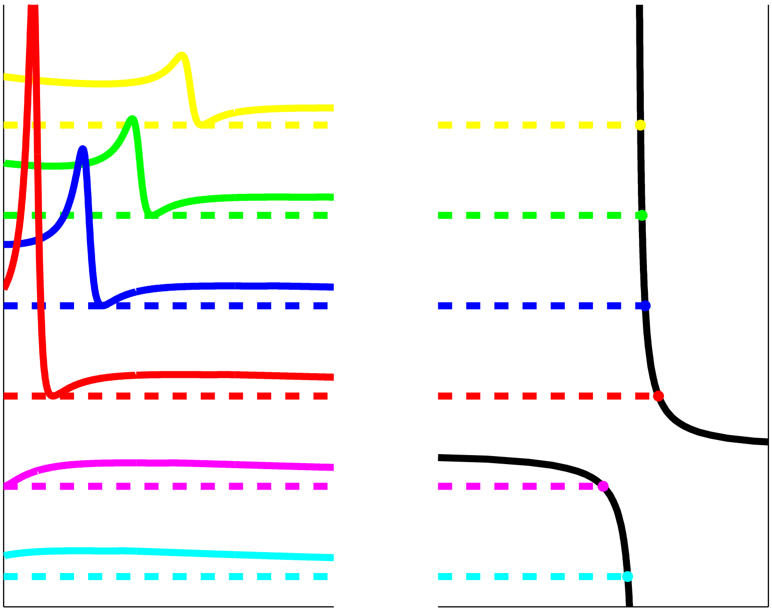
A coupled channel zero-range model for Feshbach resonances

(En zero-range model med koblede kanaler til beskrivelse af Feshbach resonanser)



23th july 2010
Bachelor's project in physics

Rasmus Sloth Hansen
20071266

Supervisor: Dmitri Fedorov

Department of Physics and Astronomy
Aarhus University

Abstract (English)

Feshbach resonances have been considered theoretically for a long time in nuclear systems and with the development of cold atoms and molecules they have become an invaluable tool to control the stability and interactions of quantum gasses.

This project describes a simple coupled channel zero-range model which can describe Feshbach resonances.

First some of the characteristics of Feshbach resonances are summarised along with their applications and some of the models used to describe them. Hereafter the zero-range model is introduced and analysed. Expressions for the scattering length and the cross section are found for elastic scattering and a numerically solvable condition for bound states is found as well. In order to make the analysis complete some threshold effects for inelastic scattering are investigated.

Finally the model is compared to data for real systems and full coupled channel calculations. This is done by calculating the parameters of the zero-range model from the available data and comparing the results to the expected. It is found that the model can describe the behaviour of the scattering length with great success and that the cross section and the bound state energies also fit very well for small energies.

Abstrakt (Dansk)

Feshbach resonancer har været i teoretikernes søgelys i lang tid i forbindelse med atomkerner, og med udviklingen indenfor kolde atomer og molekyler er de blevet et uvurderligt værktøj til at kontrollere stabilitet og vekselvirkninger i kvantegasser.

Dette projekt beskriver en simpel zero-range model med koblede kanaler, som kan beskrive Feshbach resonanser.

Først opsummeres nogle af kendetegnene for Feshbach resonanser samt deres anvendelser og nogle af de modeller, der bruges i beskrivelsen af dem. Herefter introduceres og analyseres zero-range modellen. Der bliver fundet udtryk for spredningslængden samt spredningstværsnittet for elastisk spredning, og der udledes en betingelse for bundne tilstande, der kan løses numerisk. For at gøre analysen fuldstændig undersøges nogle tærskeleffekter for inelastisk spredning.

Til sidst bliver modellen sammenlignet med data for virkelige systemer og avancerede beregninger, der tager højde for flere koblede kanaler. Dette bliver gjort ved at beregne parametrene i zero-range modellen ud fra de tilgængelige informationer og sammenligne resultaterne med det forventede. Det viser sig, at modellen kan beskrive opførslen af spredningslængden med stor succes, og at for små energier passer spredningstværsnittet og energierne for de bundne tilstande også rigtig godt.

Contents

Introduction

The goal of this Bachelor's project is to show that Feshbach resonances can be modelled by a simple coupled channel model using zero-range potentials. Before the analysis of the used model I will introduce the phenomena of Feshbach resonances and briefly discuss some other models used to describe them.

In the analysis I will first consider a very simple system with the zero-range potential before I proceed to the coupled channel model. For the coupled model I will find bound states, scattering states, and to make the analysis complete I will include a section about inelastic scattering and point out some threshold effects.

With the model established the next chapter will focus on the ability of the model to describe Feshbach resonances. First I develop some different methods to extract parameters for the zero-range model from the available data and second I will compare the model to the data itself and a full coupled channel calculation for various known resonances.

I would like to thank my supervisor Dmitri Fedorov for many good discussions, patience and invaluable ideas for my work and I would like to thank Mia Lundkvist for numerous comments on language as well as academic issues.

— 1 —

Resonances and Feshbach

Resonance as a phenomenon is known from many branches of physics. In classical physics it arises in many oscillating systems and for waves. Examples are musical instruments as flutes or driven oscillators such as a child on a swing.

Resonance phenomena also arise often in quantum mechanics and they give rise to applications such as NMR-spectroscopy and investigation of composite systems in atoms and nuclei.

During the past 80 years two of the main contributors to the description of resonances in atomic and nuclear systems are Herman Feshbach[5, 6] and Ugo Fano[4]. They developed two different approaches to treat resonances in systems due to coupling to a discrete state. Resonances in these systems are today characterised as a Fano resonance or a Feshbach resonance according to their origin.

1.1 Resonances in atoms and nuclei

Atoms and nuclei are in general not described by the same models because the mass of the electron is much smaller than that of a nucleon, but in some cases the same theory can be used for both. This is the case for low energy scattering.

One of the most interesting quantities to investigate in scattering theory is the cross section and in some cases a prominent peak is seen in the cross section, σ as a function of energy, E and this is called a resonance.

These resonances can be understood as the energies where there is a metastable bound state in the system and the origin of this bound state determines the type of the resonance.

If the state is due to the potential itself as shown in figure 1.1(a) it is called a shape-, open channel- or Fano resonance. This is the model that Fano investigated, and the origin of the resonance is simply the shape of the potential. One example of this could be the combination of an attractive potential and the centrifugal barrier.

The other possibility is to have a coupling to a potential with a bound state as it is shown in figure 1.1(b). This is called a Feshbach resonance or a closed channel resonance. The open- and closed channels are states where the separation energy is respectively smaller and bigger than the energy of the incident particles[1]. Feshbach used the idea of coupled potentials to describe resonances in nuclear physics in the two papers mentioned above.

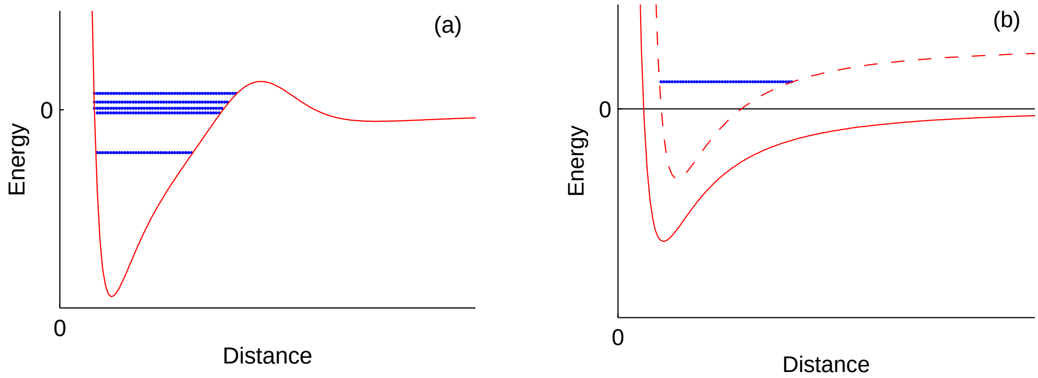


Figure 1.1: Potentials for a system with a shape resonance (a) and a Feshbach resonance (b). The bound states are indicated with blue dots. In panel (a) the three upper levels are metastable as they have $E > 0$. In panel (b) the potential of the closed channel is indicated with a dashed line.

In the context of cold atomic systems, a Feshbach resonance has a slightly different meaning today. It is most often used for the divergence of the scattering length, a, when a bound state in the closed channel approaches the threshold energy of the open channel. It is this phenomenon I will try to model in my Bachelor's project. This means that it is actually not a resonance in the original meaning, but it is closely related to a resonance as a divergence in the scattering length corresponds to a divergence for the cross section at $E = 0$ as $\sigma(E = 0) = 4\pi a^2$.

In figure 1.2 this is illustrated. The figure shows that the scattering length diverges at the value where the resonance in the cross section reaches zero. In the analysis of the zero-range model in chapter 2, I will derive expressions for both the scattering length and the cross section.

The unique feature of cold atoms is that it is possible to change the energy difference between different channels because of the Zeeman effect. This makes it possible to control the scattering length by varying the magnetic field when an open- and a closed channel have different magnetic moments.

The most common formula to fit to the experimental data is[2]:

$$a = a_{\mathrm{bg}} \left(1 - \frac{\Delta}{B - B_{\mathrm{res}}} \right) , \tag{1.1}$$

Here a_{bg} is the background scattering length, Δ is the width of the resonance, and B_{res} is the resonance position. a_{bg} gives the off-resonant value of the scattering length as the fraction approaches zero for $B - B_{\mathrm{res}} \to \pm\infty$. Δ indicates the point where $a = 0$ relative to the resonance position. This is shown in figure 1.3.

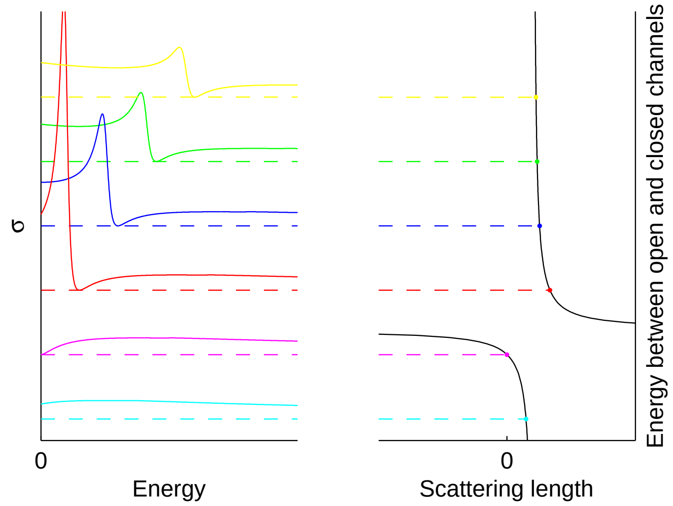


Figure 1.2: In the left panel the solid lines are the cross section, and for each colour the corresponding dashed line indicates $\sigma = 0$. In the right panel the dashed lines connect to the corresponding point for scattering length and energy difference.

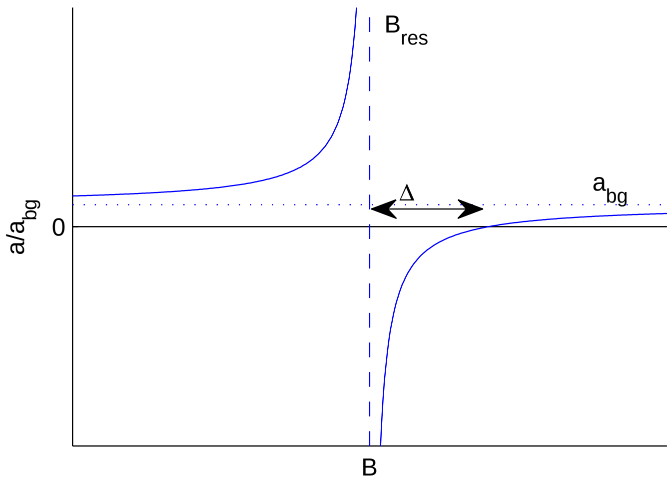


Figure 1.3: The quantities in equation (1.1) are shown for a Feshbach resonance.

1.2 Applications of Feshbach resonances in cold atoms

Feshbach resonances in cold atomic gasses have proven an invaluable tool to control the interaction between atoms. The scattering length determines not only the zero energy limit for the cross section, but also tells whether the potential is repulsive or attractive. The former corresponds to a positive a and the latter to a negative. Originally, Feshbach resonances were only considered a source of instability and were therefore avoided[12], but later the tuning of scattering length has helped to obtain stable quantum gases and Bose-Einstein condensates (BEC).

To obtain a stable BEC it is necessary to have a negative scattering length as the interaction is repulsive for positive values and this leads to a collapse of the condensate for a relatively small number of atoms. BEC's are obtained by evaporative cooling and this gives a minimum for the absolute value of the scattering length as the condensate must thermalize quite fast in order not to loose too many atoms in this process. On the other hand the magnitude of the scattering length must not be too large as this gives rise to decay due to three-body collisions. For some atomic species the scattering length has a good magnitude according to the above considerations, but for many others it is necessary to tune it with a Feshbach resonance.

Another important application is to form cold molecules from cold atoms. This is possible because the scattering length diverges as it is seen in figure 1.3 and a large negative scattering length corresponds to a weakly bound state (see also section 2.1.1). For many broad resonances there is a domain with universal behaviour which means that the system can be described by a single potential with scattering length a. This gives rise to spatially large bound states called ”quantum halos”, a system also known from nuclear physics, and Feshbach molecules give a new possibility to test the models for this phenomenon. The molecules made with Feshbach resonances are highly exited and afterwards they can be converted to deeper bound states if other properties are demanded for the molecules. This can be done by e.g. two photon Raman transitions using two lasers to drive the transition[2].

1.3 Models for Feshbach resonances

In order to understand Feshbach resonances theoretically, various models have been developed. In general these can be divided into two categories. The first is the single channel model where the resonance is placed ”by hand” and the second is the coupled model where the Feshbach resonance comes from a coupling to a bound state in a closed channel as shown in figure 1.1 (b).

Common to all the models is that they assume that the energy is so small that the atoms are in the s-state with zero electronic angular momentum.

1.3.1 Single channel model

The simplest model which can describe a Feshbach resonance contains a single zero-range potential. This can be done by giving the potential a strength proportional to the scattering length $a(B)$ which then determines the width and the position of the resonance. The most obvious way to do this would be to use the expression in equation (1.1) to find $a(B)$. This model can only be used in the domain with universality and to cover a wider range it is necessary to use more advanced models.

1.3.2 Coupled channel models

In a full coupled channel calculation it is necessary to include the Born-Oppenheimer potentials for the systems as well as the spin dependent couplings between them. This might include several different open- and closed channels in order to describe all the different spin projections and atomic species. As the exact short range behaviour of the Born-Oppenheimer potentials are often unknown these must be fitted to experimental data and this yields precise and robust models that describe energies close to threshold[2].

As the above approach gives a very complicated picture, it is desirable to have simpler models which still capture some of the essential features of the resonance.

The long range behaviour of the potential is given by the $\frac{1}{r^6}$ van der Walls potential so for small scattering energies this potential is a good approximation to the full Born-Oppenheimer potential. Using this model gives a lot of physical insight into the properties of Feshbach resonances. One of the most interesting results is the possibility of characterising a resonance as closed- or open channel dominated, where the latter has universal behaviour for a large fraction of the resonance width[2].

— 2 —

Analysis of the zero-range potential

In the previous chapter I have mentioned some methods to describe Feshbach resonances. In this chapter I will use a coupled zero-range model to describe them, but first I will introduce and analyse a single zero-range potential to show the simplicity of the model.

As I only consider two particle interactions, the system is characterised by the distance between the two particles, r and the reduced mass, m. I will only consider the relative wave function $\psi(r)$ for s-waves.

The idea of the zero-range potential is that many of the more complex potentials go to zero for large distances, and thus the wave function is approximately a solution to the free Schrödinger equation for these distances. In the zero-range potential this is taken to the extreme as the only representation of the potential is a boundary condition at zero distance. The stationary Schrödinger equation is therefore:

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi, \tag{2.1}$$

with the boundary condition:

$$(r\psi)'(0) = \frac{(r\psi)(0)}{a}, \tag{2.2}$$

A more rigid condition is that a zero-range potential can be used as an approximation if the range of the potential is much shorter than the de Broglie wavelength of the interacting particles. This is often the case for cold atoms as well as it is the case for low energy collisions in nuclear physics.

It is worth noting that the zero-range potential has different names such as contact- or delta potential and one other way to describe the zero-range potential is to use a Dirac-delta function[8].

2.1 Simple system

The simple system consists of two particles and a zero-range potential as described above. As the potential is spherically symmetric it is natural to use the spherical harmonic functions to solve the Schrödinger equation and as I only consider s-waves, the problem simplifies to solving the radial Schrödinger equation with the right boundary conditions. To make these equations even simpler I define a new function, $u(r)$:

$$\psi(r) = \frac{1}{r}u(r),$$

Now the Schrödinger equation and the boundary conditions can be written as

$$-\frac{\hbar^2}{2m}u''(r) = Eu(r), \qquad r > 0 \tag{2.3}$$

$$\left.\frac{u'}{u}\right|_{r=0} = \frac{1}{a}, \tag{2.4}$$

where a is the only parameter of the potential.

2.1.1 Bound states

I will first analyse energies less than zero which corresponds to bound states. For $E < 0$ the wave function must have the form:

$$u(r) = Ae^{-kr}, \qquad k = \sqrt{\frac{2mE}{\hbar^2}},$$

The function $u(r) = Be^{kr}$ is also a solution, but it can not be normalised. Normalisation gives $A = \sqrt{k/(2\pi)}$ and the final radial wave function is

$$\psi(r) = \sqrt{\frac{k}{2\pi}}\frac{e^{-kr}}{r},$$

Employing the boundary conditions yield

$$\left.\frac{u'}{u}\right|_{r=0} = -k = -\frac{\sqrt{-2mE}}{\hbar} = \frac{1}{a} \qquad \Rightarrow \qquad E = -\frac{\hbar^2}{2ma^2},$$

Thus one bound state is found with the energy found above if $a < 0$. If $a > 0$ there is no solution to the above equation.

2.1.2 Scattering states

The scattering states have $E > 0$, and as the potential falls off faster than $\frac{1}{r^2}$ this gives rise to asymptotic solutions of the form[9]:

$$u(r) = A\sin(\kappa r + \delta(\kappa)), \qquad \kappa = \frac{\sqrt{2mE}}{\hbar},$$

As the potential is actually zero everywhere except at $r = 0$ this is not only the asymptotic solution, but the complete solution to the Schrödinger equation.

By using the boundary conditions, $\delta(\kappa)$ can be determined:

$$\left.\frac{u'}{u}\right|_{r=0} = \kappa\frac{\cos(\delta(\kappa))}{\sin(\delta(\kappa))} = \kappa\frac{1}{\tan(\delta(\kappa))} = \frac{1}{a} \qquad \Rightarrow \qquad \delta(\kappa) = \arctan(\kappa a),$$

For low energy scattering the interesting quantities are the scattering length, a_s, and the effective range, R_{eff}. Often R_{eff} can be neglected[9]. They are defined from the limit of $\cot(\delta(\kappa))$[1]:

$$\lim_{k\to 0}(k\cot(\delta(\kappa))) = \frac{1}{a_s} + \frac{1}{2}R_{\text{eff}}k^2 + \dots,$$

For the zero-range potential $a_s = a$ and $R_{\text{eff}} = 0$ as one might expect from the name of the potential.

2.2 Coupled system

I would now like to use the zero-range potential to make a simple model of a Feshbach resonance. As mentioned earlier, Feshbach resonances are found when a bound state in a closed channel coincides with the threshold energy of a coupled open channel. Thus I must define the potential to contain some coupling constant, and to include both a closed and an open channel. The first thing to define is a wave function that can describe two channels simultaneously:

$$\psi(r) = \frac{1}{r}\begin{bmatrix} u_c(r) \\ u_o(r) \end{bmatrix},$$

As for the simple zero-range potential this wave function must satisfy the free Schrödinger equation, but as one channel is closed and the other is open their energies are different. If $E^* > 0$ is the difference in energy, the Schrödinger equations have the form:

$$-\frac{\hbar^2}{2m}u_o'' = Eu_o \qquad -\frac{\hbar^2}{2m}u_c'' = (E - E^*)u_c \quad , \tag{2.5}$$

The coupling between the two channels can be described by a coupling constant β, and the boundary conditions are now:

$$\begin{aligned} u_o'(0) &= \frac{1}{a_o}u_o(0) + \beta u_c(0) \\ u_c'(0) &= \frac{1}{a_c}u_c(0) + \beta u_o(0), \end{aligned} \tag{2.6}$$

2.2.1 Bound states

I will first analyse bound states and they must have $E < 0$. In this regime both the open and closed channels have wave functions of the form:

$$u_o(r) = Ae^{-rk}, \qquad k = \frac{\sqrt{-2mE}}{\hbar}$$

$$u_c(r) = Be^{-r\kappa}, \qquad \kappa = \frac{\sqrt{-2m(E - E^*)}}{\hbar},$$

[1]This sign convention for the scattering length is used in nuclear physics[10] whereas the opposite convention is used in atomic and molecular physics.

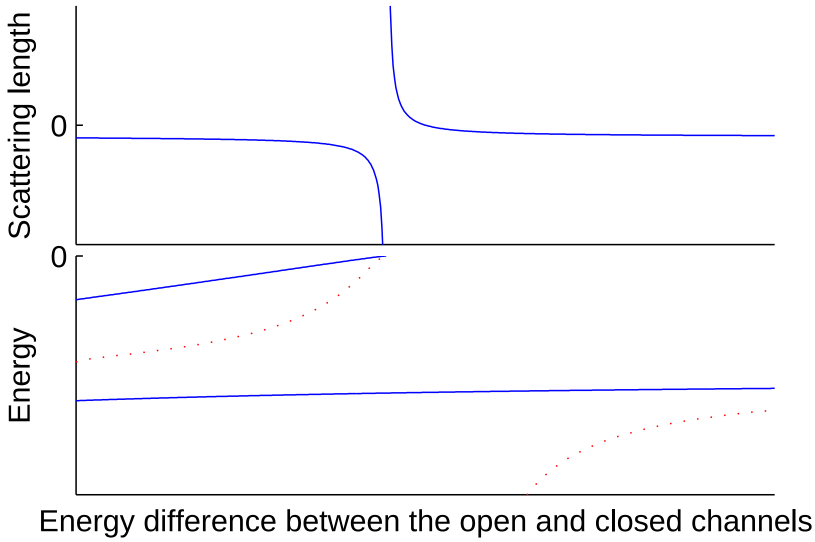


Figure 2.1: The upper panel shows the scattering length calculated with equation (2.9). The lower panel shows the bound state as a solid line found numerically and the low energy appoximation from equation (2.8) as a dotted line. $a_o < 0$ which gives rise to two bound states.

When inserted in the boundary conditions, it yields the equations:

$$\left.\begin{aligned} -kA &= \tfrac{1}{a_o}A + \beta B \\ -\kappa B &= \tfrac{1}{a_c}B + \beta A \end{aligned}\right\} \quad \Rightarrow \quad \begin{aligned} \left(k + \tfrac{1}{a_o}\right) A + \beta B = 0 \\ \beta A + \left(\kappa + \tfrac{1}{a_c}\right) B = 0 \end{aligned},$$

For these equations to have a non-zero solution, the determinant must be zero, and it gives the condition:

$$\left(k + \frac{1}{a_o}\right)\left(\kappa + \frac{1}{a_c}\right) - \beta^2 = 0, \tag{2.7}$$

This means that if the above equation is fulfilled, there is a bound state with the corresponding energy. For the case $\beta = 0$ it simplifies to the solution for two simple zero-range potentials as one might expect. If $\beta \neq 0$ the above equation is an equation of fourth degree, and it can be solved exact, but the results are four very long equations for the energy and do not give much insight.

Instead I will take the limit for $-E << E^*$ and from this I can find bound states with energies close to zero. Considering the definition of κ, this approximation corresponds to $\kappa \approx \frac{\sqrt{2mE^*}}{\hbar}$, and now equation (2.7) can be solved to give

$$E_1 = -\left(-\frac{1}{a_o} + \beta^2 \left(\frac{\sqrt{2mE^*}}{\hbar} + \frac{1}{a_c}\right)^{-1}\right)^2 \frac{\hbar^2}{2m}, \tag{2.8}$$

Another possibility is to do a numerical calculation of the bound state energies. This gives a result as close to the real bound state energy as wished. In the lower panel of figure 2.1 this is done by using a bisection method. The figure shows that for the chosen parameters it is only for a very narrow interval that equation (2.8) gives the right result. It is also worth noting that this model can describe two bound states in the case with $a_o < 0$.

2.2.2 Elastic scattering

In the energy range between 0 and E^* I expect to see different resonance effects. In the cross section I expect to find a structure resonance at the energy that corresponds to a bound state for an uncoupled closed channel. For E^* corresponding to the same energy I expect to see a Feshbach resonance in the scattering length as it is described in Chapter 1.

As for the simple zero-range potential, the wave function

$$u_o(r) = A\sin(kr + \delta(k)), \qquad k = \frac{\sqrt{2mE}}{\hbar}$$

is a solution to equation (2.5) for $E > 0$. For $u_c(r)$ the total energy is still negative and thus the solution is the same as for the bound states:

$$u_c(r) = Be^{-r\kappa}, \qquad \kappa = \frac{\sqrt{-2m(E - E^*)}}{\hbar},$$

These two solutions to the Schrödinger equation give along with the boundary conditions in equation (2.6):

$$\begin{aligned} kA\cos(\delta(k)) &= \frac{1}{a_o}A\sin(\delta(k)) + \beta B \\ -B\kappa &= \frac{1}{a_c}B + \beta A\sin(\delta(\kappa)), \end{aligned}$$

and from these equations I can find:

$$k\cot(\delta(k)) = \frac{1}{a_o} - \beta^2\left(\kappa + \frac{1}{a_c}\right)^{-1},$$

For small energies, k^2 is small and as κ can be written as a function of k^2, the Taylor series around zero for $k\cot(\delta(k))$ can be found:

$$k\cot(\delta(k)) = \frac{1}{a_o} - \beta^2\left(\frac{\sqrt{2mE^*}}{\hbar} + \frac{1}{a_c}\right)^{-1} + \beta^2\left[\left(\frac{2mE^*}{\hbar^2}\right)^{\frac{3}{4}} + \left(\frac{2mE^*}{\hbar^2}\right)^{\frac{1}{4}}\frac{1}{a_c}\right]^{-2}\frac{k^2}{2},$$

From the above expression the scattering length and effective range can be found to be

$$\frac{1}{a_{\text{eff}}} = \frac{1}{a_o} - \frac{\beta^2 a_c}{a_c\sqrt{2mE^*}/\hbar + 1} \tag{2.9}$$
$$R_{\text{eff}} = \beta^2 \left[\left(\frac{2mE^*}{\hbar^2}\right)^{3/4} + \left(\frac{2mE^*}{\hbar^2}\right)^{1/4} \frac{1}{a_c} \right]^{-2},$$

Here it is interesting that by coupling two zero-range potentials, I have obtained a system with a finite effective range. The result can also be compared to the expression for the energy close to threshold in equation (2.8). Expressing E_1 from a_{eff} yields the simple relation:

$$E_1 = -\frac{\hbar^2}{2m(-a_{\text{eff}})^2},$$

which resembles the expression for the energy of the bound state in section 2.1.1.

In figure 2.1 the scattering length is seen along with the energies of the bound states. In the limit where $a_{\text{eff}} \to -\infty$ the bound state approaches zero as one would expect. Another limit is $\beta \to 0$ where the system is decoupled and $k\cot(\delta(k)) \to \frac{1}{a_o}$ as in the simple system.

To investigate structure resonances I need an expression for the cross section. This is found from partial wave analysis to be[8]:

$$\sigma = 4\pi|f|^2 \quad , \quad f = \frac{1}{k\cot(\delta) - ik} \quad ,$$

when I only consider s-waves.

In the case of the zero-range model the cross section is thus

$$\sigma = 4\pi \left| \frac{1}{a_o} - \beta^2 \left(\kappa + \frac{1}{a_c}\right)^{-1} - ik \right|^{-2}, \tag{2.10}$$

The two expressions in equation (2.9) and equation (2.10) were used to make figure 1.2. It shows that this simple system gives rise to Feshbach resonances as a phenomenon, and that it is related to a real resonance structure in the cross section approaching zero energy. In the next section I will return to the description of data and how this model compares to full coupled channel calculations, but first I will finish the analysis of the coupled zero-range model.

2.2.3 Inelastic scattering

The last part of the energy range I will analyse is the case where $E > E^*$. In this region both u_o and u_c have positive energies, and there is a possibility of inelastic as well as elastic scattering. Here the approach with $\sin(\delta(k))$ gives equations that are complicated, and I will instead express my solutions as $e^{\pm ikr}$.

For the case of s-wave scattering, the solutions to the Schrödinger equation (2.5), are given as[3]:

$$u_o(r) = \frac{1}{2ik}\left(Se^{ikr} - e^{-ikr}\right), \qquad k = \frac{\sqrt{2mE}}{\hbar}$$
$$u_c(r) = \frac{1}{2i\kappa}Ae^{i\kappa r}, \qquad \kappa = \frac{\sqrt{2m\left(E - E^*\right)}}{\hbar},$$

As there is no incoming particle in the u_c channel, the part with $e^{-i\kappa r}$ is skipped here. Also note that S is related to the phase shift by definition $S \equiv e^{-2\eta}e^{2i\delta}$. Here the phase shift has become the complex number $\delta - i\eta$, because the problem is concerning inelastic- rather than elastic scattering.

Using the boundary conditions in equation (2.6) gives the linear system:

$$\tfrac{1}{2}S + \tfrac{1}{2} = \frac{1}{2ika_o}(S-1) + \frac{\beta A}{2i\kappa}$$
$$\tfrac{1}{2}A = \frac{A}{2i\kappa a_c} + \frac{\beta}{2ik}(S-1),$$

and solving it for S and A gives

$$S = \frac{\beta^2 a_o a_c + (ka_o i + 1)(\kappa a_c i - 1)}{\beta^2 a_o a_c + (ka_o i - 1)(-\kappa a_c i + 1)}$$
$$A = \frac{2i\beta a_o a_c \kappa}{\beta^2 a_o a_c + (ka_o i - 1)(-\kappa a_c i + 1)},$$

I would now like to find the cross section of both the elastic- and inelastic channels. For s-waves it gives[3]:

$$\sigma_{\text{elastic}} = \frac{\pi}{k^2}|S-1|^2$$
$$\sigma_{\text{inelastic}} = \frac{\pi}{k^2}\left(1 - |S|^2\right),$$

and in the case of the zero-range model:

$$\sigma_{\text{elastic}} = \frac{4\pi a_o^2(\kappa^2 a_c^2 + 1)}{1 + \beta^4 a_o^2 a_c^2 - 2\beta^2 a_o a_c + k^2 a_o^2 + 2\beta^2 a_o^2 a_c^2 k\kappa + k^2 a_o^2 \kappa^2 a_c^2 + \kappa^2 a_c^2}$$
$$\sigma_{\text{inelastic}} = \frac{4\pi\beta^2 a_o^2 a_c^2}{1 + \beta^4 a_o^2 a_c^2 - 2\beta^2 a_o a_c + k^2 a_o^2 + 2\beta^2 a_o^2 a_c^2 k\kappa + k^2 a_o^2 \kappa^2 a_c^2 + \kappa^2 a_c^2} \cdot \frac{\kappa}{k}, \tag{2.11}$$

Considering the limit where $E \approx E^*$ or $\kappa \approx 0$, it is easy to see that $\sigma_{\text{inelastic}} \propto \kappa \propto \sqrt{E}$ as it is expected for the cross section near the threshold energy[13]. This dependence is also seen in figure 2.2 in the lower insert.

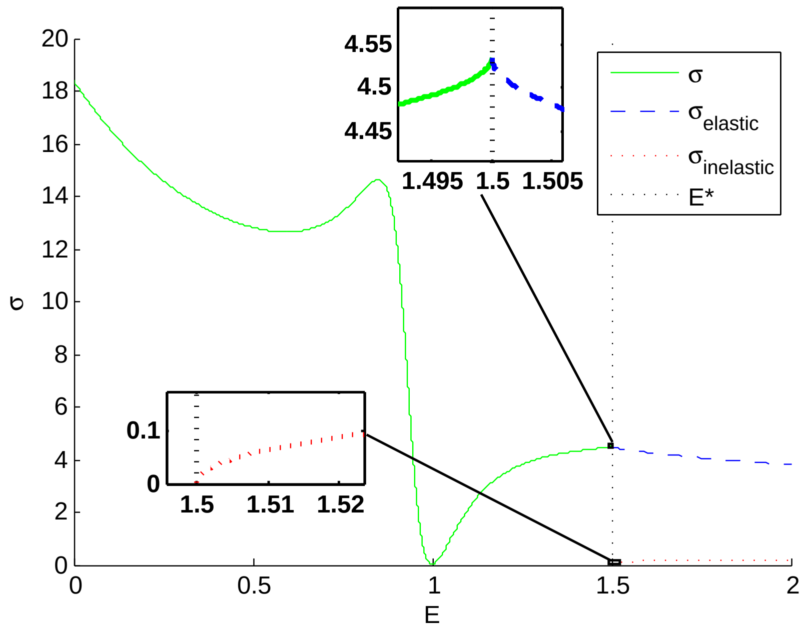


Figure 2.2: Cross section as a function of energy for $a_o = 1$, $a_c = -\sqrt{2}$, $m = 0{,}5$, $\hbar = 1$, $\beta = 0{,}3$ and $E^* = 1{,}5$.

Furthermore the elastic cross section must be continuous at $E = E^*$, and taking the limits from the right and left, this is indeed the case:

$$\sigma_{E>E^*} \to \frac{4\pi a_o^2}{1 + \beta^4 a_o^2 a_c^2 - 2\beta^2 a_o a_c + k^2 a_o^2}$$

$$\sigma_{E<E^*} = 4\pi \left| \frac{1}{a_o} - \beta^2 \left(\kappa + \frac{1}{a_c} \right)^{-1} - ik \right|^{-2} \to \frac{4\pi a_o^2}{(1 - \beta^2 a_o a_c)^2 + k^2 a_o^2},$$

On the contrary the derivative is not expected to be continuous, but rather the cross section is expected to have a Wigner cusp[13, 7] for $E = E^*$ as it is seen in the upper insert in figure 2.2. As the cross section has both non-zero right and left derivatives when differentiating with respect to κ it must have the functional form $c + d\,|E - E^*|^{1/2}$ + higher orders.

I have now analysed the zero-range potential in the whole energy range from bound states through scattering states with resonances to inelastic scattering. And the next chapter will concentrate on the ability of the model to describe Feshbach resonances.

— 3 —

Comparing the zero-range model to data and models

In the previous chapter I described and analysed the zero-range potential, and in this chapter I will relate it to observed diatomic systems. In doing this I will analyse the expression I have for the scattering length further to expose the properties of the divergence and I will take the formula that experimental data is normally fitted to and compare it to my expression. At last I will look at some systems that have been analysed with full channel calculations to compare the results.

As mentioned in chapter 1 there must be a difference between the magnetic moment for the open- and closed channel. This difference is called $\delta\mu = \mu_{\text{open}} - \mu_{\text{closed}}$ and the associated energy difference is $-\delta\mu B$. As $E^* = E_{\text{closed}} - E_{\text{open}}$ the relationship between the magnetic field B and E^* must be:

$$\delta\mu B = E^* - E_0^*$$

where E_0^* is the difference in energy at zero magnetic field.

3.1 Divergence of the scattering length

The key feature for a Feshbach resonance is the divergence of the scattering length as it is seen in figures 1.2, 1.3, and 2.1. To investigate this analytically I will need to study the expression for a_{eff} in equation (2.9):

$$\frac{1}{a_{\text{eff}}} = \frac{1}{a_o} - \frac{\beta^2 a_c}{a_c\sqrt{2mE^*}/\hbar + 1}, \tag{2.9}$$

Considering only the features of the system one might expect to find the divergence of the Feshbach resonance at

$$E^* = E_c = \frac{\hbar^2}{2ma_c^2},$$

where the closed channel would have a bound state in an uncoupled system if $a_c < 0$. Letting E^* approach E_c leads to $a_c\sqrt{2mE^*}/\hbar \to -1$ and thus the right side of equation (2.9) will diverge to infinity and the scattering length will approach zero.

To find the divergence, the right side should instead approach zero and this is fulfilled when:

$$\frac{1}{a_o} - \frac{\beta^2 a_c}{a_c\sqrt{2mE^*}/\hbar + 1} = 0 \Rightarrow E^* = \left(\beta^2 a_o - \frac{1}{a_c}\right)^2 \frac{\hbar^2}{2m},$$

It is seen that the divergence is shifted through the coupling between the open and closed channels, as it is also noted in [2].

3.2 Methods to find the zero-range parameters

I will now find different ways to relate the zero-range model to

$$a = a_{\text{bg}}\left(1 - \frac{\Delta}{B - B_{\text{res}}}\right), \tag{1.1}$$

The approaches I will investigate are a geometrical, an approximative and a numerical approach which all have some advantages and disadvantages.

3.2.1 Geometrical approach

From the analysis of the scattering length in section 3.1 I have some geometric characteristics of a_{eff}. As equation (1.1) also have a clear geometrical interpretation as shown in figure 1.3, I would like to relate them to each other.

As a_{bg} is the off resonant value of the scattering length, I can find it for the zero range model by letting $E^* \to \infty$. In this limit equation (2.9) gives $a_{\text{eff}} = a_o$.

To find Δ and B_{res} I will use the results from section 3.1. The sign of Δ tells on what side of B_{res} the zero crossing is and it can be found as:

$$\Delta = \frac{1}{\delta\mu}\left(E_c^* - E_{\text{resonant}}^*\right) = \frac{\hbar^2}{2m\delta\mu}\left(\frac{2\beta^2 a_o}{a_c} - \beta^4 a_o^2\right), \tag{3.1}$$

Lastly B_{res} is the resonant value of the magnetic field, and it can be found to be:

$$B_{\text{res}} = \frac{1}{\delta\mu}\left(E_{\text{resonant}}^* - E_0^*\right) = \frac{\hbar^2}{2m\delta\mu}\left(\beta^2 a_o - \frac{1}{a_c}\right)^2 - \frac{E_0^*}{\delta\mu}, \tag{3.2}$$

It is now possible to calculate the parameters in equation (1.1) if the zero-range model is known. As the data from experiments and other theoretical works give equation (1.1) it is useful to have the zero-range model expressed in a_{bg}, Δ, and B_{res}.

The easiest to find is $a_o = a_{\text{bg}}$ as I have already argued, since it is the off-resonant value of the scattering length. As the zero-range model contains E^*, this also needs to be found from the magnetic field:

$$E^* = E_0^* + B\delta\mu,$$

Solving equation (3.1) and equation (3.2) for β^2 and a_c gives two solutions. As a_c must be negative to have a bound state in the uncoupled closed channel I choose this solution.

$$\beta^2 = \frac{1}{a_o}\sqrt{\frac{2m}{\hbar^2}\left(B_{\text{res}}\delta\mu + E_0^*\right)}\left(1 - \sqrt{1 + \frac{\Delta\delta\mu}{B_{\text{res}}\delta\mu + E_0^*}}\right) \tag{3.3}$$

$$\frac{1}{a_c} = -\sqrt{\frac{2m}{\hbar^2}\left(B_{\text{res}}\delta\mu + E_0^*\right)\left(1 + \frac{\Delta\delta\mu}{B_{\text{res}}\delta\mu + E_0^*}\right)}, \tag{3.4}$$

Now all the quantities in the zero-range model can be found if you know the position of the Feshbach resonance, its width, the difference in magnetic moments, the reduced mass of the system, and the difference in energy of the open- and closed channels at $B = 0$.

3.2.2 Approximative approach

The geometrical approach above is quite intuitively clear and it uses the characteristics of a Feshbach resonance very directly. On the downside it lacks some mathematical rigidity and it does not show that the scattering length from the zero-range model can actually be written in the form shown in equation (1.1).

These two disadvantages can be solved by rewriting equation (2.9) and making an approximation:

$$\begin{aligned} a_{\text{eff}} &= \frac{a_o}{1 - \frac{a_c a_o \beta^2}{a_c\sqrt{2mE^*}/\hbar + 1}} \\ &= a_o\left(1 + \frac{a_c a_o \beta^2}{1 + a_c\sqrt{2mE^*}/\hbar - a_o a_c \beta^2}\right), \end{aligned} \tag{3.5}$$

At the Feshbach resonance where $B \to B_{\text{res}}$ the denominator must go to zero and as the denominator is analytic it can be expanded in a Taylor series. To substitute B for E^* I use the relation $E^* = \delta\mu B + E_0^*$ and a first order expansion gives:

$$1 + a_c\sqrt{2m\left(\delta\mu B + E_0^*\right)}/\hbar - a_o a_c \beta^2 = \frac{a_c m \delta\mu}{\hbar\sqrt{2m\left(\delta\mu B_{\text{res}} + E_0^*\right)}}\left(B - B_{\text{res}}\right), \tag{3.6}$$

It is now seen that equation (3.5) has the form of equation (1.1) in a first degree approximation.

As for the geometrical approach the position of the resonance is

$$B_{\text{res}} = \frac{\hbar^2}{2m\delta\mu}\left(\beta^2 a_o - \frac{1}{a_c}\right)^2 - \frac{E^*}{\delta\mu}, \tag{3.2}$$

and by comparing the equations (1.1) and (3.5) and using equation (3.2) to replace B_{res}, Δ can be found to be:

$$\Delta = \frac{\hbar^2}{m\delta\mu}\left(\frac{a_o\beta^2}{a_c} - \beta^4 a_o^2\right), \tag{3.7}$$

This expression only differs from the one obtained from geometric considerations in equation (3.1) by a factor of 2 in the last term. For weak coupling the last term is very small and the two expressions give almost the same.

As in the geometrical approach I need to find β and a_c from Δ and B_{res}. This can be done by solving equation (3.2) and equation (3.7):

$$\beta^2 = -\frac{\Delta\delta\mu}{\hbar a_o\sqrt{2\left(\delta\mu B_{\text{res}} + E_0^*\right)/m}} \tag{3.8}$$

$$\frac{1}{a_c} = \beta^2 a_o - \sqrt{\frac{2m}{\hbar^2}\left(\delta\mu B_{\text{res}} + E_0^*\right)}, \tag{3.9}$$

It can now be shown that the two methods give the same if the resonance is narrow so that $\Delta << B_{\text{res}}$. In this limit, equation (3.3) can be approximated since $\frac{\Delta\delta\mu}{B_{\text{res}}\delta\mu+E_0^*} << 1$ and it gives the expression in equation (3.8) as one would expect.

As a_c can be found from the expression for B_{res} and β^2 it does also reduce to the same expression in both cases if $\Delta << B_{\text{res}}$.

One weakness of both the geometrical and the approximative method is that E_0^* can not be found as the system is underdetermined. Still it is possible to see some trends from the above expressions.

The first interesting feature is that $\Delta << E_0^*$ gives the same limit as $\Delta << B_{\text{res}}$ and thus the geometrical method is better for fields close to B_{res} when E_0^* is large. The second thing to notice is that the remainder (R) in the Taylor expansion at a magnetic field B can be estimated by[11]:

$$|R| \leq \frac{a_c\delta\mu^2\Delta^2\sqrt{m}}{4\sqrt{2}\hbar((\delta\mu B)_{\text{min}} + E_0^*)^{3/2}}, \qquad (\delta\mu B)_{\text{min}} = \min\{\delta\mu B, \delta\mu B_{\text{res}}\},$$

This means that the approximative method will also become better when E_0^* is large.

3.2.3 Numerical approach

A last approach that I will not treat as thoroughly as the two first, is a numerical fit of the expression for a_{eff} from the zero-range model to the data available. I have used the Curve Fitting Toolbox included with MatLab and it uses a least squares method to find the best fit.

The strength of this method is that it can find not only a_o, a_c, and β, but also E_0^* if it has a local minima. The weakness is that it will depend on the set of points which is used for the fitting. E.g. using a uniform distribution of the points will not give as much weight to the resonance as one might want.

Some of these problems can be solved by combining the numerical method with some of the analytical results. In the next section I will show some examples of numerical fits along with the two other methods compared to available data.

Table 3.1: Data from [2]. Note that [2] uses the opposite sign convention to me for scattering length. I have used mine here..

atom(s)	B_{res}(G)	Δ(G)	a_{bg}/a_0	$\delta\mu/\mu_B$
^{6}Li	834,1	-300	1405	2,0
^{6}Li	543,25	0,1	-60	2,0
^{133}Cs	800	87,5	-1940	1,75
^{40}K ^{87}Rb	546,9	$-3{,}10$	189	2,30
^{4}0K	202,1	8,0	-174	1,68

3.3 Fitting to data

Feshbach resonances in cold atoms have been investigated both theoretically and experimentally through the last fifteen years, and [2] have collected some of the results in a table at the end of their review. In the following I will try to find the parameters of the zero-range model for the Feshbach resonances listed in table 3.1 using the various methods developed above.

3.3.1 Geometrical and approximative approach

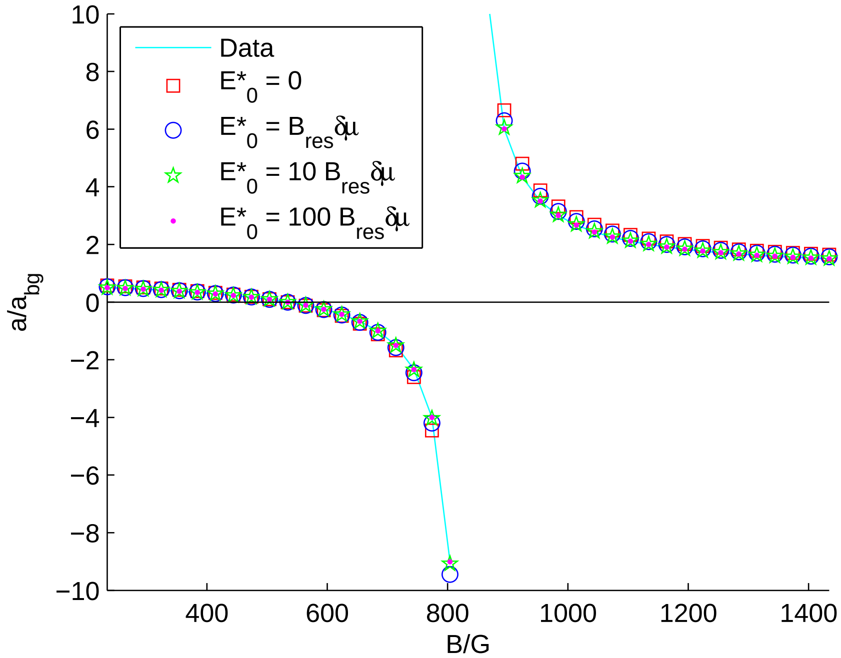
For the first two methods, all the quantities I need to do the calculations are available except the difference in energy between the open- and the closed channels at zero magnetic field, E_0^*. The systems I consider here are atomic states and all of the difference in energy often comes from the Zeeman effect. Thus it is a reasonable assumption to choose $E_0^* = 0$.

The remarks in section 3.2.2 shows that the model will fit better for higher values of E^*, but as it is seen in figure 3.1 the model fits the data quite well for all values of E_0^*. The dependence on E^* is most pronounced for the geometrical method whereas the approximative method shows almost no difference at all.

To demonstrate that the zero-range model can adapt to different types of resonances I have calculated the zero-range parameters with both methods for all the systems in table 3.1 and the results are seen in table 3.2.

Along with the parameters, the root mean square error was calculated for the set of points from figure 3.1. It is seen that the worst fit is for ^{6}Li at $834,1$G which was considered a quite good fit when looking at figure 3.1. The broad resonance for ^{6}Li at $834,1$G is one of the broadest Feshbach resonances known and it does also show some difference between the two models, but for the two narrow resonances in ^{6}Li at $543,25$G and ^{40}K ^{87}Rb the two models both give excellent results. For ^{133}Cs and ^{40}K the results show a tiny difference, but are still very good and when classifying resonances these are considered wide.

As it is clear from figure 3.1 the approximative method gives a better approximation close to B_{res} than the geometrical as it should be. The advantage for the geometrical method is that it crosses $a = 0$ at the right magnetic field. In table 3.3



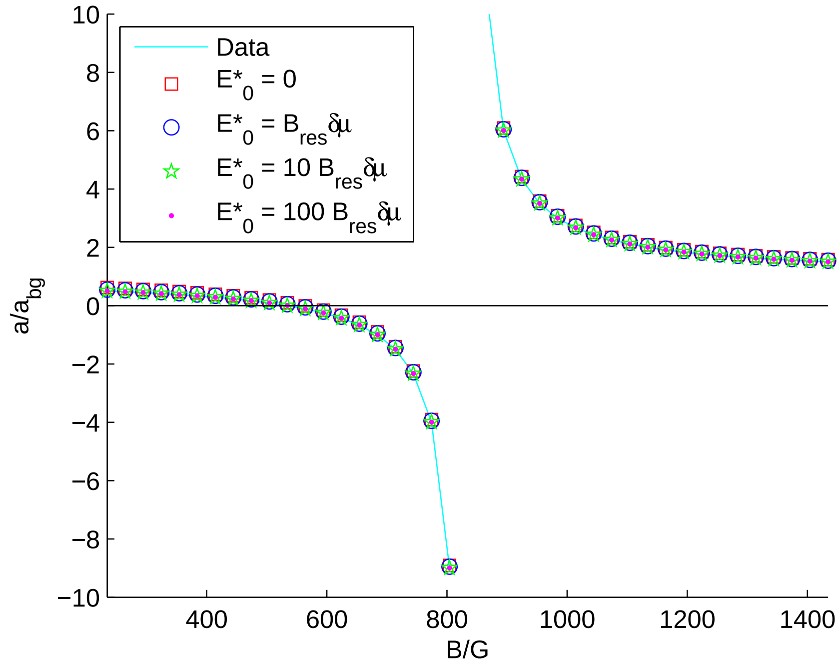


Figure 3.1: The upper panel shows a_{eff} for different choices of E_0^* for the geometrical method and the lower panel for the approximative method. The used Feshbach resonance is ^{6}Li at $B_{\text{res}} = 834,1\text{G}$.

Table 3.2: Parameters for the zero-range model. All calculations are done with $E_0^* = 0$ and the results are in atomic units if not stated otherwise. The root mean square error is found for a/a_{bg} and the points shown in figure 3.1.

atom(s)	^{6}Li	^{6}Li	^{133}Cs	^{40}K ^{87}Rb	^{40}K
B_{res}(G)	$834,1$	$543,25$	800	$546,9$	$202,1$
a_o	1405	-60	-1940	189	-174
Geometric method					
$\beta(10^{-3})$	$2,98$	$0,278$	$2,71$	$1,57$	$2,86$
a_c	$-20,0$	$-19,9$	$-3{,}53$	$-6,13$	$-13,5$
RMSE	$0,327$	$1{,}4 \cdot 10^{-4}$	$0,078$	$0,0043$	$0,029$
Approximative method					
$\beta(10^{-3})$	$2,82$	$0,278$	$2,75$	$1,57$	$2,87$
a_c	$-19,6$	$-19,9$	$-3,53$	$-6,13$	$-13,5$
RMSE	$0,093$	$4{,}6 \cdot 10^5$	$0,027$	$0,0014$	$0,010$

Table 3.3: Δ gives the magnetic field where $a = 0$ relative to B_{res}. This field is calculated in the last column from the parameters found with the approximative method in table 3.2. The actual value of Δ is also shown.

atom(s)	B_{res}(G)	Δ(G)	$\Delta_{approximation}$
^{6}Li	834,1	-300	-273
^{6}Li	543,25	0,1	0,100
^{133}Cs	800	87,5	89,9
^{40}K ^{87}Rb	546,9	$-3{,}10$	$-3{,}10$
^{4}0K	202,1	8,0	8,08

I have computed the widths from the approximative method. Again the narrow resonances give excellent results while the very broad resonance in ^{6}Li and the resonances in ^{133}Cs and ^{40}K give a small error. This means that if the resonance is characterised in an experiment by the magnetic field of the divergence and of the zero crossing, it would be better to use the geometrical- than the approximative method to find the parameters in the zero-range model.

3.3.2 Numerical approach

To compare to the numerical method I have concentrated on the broad ^{6}Li resonance as it seems to give the most problems for the two other methods. In figure 3.2 equation (1.1) has been evaluated in a set of uniformly spaced points between $B_{res} - 2\Delta$ and $B_{res} + 2\Delta$ and four fits to the points are shown. The obtained parameters are seen in table 3.4 along with the initial guesses.

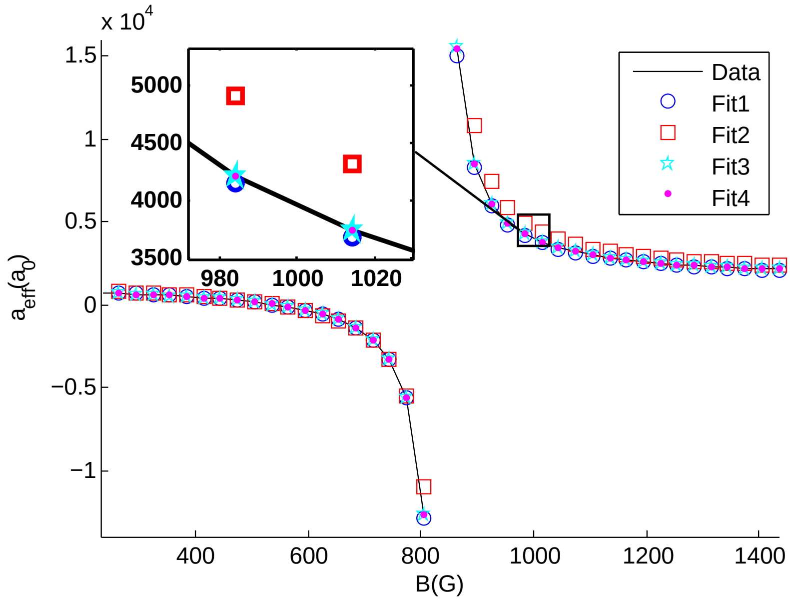


Figure 3.2: The four fits from table 3.4. The insert shows a magnification of two of the fitted points.

Table 3.4: Initial guesses and results in atomic units for numerical fitting of the resonance at $834,1$G for ^{6}Li. * means that the value has not been varied in the fitting process. ** means that the value has been calculated with the approximative approach.

		Initial guesses		
Fit	1	2	3	4
a_o	1405	1405*	1405*	1405*
a_c	-20	-20	$-0,0029302764747$	**
β	$0,003$	$0,003$	$3{,}815\,781\,291 \cdot 10^{-5}$	**
E_0^*	0	0	$10,64808510638$	$1,34$
		Fitted values		
Fit	1	2	3	4
a_o	1255	1405*	1405*	1405*
a_c	$-20,0388$	-20	$-0,0029302764747$	$-0,00826022589$**
β	$0,003148$	$0,003$	$3{,}815\,781\,291 \cdot 10^{-5}$	$6{,}406\,563\,4 \cdot 10^{-5}$**
E_0^*	$6{,}9 \cdot 10^{-10}$	$4{,}62 \cdot 10^{-10}$	$3{,}815\,781\,291 \cdot 10^{-5}$	$1,34$
RMSE	$100,4$	1417	$72,94$	$3{,}055 \cdot 10^{-5}$

The first fit is the expression for a_{eff} from equation (2.9) with the initial guesses I found for $E_0^* = 0$ from the other approaches. The fit is quite good as the root mean square error (RMSE) is a lot less than the asymptotic value of $a \approx 1000$ Bohr radii, but the result shows two problems. First, the asymptotic behaviour is not the right one as $a_o = 1255$. Second, it was not expected that $E_0^* \approx 0$ would give the best fit and as $B_{\text{res}}\delta\mu \approx 10^{-7}$a.u., a value of $6{,}9 \cdot 10^{-10}$ is essentially zero. The first problem can be solved setting a_o to the value of 1405 Bohr radii which it must have. This gives the second fit, but now the RMSE is quite high. From the figure it is also obvious that this fit is not good.

A way to solve both problems is to give new initial guesses. Using the approximative method to calculate a_c and β for $E_0^* = 10,648$a.u. gives the third fit. Here the RMSE is very low as expected, but the fitted parameters are indistinguishable from the initial guesses and it is unlikely that I have been that lucky when picking E_0^*. Furthermore the algorithm fails if E_0^* is given the initial guess $10,65$a.u. which means that it relies totally on a good initial guess. As this can only be obtained from the other two methods this numerical fit does not have much value in itself.

The advantage of the numerical method should be that it can find E_0^* and by using the formulas from the approximative approach in section 3.2.2 the scattering length can be expressed directly from the magnetic field and E_0^*. This makes it possible to find the value of E_0^* which gives the best fit in the approximative approach.

Again the fitting procedure does not change my initial guesses much, but by changing the guesses I can find a minimum of the RMSE at $E_0^* = 1{,}34$a.u.. This value is more than 10^6 times the values of B around the resonance and thus it confirms the statement that large values of E_0^* gives a good fit. The reason that higher values give larger RMSE is that the limit for precision in Matlab is reached and numerical errors start to give worse results.

As uniformly spaced points in B might not be the best choice I have tried uniformly spaced points in a to give more weight to the resonance, but it did not improve the results significantly.

To conclude on the numerical fitting, the method described here is not that useful. Besides the weakness of only fitting to the data in the points chosen it relies heavily on the initial guesses I give. Using a better numerical method it would probably be possible to make the fitting less dependent on the initial guesses, but this is beyond the scope of this project.

3.4 Comparing to full coupled channel calculations

In the previous section I showed that the zero-range model has the right behaviour around a Feshbach resonance in order to describe it.

I will now compare some of the results of the zero-range model to full coupled channel calculations. The three Feshbach resonances I will investigate are ^{6}Li at

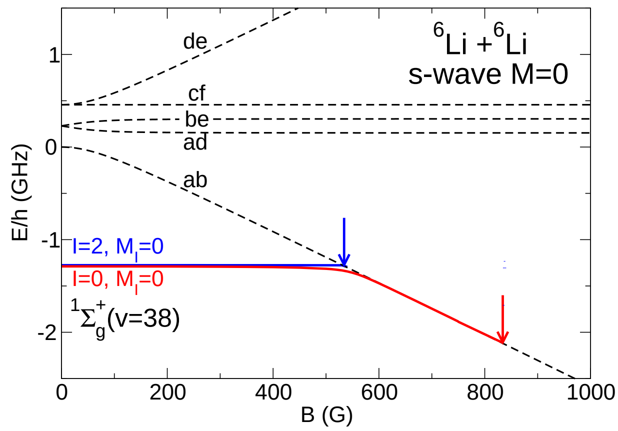


Figure 3.3: The letters a, b, c, d, e, and f are the different atomic levels in the ^{6}Li atom. a corresponds to quantum numbers $f = 1/2$ and $m_f = 1/2$ and b to $f = 1/2$, $m_f = -1/2$. The solid red and blue lines are the two last bound states from a coupled channel calculation on $^6Li_2$. The two arrows indicate the positions of the Feshbach resonances. Reprinted from [2], figure 9.

$543,25$G and $834,1$G and ^{40}K at $202,1$G. The parameters of the zero-range model when using the geometrical and approximative methods are listed in table 3.2. For ^{6}Li $a_c \approx -20$ for these two resonances and it corresponds to a bound state in the uncoupled closed channel at an energy of $E_c = 2{,}3 \cdot 10^{-7}$a.u. $= 1,5$GHz. This can be compared to the values given by [2]. The energies of the different channels are shown in figure 3.3 as well as the bound states with highest energy.

I have chosen $E_0^* = 0$ in order to find the parameters in table 3.2 for the zero-range model. For the narrow resonance this is obviously a quite good approximation, as the open channel then corresponds to the ab channel of figure 3.3 and the closed channel corresponds to a channel without magnetic moment, but with a bound state at $E_c \approx 1,5$GHz. This is roughly the same as the binding energy of the bound state in figure 3.3 which is $\approx 1,38$GHz. For the other Feshbach resonance it is less obvious from figure 3.3 that it is a good idea, as the energy of the bound state is not constant until it disappears. Though, looking in table 3.1 shows that $\Delta = -300$G, and this means that the zero-crossing for the scattering length is at $B = 534,1$G. According to the analysis of the scattering length in section 3.1 this is exactly the value of the magnetic field where $E^* = E_c$ and the bound state crosses the threshold energy of the open channel. With this in mind it is easily understood that $E_c \approx 1,5$GHz again.

Both of the energies are a little too high as $\delta\mu$ is supposed to be constant in B. As seen in figure 3.3 it is not the case for low values of B and extrapolating the slope to $B = 0$G gives the missing $\approx 0{,}15$GHz.

In order to obtain the best fit to the points a high value of E_0^* is favoured, but in this system it makes more physical sense to use $E_0^* = 0$. In a similar way a reasonable value can probably be found for other systems. Furthermore equation (1.1) might not fit experimental data perfectly and equation (2.9) could prove to be better.

For the two resonances in ^{6}Li [2] has also calculated $\sin^2(\delta(k))$ as a function of B and E which is seen in figure 3.4 and 3.6 along with the bound state energies. Doing the same calculation with the zero-range model gives figure 3.5 and 3.7. In both cases $\sin^2(\delta(k))$ gives similar results and this means that the expression for the cross section in equation (2.10) can be used for these systems. The zero-range model also gives almost the same results as the full coupled channel calculation for the bound states. The broad resonance has a large domain of universal behaviour while the narrow resonance has an extremely small universal domain[2]. This is reflected in the fact that the universal bound state energy from equation (2.8) gives a good approximation at $834,1$G while the approximation is only useful for an extremely small fraction of the width at $543,25$G.

The last resonance which is investigated with some details in [2] is for ^{40}K at $202,1$G. $\sin^2(\delta(k))$ is plotted again in figure 3.8 and the corresponding calculation from the zero-range model is found in figure 3.9. Note that the range of energy that I try to apply the model to is now 100 times larger than it is the cases in figure 3.5 and 3.7. For low energies the two plots are similar while they show different behaviour for energies about E_{vdw} which is marked on figure 3.8. E_{vdw} is the typical energy scale for the van der Wall's potential and in this energy range the short range behaviour of the potential begins to matter. With this in mind it is not surprising that the zero-range model gives a different result as it is fitted to the scattering length which only contains information about low energies.

The two dashed lines on figure 3.8 show the bound states without coupling and the two solid lines show the avoided crossing. The bound states in the zero-range model in figure 3.9 show the right overall behaviour, but they are shifted to slightly higher energies than in figure 3.8. Their assymptotic values reflect the background scattering length of -174 which gives a bound state with energy $-3,0$MHz, while the asymptotic value in figure 3.8 is $E_{-1} \approx -9$. As for figure 3.5 it is a broad open channel dominated resonance and hence the universal bound state gives a good approximation as the dashed line shows in figure 3.9.

One of the limitations of the simple system I have used here is that it can not model several resonances close to each other. An example is actually seen in figure 3.1 where the resonance at $B_{\text{res}} = 543,25$G should be visible. In this case however it does not change much for most of the B-values as the missing resonance is extremely narrow, but for other systems it can be crucial. Still the above comparisons show that the zero-range model does not only give an excellent description of the scattering length, but also describes the cross section and the bound state energy correctly for low energies in some systems.

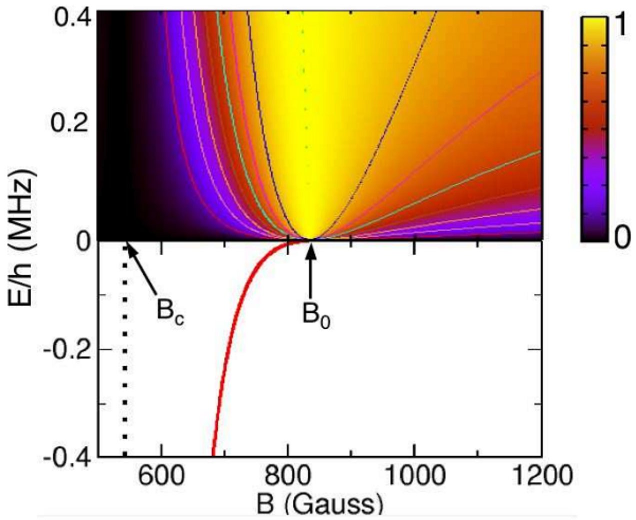


Figure 3.4: Properties of bound- and scattering states of ^{6}Li in the ab channel. The colour gradient shows the value of $\sin^2(\delta(k))$. B_0 marks the position of the Feshbach resonance at $834,1$G and B_c marks the position of the Feshbach resonance at $543,25$G. Reprinted from [2], figure 10.

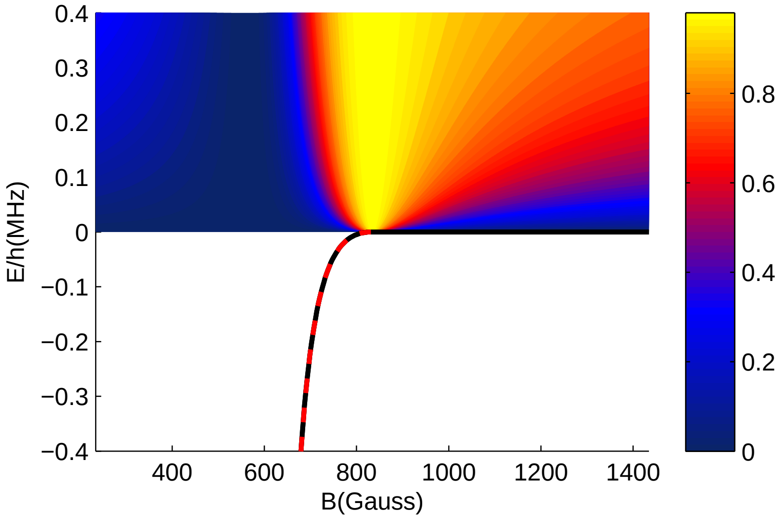


Figure 3.5: Properties of bound- and scattering states of ^{6}Li in the ab channel calculated with the zero-range model for the Feshbach resonance at $834,1$G. The colour gradient shows the value of $\sin^2(\delta(k))$. The solid line shows the energy of the bound state calculated numerically from equation (2.7). The dashed line is the universal bound state energy from equation (2.8). In the shown resolution they coincide.

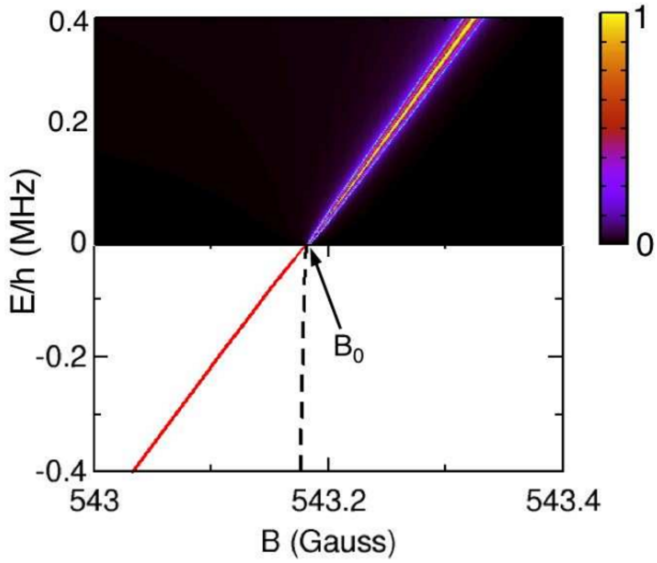


Figure 3.6: Properties of bound- and scattering states of ^{6}Li in the ab channel. The colour gradient shows the value of $\sin^2(\delta(k))$. B_0 marks the position of the Feshbach resonance at $543,18$G which is in excellent agreement with the experimentally found value of $543,25$G. The solid red line shows the energy of the bound state calculated with a coupled channel method, whereas the dashed line shows the universal bound state energy. Reprinted from [2], figure 11.

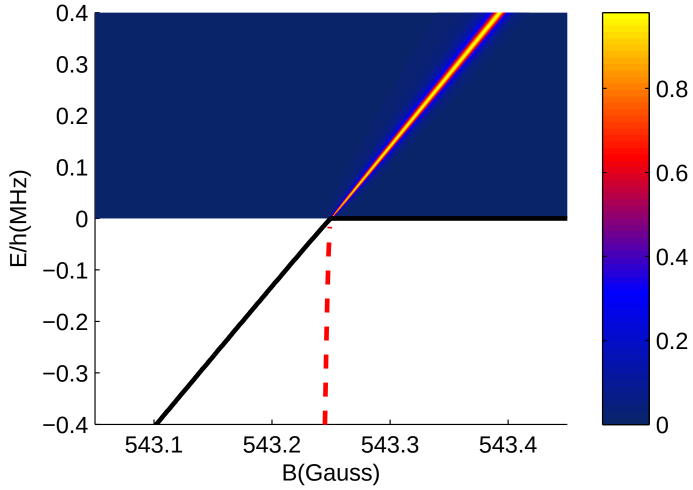


Figure 3.7: Properties of bound- and scattering states of ^{6}Li in the ab channel calculated with the zero-range model for the Feshbach resonance at $543,25$G. The colour gradient shows the value of $\sin^2(\delta(k))$. The solid line shows the energy of the bound state calculated numerically from equation (2.7). The dashed line shows the universal bound state energy from equation (2.8).

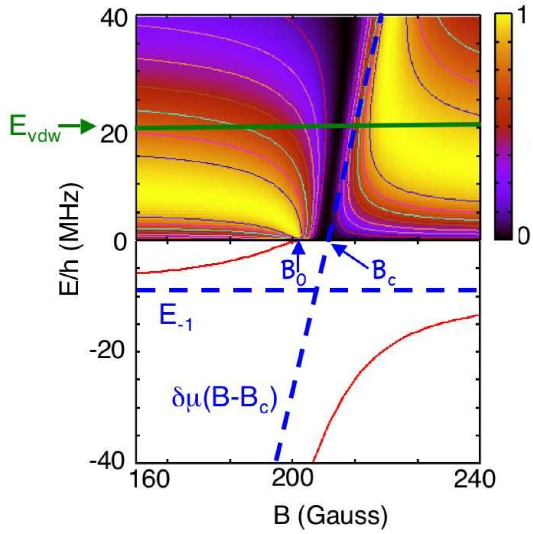


Figure 3.8: Properties of bound- and scattering states of ^{40}K for the Feshbach resonance at 202, 1G. The colour gradient shows the value of $\sin^2(\delta(k))$. B_0 marks the position of the Feshbach resonance at 202,1G. The solid red line shows the energy of the bound state calculated with a coupled channel method. The dashed lines show the "bare" bound states. Reprinted from [2], figure 13.

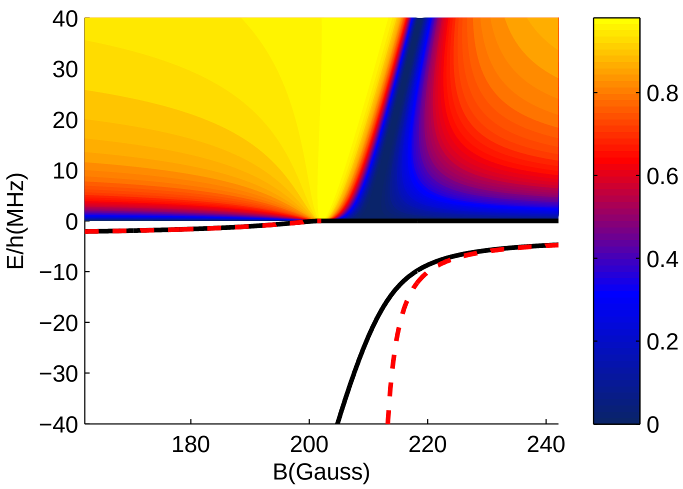


Figure 3.9: Properties of bound- and scattering states of ^{40}K for the Feshbach resonance at 202, 1G calculated with the zero-range model. The colour gradient shows the value of $\sin^2(\delta(k))$. The solid line shows the energy of the bound state calculated numerically from equation (2.7). The dashed line shows the universal bound state energy from equation (2.8).

— 4 —
Conclusion

The analysis of the zero-range model in this project has shown that it is capable of modelling Feshbach resonances and this has been demonstrated for various real systems. Furthermore two different analytical approaches to find the parameters of the zero-range model have been developed. A strictly approximative method which gives a mathematical rigid base to the theory and a geometric method which gives the possibility to conserve the exact position of the zero-crossing. Furthermore a numerical method using Curve Fitting Toolbox in Matlab has been considered, but it relied heavily on the initial guesses and thus demands a better algorithm in order to be really useful. It should be remembered though that the used points were synthetically created for the purpose and real experimental data might give different results.

Lastly, the results for the zero-range method have been compared to a full coupled channel calculation with great success for low energies. some deviation is seen for energies typical of the van der Wall's potential, but for lower energies the model show fine agreement. This is also consistent with the initial assumption that the de Broglie wavelength must be smaller than the range of the potential in order to approximate it with a zero-range potential.

As the use of Feshbach resonances develop in ultra cold atomic physics the need for simple models will grow and conceptually the one treated here is one of the simplest.

One of the analytical extensions that could be made for the zero-range model would be to investigate the wave functions for the bound states. These must be a superposition of the open- and closed channel components and their coefficients will give information about to which extent the resonance can show universal behaviour[2].

Another path could be to expand the theory to describe more complex systems with three, four, or many interacting atoms.

One thing is for sure. As the zero-range potential is the simplest possible potential except for $E = 0$ it will also in the future attract attention in low energy scattering theory as well as in many other branches of physics.

Bibliography

[1] B.H. Bransden and C.J. Joachain. *Physics of Atoms and Molecules*. Pearson Education Limited, second edition, 2003.

[2] C. Chin, R. Grimm, P. Julienne, and E. Tiesinga. Feshbach Resonances in Ultracold Gases. *ArXiv e-prints*, December 2008.

[3] Ashok Das and Adrian C. Melissinos. *Quantum Mechanics - a Modern Introduction*. Gordon and Breach Science Publishers S.A., 1986.

[4] U. Fano. Effects of configuration interaction on intensities and phase shifts. *Phys. Rev.*, 124(6):1866–1878, Dec 1961.

[5] Herman Feshbach. Unified theory of nuclear reactions. *Annals of Physics*, 5(4):357 – 390, 1958.

[6] Herman Feshbach. A unified theory of nuclear reactions. ii. *Annals of Physics*, 19(2):287 – 313, 1962.

[7] R. C. Forrey, N. Balakrishnan, V. Kharchenko, and A. Dalgarno. Feshbach resonances in ultracold atom-diatom scattering. *Phys. Rev. A*, 58(4):R2645–R2647, Oct 1998.

[8] David J. Griffiths. *Introduction to Quantum Mechanics*. Pearson Prentice Hall, second edition, 2005.

[9] Nicolai Nygaard. Low energy scattering theory, April 2010. Notes for the course Quantum Gases at Aarhus University.

[10] P. J. Siemens and A. S. Jensen. *Elements Of Nuclei: Many-body Physics With The Strong Interaction*. Addison-Wesley Pub. Co., 1987.

[11] H. Stetkær, K. Thomsen, and C. Tønnesen-Friedman. *Indledning til Matematisk Analyse II*. Institut for matematiske fag, Aarhus Universitet, 2002.

[12] William C. Stwalley. Stability of spin-aligned hydrogen at low temperatures and high magnetic fields: New field-dependent scattering resonances and predissociations. *Phys. Rev. Lett.*, 37(24):1628–1631, Dec 1976.

[13] E. P. Wigner. On the Behavior of Cross Sections Near Thresholds. *Physical Review*, 73:1002–1009, May 1948.