Chapter 2

Scattering and bound states

In this chapter we give a review of quantum-mechanical scattering theory. We focus on the relation between the scattering amplitude of a potential and its bound states [86, 87]. In the first part we consider single-channel scattering and focus on the example of the square well. In the second part we consider the situation of two coupled channels, which can give rise to a Feshbach resonance.

2.1 Single-channel scattering: an example

We consider the situation of two atoms of mass $m$ that interact via the potential $V(r)$ that vanishes for large distances between the atoms. The motion of the atoms separates into the trivial center-of-mass motion and the relative motion, described by the wave function $\psi(r)$ where $r \equiv x_1 - x_2$, and $x_1$ and $x_2$ are the coordinates of the two atoms, respectively. This wave function is determined by the time-independent Schrödinger equation

$$\left[ -\frac{\hbar^2 \nabla^2}{m} + V(r) \right] \psi(r) = E \psi(r), \quad (2.1)$$

with $E$ the energy of the atoms in the center-of-mass system. Solutions of the Schrödinger equation with negative energy correspond to bound states of the potential, i.e., to molecular states. To describe atom-atom scattering we have to look for solutions with positive energy $E = 2\epsilon_k$, with $\epsilon_k \equiv \hbar^2 k^2/2m$ the kinetic energy of a single atom with momentum $\hbar k$. Since any realistic interatomic interaction potential vanishes rapidly as the distance between the atoms becomes large, we know that the solution for $r \to \infty$ of Eq. (2.1) is given by a superposition of incoming and outgoing plane waves. More precisely, the scattering wave function is given by an
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Figure 2.1: Schematic representation of two-atom scattering in the center-of-mass reference frame. The atoms are initially in a plane-wave state with relative momentum $\hbar \mathbf{k}$, and scatter into the spherical wave with relative momentum $\hbar \mathbf{k}'$. Due to energy conservation we have that $k = k'$. The angle between $\mathbf{k}$ and $\mathbf{k}'$ is denoted by $\theta$. The region where the interaction takes place is indicated by the black circle.

incoming plane wave and an outgoing spherical wave and reads

$$\psi (\mathbf{r}) \sim e^{i \mathbf{k} \cdot \mathbf{r}} + f (\mathbf{k}', \mathbf{k}) \frac{e^{i \mathbf{k}' \cdot \mathbf{r}}}{r},$$

(2.2)

where the function $f (\mathbf{k}', \mathbf{k})$ is known as the scattering amplitude. The interatomic interaction potential depends only on the distance between the atoms and hence the scattering amplitude depends only on the angle $\theta$ between $\mathbf{k}$ and $\mathbf{k}' \equiv k' \hat{\mathbf{r}}$, and the magnitude $k$. Because of energy conservation we have that $k' = k$. The situation is shown schematically in Fig. 2.1.

Following the partial-wave method we expand the scattering amplitude in Legendre polynomials $P_l(x)$ according to

$$f (\mathbf{k}', \mathbf{k}) = \sum_{l=0}^{\infty} f_l (k) P_l (\cos \theta).$$

(2.3)

The wave function is expanded in a similar manner as

$$\psi (r, \theta) = \sum_{l=0}^{\infty} R_l (k, r) P_l (\cos \theta),$$

(2.4)
with \( R_l(k, r) = u_l(k, r)/r \) the radial wave function and \( u_l(k, r) \) determined by the radial Schrödinger equation

\[
\left[ \frac{d^2}{dr^2} - \frac{l(l + 1)}{r^2} - \frac{m V(r)}{\hbar^2} + k^2 \right] u_l(k, r) = 0 .
\]

By expanding also the incident plane wave in partial waves according to

\[
e^{i k \cdot r} = \sum_{l=0}^{\infty} \frac{(2l + 1)i^l}{kr} \sin \left( k r - \frac{l \pi}{2} \right) P_l(\cos \theta) ,
\]

we can show that to obey the boundary condition in Eq. (2.2), the partial-wave amplitudes \( f_l(k) \) have to be of the form

\[
f_l(k) = \frac{2l + 1}{2i k} \left( e^{2i \delta_l(k)} - 1 \right) ,
\]

where \( \delta_l(k) \) is the so-called phase shift of the \( l \)-th partial wave.

For the ultracold alkali atoms, we are allowed to consider only \( s \)-wave \((l = 0)\) scattering, since the colliding atoms have too low energies to penetrate the centrifugal barrier in the effective hamiltonian in Eq. (2.5). Moreover, as we see later on, the low-energy effective interactions between the atoms are fully determined by the \( s \)-wave scattering length, defined by

\[
a = - \lim_{k \downarrow 0} \frac{\delta_0(k)}{k} .
\]

From Eq. (2.7) we find that the \( s \)-wave scattering amplitude is given by

\[
f_0(k) = \frac{1}{k \cot \delta_0(k) - ik} .
\]

As explained above, we take only the \( s \)-wave contribution into account, which gives for the scattering amplitude at zero-momentum

\[
f(0, 0) \simeq -a .
\]

To illustrate the physical meaning of the \( s \)-wave scattering length, we now calculate it explicitly for the simple case that the interaction potential is a square well. We thus take the interaction potential of the form

\[
V(r) = \begin{cases} 
V_0 & \text{if } r < R; \\
0 & \text{if } r > R,
\end{cases}
\]
with \( R > 0 \). With this potential, the general solution of Eq. (2.5) for \( l = 0 \) is given by

\[
\begin{align*}
u^<(r) &= A e^{ik^<r} + B e^{-ik^<r}, \quad \text{for } r < R; \\
u^>(r) &= C e^{ikr} + D e^{-ikr}, \quad \text{for } r > R,
\end{align*}
\]

with \( k^< = \sqrt{k^2 - mV_0/\hbar^2} \). Since the wave function \( \psi(r) \) has to obey the Schrödinger equation at the origin we have to demand that the function \( u^<(r) \) vanishes at this point. This leads to the boundary condition \( B = -A \). By comparing the explicit form of the wave function \( u^>(r) \) with the \( s \)-wave component of the general scattering wave function for \( r \to \infty \), we find that

\[
e^{2i\delta_0(k)} = -\frac{C}{D}.
\]

Hence, we determine the phase shift by demanding that the wave functions for \( r < R \) and \( r > R \) join smoothly. This leads to the equations

\[
\begin{align*}
A \left( e^{ik^<R} - e^{-ik^<R} \right) &= -e^{2i\delta_0(k)} e^{ikR} + e^{-ikR}, \\
A \left( k^< e^{ik^<R} + k^< e^{-ik^<R} \right) &= -e^{2i\delta_0(k)} ke^{ikR} - ke^{-ikR},
\end{align*}
\]

where we have chosen the normalization such that \( D = 1 \). Multiplication of the above equations with \( e^{-i\delta_0(k)} \) and dividing the result leads to

\[
k \tan(k^<R) = k^< \tan(\delta_0(k) + kR),
\]

from which it follows that

\[
\delta_0(k) = -kR + \tan^{-1} \left[ \frac{k}{k^<} \tan(k^<R) \right].
\]

Note that for a repulsive hard-core potential we have that \( V_0 \to \infty \) and therefore, with the use of the definition in Eq. (2.8), that the scattering length \( a = R \). This immediately gives a physical picture for a positive \( s \)-wave scattering length: at low energy and momenta the details of the potential are unimportant and we are allowed to model the potential with an effective hard-core potential of radius \( a \). For a fully repulsive potential the scattering length is always positive. For a potential with attractive parts the scattering length can be both negative and positive, corresponding to attractive and repulsive effective interactions, respectively.

This is seen by explicitly calculating the scattering length for our example in the case that \( V_0 < 0 \). As its definition in Eq. (2.8) shows, the scattering length is determined by the linear dependence of the phase shift on the magnitude of the
2.1. SINGLE-CHANNEL SCATTERING: AN EXAMPLE

Figure 2.2: Scattering length (solid line) and effective range (dashed line) for an attractive square well in units of the range of the potential, as a function of the dimensionless parameter \( \gamma = R \sqrt{m|V_0|/\hbar^2} \).

Relative momentum \( \hbar k \) of the scattering atoms for small momentum. Generally, the phase shift can be expanded according to [86–88]

\[
k \cot(\delta_0(k)) = -\frac{1}{a} + \frac{1}{2} r_{\text{eff}} k^2 + \cdots,
\]

from which the scattering length is determined by

\[
a = R \left( 1 - \frac{\tan \gamma}{\gamma} \right),
\]

with \( \gamma = R \sqrt{m|V_0|/\hbar^2} \) a dimensionless constant. The parameter \( r_{\text{eff}} \) is the so-called effective range and is, in our example of the square-well potential, given by

\[
r_{\text{eff}} = R \left[ 1 + \frac{3 \tan \gamma - \gamma (3 + \gamma^2)}{3 \gamma (\gamma - \tan \gamma)^2} \right].
\]

In Fig. 2.2 the scattering length is shown as a function of \( \gamma \) by the solid line. Clearly, the scattering length can be both negative and positive, and becomes equal to zero at values of \( \gamma \) such that \( \gamma = \tan \gamma \). In the same figure, the effective range is shown by the dashed line. Note that the effective range diverges if the scattering length becomes equal to zero. This is because the expansion in Eq. (2.17) is ill-defined for \( a = 0 \). At values of \( \gamma = (n + 1/2)\pi \) with \( n \) a positive integer the scattering length
diverges and changes sign. This behaviour is called a potential or shape resonance and in fact occurs each time the potential is just deep enough to support a new bound state. Therefore, for large and positive scattering length the square well has a bound state with an energy just below the continuum threshold. It turns out that there is an important relationship between the energy of this bound state and the scattering length.

To find this relation we have to determine the bound-state energy by solving the Schrödinger equation for negative energy $V_0 < E < 0$. This leads to solutions

\[
\begin{align*}
  u^<(r) &= A \left( e^{i k^< r} - e^{-i k^< r} \right), \quad \text{for } r < R; \\
  u^>(r) &= B e^{-\kappa r}, \quad \text{for } r > R,
\end{align*}
\]

with $k^< = \sqrt{m(E - V_0)/\hbar^2}$ and $\kappa = \sqrt{m|E|/\hbar^2}$. Demanding again that these solutions join smoothly at $r = R$, we find the equation for the bound-state energy

\[
\sqrt{\frac{m}{\hbar^2}} |E_m| = -\sqrt{\frac{m}{\hbar^2}} (E_m - V_0) \cot \left( \sqrt{\frac{m}{\hbar^2}} (E_m - V_0) \right). \tag{2.21}
\]

We can show that for values of $\gamma$ such that $(n - 1/2)\pi < \gamma < (n + 1/2)\pi$ this equation has $n$ solutions for $V_0 < E_m < 0$ [87].

For small binding energy $|E_m| \ll |V_0|$ we have from the equation for the bound-state energy that

\[
\sqrt{\frac{m}{\hbar^2}} |E_m| \simeq -\gamma \cot \gamma / R \simeq 1/a, \tag{2.22}
\]

where we made use of the fact that $\gamma$ has to be close to the resonant values $(n + 1/2)\pi$ in this case. This leads to the desired relation between the energy of the molecular state and the scattering length given by

\[
E_m = -\frac{\hbar^2}{ma^2}. \tag{2.23}
\]

This result does not depend on the specific details of the potential and it turns out to be quite general. Any potential with a large positive scattering length has a bound state just below the continuum threshold with energy given by Eq. (2.23). Moreover, the relation will turn out to hold also in the multichannel case of a Feshbach resonance as we will see in Section 2.3. Before discussing this situation, we first turn to some concepts of scattering theory which are of importance for the remainder of this thesis.

### 2.2 Single-channel scattering: formal treatment

Let us give a more formal treatment of the scattering theory described above. In a basis-independent formulation the Schrödinger equation we have solved reads,

\[
\left[ \hat{H}_0 + \hat{V} \right] |\psi\rangle = E |\psi\rangle, \tag{2.24}
\]
with $\hat{H}_0 = \hat{p}^2/m$ the kinetic energy operator for the atoms. To describe scattering, we have to look for solutions which asymptotically represent an incoming plane wave, and an outgoing spherical wave. In the absence of the potential $\hat{V}$ there is no scattering, and hence we demand that the solution of Eq. (2.24) reduces to a plane wave in the limit of vanishing potential. The formal solution that obeys this condition is given by

$$|\psi_{k}^{(+)\rangle} = |k\rangle + \frac{1}{E^{+} - \hat{H}_0} \hat{V} |\psi_{k}^{(+)\rangle},$$  \hspace{1cm} (2.25)$$

where $|k\rangle$ represents the incoming plane wave and we recall that $E = 2\epsilon_k$ is the kinetic energy of the atoms. This energy is made slightly complex by the usual limiting procedure $E^{+} = \lim_{\eta \to 0} E + i\eta$. Moreover, we have for the scattering amplitude that

$$f(k', k) = -\frac{m}{4\pi \hbar^2} \langle k' | \hat{V} |\psi_{k}^{(+)\rangle}.$$  \hspace{1cm} (2.26)$$

To determine the scattering amplitude directly, we introduce the two-body T(ransition) matrix by means of

$$\hat{V} |\psi_{k}^{(+)\rangle} = \hat{T}^{2B}(E^{+}) |k\rangle.$$  \hspace{1cm} (2.27)$$

Multiplying the formal solution in Eq. (2.25) by $\hat{V}$ we have that

$$\hat{T}^{2B}(E^{+}) |k\rangle = \hat{V} |k\rangle + \hat{V} \frac{1}{E^{+} - \hat{H}_0} \hat{T}^{2B}(E^{+}) |k\rangle.$$  \hspace{1cm} (2.28)$$

Since this equation holds for an arbitrary plane wave $|k\rangle$ and because these plane waves form a complete set of states we have the following operator equation for the two-body T-matrix

$$\hat{T}^{2B}(z) = \hat{V} + \hat{V} \frac{1}{z - \hat{H}_0} \hat{T}^{2B}(z).$$  \hspace{1cm} (2.29)$$

This equation is called the Lippmann-Schwinger equation and from its solution we are able to determine the scattering properties of the potential $\hat{V}$. To see this we first note that from the definition of the T-matrix in Eq. (2.27), together with Eq. (2.26), it follows immediately that

$$f(k', k) = -\frac{m}{4\pi \hbar^2} \langle k' | \hat{T}^{2B}(2\epsilon_k^{+}) |k\rangle.$$  \hspace{1cm} (2.30)$$

Therefore, we indeed see that the two-body T-matrix completely determines the scattering amplitude. The Lippmann-Schwinger equation for the two-body T-matrix can be solved in perturbation theory in the potential. This results in the so-called Born series given by

$$\hat{T}^{2B}(z) = \hat{V} + \hat{V} \hat{G}_0(z) \hat{V} + \hat{V} \hat{G}_0(z) \hat{V} \hat{G}_0(z) \hat{V} + \cdots,$$  \hspace{1cm} (2.31)$$
where
\[ \hat{G}_0(z) = \frac{1}{z - \hat{H}_0}, \]  
(2.32)
is the noninteracting propagator of the atoms. By using, instead of the true interatomic interaction potential, a pseudopotential of the form
\[ V(x - x') = \frac{4\pi ah^2}{m}\delta(x - x'), \]  
(2.33)
the first term in the Born series immediately yields the correct result for the scattering amplitude at low energies and momenta, given in Eq. (2.10). Such a pseudopotential should therefore not be used to calculate higher-order terms in the Born series, but should be used only in first-order perturbation theory.

The poles of the T-matrix in the complex-energy plane correspond to bound states of the potential. To see this we note that the formal solution of the Lippmann-Schwinger equation is given by
\[ \hat{T}^{2B}(z) = \hat{V} + \hat{V} \frac{1}{z - \hat{H}} \hat{V}. \]  
(2.34)
After insertion of the complete set of eigenstates \( |\psi_\alpha\rangle \) of \( \hat{H} = \hat{H}_0 + \hat{V} \) we have
\[ \hat{T}^{2B}(z) = \hat{V} + \sum_\alpha \hat{V} \frac{|\psi_\alpha\rangle\langle\psi_\alpha|}{z - \epsilon_\alpha} \hat{V}, \]  
(2.35)
where the summation over \( \alpha \) is discrete for the bound-state energies \( \epsilon_\alpha < 0 \), and represents an integration for positive energies that correspond to scattering solutions of the Schrödinger equation, so explicitly we have that
\[ \hat{T}^{2B}(z) = \hat{V} + \sum_k \hat{V} \frac{|\psi_k\rangle\langle\psi_k|}{z - \epsilon_k} \hat{V} + \int \frac{dk}{(2\pi)^3} \hat{V} \frac{|\psi_k^{(+)}\rangle\langle\psi_k^{(+)}|}{z - 2\epsilon_k} \hat{V}. \]  
(2.36)
From this equation we clearly see that the two-body T-matrix has poles in the complex-energy plane, corresponding to the bound states of the potential. In addition, the T-matrix contains a branch cut on the positive real axis due to the continuum of scattering states.

As an example, we note that for s-wave scattering the T-matrix \( T^{2B}(2\epsilon_k^+) \equiv \langle k' | \hat{T}^{2B}(2\epsilon_k^+) | k \rangle \) is independent of the angle between \( k' \) and \( k \). From the relation between the T-matrix and the scattering amplitude, and the expression for the latter
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in terms of the phase shift, we have for low positive energies

\[ T^{2B}(E^+) = - \frac{4\pi \hbar^2}{m} \frac{1}{\sqrt{\frac{mE}{\hbar^2}}} \cot \left( \delta \left( \sqrt{\frac{mE}{\hbar^2}} \right) \right) - i \frac{\sqrt{mE}}{\hbar} \]

\[ \simeq \frac{4\pi a\hbar^2}{m} \left[ \frac{1}{1 + ia \sqrt{\frac{mE}{\hbar^2}} - \frac{ar_{\text{eff}}mE}{2\hbar^2}} \right], \quad (2.37) \]

where we made use of the expansion in Eq. (2.17). From this result we deduce by analytic continuation that

\[ T^{2B}(z) \simeq \frac{4\pi a\hbar^2}{m} \left[ \frac{1}{1 - a \sqrt{\frac{-mz}{\hbar^2}} - \frac{ar_{\text{eff}}mz}{2\hbar^2}} \right]. \quad (2.38) \]

Clearly, for large and positive scattering length the T-matrix has a pole at negative energy \( E_m = -\hbar^2/ma^2 \), in complete agreement with our previous discussions.

Summarizing, we have found that the scattering length of an attractive potential well can have any value and depends strongly on the energy of the weakest bound state in the potential. In principle therefore, if we have experimental access to the energy difference of this bound state and the continuum threshold we are able to experimentally alter the scattering length and thereby the effective interactions of the atoms. In the single-channel case this is basically impossible to achieve. In a multichannel system, however, the energy difference is experimentally accessible, which makes the low-energy effective interactions between the atoms tunable. In the next section we discuss this situation.

2.3 Example of a Feshbach resonance

We consider now the situation of atom-atom scattering where the atoms have two internal states [89]. These states correspond, roughly speaking, to the eigenstates of the spin operator \( S \) of the valence electron of the alkali atoms. The effective interaction potential between the atoms depends on the state of the valence electrons of the colliding atoms. If these form a singlet the electrons are in principle allowed to be on top of each other. For a triplet this is forbidden. Hence, the singlet potential is generally much deeper than the triplet potential.

Of course, in reality the atom also has a nucleus with spin \( I \) which interacts with the spin of the electron via the hyperfine interaction

\[ V_{\text{hf}} = \frac{a_{\text{hf}}}{\hbar^2} I \cdot S, \quad (2.39) \]
with $a_{\text{hf}}$ the hyperfine constant. The hyperfine interaction couples the singlet and triplet states. Moreover, in the presence of a magnetic field the different internal states of the atoms have a different Zeeman shift. In an experiment with magnetically-trapped gases, the energy difference between these states is therefore experimentally accessible. Putting these results together, we can write down the Schrödinger equation that models the above physics

$$\left( -\frac{\hbar^2 \nabla^2}{m} + V_T(r) - E + \frac{V_{\text{hf}}}{m} \right) \psi_T(r) - \frac{\hbar^2 \nabla^2}{m} + \Delta \mu B + V_S(r) - E \left( \psi_S(r) \right) = 0. \quad (2.40)$$

Here, $V_T(r)$ and $V_S(r)$ are the interaction potentials of atoms with internal state $|T\rangle$ and $|S\rangle$, respectively, and $\Delta \mu B$ is their difference in Zeeman energy due to the interaction with the magnetic field $B$, with $\Delta \mu$ the difference in magnetic moment. In agreement with the above remarks, $|T\rangle$ is referred to as the triplet channel, whereas $|S\rangle$ is referred to as the singlet channel. The potentials $V_T(r)$ and $V_S(r)$ are the triplet and singlet interaction potentials, respectively.

As a specific example, we use for both interaction potentials again square well potentials,

$$V_{T,S}(r) = \begin{cases} -V_{T,S} & \text{if } r < R \\ 0 & \text{if } r > R \end{cases}, \quad (2.41)$$

where $V_{T,S} > 0$. For convenience we have taken the range the same for both potentials. Furthermore, we assume that the potentials are such that $V_T < V_S$ and that $V_S$ is just deep enough such that it contains exactly one bound state. Finally, we assume that $0 < V_{\text{hf}} \ll V_T, V_S, \Delta \mu B$. The potentials are shown in Fig. 2.3.

To discuss the scattering properties of the atoms, we have to diagonalize the hamiltonian for $r > R$, in order to determine the incoming channels, which are superpositions of the triplet and singlet states $|T\rangle$ and $|S\rangle$. Since the kinetic energy operator is diagonal in the internal space of the atoms, we have to find the eigenvalues of the hamiltonian

$$H^\perp = \begin{pmatrix} 0 & V_{\text{hf}} \\ V_{\text{hf}} & \Delta \mu B \end{pmatrix}. \quad (2.42)$$

These are given by

$$\epsilon^\perp = \frac{\Delta \mu B}{2} \pm \frac{1}{2} \sqrt{(\Delta \mu B)^2 + (2V_{\text{hf}})^2}. \quad (2.43)$$

The hamiltonian $H^\perp$ is diagonalized by the matrix

$$Q(\theta) = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix}, \quad (2.44)$$
according to
\[
Q(\theta^\rightarrow)H^\rightarrow Q^{-1}(\theta^\rightarrow) = \begin{pmatrix}
\epsilon^\geq & 0 \\
0 & \epsilon^\geq
\end{pmatrix},
\] (2.45)
which determines \(\tan \theta^\rightarrow = -2V_{hf}/\Delta \mu B\). We define now the hyperfine states \(|\uparrow\rangle\) and \(|\downarrow\rangle\) according to
\[
\begin{pmatrix}
|\uparrow\rangle \\
|\downarrow\rangle
\end{pmatrix} = Q(\theta^\rightarrow) \begin{pmatrix}
|T\rangle \\
|S\rangle
\end{pmatrix},
\] (2.46)
which asymptotically represent the scattering channels. In this basis the Schrödinger equation for all \(r\) reads
\[
\begin{pmatrix}
-\frac{\hbar^2 \nabla^2}{m} + V_{\uparrow\uparrow}(r) - E \\
V_{\uparrow\downarrow}(r)
\end{pmatrix}
\begin{pmatrix}
V_{\uparrow\uparrow}(r) \\
V_{\uparrow\downarrow}(r)
\end{pmatrix}
= \frac{-\hbar^2 \nabla^2}{m} + \epsilon^\geq - \epsilon^\leq + V_{\downarrow\downarrow}(r) - E
\times \begin{pmatrix}
\psi_{\uparrow}(r) \\
\psi_{\downarrow}(r)
\end{pmatrix} = 0,
\] (2.47)
where the energy \(E\) is measured with respect to \(\epsilon^\geq\) and we have defined the potentials according to
\[
\begin{pmatrix}
V_{\uparrow\uparrow}(r) & V_{\uparrow\downarrow}(r) \\
V_{\uparrow\downarrow}(r) & V_{\downarrow\downarrow}(r)
\end{pmatrix} = Q(\theta^\rightarrow) \begin{pmatrix}
V_T(r) & 0 \\
0 & V_S(r)
\end{pmatrix} Q^{-1}(\theta^\rightarrow).
\] (2.48)
Since all these potentials vanish for \(r > R\) we can study scattering of atoms in the states \(|\uparrow\rangle\) and \(|\downarrow\rangle\). Because the hyperfine interaction \(V_{hf}\) is small we have that \(\epsilon^\geq \simeq \Delta \mu B\) and \(\epsilon^\leq \simeq 0\). Moreover, for the experiments with magnetically-trapped gases we always have that \(\Delta \mu B \gg k_B T\) where \(k_B\) is Boltzmann’s constant and is \(T\) the temperature. This means that in a realistic atomic gas, in which the states \(|\uparrow\rangle\) and \(|\downarrow\rangle\) are available, there are in equilibrium almost no atoms that scatter via the latter state. Because of this, the effects of the interactions of the atoms will be determined by the scattering amplitude in the state \(|\uparrow\rangle\). If two atoms scatter in this channel with energy \(E \simeq k_B T \ll \Delta \mu B\) they cannot come out in the other channel because of energy conservation. Therefore, the index \(\uparrow\) refers to an open channel, whereas \(\downarrow\) is associated with a closed channel. Note that, since we describe a collision of two atoms in the center-of-mass frame, the open and closed channel are two-atom states. The situation is further clarified in Fig. 2.3.

To calculate the \(s\)-wave scattering length in the open channel we have to solve the Schrödinger equation. In the region \(r > R\) the solution is of the from
\[
\begin{pmatrix}
u_{\uparrow}(r) \\
\nu_{\downarrow}(r)
\end{pmatrix} = \begin{pmatrix}
Ce^{ikr} + De^{-ikr} \\
Fe^{-kr}
\end{pmatrix},
\] (2.49)
Figure 2.3: Feshbach resonance in a two-channel system with square-well interaction potentials. The triplet potential \( V_T(r) \) is indicated by the thick dashed line. The singlet potential that contains the bound state responsible for the Feshbach resonance is indicated by the thin dashed line. Due to the Zeeman interaction with the magnetic field, the energy difference between the singlet and triplet is equal to \( \Delta \mu B \). The interactions in the open and closed hyperfine channels are indicated by \( V_{\uparrow \uparrow}(r) \) and \( V_{\downarrow \downarrow} \), respectively.

where \( \kappa = \sqrt{m(\epsilon_\uparrow - \epsilon_\downarrow)/\hbar^2 - k^2} \) and, because we have used the same notation as in Eq. (2.12), the s-wave phase shift is again determined by Eq. (2.13). In the region \( r < R \) the solutions are of the form

\[
\begin{pmatrix}
u_\uparrow(r) \\ \nu_\downarrow(r)
\end{pmatrix} = \begin{pmatrix} A \left( e^{ik_\uparrow r} - e^{-ik_\uparrow r} \right) \\ B \left( e^{ik_\downarrow r} - e^{-ik_\downarrow r} \right) \end{pmatrix},
\]

(2.50)

where

\[
k_\uparrow = \sqrt{m(\epsilon_\uparrow - \epsilon_\downarrow)/\hbar^2 + k^2};
\]

\[
k_\downarrow = \sqrt{m(\epsilon_\downarrow - \epsilon_\downarrow)/\hbar^2 + k^2},
\]

(2.51)

and

\[
\epsilon_\pm = \frac{\Delta \mu B - V_T - V_S}{2} \mp \frac{1}{2} \sqrt{(V_S - V_T - \Delta \mu B)^2 + (2V_{hf})^2}.
\]

(2.52)

are the eigenvalues of the matrix

\[
H^< = \begin{pmatrix} -V_T & V_{hf} \\ V_{hf} & \Delta \mu B - V_S \end{pmatrix}.
\]

(2.53)

In order to determine the phase shift we have to join the solution for \( r < R \) and \( r > R \) smoothly. This is done most easily by transforming to the singlet-triplet
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The depth of the triplet and singlet channel potentials is $V_T = \hbar^2/mR^2$ and $V_S = 10\hbar^2/mR^2$, respectively. The hyperfine coupling is $V_{hf} = 0.1\hbar^2/mR^2$. The dotted line shows the background scattering length $a_{bg}$.

Indeed, solving the equation for the binding energy in Eq. (2.21) with $V_0 = -V_S$ we find that $|E_m| \simeq 4.62\hbar^2/mR^2$, which is approximately the position of the resonance in Fig. 2.4. The difference is due to the fact that the hyperfine interaction leads to a shift in the position of the resonance with respect to $E_m$.

The magnetic-field dependence of the scattering length near a Feshbach reso-
Figure 2.5: Bound-state energy of the molecular state near a Feshbach resonance for two coupled square-well interaction potentials. The solid line and the inset show the result for $V_{\text{hf}} = 0.1\hbar^2/mR^2$. The dashed line corresponds to $V_{\text{hf}} = 0$. The other parameters are the same as in Fig. 2.4.

This explicitly shows that the scattering length, and therefore the magnitude of the effective interatomic interaction, may be altered to any value by tuning the magnetic field. The off-resonant background scattering length is denoted by $a_{\text{bg}}$ and is, in our example, approximately equal to the scattering length of the triplet potential $V_T(r)$. Using the expression for the scattering length of a square well in Eq. (2.18) for $D = 1$, we find that $a_{\text{bg}} \approx -0.56R$. Furthermore, we have for our example that the position of the resonance is given by $B_0 \approx 4.63\hbar^2/m\Delta\mu R^2$ and that the width is equal to $\Delta B \approx -0.05\hbar^2/m\Delta\mu R^2$.

Next, we calculate the energy of the molecular state for the coupled-channel case which is found by solving Eq. (2.47) for negative energy. In particular, we are interested in its dependence on the magnetic field. In the absence of the hyperfine coupling between the open and closed channel we simply have that $\epsilon_m(B) = E_m + \Delta\mu B$. Here, $E_m$ is the energy of the bound state responsible for the Feshbach resonance, that is determined by solving the single-channel Schrödinger equation for the singlet potential. This bound-state energy as a function of the magnetic field is shown in Fig. 2.5 by the dashed line. A nonzero hyperfine coupling drastically changes this result. For our example the bound-state energy is easily calculated. The result is shown by the solid
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line in Fig. 2.5 for the same parameters as before. Clearly, close to the resonance the
dependence of the bound-state energy on the magnetic field is no longer linear, as the
inset of Fig 2.5 shows. Instead, it turns out to be quadratic. Moreover, the magnetic
field $B_0$ where the bound-state energy is equal to zero is shifted with respected to the
case where $V_{hf} = 0$. It is at this shifted magnetic field that the resonance is observed
experimentally. Moreover, for magnetic fields larger than $B_0$ there no longer exists
a bound state and the molecule now decays into two free atoms due to the hyperfine
coupling, because its energy is above the continuum threshold.

Close to resonance the energy of the molecular state turns out to be related to the
scattering length by

$$\epsilon_m(B) = -\frac{\hbar^2}{m[a(B)]^2},$$

as in the single-channel case. As we will see in the next chapters, the reason for this is
that close to resonance the effective two-body T-matrix again has a pole at the energy
in Eq. (2.56). This important result will be proven analytically in Chapter 4. First,
we derive a description of the Feshbach resonance in terms of coupled atomic and
molecular quantum fields.