

Chapter 2

The 155 G ^{85}Rb Feshbach resonance

2.1 Introduction

This Chapter provides a brief overview of a Feshbach resonance in the collisions of ^{85}Rb atoms. In addition to allowing the creation of ^{85}Rb Bose-Einstein condensates, the Feshbach resonance also made possible a variety of experiments involving changes to the self-interaction of the BEC. The effects of this variable self-interaction were numerous and they form the subject matter for the rest of this thesis.

2.2 Atomic interactions in a BEC

One of the most interesting properties of Bose-Einstein condensates in dilute atomic gases is the existence of interactions between the constituent atoms. Although the BEC is typically 5 orders of magnitude less dense than air, the interatomic interactions strongly affect a number of the properties of the condensate. The interactions in a BEC have been successfully described by mean-field theory [5], in which each BEC atom moves in an effective mean-field due to the other atoms. The mean-field interaction is mediated by the elastic collisions between atoms.

The well-known Gross-Pitaevskii (GP) equation can be used to describe a condensate in the limit of zero temperature and neglecting all correlations between the

atoms. The GP equation for a trapped BEC has the form

$$i\hbar\frac{\partial}{\partial t}\Phi(\vec{r},t) = \left[-\frac{\hbar^2\nabla^2}{2m} + V_{\text{ext}}(\vec{r}) + g|\Phi(\vec{r},t)|^2 \right] \Phi(\vec{r},t), \quad (2.1)$$

where Φ is the BEC order parameter, V_{ext} is the trap potential energy, and the coefficient $g = \frac{4\pi\hbar^2a}{m}$ characterizes the pair-wise interatomic interactions in the BEC through the s-wave elastic scattering length, a . The solution to the GP equation (2.1) is the condensate order parameter, Φ , which for most purposes can be regarded as the macroscopic wavefunction of the BEC atoms. The GP equation has the form of a nonlinear Schrodinger equation, where the nonlinear term arises from the mean-field interaction of one atom with all of the others. The mean-field interaction term, often called the self-interaction energy of the condensate, depends on the density of atoms and the scattering length. Thus, the GP equation predicts that the sign and magnitude of a determine the strength of the self-interaction and whether this interaction is attractive or repulsive.

For controlling the BEC self-interaction, it would clearly be desirable to find some method to change the scattering length. Almost one decade ago, it was suggested that the scattering length could be influenced using an external magnetic field [6]. The magnetic field would allow one to shift the energy of a molecular bound state to near-degeneracy with the energy of a colliding pair of atoms, thereby altering the elastic scattering properties. Such an effect is called a Feshbach resonance and was first studied in nuclear scattering. The physics of Feshbach resonances will be discussed in the rest of this Chapter.

2.3 Feshbach resonance

2.3.1 Simple picture of the resonance

In a simplified picture, a Feshbach resonance occurs when the energy of a bound state of the interatomic potential is equal to the kinetic energy of a colliding pair of atoms. Assuming a finite kinetic energy, such a degeneracy can occur only when the

bound state exists in a potential that has a higher threshold energy than that of the colliding atom pair. This condition can be satisfied in ultracold gases of alkali atoms, due to the low collision energy of the atoms and the existence of atomic hyperfine structure. Since the different hyperfine states generally possess different spin configurations and magnetic moments, one can sometimes tune the bound state energy into resonance with the colliding atom energy via the different Zeeman shifts in an external magnetic field. Assuming that both colliding atoms are in the lower hyperfine state, it may happen that an interatomic potential associated with the upper hyperfine state supports a bound state nearby in energy, as shown schematically in Figure 2.1.

The schematic curves in Figure 2.1 show the potential energy of the atoms as a function of their internuclear separation, R . Neglecting the Zeeman interaction, the large R asymptotic energy is determined entirely by the sum of the hyperfine energies for the colliding atoms. Each asymptote is called a collision channel and different channels are labeled by the hyperfine quantum numbers (F, m_F) for the atom pair.

If two atoms begin an elastic collision in the lower channel with kinetic energy much smaller than the hyperfine splitting, ΔE_{HF} , the atoms cannot exit the collision in the upper channel because of energy conservation. Thus, the upper channel is energetically “closed”, while the lower channel is “open”. In the case of ^{85}Rb experiments, the hyperfine splitting of 140 mK greatly exceeds the kinetic energy of the degenerate gas sample, which is <10 nK. This means that the Feshbach resonance will be “well-resolved” because the energy spread of the BEC atoms is far smaller than the energy difference between the two hyperfine states.

In addition to low collision energy and hyperfine structure, another requirement for the existence of a Feshbach resonance is a coupling between the open and closed channels. The coupling is provided by the Coulomb (or exchange) interaction, which couples together different hyperfine states at short internuclear distance [7]. As the atoms move together during a collision, the strong electrostatic interaction between the

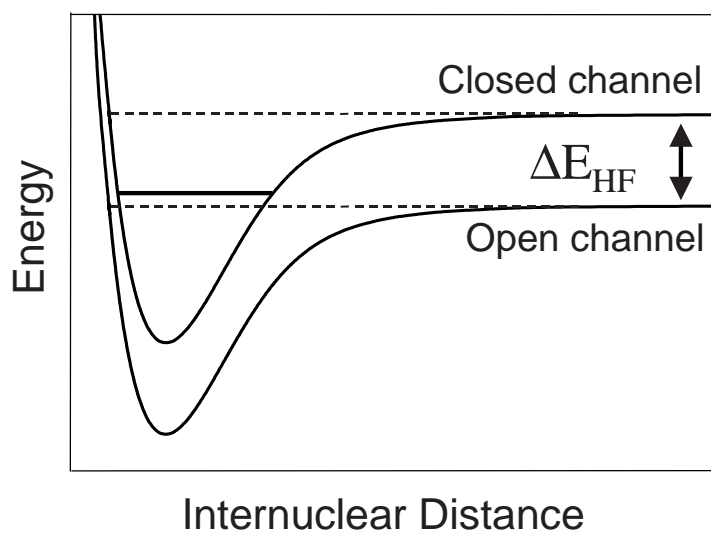


Figure 2.1: A simplified representation of the interatomic potentials involved in a Feshbach resonance. The solid lines represent the potential energy versus internuclear separation for the colliding atoms. The dashed lines show the threshold or asymptotic energies of the potential curves, which are separated by the hyperfine splitting, ΔE_{HF} . A bound state of the upper potential, shown by the short horizontal line, is nearly degenerate with the threshold energy of the lower potential. The definition of energetically open and closed channels is given in the text.

nuclei and the electron clouds overwhelms the relatively weak hyperfine interaction, allowing a spin flip to occur. Due to the symmetry of the binary system, the total spin projection quantum number $m_{F(tot)}=m_{F(1)}+m_{F(2)}$ is conserved, but the total spin $F_{tot}=F_1+F_2$ is not. The symmetry requirement determines whether a given closed channel can couple to the open channel.

2.3.2 Real ^{85}Rb Feshbach resonance

It turns out that the idealized picture of the Feshbach resonance caused by the interaction of a *single* closed channel with the open channel is too simplistic. Because of the complicated hyperfine structure of alkali atoms, any real resonance must involve coupling of the open channel to a number of different closed channels. As discussed in section 2.3.1, the symmetry of the Hamiltonian describing the colliding atoms dictates that only those channels with the same total spin projection as the open channel can be coupled. For the 155 G ^{85}Rb Feshbach resonance, the open channel is $|F_1, m_{F(1)}\rangle + |F_2, m_{F(2)}\rangle = |2, -2\rangle + |2, -2\rangle$. The symmetry requirement that $m_{F(tot)} = -4$ restricts the number of closed channels to four. We list the relevant ^{85}Rb closed channels in order of increasing threshold energy in Table 2.1.

Table 2.1: Closed channels involved in the ^{85}Rb Feshbach resonance. Each channel is a sum of two different hyperfine states, as indicated by the quantum numbers in the second column. The threshold energies and magnetic moments of the closed channels relative to the open channel are calculated using the Breit-Rabi equation at a magnetic field of 175 G. Note that $\Delta E_{\text{HF}} = 3.036$ GHz.

Label	Closed channel	Energy/ ΔE_{HF} at B=175 G	Magnetic moment (MHz/G)
(a)	$ 2, -1\rangle + 3, -3\rangle$	0.840	-2.72
(b)	$ 2, -2\rangle + 3, -2\rangle$	0.900	-1.57
(c)	$ 3, -1\rangle + 3, -3\rangle$	1.799	-3.22
(d)	$ 3, -2\rangle + 3, -2\rangle$	1.800	-3.14

All of these closed channels can potentially interact with the open channel. There-

fore the simplified picture of a Feshbach resonance given in Figure 2.1 is inadequate. In fact, to describe the resonance when the magnetic field approaches the resonance value, one must include the effects of multi-channel coupling [7, 8, 9]. In a coupled-channels approach, the wavefunction of the colliding atom pair is expanded as a sum of the open channel state and the four closed channel states. The expansion coefficients are dependent on collision energy, magnetic field, and the internuclear separation of the colliding atoms. When one substitutes the expanded wavefunction into the Schrodinger equation containing an approximate Hamiltonian for the interatomic interactions, one obtains a set of coupled equations that describe the elastic collision. By solving these equations, one can accurately determine the most important property of the elastic collision – the scattering length, a . The existence of the Feshbach resonance profoundly affects the scattering length by introducing a magnetic field dependence to a .

2.3.3 Variable scattering length

A well-known feature of low energy scattering from an attractive potential well is resonance scattering [10, 11]. Resonance scattering occurs when a bound state of the potential is very close to the collision energy of the atoms. The presence of the bound state near zero energy profoundly affects the scattering physics. This is because the colliding atoms can make a transition to the bound state and dwell there briefly before moving apart again after the collision. The biggest effect on the scattering occurs when the two levels have exactly the same energy, which causes the elastic cross section and scattering length to reach infinite values. In a Feshbach resonance, one can adjust the energy of a bound state relative to the collision energy by tuning the magnetic field. Even though the bound state exists in a different interatomic potential from that of the colliding atoms, the variable bound state energy can still dramatically alter the scattering length.

From the coupled-channels scattering theory of Feshbach resonances, one can

derive an approximate analytic expression for the variation of the scattering length with magnetic field [7]. In terms of the Feshbach resonance parameters, the scattering length is [7, 12]

$$a = a_{\text{bg}} \left(1 - \frac{\Delta}{B - B_{\text{peak}}} \right), \quad (2.2)$$

where B_{peak} is the resonance position and is defined to be the magnetic field where the magnitude of a becomes infinite, a_{bg} is the background scattering length, and Δ is the resonance width in magnetic field. Although equation (2.2) is only approximate, we have found that the analytic expression works very well. In fact, the scattering length from equation (2.2) agrees with a calculated from a full coupled-channels theory to better than 1% percent from 155 G to 250 G [13]. Figure 2.2 displays the scattering length predictions from equation (2.2).

2.3.4 Bound state properties for the ^{85}Rb Feshbach resonance

Very near the ^{85}Rb Feshbach resonance on the high B-field side, the scattering length is large and positive. From zero-energy scattering theory [10, 11], we know that when a is much bigger than the effective range of the attractive potential well ($a \gg R_{\text{eff}} \sim 25 a_0$), there must exist a weakly bound state just below the threshold energy. The binding energy of the weakly bound state bears a simple relationship to the scattering length:

$$\epsilon_{\text{bind}} = -\hbar^2/(ma^2), \quad (2.3)$$

where m is the atomic mass. The arguments leading to this result are very general, so the equation must be valid as long as a is big. It is therefore not necessary to deal with a complicated coupled-channels calculation of ϵ_{bind} in the large scattering length regime, provided that the parameters of the Feshbach resonance are well known and one can use equation (2.2) to determine the scattering length.

However, to obtain the full magnetic field dependence of the molecular binding

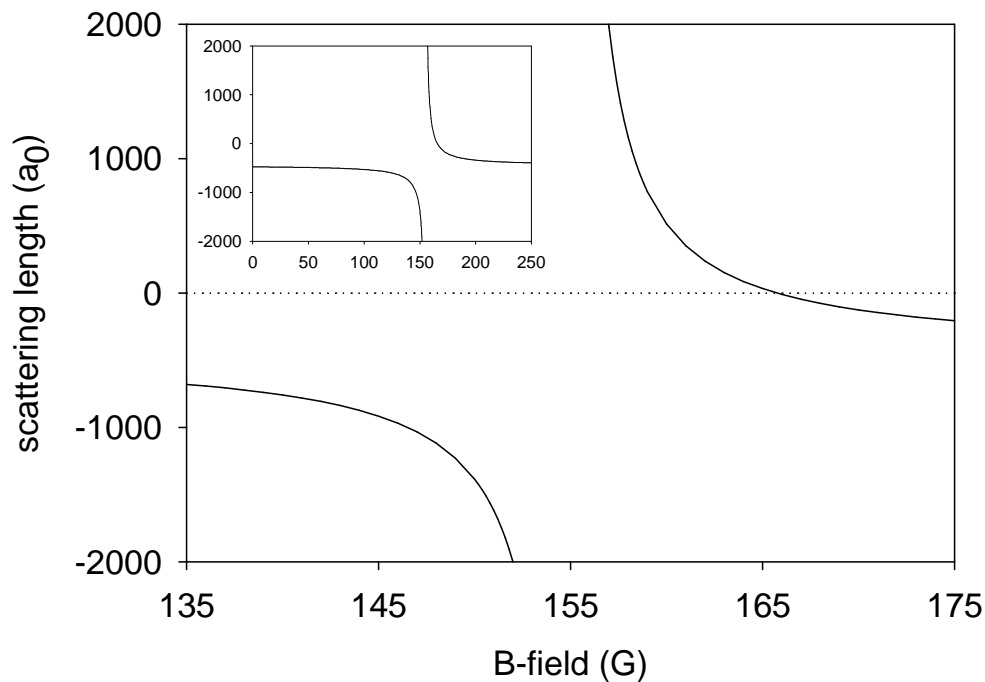


Figure 2.2: Magnetic field dependence of scattering length near the Feshbach resonance. The solid line is the scattering length calculated from equation (2.2) with the current best values for the resonance parameters (see Chapter 7). For the resonance position and width, we have $B_{\text{peak}}=155.041$ G and $\Delta=10.709$ G, respectively. The value of the background scattering length is $-443 a_0$. The horizontal dashed line indicates zero scattering length, which occurs at $B_{\text{zero}}=165.75$ G. In the inset, we show the scattering length variation over a larger range of B-field.

energy, a coupled-channels calculation is needed [9]. When the interactions between all of the channels are accounted for, one obtains a rather complicated magnetic field dependence in ϵ_{bind} . The coupling matrix element between the open channel and each closed channel varies strongly with B-field, which leads to a nonlinear magnetic field dependence of the binding energy. Figure 2.3 shows this dependence along with the scattering length variation for magnetic fields above the ^{85}Rb Feshbach resonance.

In addition to the binding energy, another important property of the molecular state is the spatial size of the wavefunction. Zero-energy scattering theory provides a useful prediction for the shape of the molecular state wavefunction. Outside the effective range of the potential, the wavefunction for the molecular state can be shown to have the form [10]

$$\phi(r) \sim \frac{\exp(-r/a)}{r}, \quad (2.4)$$

where $a \gg R_{\text{eff}}$ is the large, positive scattering length and R_{eff} is the range of the potential. Equation (2.4) shows that the decay of the bound state occurs over a length scale equal to the scattering length, which can easily exceed the potential range by several orders of magnitude. This behavior is possible because of the proximity of the bound state to zero energy. The elongated spatial size of the molecule has some bizarre consequences. For instance, when the scattering length is very large, the atoms in the weakly bound molecule spend the majority of their time at internuclear separations that are best described by the hyperfine basis. The molecular state is far too large to be labeled according to the conventional singlet/triplet molecular quantum numbers.

It is worth emphasizing that the characteristics of the weakly bound molecular state are completely different from those of the single closed channel state of conventional Feshbach theory. For instance, the weakly bound state extends far past the short-range part of the interatomic potential. The size of the weakly bound state is basically given by the scattering length when $a \gg 0$. In contrast, the closed channel bound state

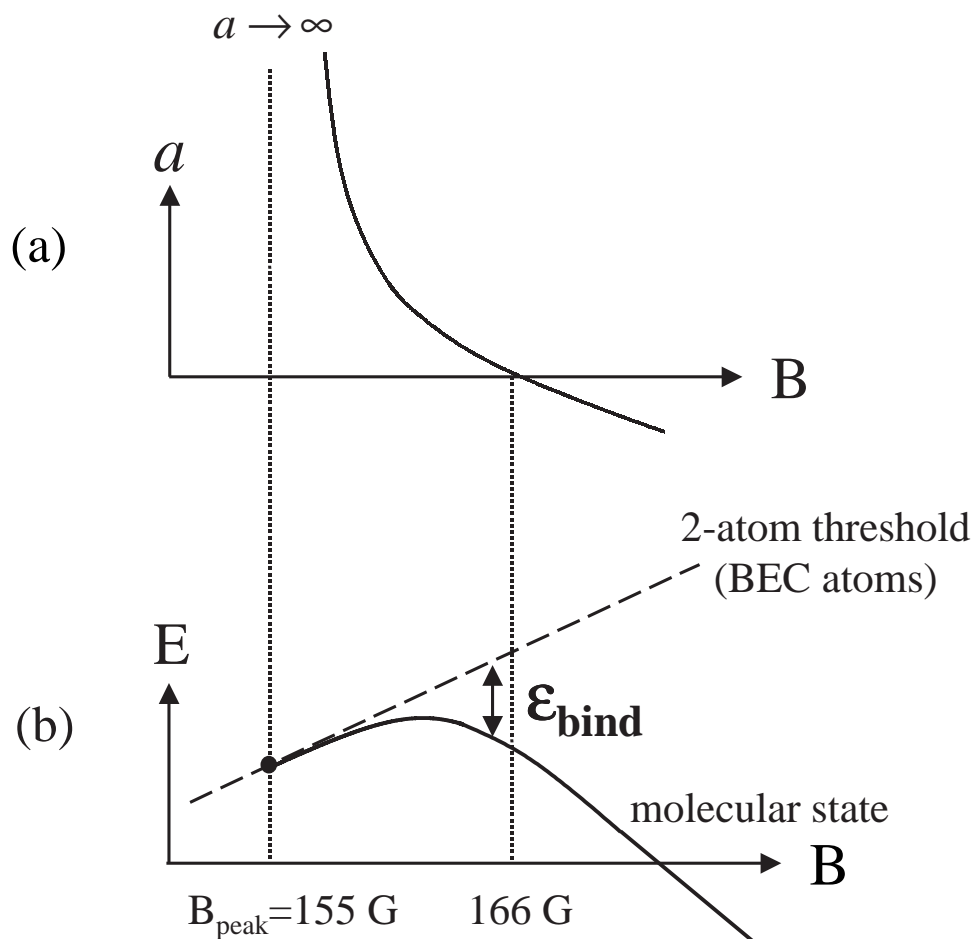


Figure 2.3: Schematic representation of the Feshbach resonance in ^{85}Rb . **(a)** Variation of scattering length for $B > B_{\text{peak}}$. The two vertical dotted lines indicate the range of magnetic field where $a > 0$. **(b)** Dependence of atomic and molecular energies on B-field. The dashed line shows the colliding atom threshold energy, while the solid curve is the molecular state energy, which intersects the atomic threshold at B_{peak} . For magnetic fields significantly above resonance, the molecular energy decreases linearly with B-field at a rate that is very similar to the magnetic moments of closed channels (c) and (d), as listed in Table 2.1.

is confined to the part of the interatomic potential where molecular forces dominate, which is roughly $25 a_0$ in extent. Another property of the weakly bound state that sets it apart from the closed channel state is the magnetic field dependence. While the closed channel state exhibits a linear variation of energy versus B-field, the weakly bound state shifts in a highly nonlinear fashion (see Figure 2.3).

2.3.5 Physical relevance of weakly bound state

Prior to the publication of our recent measurements of the molecular state binding energy (see [4] and also Chapters 6-7), the existing theoretical descriptions of alkali atom Feshbach resonances [14, 15] were mostly based on the simple picture of a single closed channel coupled to the open channel (see section 2.3.1). In the course of our studies of ^{85}Rb condensates, we found that the simple picture was totally incorrect — it failed to describe the atom-molecule oscillation data in Chapter 6. Our measurements clearly demonstrated the physical relevance of the weakly bound molecular state. Several new theoretical models for the ^{85}Rb Feshbach resonance are currently being developed [9, 16, 17, 18] to describe the data.