Energy spectrum of two atoms interacting via a short-range potential in higher partial waves

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By

YI LIANG, B. Sc., M. Sc.

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AUTHOR:	Yi Liang, B. Sc. Zhejiang University Hangzhou, P. R. China, 2004
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Abstract

We study a two-atom system interacting via a short-range potential, and trapped by an optical lattice, in higher partial waves. These atoms may be made to interact strongly near a Feshbach resonance. Our main purpose is to find the relation between energy levels of the system and the scattering parameters in higher partial waves. We check our analytical results by numerical calculations and find the conditions under which this method is applicable for the d-wave.

To my family.

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Table of Contents

List of Figures

List of Tables

Chapter 1

Introduction

Ultracold atoms are maintained at micro to nano Kelvin temperatures. The quantum-mechanical properties become dominant at these temperatures and the atoms obey quantum laws. Nevertheless, ultra-cold atoms may be trapped magnetically, or in optical lattices [1]. The dimensionality of the trap, and the interaction between the atoms may be controlled. Ultracold physics has enormous prospects in many fields of physics. Hence abundant research has been done in this area, especially after the discovery of Bose-Einstein condensation (BEC) [[2], [3]].

After the theoretical suggestion [4] and the experimental realization [5] for systems of ultracold gases in optical lattices, these have become popular research topics [1]. An optical lattice is a periodic intensity pattern formed by the interference of counter-propagating laser beams. The electric fields of the lasers induce an electric dipole moment in the atom, the atoms can be trapped by the optical lattice. In these systems the trap potential can be approximated by a harmonic potential, and the two-particle interaction strength may be tuned with high precision [6]. All these properties have made them ideal model systems for low-temperature physics.

We have studied a system of ultracold atoms trapped in an optical lattice in this thesis. At low temperatures, scattering parameters such as scattering length and effective range determine the properties of the system, such as the stability of Bose-

Einstein condensates, and the formation of degenerate Fermi gases. Because of the importance of these scattering parameters in understanding collisions between ultracold atoms, we study the relation between the energy levels of trapped atoms and the shape-independent scattering parameters for various partial waves. Since the system consists of dilute ultracold atoms, we study the two-body scattering, as being more important than 3-body collisions.

Abundant studies have been done in this area. A semiclassical approximation to scattering length for s-wave scattering has been derived by Gribakin and Flambaum in 1993 [7] for the inverse law potential. Flambaum *et al.* [8] and Gao [9] showed that there is an approximate relationship between the scattering length and the effective range, given a power-law potential. In a very dilute gas, two particles cannot see the details of the potential, but only sample the extreme tail. Hence it is proper to use any short-range potential that can reproduces the shape-independent scattering parameters. For slow particles at low temperatures only a few partial waves need to be considered. Hence to determine the scattering length, we need to study the short-range interaction between these atoms.

By sweeping a static magnetic field near a Feshbach resonance(FR), which we discuss in Chapter 4, the interaction between atoms may be significantly enhanced in a particular partial wave [10]. Hence it is now possible to achieve strong correlations between atoms even though these particles are very dilute. Recently substantial theoretical and experimental work on the "dressed state" have been done. The researches are first on s-wave Feshbach resonance between two Fermions of different internal hyperfine spins [[11], [12]]. Yip has extended the study to two identical fermions under a p-wave Feshbach resonance [13]. Yip also got a general expression for the energy spectrum in a unpublished paper [14]. It was stated that the energy spectrum is only valid for $l < 2$ case Feshbach resonance.

Chapter 2 is a review of standard scattering theory. An effective-range expansion for two-body scattering is given. We also review the conditions for the validity of this expansion. In Chapter 3 we discuss the formula for the scattering length for particles in a model potential. The model potential has the $\sim 1/r^6$ form at large distances, and is cut off at short distances by a hard core. The expression for s-wave scattering length is given by Pethick and Smith [15]. We extend their result to $l = 1$. In Chapter 4 we discuss a system of two atoms trapped in a harmonic potential near a Feshbach resonance. These atoms could, under appropriate conditions, be bosonic or fermionic. We argue that even though the scattering parameters may not exist for a long range $1/r^6$ interatomic potential, there is a relation between these parameters and the energy levels for higher partial waves, in the presence of coupling to a Feshbach resonance. Using a method first formulated by Jonsell[16], we obtain the energy spectrum for a given l. Yip's result for p-wave resonance is verified, and extended to higher partial waves. The d-wave energy spectrum is checked by direct numerical integration of the Schrödinger equation. The analytical formula is not accurate for the ground state in a narrow band across the resonance as Yip stated, and we explain this limitation in Appendix A. At the end of this thesis are two appendices. Appendix A shows why our method is valid in deducing the result when $l = 2$, and why it is inapplicable in a narrow band at resonance for the ground state. Appendix B contains the formulas of scattering length and effective range for an attractive square-well potential, as derived by Prof. Akira Suzuki.

Chapter 2

Effective Range Expansion

This whole chapter is a review of standard material for the quantum scattering problem. The matter we review here is crucial for our discussion in the following chapters.

In a central field $U(r)$ of a fixed center of force, the problem of two-body elastic collision amounts to the scattering of a single particle with a reduced mass. In this chapter we use a coordinate system in which the center of mass is at rest, and m will denote the reduced mass of the colliding particles.

2.1 general theory for scattering

The scattering wave function corresponding to a plan wave incident along the z direction, has an asymptotic form

$$\psi \approx e^{ikz} + f_k(\theta)e^{ikr}/r, \tag{2.1}$$

where$f_k(\theta)$ is called the scattering amplitude for the relative wave number k. The cross section for scattering through angles in the range from θ to $\theta + d\theta$ is:

$$d\sigma = 2\pi \sin\theta |f(\theta)|^2 d\theta. \tag{2.2}$$

For particles scattered by a central potential $U(r)$, the wave function must be axially symmetric about the direction of the incident particles, which is the *z axis* in our case. Therefore the wave function could be represented as a summation of functions that are independent of the azimuthal angle ϕ round the *z axis*.

$$\psi = \sum_{l=0}^{\infty} A_l P_l(\cos\theta) R_{k,l}(r), \tag{2.3}$$

where the A_l are constants and the $R_{k,l}$ are radial functions satisfying the equation

$$\frac{1}{r}\frac{d^2}{dr^2}(rR_{kl}) + \left[k^2 - \frac{l(l+1)}{r^2} - \frac{2m}{\hbar^2}U(r)\right]R_{k,l} = 0. \tag{2.4}$$

From the solution of this equation, we can obtain the asymptotic expression for ψ

$$\psi \approx \frac{1}{2ikr}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)\left[(-1)^{l+1}e^{-ikr} + S_l e^{ikr}\right], \tag{2.5}$$

where the notation

$$S_l = exp(2i\delta_l) \tag{2.6}$$

is called the scattering matrix. Hence the scattering amplitude can be written as

$$f_k(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)[S_l - 1]P_l(\cos\theta) = \sum_l (2l+1) f_l P_l(\cos\theta), \tag{2.7}$$

where

$$f_l = \frac{1}{2ik}(S_l - 1) = \frac{1}{2ik}(e^{2i\delta_l} - 1) = \frac{1}{k\cot\delta_l - ik}. \tag{2.8}$$

The cross-section for the l^{th} partial wave is

$$\sigma_l = 4\pi(2l+1)|f_l|^2.$$

2.2 Scattering of slow particles by a short range potential

2.2.1 effective range expansion

In the limit of slow particle scattering, the relative velocity could be so small that the wave length of these particles are large compared with the range b of the potential $U(r)$ $(i.e. kb \ll 1)$; we can call this a short-range scattering problem. Besides, the energy is small compared to the field within that range, hence we can neglect the energy term in the Schrodinger equation within the range of the potential. A relation between the scattering phase shift and the wave number k can be found. In this subsection we will discuss this relation which is called the **effective-range expansion**. In the range $r \leq b$ we can neglect the term in k^2 in the exact Schrodinger equation for the radial functions, since the velocity is so slow that the energy term in the Schrodinger equation is less significant than the $U(r)$ term. So we get the equation as:

$$R_l'' + 2\frac{R_l'}{r} - l(l+1)\frac{R_l}{r^2} = 2mU(r)\frac{R_l}{\hbar^2}. \tag{2.9}$$

For the range $b \ll r \ll 1/k$, the term in $U(r)$ may also be omitted, thus the equation reduces to:

$$R_l'' + 2\frac{R_l'}{r} - l(l+1)\frac{R_l}{r^2} = 0. \tag{2.10}$$

The general solution for this equation is

$$R_l = c_1 r^l + \frac{c_2}{r^{l+1}}, \tag{2.11}$$

where c_1 and c_2 are constants, they are different for different l, and can only be determined by solving the Schrodinger equation for a particular potential $U(r)$ in principle. At greater distances, when we consider the wave at a range of distance $r \sim 1/k$. We can still omit the term in U(r) from Schrodinger's equation, but the term in k^2 is comparable to the angular momentum term in the Schrodinger equation, so it should be kept. The equation turns out to be

$$R_l'' + 2\frac{R_l'}{r} + \left[k^2 - \frac{l(l+1)}{r^2}\right] R_l = 0, \tag{2.12}$$

i.e. the radial equation for free particles.

We can write the general solution of this equation as

$$R_l = c_1 \frac{(2l+1)!!}{k^l} j_l(kr) - c_2 \frac{k^{l+1}}{(2l-1)!!} n_l(kr). \tag{2.13}$$

We know the leading terms for Spherical Bessel functions when the variables are small:

$$\lim_{x \to 0} j_l(x) = \frac{x^l}{(2l+1)!!};$$

$$\lim_{x \to 0} n_l(x) = -\frac{(2l-1)!!}{x^{l+1}}.$$

so for the region where $kr \ll 1$ this solution becomes (2.11). With this normalization, the solution in the region $kr \ll 1$ will join to the solution in the region $kr \sim 1$.

On the other hand, when the argument of Spherical Bessel Function is large, they can be written in their asymptotic forms

$$\lim_{x \gg 1} j_l(x) = \frac{\sin(x - \frac{l\pi}{2})}{x};$$

$$\lim_{x \gg 1} n_l(x) = -\frac{\cos(x - \frac{l\pi}{2})}{x}.$$

So when $kr \gg 1$ we have

$$r R_l \approx C_l \sin(kr - \frac{l\pi}{2} + \delta_l), \tag{2.14}$$

where C_l is a constant. We can see that this is the same solution as in (2.5), with

$$\tan\delta_l = \frac{c_2}{c_1}\frac{k^{2l+1}}{(2l-1)!!(2l+1)!!}. \tag{2.15}$$

δ_l is called scattering *phase shift*. For a free particle, δ_l is zero, which means no scattering. A repulsive potential produces a wave function which is pushed out from the origin and accordingly δ_l is negative. Likewise, a weakly attractive potential attracts the wave function back to the origin and the accordingly δ_l is positive.

Comparing *Eq.*(2.15) to *Eq.*(2.8), it's easy to get the formula

$$Im(1/f_l) = -k. \tag{2.16}$$

According to *Eq.*(2.8)

$$f_l = \frac{1}{2ik}(e^{2i\delta_l} - 1) \approx \delta_l/k. \tag{2.17}$$

So in the limit of low energies, the partial wave scattering amplitudes behave as

$$f_l \sim k^{2l}. \tag{2.18}$$

Thus all the partial amplitudes with $l \neq 0$ are small compared to the partial wave amplitude of *s-wave* scattering. Equation (2.16) means the amplitude f_l must have the form

$$f_l = \frac{1}{(g_l - ik)}, \tag{2.19}$$

where g_l is a real quantity; comparing *Eq*(2.19) with *Eq*(2.8) we have

$$g_l = k\cot\delta_l. \tag{2.20}$$

For a given potential, g_l is a function of k. However, from (2.12) we can see k is involved in the equation as k^2 term, so g_l is a real function determined only by the absolute value of k, or we can say g_l is a real function of k^2, and therefore can be expanded in integral powers of k^2. So if the relation $Eq(2.18)$ is valid, we can expand $k^{2l+1}\cot\delta_l$ from the zero-order term of k^2 as

$$k^{2l+1}\cot\delta_l = -\frac{1}{a_l} + \frac{r_l k^2}{2} + O(k^4). \tag{2.21}$$

This formula is called effective range expansion. We will discuss the meaning of a_l and r_l in the following sections.

2.2.2 The meaning of scattering length

First let's discuss the meaning of a_l in the effective range expansion, a_l is called scattering length. When $k \sim 0$, it is easy to see from *Eq.*(2.21) that

$$k^{2l+1} \cot \delta_l = \frac{-1}{a_l}, \tag{2.22}$$

which can also be written as

$$\tan \delta_l = -k^{2l+1} a_l. \tag{2.23}$$

On the other hand, when the wave is outside the action of potential, the radial functions R_l have this form [17]

$$R_l \propto j_l(kr) - \tan \delta_l n_l(kr). \tag{2.24}$$

To extent this wave to the region around origin, recall the limiting form of the Spherical Bessel function for small variables, the extension of outer-range radial wave is proportion to

$$\left[\frac{(kr)^l}{(2l+1)!!} + \frac{(2l-1)!!}{kr}^{l+1} \tan \delta_l \right]. \tag{2.25}$$

Thus the intercept of the wave on the *r-axis* can be determined by:

$$\tan \delta_l = -\frac{(kI_l)^{2l+1}}{(2l+1)!!(2l-1)!!}, \tag{2.26}$$

where I_l is the intercept as $k \rightarrow 0$,

$$I_l = \Big[(2l+1)!!(2l-1)!! \; a_l \Big]^{1/(2l+1)}. \tag{2.27}$$

Hence I_l is proportion to $a_l^{1/2l+1}$, since (2l+1) is an odd number, I_l has the same sign as a_l. For $l = 0$

$$I_0 = a_0 = -\frac{\tan \delta_0}{k} = -\frac{c_2}{c_1}. \tag{2.28}$$

As we've discussed before for a free particle, the phase shift δ_0 equals zero, hence the intercept is also zero. For a weakly attractive potential, the wave function is attracted back to the origin, so the extension of outer wave has a small positive *phase shift* δ_0, hence the intercept is negative. If the attractive potential is more and more attractive, the *phase shift* will become larger and larger until the the outer wave become horizontal, at this point $\delta_0 = \pi/2$, and the intercept $I_0 \to \infty$ the solution is that of a confined particle, which is, a zero-energy bound state accompanied by an infinite scattering length. Moreover, if the potential strength

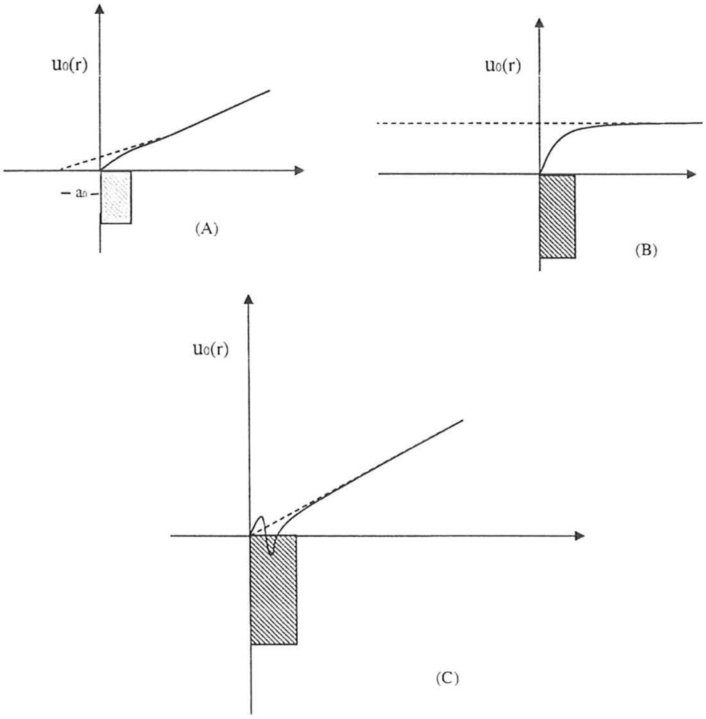

Figure 2.1: This figure shows the relation between the scattering length and s wave function for attractive potentials of differing strengths. The dashed curve is the extrapolation of the outer wave function to the point where it intersects the r axis. As we state in 2.2.2, this intercept is the scattering length. (A) Weak attraction, $a_0 < 0$; (B) Stronger attraction, $a_0 \sim \infty$; (C) Attractive enough for two bound states.

continues to increase, even more bound states are supported and the cycle repeats. From the relation $\tan\delta_0 = -ka_0$ we can see that if the potential is strong enough to have a bound state at $k = 0$, the phase shift must be π rather than 0.

Actually there is a general relation called **Levinson's theorem** to describe this cycle [18].

$$\delta_l(k=0) - \delta_l(k=\infty) = n\pi. \tag{2.29}$$

This theorem relates the difference of the phase shifts at zero and infinite energy, to the number of bound states n.

2.2.3 The meaning of effective range

In the effective range expansion given by Eq.(2.21), r_l is called effective range. We now discuss the expression of effective range and the physical meaning of it [19]. The method used here is first introduced by Bethe[[20], [21]].

We first consider a potential of this form

$$U(r) = -\frac{\alpha}{r^s},$$

where α is constant. For the range where $kr \ll 1$ we can neglect both the kinetic term and the potential, so we have

$$\frac{d^2u_l}{dr^2} + \left[\frac{\alpha}{r^s} - \frac{l(l+1)}{r^2}\right]u_l = 0. \tag{2.30}$$

By substituting

$$x = \left[2\alpha^{1/2}/(s-2)\right]r^{-\frac{1}{2}(s-2)};$$

$$u_l = r^{1/2}K_l(x).$$

The former equation reduces to

$$\frac{d^2K_l}{dx^2} + \frac{1}{x}\frac{dK_l}{dx} + \left[1 - \left(\frac{2l+1}{s-2}\right)^2\frac{1}{x^2}\right]K_l = 0. \tag{2.31}$$

The general solution of this kind of equation can be expressed in terms of Bessel functions as

$$K_l = AJ_{(2l+1)/(s-2)}(x) + BJ_{-(2l+1)/(s-2)}(x). \tag{2.32}$$

Hence the asymptotic form of u_l for large distance, which means at small x, can be obtained from the Taylor expansion of the Bessel function

$$J_n(x) = \sum_{r=0}^{\infty}\frac{(-1)^r x^{n+2r}}{2^{n+2r}r!\Gamma(n+r+1)}.$$

Then we have u_l in this form

$$u_l = A\big[r^{-l} + a_1 r^{-(4s-2)} + \dots\big] + B\big[r^{l+1} + b_1 r^{l-s+3} + \dots\big]. \tag{2.33}$$

In order to obtain an expression of effective range applicable to $l = 0$ and higher-order phase shifts, we introduce a generalized procedure.

The asymptotic form of u_l is the solution of equation:

$$\frac{d^2 u_l}{dr^2} + \left[k^2 - U(r) - \frac{l(l+1)}{r^2}\right] u_l = 0. \tag{2.34}$$

The solution which vanishes at $r = 0$ can now be written

$$u_l(r) \sim c_l[\cot\delta_l S_l(r) + C_l(r)], \tag{2.35}$$

where

$$\begin{aligned} S_l(r) &= krj_l(kr) \\ &\sim \sin(kr - \frac{l\pi}{2}) \quad as \quad r \to \infty; \\ &\to \frac{1}{2}(2kr)^{l+1} l!/(2l+1)! \quad as \quad r \to 0, \end{aligned} \tag{2.36}$$

$$\begin{aligned} C_l(r) &= -krn_l(kr) \\ &\sim \cos(kr - \frac{l\pi}{2}) \quad as \quad r \to \infty; \\ &\to (2kr)^{-l} l!/(2l)!/l! \quad as \quad r \to 0. \end{aligned} \tag{2.37}$$

Define the asymptotic solution w_l by subtracting the terms in the power series expansion of C_l which will diverge at the origin. For $l \leq 2$ we can take

$$w_l = c_l\big[\cot\delta_l S_l(r) + C_l(r) - A_l/r^l\big], \tag{2.38}$$

where

$$A_l = (2k)^{-l}(2l)!/l!, \qquad \text{Butfor} \quad l = 0, \quad C_0 = 1, \quad A_0 = 0.$$

When $l > 2$, more than one term need to be subtracted, here our discussion is limited to $l \leq 2$. By choosing $c_l = k^l$ we can make w_l finite as $k \to 0$. The general wave when we take the potential into account satisfies

$$\frac{d^2 u_{l,1}}{dr^2} + \left[k_1^2 - U(r) - \frac{l(l+1)}{r^2}\right] u_{l,1} = 0; \tag{2.39}$$

$$\frac{d^2 u_{l,2}}{dr^2} + \left[k_2^2 - U(r) - \frac{l(l+1)}{r^2}\right] u_{l,2} = 0. \tag{2.40}$$

Here $u_{l,1}, u_{l,2}$ are for k_1, k_2 correspondingly. Multiplying (2.39) and (2.40) by $u_{l,2}$ and $u_{l,1}$ respectively, subtracting and integrating, we have

$$\left[u_{l,2}\frac{du_{l,1}}{dr} - u_{l,1}\frac{du_{l,2}}{dr}\right]_a^b = (k_2^2 - k_1^2)\int_a^b u_{l,1}u_{l,2}dr. \tag{2.41}$$

On the other hand, the equation for w_l is modified to

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2}\right] w_l = -A_l r^{-l} k^2. \tag{2.42}$$

So for wave outside the range of the action for potential, using $w_{l,1}$ and $w_{l,2}$ as the solution respectively, according to (2.38) the corresponding equation with $U(r) = 0$ is

$$\begin{aligned}\left[w_{l,2}\frac{dw_{l,1}}{dr} - w_{l,1}\frac{dw_{l,2}}{dr}\right]_a^b &= (k_2^2 - k_1^2)\int_a^b w_{l,1}w_{l,2}dr \\ &+ \int_a^b r^{-l}\left(k_2^{l+2}A_{l,2}w_{l,1} - k_1^{l+2}A_{l,1}w_{l,2}\right)dr.\end{aligned} \tag{2.43}$$

By subtracting (2.43) from (2.41) and take $a = 0, b \to \infty$ the difference between the integrated terms vanishes and we have the equation as for large R

$$\begin{aligned}&\int_0^R r^{-l}\big(k_1^{l+2}A_{l,1}w_{l,2}-k_2^{l+2}A_{l,2}w_{l,1}\big)dr\\&=(k_2^2-k_1^2)\int_0^R\big(u_{l,1}u_{l,2}-w_{l,1}w_{l,2}\big)dr.\end{aligned}\tag{2.44}$$

Integrating the left hand side of this equation, we then obtain

$$\begin{aligned}&k_1^2k_2^{2l-1}\cot\delta_l^{(2)}-k_2^2k_1^{2l-1}\cot\delta_l^{(1)}\\&=(k_2^2-k_1^2)\int_0^\infty\big(u_{l,1}u_{l,2}-w_{l,1}w_{l,2}\big)dr.\end{aligned}\tag{2.45}$$

When $k_2 \rightarrow k_1 = k$ we have

$$\frac{d^2}{dk^2}\Big(k^{2l+1}\cot\delta_l\Big)-2k^{2l-1}\cot\delta_l=\int_0^\infty\big(w_l^2-u_l^2\big)dr.\tag{2.46}$$

Notice the limit cannot be taken on the right-hand side as $k \rightarrow 0$, since w_l^2 has a term

$$-2A_lS_lk^{2l}r^{-l}\cot\delta_l\rightarrow\frac{r}{(2l+1)a_l}\quad as\quad k\rightarrow 0,$$

which goes to infinity as $r \rightarrow \infty$. On the other hand, according to (2.36), we can do the integral

$$\int_0^\infty r^{-l}S_ldr=\big[r^{-l}S_{l-1}\big]_0^\infty/k=2^lk^{l-1}l!/(2l)!,$$

so we have

$$2A_lk^{2l}\cot\delta_l\int_0^\infty S_lr^{-l}dr=2k^{2l-1}\cot\delta_l.\tag{2.47}$$

Then (2.46) can be written as

$$\frac{d}{dk^2}(k^{2l+1}\cot\delta_l)=\int_0^\infty\big(w_l^2-u_l^2+2k^{2l}A_lr^{-l}S_l\cot\delta_l\big)dr.\tag{2.48}$$

Comparing this equation with (2.21) we have the expression for the effective range

$$r_l = 2\int_0^\infty \left(w_{l,0}^2 - u_{l,0}^2 + 2k^{2l}A_l r^{-l} S_l \cot\delta_l\right) dr. \tag{2.49}$$

where $w_{l,0}$ and $u_{l,0}$ are the first term approximation of the expansion of w_l and u_l with k respectively, they are both function of r.

In order to see the meaning of effective range, let's consider the case $l = 0$. See Fig(2.1), for low energy limit, we choose $k \sim 0$, in this case (2.48) gives

$$k\cot\delta_0 = -\frac{1}{a_0} + k^2 \int_0^\infty \left(w_0^2 - u_0^2\right) dr + O(k^4), \tag{2.50}$$

where we use w_0 and u_0 as shortened form of $w_{0,0}$ and $u_{0,0}$ respectively.

This is the effective range expansion for $l = 0$. This formula would only be valid provided a_0 and r_0 exist, we will discuss the condition for the existence of these terms in the next section. By comparing (2.38) and (2.21) we get a formula for effective range of the scattering potential in s-waves.

$$r_0 = 2\int_0^\infty \left(w_0^2 - u_0^2\right) dr. \tag{2.51}$$

Since u_0 and w_0 are only different within the action range of potential, r_0 has the same order as the range of potential, it can be viewed as a measurement of the distance where the actual solution merges into the asymptotic solution. Any potential function which contains at least two adjustable constants can give us the experimental values of a_0 and r_0, in another words, these two terms are independent of the shape of the potential.

2.3 Constraint condition for the validity of effective range expansion

In this section we discuss when the scattering length and effective range exist. As we can see in previous sections, when we derive the effective range expansion, we neglect the potential for large r, so we may deduce that the potential has to decrease rapidly enough to make sure our approximation is valid. Now let's see how rapidly the decrease need to be.

2.3.1 Constraint condition for the validity of a_l

The *scattering length* a_l in *Eq.*(2.21) may be either positive or negative. In the discussion of *section 2.2* we have tacitly assumed that the field $U(r)$ decreases sufficiently rapidly at large distances ($r \gg r_c$) for the legitimacy of the approximation we made. Since we neglect $U(r)$ in our derivation of the general solution in the range $r_c \ll r \ll 1/k$, $U(r)$ must decrease rapidly enough. The second term of R_l in (2.11) is small term at large distance, and it$\sim$ $l(l+1)/r^2$ in (2.12), to retain this term in equation (2.12), it must be large compared with the multiplication of the first term of R_l in (2.11) and $U(r)$, which$\sim$ $U(r)r^l$. Thus $U(r)$ must decrease more rapidly than $1/r^{2l+3}$. In conclusion, if the potential $U(r) \sim 1/r^s$ at large distances, then for the existence of a_l we must have:

$$s > 2l + 3. \tag{2.52}$$

2.3.2 constraint condition for the validity of r_l

To examine how the decreasing speed of $U(r)$ at large distance affect the phase shift,

Thus the limit for $k \rightarrow 0$ will only exist provided $U(r)$ falls off sufficiently rapidly. We've assumed that $U(r)$ falls off faster than $r^{-(2l+3)}$ in order the scattering length exist. As can be seen from (2.33) the asymptotic form of $u_l^{(0)}$ will contain terms of order r^{l+1}, r^l, and r^{l-s+3}, whereas according to (2.38), $w_l^{(0)}$ will only contain the first two. So at the upper limits of the integral in (2.49) a term of order r^{2l-s+4} will arise. which makes the integral converge only if

$$s > 2l + 5, \tag{2.53}$$

this is the constraint condition for the validity of r_l.

Chapter 3

Scattering length for a model potential

Pethick and Smith gave a formula of s-wave scattering length for a model potential [15]. In the chapter, I will extend their discussion to higher level of angular momentum and find out how far we can go. A model potential as

$$\begin{aligned} U(r) &= \infty \quad for \quad r \leq r_c; \\ U(r) &= -\frac{C_6}{r^6} \quad for \quad r > r_c, \end{aligned} \tag{3.1}$$

has the van der Waals form$\sim 1/r^6$ at large distances, and is cut off at short distances by a hard core of radius r_c. This simplified model represents some essential features of the scattering at a potential with many bound states, as in alkali atoms. The core radius r_c is a way of parameterizing the behavior of the potential at short distance.

3.1 expression of scattering length

The general Schrodinger equation for $\chi = u_l = rR_l$ as we used in section*2.2.3* is

$$\frac{d^2\chi_l}{dr^2} + \left[k^2 - \frac{l(l+1)}{r^2} - \frac{2m_r}{\hbar^2}U(r)\right]\chi_l(r) = 0. \tag{3.2}$$

Put $r_0 = \left(\frac{2\mu}{\hbar^2}C_6\right)^{1/4}$ into above equation, and since we are considering scattering at very low energies, k can be set to zero. Thus outside the range of action, the the equation becomes:

$$\frac{d^2\chi_l}{dr^2} - \frac{l(l+1)}{r^2}\chi_l + \frac{r_0^4}{r^6}\chi_l = 0, \quad for \quad r > r_c. \tag{3.3}$$

We first introduce a dimensionless variable $x = r/r_0$. Then the above equation turns out to be

$$\frac{d^2\chi(x)}{dx^2} + \frac{1}{x^6}\chi(x) - \frac{l(l+1)}{x^2}\chi_l(x) = 0. \tag{3.4}$$

In order to turn the differential equation to one whose solutions are known, we set

$$\chi = x^\beta f(x^\gamma) \tag{3.5}$$

and try to choose values of β and γ that will result in a known differential equation for $f = f(y)$ with $y = x^\gamma$. By choosing $\beta = 1/2$ and $\gamma = -2$, introducing a new variable $\rho = y/2$, and writing $f(y) = g(\rho)$, we obtain a new equation for $g(\rho)$

$$\frac{d^2g}{d\rho^2} + \frac{1}{\rho}\frac{dg}{d\rho} + \left(1 - (\frac{l+\frac{1}{2}}{2\rho})^2\right)g(\rho) = 0. \tag{3.6}$$

This equation is the standard Bessel's equation. The general solution of this equation may be written as a linear combination of the Bessel functions $J_{\frac{2l+1}{4}}(\rho)$ and $J_{-\frac{2l+1}{4}}(\rho)$. So we get the solution as

$$g = AJ_\nu(\rho) + BJ_{-\nu}(\rho), \tag{3.7}$$

where

$$\nu = \frac{2l+1}{4}, \qquad \rho = \frac{1}{2}\left(\frac{r_0}{r}\right)^2. \tag{3.8}$$

Then we get the general solution for equation (3.2) as

$$\chi_l(r) = \sqrt{\frac{r}{r_0}}\left[AJ_\nu(\rho) + BJ_{-\nu}(\rho)\right]. \tag{3.9}$$

Because we are using a hard core potential, χ must vanish at $r = r_c$. Hence we can obtain

$$\chi_l(r_c) = 0 \quad\Longrightarrow\quad AJ_\nu(\rho_c) + BJ_{-\nu}(\rho_c) = 0 \quad\Longrightarrow\quad \frac{A}{B} = -\frac{J_{-\nu}(\rho_c)}{J_\nu(\rho_c)}. \tag{3.10}$$

Thus the general solution can be written as

$$\chi_l(r) = \sqrt{\frac{r}{r_0}}B\left[J_{-\nu}(\rho) - \frac{J_{-\nu}(\rho_c)}{J_\nu(\rho_c)}J_\nu(\rho)\right], \tag{3.11}$$

For alkali atoms, the interatomic potentials become repulsive for $r \leq 10a_0$, and therefore $10a_0$ is an appropriate choice for the magnitude of r_c. On the other hand, $r_0 \sim 100a_0$, so the condition $r_0 \gg r_c$ is satisfied, so $\rho_c \gg 1$. As we shall discuss below, this condition implies that the potential has many bound states. The ratio of A/B can be further evaluated by using the asymptotic form of Bessel function

$$J_p(z) \simeq \sqrt{\frac{2}{\pi z}}\cos\left[z - (p + \frac{1}{2})\frac{\pi}{2}\right], \tag{3.12}$$

which valid for large z. Thus we obtain the fraction of A/B is

$$\frac{A}{B} = -\frac{\cos\left(\rho_c + (\nu - 1/2)\frac{\pi}{2}\right)}{\cos\left(\rho_c - (\nu + 1/2)\frac{\pi}{2}\right)}. \tag{3.13}$$

So the general solution can be written as

$$\chi_l(r) = B\sqrt{\frac{r}{r_0}}\left[J_{-\nu}(\rho) - \frac{\cos\left(\rho_c + (\nu - 1/2)\frac{\pi}{2}\right)}{\cos\left(\rho_c - (\nu + 1/2)\frac{\pi}{2}\right)}J_\nu(\rho)\right] \tag{3.14}$$

To determine the scattering length, we must examine the wave function χ at large distances $r \gg r_0$, that is for small values of ρ. The Taylor expansion of the Bessel function give us the approximation that can be used when the variable is small

$$J_p(z) \simeq \frac{z^p}{2^p\Gamma(1+p)} \qquad z \ll 1, \tag{3.15}$$

thus χ_l can be further written as

$$\chi_l(r) \simeq B\sqrt{\frac{r}{r_0}}\left[\frac{\rho^{-\nu}}{2^{-\nu}\Gamma(1-\nu)} - \frac{\cos\left(\rho_c + (\nu - 1/2)\frac{\pi}{2}\right)}{\cos\left(\rho_c - (\nu + 1/2)\frac{\pi}{2}\right)}\frac{\rho^{\nu}}{2^{\nu}\Gamma(1+\nu)}\right] \qquad r \gg r_0. \tag{3.16}$$

Using the expression for ρ we finally get an expression for χ_l when r is large

$$\chi_l(r) \simeq B\frac{2^{(2l+1)/2}}{\Gamma(\frac{3-2l}{4})}(\frac{r}{r_0})^{l+1}\left[1 - 2^{-(2l+1)}\frac{\Gamma\left(\frac{3-2l}{4}\right)\cos\left(\rho_c + (\nu - 1/2)\frac{\pi}{2}\right)}{\Gamma\left(\frac{2l+5}{4}\right)\cos\left(\rho_c - (\nu + 1/2)\frac{\pi}{2}\right)}\left(\frac{r}{r_0}\right)^{-(2l+1)}\right] \tag{3.17}$$

On the other hand, since we are considering wave function at large distance, the $\frac{1}{r^6}$ term in Schrodinger equation can be neglected. Thus the Schrodinger equation for χ_l reduces to

$$\frac{d^2\chi_l}{dr^2} + \left[k^2 - \frac{l(l+1)}{r^2}\right]\chi_l(r) = 0. \tag{3.18}$$

The general solution of this equation is

$$\begin{aligned}\chi_l(r) &\simeq C_l(k)(kr)\left[j_l(kr) - \tan\delta_l n_l(kr)\right]\\ &\propto r^{(l+1)}\left[1 + (2l+1)[(2l-1)!!]^2\frac{\tan\delta_l}{(kr_0)^{2l+1}}\right] \qquad \textit{when} \quad kr \ll 1,\end{aligned} \tag{3.19}$$

where $C_l(k)$ is independent of r but is a function of k, j_l and n_l are Spherical Bessel functions, we've used the expansion for the Spherical Bessel function in the second step.

By comparing (3.17) and (3.19), it's easy to get this relation

$$k^{(2l+1)}\cot\delta_l = -(2l+1)[(2l-1)!!]^2\left(\frac{2}{r_0}\right)^{2l+1}\frac{\Gamma\left(\frac{5+2l}{4}\right)}{\Gamma\left(\frac{3-2l}{4}\right)}\frac{\cos\left(\rho_c-(\nu+1/2)\frac{\pi}{2}\right)}{\cos\left(\rho_c+(\nu-1/2)\frac{\pi}{2}\right)}$$

and from the effective range expansion formula we know that

$$k^{(2l+1)}\cot\delta_l \simeq -\frac{1}{a_l} \qquad \mathit{when} \quad k\to 0, \tag{3.20}$$

so we have the expression for the scattering length a_l

$$a_l = \left(\frac{r_0}{2}\right)^{2l+1}\frac{1}{(2l+1)!!(2l-1)!!}\frac{\Gamma\left(\frac{3-2l}{4}\right)}{\Gamma\left(\frac{2l+5}{4}\right)}\frac{\cos\left(\rho_c+(\nu-1/2)\frac{\pi}{2}\right)}{\cos\left(\rho_c-(\nu+1/2)\frac{\pi}{2}\right)}. \tag{3.21}$$

3.2 discussion

Eq.(3.21) can be further written as

$$a_l = \left(\frac{r_0}{2}\right)^{2l+1} \frac{1}{(2l+1)!!(2l-1)!!} \frac{\Gamma(\frac{3-2l}{4})}{\Gamma(\frac{5+2l}{4})} \cos(\pi\nu) \left[1 - \tan(\pi\nu)\tan(\theta_l)\right], \quad (3.22)$$

where

$$\rho_c = \frac{1}{2}\left(\frac{r_0}{r_c}\right)^2, \qquad \nu = \frac{(2l+1)}{4}, \quad \text{and} \quad \theta_l = \rho_c - (\nu + \frac{1}{2})\frac{\pi}{2}. \quad (3.23)$$

This equation leads us to several conclusions. Notice the scale of the scattering length is set by r_0^{2l+1}, which is in agreement with the discussion in section(2.2.2). Besides, the scattering length can be either positive or negative, and the scattering length depends on the details of the short range part of the interaction, which is r_c in this case.

It can be seen from (3.23) and (3.24) that

$$a_l = \frac{(-1)^l}{\sqrt{2}}\left(\frac{r_0}{2}\right)^{2l+1} \frac{1}{(2l+1)!!(2l-1)!!} \frac{\Gamma(\frac{3-2l}{4})}{\Gamma(\frac{5+2l}{4})} \left[1 + (-1)^{l+1}\tan(\theta_l)\right]. \quad (3.24)$$

When $l = 0$ this equation reduces to

$$a_0 = r_0 \frac{\Gamma(3/4)}{2\sqrt{2}\Gamma(5/4)} \Big[1 - \tan(\rho_c - 3\pi/8)\Big], \quad (3.25)$$

which is in agreement with Pethick and Smith's result [15].

Moreover, we can also generalize their discussion about the number of the bound states, from (3.25) we know

$$\begin{aligned} a_l &\propto [1 - \tan(\theta_l)] \qquad l \text{ is even}, \\ a_l &\propto -[1 + \tan(\theta_l)] \qquad l \text{ is odd}. \end{aligned} \quad (3.26)$$

Whenever the scattering length tends to minus infinity a bound state appears. Hance the number of bound states is given by the integer part of θ_l/π.

All values of ρ_c are in a range that is much greater than π, by assuming that they are all equally probable, we can make statistical arguments about the relative likelihood of attractive and repulsive interactions for general l, like Pethick and Smith did in their book [15]. From (3.27) we see that for even values of l the scattering length a_l is positive unless θ_l lies in the interval between $n\pi + \pi/4$ and $n\pi + \pi/2$ with n being an integer. There is a 'probability' 3/4 of the scattering length being positive, and hence repulsive interactions should be three times more common than attractive ones on average. On the other hand, for odd values of l, the scattering length is negative unless θ_l lies in the interval between $\nu\pi + \pi/2$ and $\nu\pi + 3\pi/4$ with ν being an integer. So the 'probability' of the scattering length being positive is 1/4. This result agree with Dickinson's result for $l = 1$ [22], where he uses the WKB method to obtained a solution in short-range which is not applicable in our case, since our model potential is too steep for WKB method.

So far our derivation looks good, but it is a quite limited method. According to (2.3.1) the effective range expansion and the scattering length only exist when $s > 2l + 3$ for a potential $\propto \frac{1}{r^s}$. This means that the condition

$$l < \frac{s-3}{2} \tag{3.27}$$

has to be satisfied. In our case $s = 6$, so l can only be 0 or 1.

Chapter 4

Energy spectrum of two atoms in a harmonic trap near a Feshbach resonance

Substantial research has been done in studying ultracold trapped atomic gases. Generally, the scattering between two neutral atoms in higher partial waves is suppressed due to the centrifugal barrier. However, by sweeping a static magnetic field near a Feshbach resonance (FR) at a higher partial wave [[23], [24]], one can control the interaction between the two particles. These atoms could be bosonic or fermionic under appropriate conditions. When the relative energy of the scattering atoms is near the energy of a quasi-bound molecular state with a nonzero angular momentum, the scattering is enhanced.

A Feshbach resonance was first observed for bosons interacting in the *s*-state [25]. Later, these were also observed [24] at higher partial waves. For fermions, two spin polarized fermions in a single channel ultra-cold gas may also interact in a relative odd-l state , or when the two atoms are in distinct spin states they may interact in an even-l state. Regal et al. [23] first observed the single-channel *p*-wave FR between ^{40}K atoms, while the fermionic *s*-wave between these atoms in distinct spin states was observed by the same group a little earlier [26].

For two atoms in a spherical harmonic potential(HO), when the range of the interaction between these two atoms is much smaller than the average inter-particle distance in the HO, i.e. the oscillator length, the energy spectrum near a s-wave FR is found to be universal[27, 16, 28]. This remarkable result is obtained in a one-channel approximation, and fits the data even with the first term in the effective range expansion. The spectrum has been checked experimentally [29] in the limit of low tunneling for fermionic ^{40}K atoms in an optical trap in two distinct spin states near the Feshbach resonance.

Yip [13] has calculated the spectrum of two identical fermions in a HO near a *p*-wave FR. For higher partial waves, however, Yip stated that the energy spectrum could not be expressed in terms of the parameters in the scattering amplitude and the oscillator constant. By using a method first formulated by Jonsell [16] for $l = 0$, we proceeded to do this, I shall show how this may be done under certain restrictions for $l = 2$ in the following sections.

4.1 Two-body problem

4.1.1 Two-channel model of Feshbach resonance

First recall the the well-known results for two-channel scattering, following the treatment and notation of Cohen-Tannoudji [30].

For a two atom system, there is one channel for the 2 atoms to collide with a very small positive energy E. This channel is called an *open* channel, and the wave function for this channel is denoted as ϕ_k^+. We can take the energy of the dissociation threshold of the open channel as the zero of energy. There is another channel above the open channel, where the scattering states with energy E cannot exist because E is below the dissociation threshold of this channel, we call this channel the *closed* channel. A bound state ϕ_{res} exists in the closed channel with an energy E_{res} above the collision energy E of the open channel. ϕ_k^+ and ϕ_{res} are called bare states. Since the atom-atom interaction has off-diagonal elements between different channels, the wave function of each channel does not evolve independently from the others.

The incoming state with energy E of the 2 colliding atoms in the open channel is coupled by an interaction W to the bound state ϕ_{res} with energy E_{res} of the closed channel. Thus a pair of colliding atoms can make a virtual transition to the bound state and come back to the colliding state. The duration of this virtual transition scales as $\hbar/|E - E_{res}|$, i.e. as the inverse of the detuning between the collision energy E and the energy E_{res}. When E is close to E_{res}, the virtual transition may last a very long time and this enhances the scattering amplitude. The total magnetic moment of the atoms are not the same in the 2 channels, because they have different spin configurations. By sweeping a magnetic field, the energy difference between the 2 channels can be adjusted, and the energy E may be close to E_{res}.

The wave function ψ of the two-channel problem is a column matrix with two components ϕ_{op} and ϕ_{cl}

$$\psi = \begin{pmatrix} \phi_{op} \\ \phi_{cl} \end{pmatrix}.$$

These two components ϕ_{op} and ϕ_{cl} of the scattering states are called dressed states, because they include the effect of the coupling potential $W(r)$.

The Hamiltonian H for a two-channel model is a 2×2 matrix, with the diagonal elements H_{op} and H_{cl}, and the non-diagonal coupling given by the short range spin exchange potential W.

$$\mathbf{H} = \begin{pmatrix} H_{op} & W(r) \\ W(r) & H_{cl}. \end{pmatrix}$$

Here $H_{op} = (-\nabla^2 + V_{op})$, with V_{op} given by the van der Waals power law potential whose asymptotic fall-off goes like r^{-6}. The closed channel Hamiltonian, by neglecting all eigenstates of H_{cl} than ϕ_{res}, may be expressed as $H_{cl} = E_{res}|\phi_{res} >< \phi_{res}|$, with the resonance energy at E_{res}. So the wave function ψ satisfys

$$\begin{pmatrix} H_{op} & W(r) \\ W(r) & H_{cl}, \end{pmatrix} \begin{pmatrix} \phi_{op} \\ \phi_{cl} \end{pmatrix} = E \begin{pmatrix} \phi_{op} \\ \phi_{cl} \end{pmatrix}. \tag{4.1}$$

As shown by Cohen-Tannoudji [30], it is easy to prove that the two-channel scattering problem can be described entirely in the open channel by a Lippman-Schwinger equation where the (relative) outgoing wave of the dressed atoms $|\phi_{op}^k >$ is equal to a sumation of the bare state and the open channel $|\phi_k^+ >$, in which the incident wave is distorted by the open channel potential V_{op}, and an extra item from the effective interaction. Explicitly, it is given by

$$|\phi_{op}^k >= |\phi_k^+ > + G_{op}^+(E) V_{eff} |\phi_k^+ > \ , \tag{4.2}$$

where

$$V_{eff} = W \frac{|\phi_{res} >< \phi_{res}|}{E - E_{res} - < \phi_{res}| W G_{op}^+(E) W |\phi_{res} >} W \ . \tag{4.3}$$

This is a single channel scattering by the effective potential V_{eff}. Here $G_{op}^+(E) = (E - H_{op} + i\epsilon)^{-1}$ is is a Green function of H_{op}. Notice the term $+i\varepsilon$, where is a positive number tending to 0, ensures that the Green function has the asymptotic behavior of an outgoing scattered state for $r \longrightarrow \infty$.

As $k \longrightarrow 0$, the large-r behaviour of the first term on the RHS of Eq.(4.2) gives the background scattering length, and the second term yields the energy-dependent scattering length that dominates near the Feshbach resonance. As we have stated in section *2.3*, for higher partial waves $l \geq 2$, and $V_{op}(r) = -(\hbar^2/M)C_6/r^6$, the background scattering length does not exist [17, 9]. Indeed, the phase shift caused by this potential is vanishingly small for small k. This background phase shift, denoted by $\delta_l^{bg}(k)$, is given by [31]

$$\tan\delta_l^{bg}(k) = \frac{\pi}{2}2^{-5}C_6\frac{\Gamma(5)\Gamma(l-3/2)}{\Gamma^2(3)\Gamma(l+7/2)}\,|k|^3k\ . \tag{4.4}$$

The distortion in the incident wave ϕ_k^+ for small k may therefore be neglected, and the scattering for the higher partial waves at low energies is governed by the energy-dependent short range potential V_{eff}. As usual, its energy denominator may be related to the Zeeman splitting due to a sweeping magnetic field, giving rise to a large variation of the scattering length a_l near the FR. We may then express the flow of the energy levels as a function of the scattering length, assuming a fixed effective range r_l in the expansion (4.5). This we proceed to do, generalising a method first proposed by Jonsell [16] for $l = 0$. We confine our treatment to $m_l = 0$.

4.1.2 Discussion of validity

In calculating the p wave spectrum, Yip used an effective range expansion for higher partial waves [19]

$$k^{2l+1}\cot\delta_l(k) = -\frac{1}{a_l} + \frac{1}{2}r_lk^2, \tag{4.5}$$

with $l = 1$. Note that the scattering length a_l and the effective range r_l have the dimensions of $(L)^{2l+1}$ and $(L)^{-2l+1}$ respectively. As we have discussed in section *2.3.1*, for single channel elastic scattering by a power-law potential r^{-n}, and *without any virtual transition to other channels like an excited quasi-molecular state*, a_l in Eq.(4.5) is only defined if $n > (2l+3)$ [17]. Similarly from the conclusion in section *2.3.2*, for the effective range r_l to exist, the restriction is even more severe effective: $n > (2l+5)$. Taking $n = 6$ for the asymptotic behavior of the interatomic potential, we see that for $l = 1$, only a_1 exists, but not r_1. For $l = 2$, neither a_2, nor r_2 is defined [17, 9].

The situation changes, however, for dressed atoms near a Feshbach resonance. As we have shown in section *4.1.1*, the open scattering channel is coupled to a resonance in the closed channel through a spin-dependent *two-body* interaction W that depends on the relative distance r between the two atoms [32]. One part is the long range tensor interaction between the two dipoles that falls off as r^{-3}. The other is the spin-exchange interaction between the two valence electrons of the alkali atoms that are closer than the coupling distance r_u. For $r < r_u$, the nuclear and electronic spins that were otherwise coupled in an isolated atom get uncoupled due to one atom's proximity to the other. The resulting spin-exchange interaction has a range r_u which is smaller than the so-called van der Waals distance, a measure of the length scale for the r^{-6} potential. The coupling potential W may therefore be regarded as of shorter range than r^{-6} in cases where the spin exchange interaction is dominant.

As we state in *4.1.1*, the elimination of a closed channel results in an additional effective potential V_{eff} in the single-channel formalism. As is apparent, from (4.3), the effective potential V_{eff}, which dominates the open channel scattering near the Feshbach resonance, contains W, which we introduced in (4.1), quadratically. Thus the effective range expansion should be valid for the higher partial waves for this short-range potential.

Making this assumption, we obtain the eigenvalue spectrum of two interacting atoms in a harmonic potential for the l-th partial wave in the following sections. Our eigen-spectrum formula reduces to the known ones [27, 16], and [13] for $l = 0$ and $l = 1$. For a given choice of the effective range r_l, the flow of the energy levels is plotted as a function of a_l/L for $l = 2$ on the assumption that the range of the interaction is much smaller than the oscillator length L, so long as the ground state energy E_2 is not too close to zero.

4.2 Energy spectrum in an harmonic trap

Each particle, of mass M, moves in a harmonic potential $(1/2)M\omega^2r^2$. Making the usual transfomations to relative and CM co-ordinates, $\mathbf{r} = (\mathbf{r}_1 - \mathbf{r}_2)$, and $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, and their corresponding canonical momenta $\mathbf{p}, \mathbf{P}$, we obtain, for the noninteracting particles,

$$H_0 = \left(\frac{P^2}{2M_{cm}} + \frac{1}{2}M_{cm}\omega^2R^2\right) + \left(\frac{p^2}{2\mu} + \frac{1}{2}\mu\omega^2r^2\right) , \tag{4.6}$$

where $M_{tot} = 2M$, $\mu = M/2$. Consider the relative motion of these two trapped particles, interacting through a short range effective potential $V_s(r)$. This is the single-channel equivalent of the potential $W^2(r)$ of Eq.(4.3), with the energy dependence in the denominator being absorbed in the rapidly varying scattering length parametrized by the Zeeman splitting. The two-body Schrödinger equation in each partial wave l for the radial wave function $u_l(r) = r\psi_l(r)$ with energy E_l may be expressed in dimensionless variables $x = r/(\sqrt{2}\ L)$, where $L = \sqrt{\hbar/(M\omega)}$, and $\eta_l = 2E_l/(\hbar\omega)$. It is given by

$$-\frac{d^2u_l}{dx^2} + \frac{l(l+1)}{x^2}u_l + \frac{2V_s}{\hbar\omega}u_l + x^2u_l = \eta_l u_l \ . \tag{4.7}$$

We find the energy spectrum of the above equation without specifying the specific form of V_s by generalising a method first adopted by Jonsell [16] for $l = 0$. Let the range of the short range potential $V_s(r)$ be given by b. For $r > b$, taking $V_s = 0$, the solution of Eq.(4.7) is given by

$$u_l = e^{-x^2/2}\left[c_1' x^{l+1} M\left(\frac{2l+3-\eta_l}{4}, l+\frac{3}{2}; y\right) + c_2' x^{-l} M\left(\frac{-2l+1-\eta_l}{4}, \frac{1}{2}-l; y\right)\right] , \tag{4.8}$$

where $y = x^2$, and $M(\alpha, \gamma; z)$ is the confluent hypergeometric function [17], it is also called Kummer's function [33]. Since, for large z, $M(\alpha, \gamma; z)$ behaves as

$$M(\alpha, \gamma; z) \sim \frac{\Gamma(\gamma)}{\Gamma(\alpha)} z^{\alpha-\gamma} \mathrm{e}^{z} \,, \tag{4.9}$$

the wave function behaves as

$$u_l = \left[c_1' \frac{\Gamma(3/2+l)}{\Gamma((3+2l-\eta_l)/4)} + c_2' \frac{\Gamma(1/2-l)}{\Gamma((1-2l-\eta_l)/4)} \right] x^{-(1+\eta_l)/2} \mathrm{e}^{x^2/2} \tag{4.10}$$

for large x. In order to get a convergent solution, we must have

$$\frac{c_2'}{c_1'} = -\frac{\Gamma(3/2+l)}{\Gamma(1/2-l)} \frac{\Gamma((1-2l-\eta_l)/4)}{\Gamma((3+2l-\eta_l)/4)} \,. \tag{4.11}$$

Since

$$\frac{\Gamma(3/2+l)}{\Gamma(1/2-l)} = (-1)^l \left(l + \frac{1}{2} \right) \frac{[(2l-1)!!]^2}{2^{2l}} \,, \tag{4.12}$$

we obtain

$$\frac{c_2'}{c_1'} = -(-1)^l \left(l + \frac{1}{2} \right) \frac{[(2l-1)!!]^2}{2^{2l}} \frac{\Gamma((1-2l-\eta_l)/4)}{\Gamma((3+2l-\eta_l)/4)} \,. \tag{4.13}$$

We now relate this ratio to the scattering length a_l to determine the eigenvalue η_l. Note that if the range b of V_s is very small, as we approach $r \to b^+$, the oscillator potential may be neglected. *This assumption is crucial for our derivation, and is justified in some detail in Appendix A for* $l = 2$. Thus $u_l(r)$ for positive energy may be regarded as the phase-shifted scattering solution due to V_s, given by

$$u_l(r) = A_l kr \left[j_l(kr) - n_l(kr) \tan \delta_l \right] \,, \tag{4.14}$$

$E_l = \hbar^2 k^2 / M$. For $r > b$, but still small, $u_l(r)$ behaves as

$$u_l(r) \longrightarrow B_l r^{l+1} \left[1 + (2l+1)[(2l-1)!!]^2 \frac{\tan \delta_l}{(kr)^{2l+1}} \right] \,, \tag{4.15}$$

where

$$B_l = \frac{A_l k^l}{(2l+1)!!} \ . \tag{4.16}$$

We match u_l, given by Eq.(4.15) with that obtained from Eq.(4.8) for small x. For $z \rightarrow 0$, and $\gamma \neq 0$, the Kummer function $M(\alpha, \gamma; z)$ is unity; hence the solution given by Eq.(4.8) behaves as

$$u_l(x) = c_1' x^{l+1} \left(1 + \frac{c_2'}{c_1'} x^{-2l-1}\right) \ . \tag{4.17}$$

When this is matched to Eq.(4.15), we obtain

$$\frac{c_2'}{c_1'} = (2l+1)[(2l-1)!!]^2 \frac{\tan \delta_l}{(\sqrt{2}kL)^{2l+1}} \ . \tag{4.18}$$

Equating Eqs(4.13, 4.18), and using the effective range expansion (4.5), we obtain

$$\frac{1}{\sqrt{2}} \frac{\Gamma((1-2l-\eta_l)/4)}{\Gamma((3+2l-\eta_l)/4)} = (-2)^l \frac{\tilde{a}_l}{1 - \tilde{a}_l \tilde{r}_l \eta_l / 4} \ . \tag{4.19}$$

In the above, we have defined the dimensionless quantities

$$\tilde{a}_l = \frac{a_l}{L^{2l+1}} \ , \qquad \tilde{r}_l = L^{2l-1} r_l \ . \tag{4.20}$$

If we set $l = 1$ and $L = l_r/\sqrt{2}$ following Yip [13], we recover his result, specifically, his Eq.(13);

$$-\frac{l_r^3}{v} + \frac{1}{2} l_r (2c) \eta_1 = 8 \frac{\Gamma((5-\eta_1)/4)}{\Gamma((-1-\eta_1)/4)} \ , \tag{4.21}$$

where we have put $a_1 = v$ and $r_1 = 2c$. Similarly, by setting $l = 0$ in Eq.(4.19) we recover the spectrum of the $l = 0$ states as given by Busch [27]. Note that Eq.(4.19) has been obtained with no mention of any specific shape of the potential, and is valid for *any* short-range two-body potential.

4.3 Results and Discussion

Before discussing the spectra, we comment on the choice of the effective range parameter. For $l = 1$, Yip had set the scaled effective range $\tilde{r}_1 = -64/\sqrt{2}$ from experimental data [34]. From a theoretical point of view, to see if this may be generated by a potential whose range is much smaller than the oscillator length L, we take a square-well potential. Even though the energy spectra for $l = 1$ and $l = 2$ are extremely sensitive to the choice of the effective range, we find that the levels are practically unchanged by introducing the next term in the expansion, which is shape-dependent.

The shape of the potential should not matter unless the leading shape-dependent term in the effective range expansion (proportional to k^4) affects the energy spectrum. We have verified that the spectra in Figs 4.1−4.5 remain virtually unchanged when this term is included. In the Appendix B, the analytical expressions for the scattering length and the effective range for any given partial wave are given. At a resonance, $a_l = \pm\infty$, hence it follows from Eq.(B.2) that $j_{l-1}(s) = 0$. Therefore, from Eq.(B.3) we get $r_0 = b$, $r_1 = -3/b$, and $r_2 = -15/b^3$. For Yip's choice of $r_1 L = \tilde{r_1} = -64/\sqrt(2)$, it follows that $b/L = \tilde{b} \simeq 1/15$, fulfilling the condition that $b << L$. Unlike the case $l = 1$, we do not have guidance from experiment for the choice of $\tilde{r_2}$, so we estimate it from the square-well potential arranging $\tilde{b} = 1/15$, 1/30, or 1/10. Furthermore, we find that for the square-well example, although the scattering length is highly sensitive to the choice of the strength parameter s defined by Eq.(B.1), the effective range hardly changes as s is varied over a narrow range to accommodate the variation in the scattering length. So we can plot the energy spectrum given by Eq.(4.19) as a function of the scaled scattering length $\tilde{a}_l$ for $l = 0 - 2$, keeping the effective range $\tilde{r}_l$ fixed. The same energy spectra look quite different when plotted against the inverse of the scattering length, $1/\tilde{a}_l$. For $l = 1$, we reproduce Yip's result, taking the first two terms in the effective-range expansion into account.

Figs. (4.2-4.5) show that away from the resonance ($\tilde{a}_l \rightarrow \pm\infty$), the energy

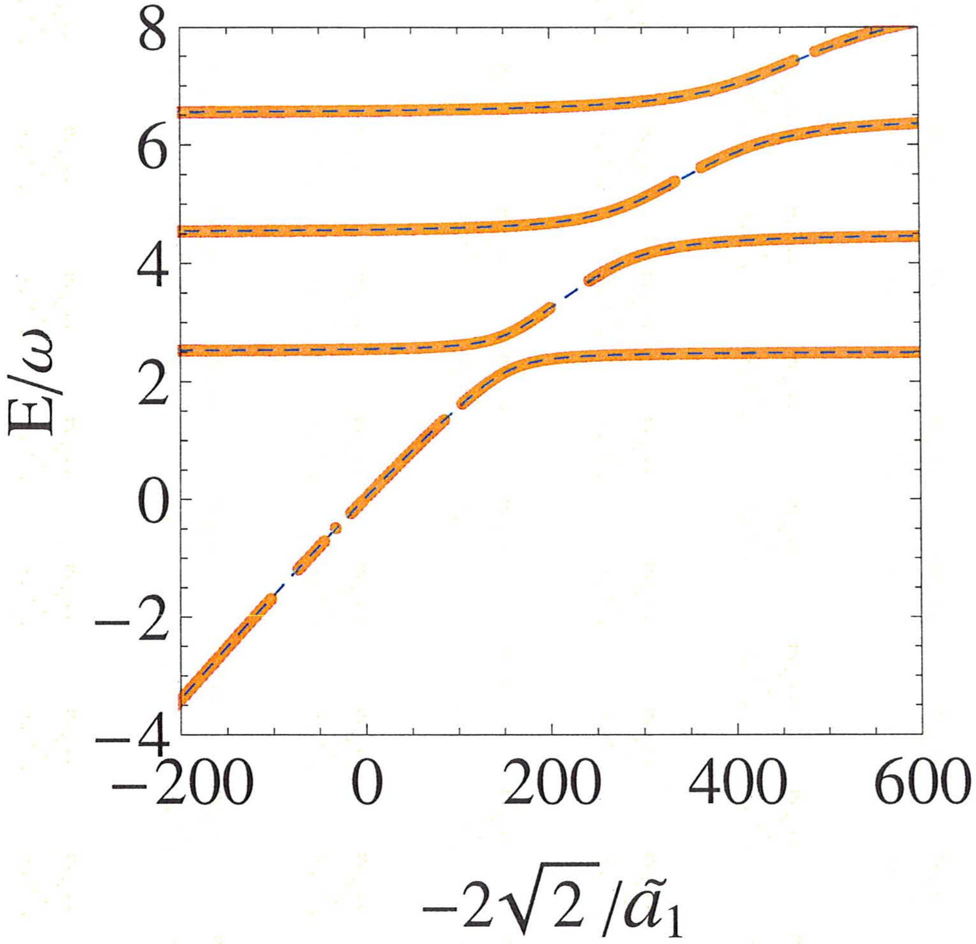

Figure 4.1: The $l = 1$ energy levels vs $-2\sqrt{2}/\tilde{a}_1$. The blue dashed curves are for the fixed effective range $\tilde{r}_1 = -64/\sqrt{(2)}$ as Yip used in his paper, while the orange curves are results from Eq.(4.19) using the scattering length and effective range of a square-well potential.

plots against $\tilde{a}_l$ have similar shapes. Whereas the $l = 0$ plots remain essentially unchanged when $\tilde{r}_0$ is varied over a wide range, the higher partial waves become more and more sensitive to the choice of the effective range. This is apparent from Figs 4.3-4.5. In all three, the lowest energy state tends to $-\infty$ as $\tilde{a}_l \rightarrow 0$. When $\tilde{a}_l \rightarrow \pm\infty$, the $l = 0$ energy levels tend to the limit $(2n + 1/2), n = 0, 1, 2..$ in units of the oscillator spacing. By contrast, for $l \neq 0$, all but the lowest energy level go to the noninteracting values $(2n + l + 3/2)$ in the zero range limit. All energies are

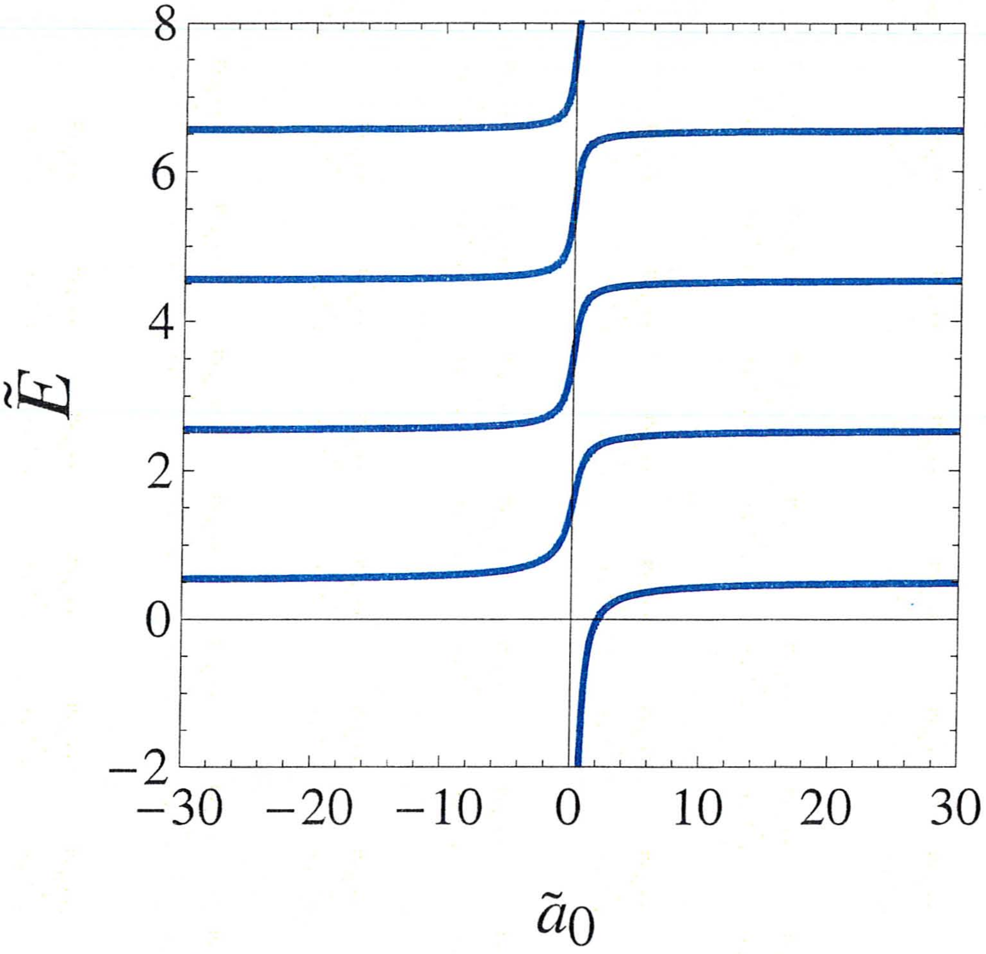

Figure 4.2: Plot of the $l = 0$ energy levels E in units of $\hbar\omega$ versus the s-wave scattering length a_0 in units of the oscillator length L. The scaled effective range is fixed at 1/15. The plots change negligibly even for zero range.

in units of the oscillator spacing. At resonance, the lowest energy level for $l \neq 0$ tends to zero as the range of the potential is decreased.

In Fig. 4.6, we see that the higher energy levels show strong bends away from the resonance, a feature even more pronounced than for the $l = 1$ case shown in [13].

To confirm that the analytical result (4.19) does produce the energy spectrum for $l = 2$ accurately for the range of the scattering parameters shown in Fig. 4.4,

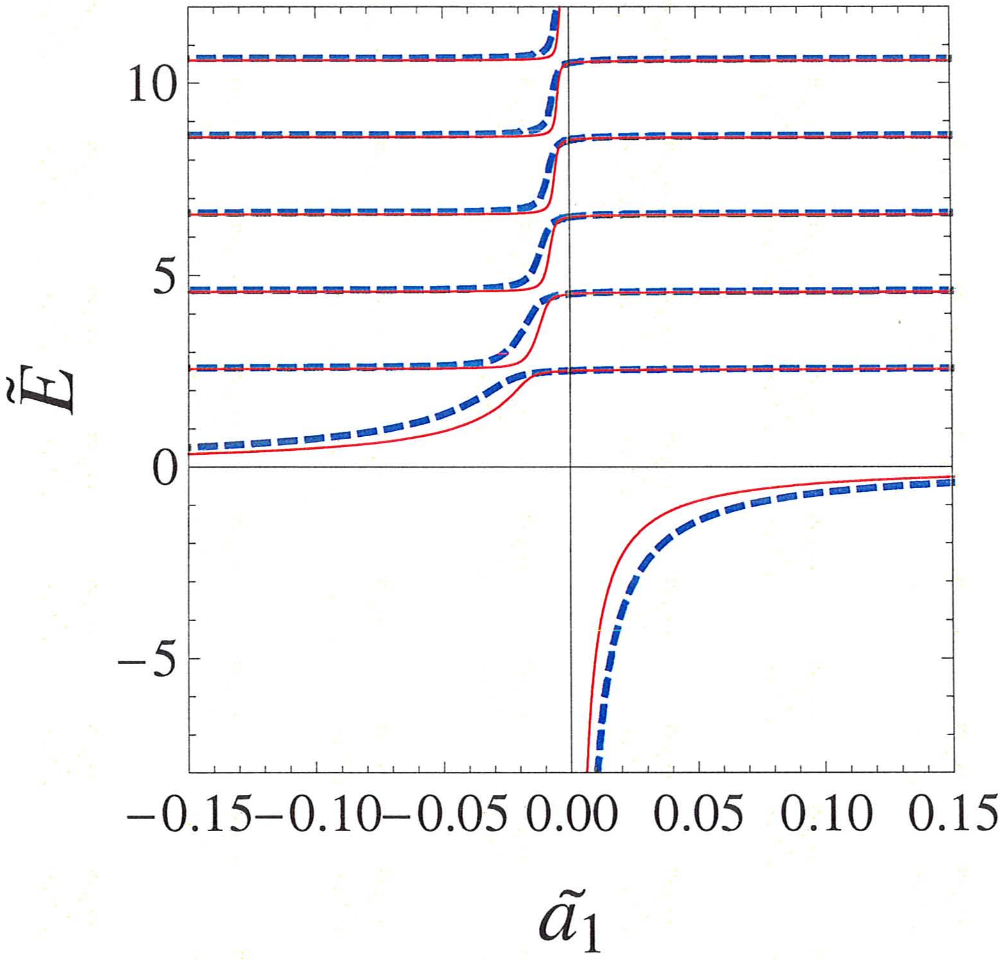

Figure 4.3: The $l = 1$ energy levels vs the scaled p-wave scattering length $\tilde{a}_1$. The dashed curves are for the effective range $\tilde{r}_1 = -30$, while the continuous curves are for $\tilde{r_1} = -45$.

we solved Eq.(4.7) numerically to determine E_2. For V_s, a square-well potential was taken with $\tilde{b} = 1/15$, kept fixed. The scattering length $\tilde{a}_2$ was varied as shown by changing the depth of the potential.

In Fig. 4.4, the dashed curves and lines are plotted using the analytical formula (4.19). The superposed dots are from the data of Table 4.1, which show the results for the eigenvalues obtained by the numerical integration of Eq.(4.7). The agreement is excellent, confirming the expectation of Appendix A.

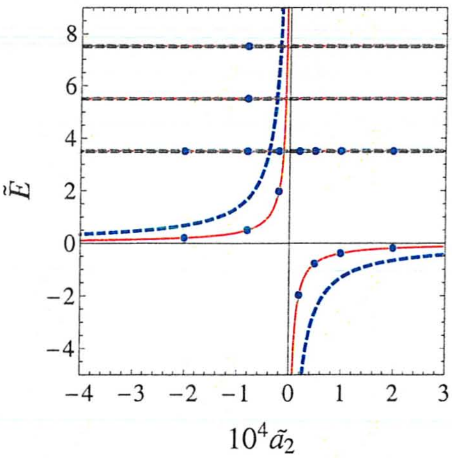

Figure 4.4: The $l = 2$ energy levels vs the scaled d-wave scattering length. The blue dashed line is for $\tilde{r}_2 = -15 \times 10^3$, while the continuous red line is for $\tilde{r}_2 = -15 \times 10^4$. See text for the choice of the effective range parameters.

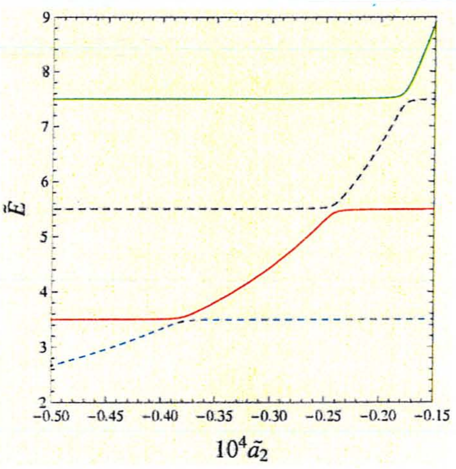

Figure 4.5: Amplified version of Fig 4.4, showing that the levels do not actually cross, but bend sharply in Fig 4.4.

Table 4.1: Comparison of energy η_2 obtained numerically from Eq. (4.7) and from the analytical formula (4.19). The $\tilde{b}$ of the square-well potential is kept fixed at 1/15. The units are $E/\hbar\omega$; the top two lines are for the ground state, the lower two lines are for the first excited state.

$10^4\tilde{a}_2$	-2	-0.8	-0.2	0.2	0.5	1	2	100	10^5	10^8
N^1	0.1992	0.4952	1.9726	-1.9772	-0.7887	-0.3945	-0.1956	-0.0022	0.0017	0.0017
A^2	0.1975	0.4939	1.9762	-1.9731	-0.7894	-0.3951	-0.1976	-0.0040	-0.0001	-0.0001
N	3.5002	3.5010	3.5012	3.5001	3.5001	3.5001	3.5002	3.5002	3.5002	3.5002
A	3.5002	3.5002	3.5003	3.5001	3.5001	3.5001	3.5002	3.5002	3.5002	3.5002

Table 4.1 shows, however, that the agreement with numerical integration becomes poor for the ground state as its energy approaches zero (which happens for large values of $\tilde{a}_2$). This limitation is understandable from Eq.(A.4) derived in Appendix A and the discussion that follows it.

In summary, we have argued in this chapter that it is legitimate to use the effective range formalism for higher partial waves in the vicinity of a Feshbach resonance, even though these parameters may not exist for a long range $1/r^6$

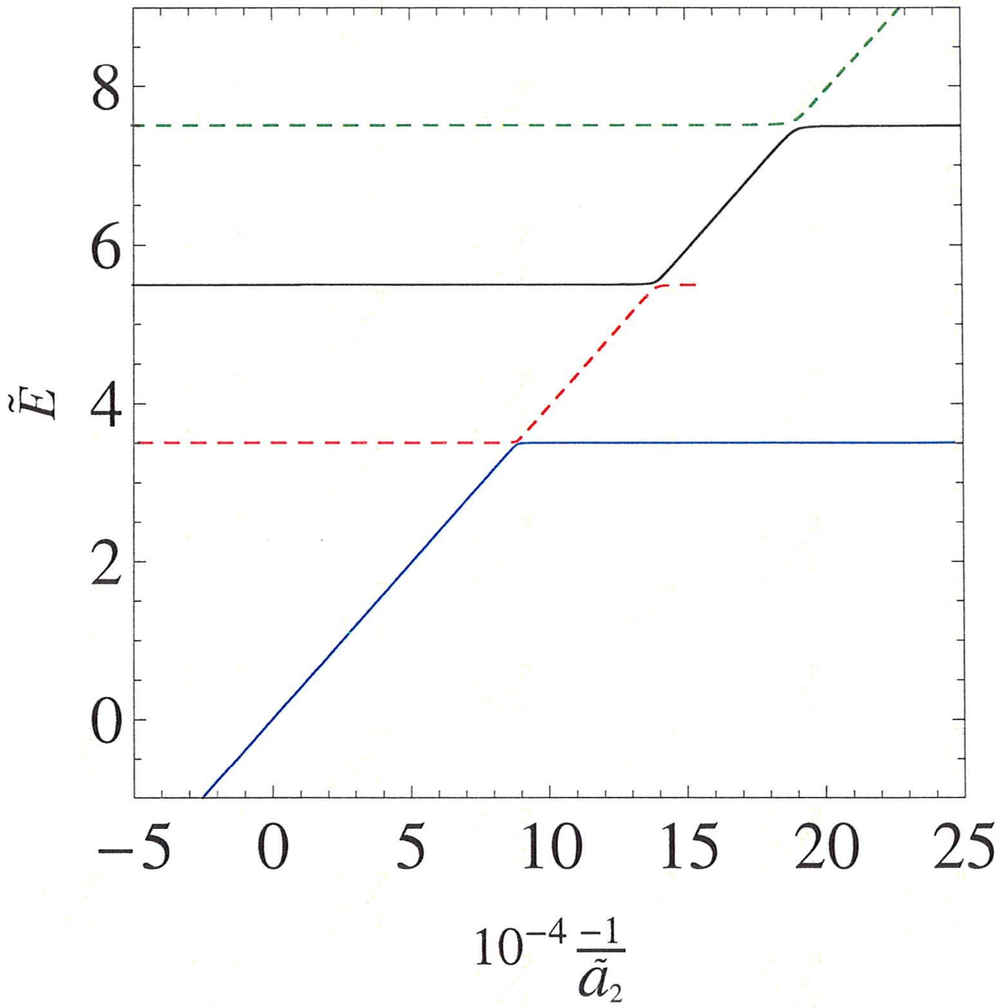

Figure 4.6: Plot of the excited state $l = 2$ energy levels vs the inverse of the scattering length in dimensionless units. This figure should be compared to Fig. 4.4.

interatomic potential. Next, we have derived a general equation (4.19), valid for any partial wave, relating the eigenenergies to the effective range parameters. This is known to be valid for $l = 0$ and $l = 1$ as long as the range of the potential is much shorter than the oscillator length. We have shown that it is also applicable for $l = 2$, so long as the ground state energy is not too close to zero. Our Eq.(A.4) in Appendix A, derived for the matching distance for $l = 2$ shows the limitation of the shape-independent parameters. At resonance, since both the terms on the RHS vanish, the analytical result (4.19) is not valid. For $l > 2$, the restriction is even more severe.

Appendix A

Limitation of the analytical result

The energy spectrum Eq.(4.19) is obtained when the ratio c_2'/c_1' from (4.8) with the oscillator potential present was equated to the corresponding ratio from the scattering solution (4.15) without the confining potential. In doing so, we assumed that this matching was done at a small enough distance (still larger than the range b of $V_s(r)$) that the oscillator potential could be neglected. In this appendix, we justify this assumption by taking the specific example of $l = 2$. To do this, we need to write Eq.(4.17) in more detail, and examine the neglected terms in the expansion of Eq.(4.8). For $l = 2$, for small x, this is given by

$$u_2(x) = c_1' \left[x^3 - \frac{\eta_2}{4} x^5 + ... + \frac{c_2'}{c_1'} \left(x^{-2} + \frac{\eta_2}{6} + \frac{1}{24}(\eta_2^2 - 6)x^2 + ... \right) \right] . \tag{A.1}$$

It is in the coefficient $\frac{(\eta_2^2-6)}{24}$ of the x^2 term that the oscillator presence is felt; without the oscillator, this coefficient is $\frac{\eta_2^2}{24}$. In Eq.(4.17), we neglect this term of order x^2, and yet retain the leading term x^3 of the regular solution, even though x is small. This can only be justified if the matching distance x satisfies the inequality

$$x^3 \gg \left|\frac{c_2'}{c_1'}\right| \frac{x^2}{4} . \tag{A.2}$$

To check this, we substitute above the expression (4.18) for c_2'/c_1', which, for $l = 2$, gives the condition

$$x \gg \frac{45}{4} \frac{|\tan \delta_2|}{(\sqrt{2}kL)^5} . \tag{A.3}$$

To estimate the RHS, we use Eq.(4.5), and put $k^2 = \frac{M}{\hbar^2}E_2$. We then get, for the condition (A.2)

$$x \gg 2 \left| \left(-\frac{1}{\tilde{a}_2} + \frac{1}{2}\tilde{r}_2 \frac{E_2}{\hbar\omega} \right)^{-1} \right| \tag{A.4}$$

From Figs. 3 and 4, we see that $\left\| \frac{1}{\tilde{a}_2} \right\|$ is of the order of 10^4 (either sign), and $\|\tilde{r}_2\|$ is -15×10^3 or ten times larger. The energy $E_2/\hbar\omega$ is of order unity. Unless there is some accidental cancellation , the RHS of Eq.(A.4) is very small, of the order of 10^{-4}. On the LHS of Eq.(A.4), x stands for the matching distance (in units of L, which is slightly larger than $\tilde{b} = 1/15$. Therefore the inequality condition (A.4) is easily satisfied. When, however, $E_2 \to 0$ and $\tilde{a}_2 \to \pm\infty$, (A.4) is not satisfied, and our formula (4.21) breaks down.

Appendix B

Scattering parameters for square-well potential

Consider an attractive square-well potential of depth V_0 and range b. Define the strength parameter

$$s = (\sqrt{MV_0/\hbar^2}\ )\ b\ . \tag{B.1}$$

In a given partial wave l, the expressions for the scattering length a_l and the effective range r_l are given by

$$a_l = -\frac{b^{2l+1}}{(2l-1)!!(2l+1)!!}\frac{j_{l+1}(s)}{j_{l-1}(s)}\ , \tag{B.2}$$

$$r_l = \frac{(2l-1)!!(2l+1)!!}{b^{2l-1}}\left[-\frac{1}{2l-1} + \frac{2l+1}{s^2}\frac{j_{l-1}(s)}{j_{l+1}(s)} - \frac{1}{2l+3}\left(\frac{j_{l-1}(s)}{j_{l+1}(s)}\right)^2\right]\ . \tag{B.3}$$

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