_b \) within a closed channel the scattering length \( a \) can diverge.

The divergence of the scattering length occurs when the bound state in the closed channel shifts into resonance with the energy of the open channel. Due to the difference in magnetic field dependence of the open and closed channel, the closed channel can be moved relative to the energy of the open channel by applying an external magnetic field. The bound state in the closed channel is resonant at a certain magnetic field \( B_0 \), when there is a coupling between the open and the closed channel. At the resonance at magnetic field \( B_0 \) the scattering length diverges as shown in Fig. 2.5.

The theory of Feshbach resonances \([\text{Fes58, Fes62}]\) was originally developed for nuclear physics, where the resonances do not depend on an external magnetic field but on the energy of the scatterers. The application of Feshbach resonances to alter the sign and the strength of the interaction in ultracold atoms by changing an external field was proposed by \([\text{Tie92, Tie93}]\). The first experimental observation of this effect in ultracold atoms were made in \(^{23}\text{Na}\) \([\text{Ino98}]\) and in \(^{85}\text{Rb}\) \([\text{Cou98}]\). A detailed review of Feshbach resonances in ultracold atoms is given in \([\text{Chi10}]\).

If only one closed channel is present the scattering length can be expressed as the sum of a resonant part \( a_{\text{res}} \) and the background scattering length \( a_{\text{bg}} \) originating from the open channel:

\[
a(B) = a_{\text{bg}} + a_{\text{res}}(B).
\]
2.5. Feshbach resonances

Figure 2.4: Two-channel model for a Feshbach resonance. When two atoms collide at energy $E$ in the open (entrance) channel (black curve), they can couple resonantly to a bound state with binding energy $E_b$ within a molecular potential (closed channel) (red curve). The coupling leads to a diverging scattering length. If there is a difference in magnetic moment of the open and the closed channel, the energy of the bound state in the closed channel can be tuned to cross the energy threshold of the two atoms by changing the magnetic field.

The $s$-wave scattering in absence of inelastic two-body channels is described by [Moe95]

$$ a(B) = a_{bg} \left( 1 - \frac{\Delta B}{B - B_0} \right), \quad (2.28) $$

with the off-resonant background value of the scattering length $a_{bg}$, the Feshbach resonance position $B_0$ and its width $\Delta B$. The width is defined via the position of the zero-crossing of the Feshbach resonance $B(a = 0) = B_0 + \Delta B$. The behaviour of the scattering length around a Feshbach resonance is shown in Fig. 2.5. The scattering cross section is given by:

$$ \sigma = g \frac{4\pi a^2}{1 + k^2a^2} = g\frac{4\pi a_{bg}^2 \left( 1 - \frac{\Delta B}{B - B_0} \right)^2}{1 + k^2a_{bg}^2 \left( 1 - \frac{\Delta B}{B - B_0} \right)^2}, \quad (2.29) $$

where $k$ is the momentum and $g$ is a symmetry factor. It is $g = 1$, except for the case of two identical atoms (same species and same state) in a Maxwellian gas [Chi10]. The difference in magnetic moment between the open and the closed channel $\Delta \mu = \mu_0 - \mu_c = -\partial E_b/\partial B$ describes the coupling strength $C$ between the open and the closed channel.

$$ C \equiv a_{bg} \Delta B \Delta \mu. $$

Further useful expressions to describe a Feshbach resonance are the length scale [Pet04]

$$ R^* \equiv \frac{\hbar^2}{2m_r a_{bg} \Delta B \Delta \mu}, $$

the width

$$ \Gamma \equiv \frac{\hbar^2k}{m_r R^*} = 2Ck $$
2. Theoretical Background

Figure 2.5: Divergence of the s-wave scattering length \( a \) around a Feshbach resonance at the magnetic field \( B_0 \).

and the resonance strength which can be described by a dimensionless parameter [Chi10]:

\[
\begin{align*}
    s_{\text{res}} &= \frac{R^*}{r_0} \\
    E_b &= \frac{\hbar^2}{2m_a a^2}.
\end{align*}
\]  

Further away from the resonance and for positive values of \( a \) the energy is proportional to the magnetic field \( B \), with a slope depending on the difference of the magnetic moments of the open and closed channel. The quadratic dependence close to the Feshbach resonance is caused by the coupling between open and closed channel.

To calculate the exact position and widths of Feshbach resonances the potentials of the involved channels are needed and their coupling has to be computed. In general this requires the (numerical) solving of a large number of coupled equations using coupled channel calculations (CC). Simple models like the asymptotic bound state model (ABM) and the multichannel quantum defect theory (MQDT) are useful to assign resonances and allow for the calculation of approximate resonance positions with less computational effort than needed for CC. In the experiments presented in this thesis we used the ABM to assign and locate Feshbach resonances. The following section gives a brief introduction to this model.

2.6 Asymptotic bound state model

The asymptotic bound state model (ABM) was initially developed (see [Tie10b] and references therein) to assign features observed in experiments with \(^6\text{Li} - ^{40}\text{K} \) [Wil08] to the bound states and closed channels causing the Feshbach resonances. The main idea is that the two-body Hamiltonian in Eq. 2.4 is diagonalized and the energy of the bound molecular states is varied to fit known resonances. The input parameters are the singlet \( a_s \) and the triplet scattering length \( a_t \) and the \( C_6 \) coefficient to describe the
van der Waals tail of the interatomic potential. It is not necessary to solve the radial Schrödinger equation.

The model is called asymptotic because it is assumed that the detailed behaviour of the potential at small interatomic distances can be neglected as the main contribution to the position of Feshbach resonances stems from the asymptotic behaviour of the atoms. In the course of diagonalizing the Hamiltonian, the overlap between the wavefunction in the singlet $V_s$ and the triplet potential $V_t$ needs to be computed. This overlap is $\approx 1$. For a first calculation of the position of Feshbach resonances there are thus only three input parameters necessary. The calculation can be improved by optimizing the overlap and the bound state energies of the molecular bound states to fit data determined in experiments. With the improved assumptions for the energies and the overlap, the position of other Feshbach resonances can be determined. The ABM has the advantage that all possible resonances, however narrow, will be predicted with relatively little computational effort. These results can then be used as input for the exact coupled channel calculations. The assignment of $s$- and $p$-wave is also immediately clear with ABM.

The ABM has been applied to mixtures of $^6$Li - $^{40}$K [Wil08, Tie10c], $^{85}$Rb - $^{87}$Rb, $^6$Li - $^{87}$Rb [Li08], $^6$Li - $^{85}$Rb [Deh10], $^{40}$K - $^{87}$Rb [Tie10c], $^3$He* - $^4$He* [Goo10] and to $^{23}$Na [Kno11]. The original ABM has been extended to also include dipole-dipole interactions and overlapping resonances [Goo10], and radio-frequency induced resonances [Tsc10]. The ABM is also used to calculate the widths of resonances [Tie10c]. This involves rewriting the Hamiltonian in terms of the closed and open channel contributions and extracting the coupling between them. For the individual mixtures and species some adaptations have to be made, it turns out that for $^6$Li - $^{40}$K one bound state is sufficient. In $^{40}$K two bound states play a role as well as the large background scattering length (see Sec. 5.3.3).

In our experiment we used the ABM together with values of the four resonances known at that time as well as the input parameters $a_s$, $a_t$ and $C_6$ from molecule spectroscopy [Fal08] to get initial predictions for Feshbach resonances in the hyperfine state mixtures of $^{40}$K. Once new measurements were obtained, the overlap and binding energies were optimised (see Sec. 5.3.3) and further predictions for other hyperfine state mixtures were calculated.

## 2.7 Trapped fermions

We use magnetic and optical traps to confine the $^{40}$K. These trapping potentials are described in detail in the appendices A and B. The potential has an effect on the density of states and with that on the Fermi energy $E_F$. As depicted in Fig. 2.1, the Fermi energy $E_F$ is defined as the energy of the highest state in a potential occupied at $T = 0$. The Fermi temperature is defined accordingly as $T_F = E_F/k_B$. For an ideal gas in a trapping potential $U(r)$, the density of states is

$$g(\epsilon) = \frac{1}{\hbar^3} \int \delta \left( \epsilon - \left[ \frac{p^2}{2m} + U(r) \right] \right) dp dr. \quad (2.31)$$
From the definition of the Fermi energy follows the total number of atoms $N$:

$$N \equiv \int_{0}^{E_{F}} g(\epsilon) \, d\epsilon. \quad (2.32)$$

With Eq. [2.31] and [2.32] and a known potential the Fermi energy $E_{F}$ can be calculated. The optical dipole trap used in our experiment, can be approximated at low temperatures by a harmonic potential\(^*\), with

$$U_{ODT}(x, y, z) = \frac{m}{2}(\omega_{r}^{2}x^{2} + \omega_{r}^{2}y^{2} + A\omega_{z}^{2}z^{2})$$

this results in the density of states [But97]

$$g_{ODT}(\epsilon) = \frac{\epsilon^{2}}{2A(\hbar\omega_{r})^{3}} \quad (2.33)$$

and

$$E_{F} = \hbar\omega_{r}(6AN)^{1/3}, \quad (2.34)$$

where $A = \omega_{z}/\omega_{r}$ is the aspect ratio of the optical dipole trap, and the trapping frequencies are determined by the mass of the atoms and the laser detuning as described in Appendix A\(^*\). For the linear magnetic trap as employed in the experiment (see Sec. 3.5.1 and B.3) with a potential of the form

$$U_{MT}(x, y, z) = \frac{U_{0}}{2}x^{2} + y^{2} + 4z^{2},$$

the density of states is given by [Bag87]:

$$g_{MT}(\epsilon) = \frac{16\sqrt{2}}{105\pi} \left(\frac{2\sqrt{m}}{\hbar U_{0}}\right)^{3} \epsilon^{7/2}. \quad (2.35)$$

The Fermi energy in this case is

$$E_{F} \approx 1.5962N^{2/9} \left(\frac{hU_{0}}{\sqrt{m}}\right)^{2/3}. \quad (2.36)$$

### 2.7.1 Fermi Degenerate Density Distribution

For an ideal gas below the Fermi temperature $T_{F}$ the distribution is a Fermi-Dirac distribution

$$f_{FD}(\epsilon) = \frac{1}{\zeta e^{\mu/k_{B}T} + 1}, \quad (2.37)$$

with the fugacity $\zeta \equiv \exp(\mu/k_{B}T)$ depending on the chemical potential $\mu$.

To calculate the density distribution of a degenerate gas in a potential, a semiclassical approximation can be used as long as the thermal energy of the gas $k_{B}T$ is

\(^*\)The atoms in the optical dipole trap are in a Gaussian potential, which can be approximated harmonically for low atom temperatures. The density distribution for thermal atoms in a Gaussian potential is described in Appendix A\(^*\).
2.7. Trapped fermions

much larger than the spacing \(\hbar \omega\) of the (quantum mechanical) levels of the trapping potential \(U(r)\). In this case the density distribution is given by:

\[
n_{FD}(r) = \frac{1}{\hbar^3} \int \frac{1}{e^{\mathcal{H}(p,r) - \mu} / k_B T + 1} \, dp.
\]  

Integration over all possible momenta \(p\) results in the density distribution of a degenerate cloud of fermions at finite temperatures \(0 < T < T_F\):

\[
n_{FD}(r) = -\left(\frac{2\pi mk_B T}{\hbar}\right)^{3/2} \text{Li}_{3/2}(-\zeta e^{U(r) / k_B T}),
\]  

with the polylogarithm function (Jonquière’s function) \(\text{Li}_n(x) \equiv \sum_{k=1}^{\infty} x^k / k^n\). The number of atoms for a harmonic confinement is obtained by integrating Eq. 2.39 over \(r\):

\[
N = -\frac{1}{A} \left(\frac{k_B T}{\hbar \omega}\right)^3 \text{Li}_3(-\zeta).
\]

Combining this result with the Fermi energy \(k_B T_F\) in a harmonic trap Eq. 2.34 the fugacity depends only on \(T/T_F\):

\[
\frac{T}{T_F} = (-6 \text{Li}_3(-\zeta))^{-1/3}
\]

In the experiments we determine the density distribution by means of absorption imaging (see 3.8.3) along the axial direction of the dipole trap. This results in a projection of the atom density on a two-dimensional optical density profile, which we can calculate for a harmonic potential by integrating Eq. 2.34 over \(y\).

The imaging is usually done after releasing the atoms from the trap and some expansion of the cloud in time-of-flight. In the case of a harmonic trap it has been shown [Bru00], that the description of an ideal Fermi gas after free expansion only requires a rescaling of the spatial coordinates \(x_i\) in the density distribution Eq. 2.39, similar to the bosonic case [Cas96, Kag96]. The rescaled coordinates \(x'_i(t)\) are given by

\[
x'_i(t) = \frac{x_i(0)}{\sqrt{1 + \omega_i^2 t^2}},
\]

when the harmonic trapping potential with trapping frequencies \(\omega_i\) is switched off at \(t = 0\). For a harmonic trap the cloud maintains the aspect ratio and shape it had in the trap after free expansion. This shape invariance only holds for harmonic potentials and simplifies the analysis of the absorption images tremendously. From the absorption images the number of atoms and the temperature of the cloud can be determined using the rescaled density profiles [But97, DeM01].

\[\parallel\]The axial (z-) direction of the dipole trap corresponds to the y-axis in the coordinate system of the experiment as depicted in Fig. 3.2.