

The Two-Body Universal Energy Spectrum of Interacting Ultracold Atoms Near Feshbach Resonances

by

Alex C. Han

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Abstract

In this undergraduate thesis, we discuss the two-body quantum mechanical problem of two ultracold bosonic atoms at low energy limit, interacting through a square potential with and without an external confinement. The two-body s -wave scattering length is introduced in terms of the radial wavefunction. In free space with no confinement, the interaction-scattering length relation is calculated and compared in 3- and 1-dimensions; we show the recurring resonance regions where the scattering length diverges and the existence of dimer bound state with positively large scattering length. Lastly, in the case of a 3-dimensional isotropic harmonic confinement, again under the ultracold limit, we obtain the universal (s -state) energy spectrum of the two atoms in terms of the scattering length.

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Chapter 1

Introduction and Motivation

Ultracold atom physics has been a field of intense research and attracted great deal of interests from both theoretical and experimental areas since the experimental achievements such as laser trapping and cooling of atoms and the first Bose-Einstein Condensation of Rubidium atoms [1]. As the temperature cools down very close to absolute zero, the thermal motion of atoms is greatly suppressed and the quantum nature of matter becomes very apparent, which provides researchers a clean playground for exploring atomic and many-body quantum effects in quantum gases. Quantum gases of ultracold atoms are of special attention due to their ultracold temperatures where collisions of the atoms happen at very low energies, and the quantum (wave) nature of the matter dominates their behaviours. Novel quantum phases have also been studied for ultracold atomic gases, such as the exhibition of superfluidity and Mott-insulator phase [2].

The wheel of ultracold atom research spins forward through advances in experimental techniques such as optical lattices and Feshbach resonance scattering methods, where optical lattices are constructed by counter-propagating laser beams and form periodic trapping potential with experimentally controlled trap size; while Feshbach resonance scattering methods are used to tune the interaction between ultracold atoms [3]. With these experimental abilities of control over the system parameters, more and more theoretical research has been in place in order to fully understand the underlying principles, and to give support and predictions for future experimental works.

In view of these recent development to study quantum many-body systems, new doors have been opened for few-body physics at ultracold temperatures. The few-body problems focus more on the details of the quantum mechanical scattering of a small number (usually two or three) of ultracold atoms. In addition, the confinement for these atoms, namely optical traps, are usually easy to deal with theoretically. The optical confinement is in essence in the shape of a harmonic

oscillator potential, whose quantum mechanical properties are well known in textbooks on modern quantum physics. At appropriate conditions, the interaction potential between atoms can also be very well represented by the quantity called the two-body s -wave scattering length. One among many of its interesting properties of the scattering length, is that its scale of value can vary from as small as typical cold atom interaction range (angstroms) to as large as comparable to the harmonic oscillator length of the laser trap [4], where the physics of the situation is greatly simplified in terms of this scattering length alone and the system has, namely, universal properties: the details of the interaction are unimportant and same physics apply for given scattering length.

The universal properties apply for both fermionic and bosonic ultracold atoms. In this research project, we focus on the bosonic atoms due to the ease of theoretical calculations on the symmetric requirement of the two-body wavefunction. In addition, the s -partial-wave approximation is valid for bosonic atoms whereas the behaviours of fermionic atoms are dominated by p -waves due to their spins.

In summary, in this undergraduate research project we focus on the study of two interacting bosonic atoms at very low energies and their scattering properties. In the following sections we first reduce the two-body problem in general to a one-body problem and then study it in terms of the s -wave scattering length. Then we will look at a specific problem of a 3-dimensional isotropic harmonic trapping potential and solve the energy spectrum of the s -states in terms of the scattering length alone (universal spectrum).

Chapter 2

The Two-Body Problem

2.1 Reduction to One-Body Problem

The two-body low energy scattering formalism has been associated with nuclear interactions in the past, but it is borrowed and utilized here in the context of ultracold atoms. Physically, we concern ourselves with two interacting bosonic atoms may or may not be in a confinement. We first of all pose the two-body problem by writing down the Schrodinger's equation as the energy eigenvalue problem for the stationary states:

$$H\psi(\mathbf{r}_1, \mathbf{r}_2) = E_{12}\psi(\mathbf{r}_1, \mathbf{r}_2)$$

$$H = -\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + V_{12}(\mathbf{r}_1 - \mathbf{r}_2) + V_{trap}(\mathbf{r}_1) + V_{trap}(\mathbf{r}_2) \quad (2.1)$$

where the Hamiltonian involves the kinetic energies of atoms denoted 1 and 2, the interaction potential between them V_{12} and there might also be a confinement providing a trapping potential V_{trap} . The eigen-energies are continuous if there is no trap and is quantized in traps.

Similar to the method a two-body problem has been solved in the classical mechanics, we introduce the centre of mass frame of reference and the relative motion of the two particles, by a separation of spatial wavefunction $\psi(\mathbf{r}_1, \mathbf{r}_2) = \psi_\mu(\mathbf{r})\psi_M(\mathbf{R})$ with new variables and masses

$$\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \quad M = m_1 + m_2, \quad \mu = \frac{m_1m_2}{m_1 + m_2} \quad (2.2)$$

Now, assuming the interaction is isotropic, as most practical cases are, then $V_{12}(\mathbf{r}_1 - \mathbf{r}_2) = V_{12}(|\mathbf{r}_1 - \mathbf{r}_2|) = V_{12}(r)$. And change of variables makes $\frac{1}{m_1}\nabla_1^2 + \frac{1}{m_2}\nabla_2^2 = \frac{1}{M}\nabla_R^2 + \frac{1}{\mu}\nabla_r^2$, then the Hamiltonian becomes

$$H = -\frac{\hbar^2}{2M}\nabla_R^2 - \frac{\hbar^2}{2\mu}\nabla_r^2 + V_{12}(r) + V_{trap}(\mathbf{R}) + V_{trap}(\mathbf{r}) \quad (2.3)$$

Note here we rely on the trapping potential to be "nice" such that $V_{trap}(\mathbf{r}_1) + V_{trap}(\mathbf{r}_2) = V_{trap}(\mathbf{R}) + V_{trap}(\mathbf{r})$ (and to be seen in Chapter 3 that a 3-dimensional isotropic harmonic will satisfies this condition as well). The original Schrodinger's equation then decouples into two separate Schrodinger's equations for the centre of mass motion and the relative motion (with $E_{12} = E_M + E_\mu$)

$$\left[-\frac{\hbar^2}{2M}\nabla_R^2 + V_{trap}(\mathbf{R}) \right] \psi_M(\mathbf{R}) = E_M \psi_M(\mathbf{R}) \quad (2.4)$$

$$\left[-\frac{\hbar^2}{2\mu}\nabla_r^2 + V_{trap}(\mathbf{r}) + V_{12}(r) \right] \psi_\mu(\mathbf{r}) = E_\mu \psi_\mu(\mathbf{r}) \quad (2.5)$$

where we note that the equation for the motion of the centre of mass is exactly solvable if the given trapping potential is exactly solvable, and the problem of finding the eigen-energies is reduced to solving the problem posed by equation (2.5).

At low energy limit, the momenta (k) of the atoms are extremely low and thus the de Broglie wavelengths ($2\pi/k$) of the atoms are extremely large, resulting in the poor resolution of the interaction potential the atom scatters. Effectively then, we can write the s -wave approximation in the partial wave expansion of the relative motion wavefunction, assuming azimuthal symmetry, $\psi_\mu(\mathbf{r}) = \psi_\mu(r, \theta) = \sum_l \frac{u_l(r)}{r} P_l(\cos \theta)$ and let $l = 0$ (retain only s -wave term), then

$$\psi_\mu(\mathbf{r}) = \psi_\mu(r) = \frac{u_0(r)}{r} \quad (2.6)$$

and if the trapping potential is also isotropic, then equation (2.5) becomes

$$\left[-\frac{\hbar^2}{2\mu}\nabla_r^2 + V_{trap}(r) + V_{12}(r) \right] \psi_\mu(r) = E_\mu \psi_\mu(r) \quad (2.7)$$

writing out the Laplacian operator in polar form and insert the ansatz in equation (2.6), we have

$$\left[-\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} + V_{trap}(r) + V_{12}(r) \right] (r\psi_\mu(r)) = E_\mu(r\psi_\mu(r)) \quad (2.8)$$

which is in form a 1-dimensional scattering problem, with boundary conditions specified by the interaction term and the trapping potential term.

In order to proceed, we now look at the interaction potential and justify that a good effective model is an isotropic square potential for V_{12} , namely

$$V_{12}(r) = \begin{cases} V_0 & \text{for } 0 < r < r_0 \\ 0 & \text{for } r > r_0 \end{cases} \quad (2.9)$$

where the range of the potential is r_0 , and the strength V_0 can be either positive, zero or negative. The features of this square potential include: (i) isotropy - justified in most ultracold atom interactions; in addition, the low energy limit also implies a low angular resolution of the object the atoms scatters; (ii) finite range - for typical ultracold atoms, the interaction is dominated by van der Waals interaction potential, which can be thought of essentially zero after a certain finite distance, combined with the large de Broglie wavelength, the interaction can be considered negligible after a finite range r_0 ; (iii) uniform potential value inside - again justified by the long de Broglie wavelength (comparing to r_0), and the scattering atom can't "feel" the details of the interaction inside r_0 .

As a summary of the preconditions that we used to reduce problem of equation (2.1) to that of equation (2.8), we require

- An isotropic, finitely ranged, (square) interaction,
- A "nice" trapping potential (if any): isotropic and is felt by the two atoms separately (namely the requirement that $V_{trap}(\mathbf{r}_1) + V_{trap}(\mathbf{r}_2) = V_{trap}(\mathbf{R}) + V_{trap}(\mathbf{r})$), and
- Ultra-low energy levels at which the s -wave approximation is valid.

2.2 The S -wave Scattering Length

In this section we introduce the concept of two-body s -wave scattering length. The definition is rooted in the low energy limit of the Schrodinger's equation. Let's consider the case where there is no external confinement, and outside the interaction range r_0 we take the limit of energy going to zero in equation (2.8)

$$-\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} u_{(0)}(r) = 0 \quad (2.10)$$

where we denoted $u(r) = r\psi_\mu(r)$. The solution to above differential equation is linear in r and can be written in the form [5]

$$u_{(0)}(r) = \text{const}(r - a) \quad (2.11)$$

therefore, the solution to equation (2.8) with no confinement and outside the interaction range r_0 must go to $u_{(0)}(r)$ under low energy limit. i.e.

$$\lim_{k \rightarrow 0} u(r) = \text{const}(r - a) \quad (2.12)$$

which is to say

$$\lim_{k \rightarrow 0} \frac{u'(r)}{u(r)} = \frac{1}{r - a} \quad (2.13)$$

The parameter a here is defined to be the s -wave scattering length. Graphically, we can set $r = r_0$ and a is just the intercept of the tangent line to $u(r)$ at r_0 , shown by rearranging the terms in above equation, at low k limit,

$$u'(r_0)(a - r_0) + u(r_0) = 0 \quad (2.14)$$

Note that we can set $r = 0$ in equation (2.13). Even though the radial wavefunction is *NOT* $u(r)$ there, it does not violate the equality of equation (2.13). Then we have a more compact definition for the scattering length

$$\lim_{k \rightarrow 0} \frac{u'(0)}{u(0)} = -\frac{1}{a} \quad (2.15)$$

In free space, outside the interaction $u(r)$ has the asymptotic function form $u(r) \sim \sin(kr - \delta(k))$ with s -wave phase shift $\delta(k)$, thus equation (2.15) has a more often seen form [6],

$$\lim_{k \rightarrow 0} k \cot(\delta(k)) = -\frac{1}{a} \quad (2.16)$$

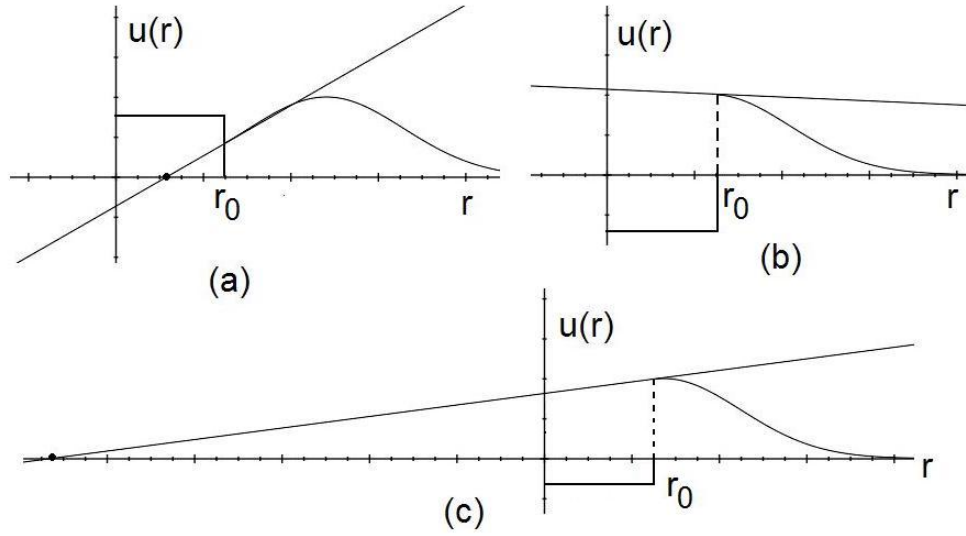


Figure 2.1: Different situations in 3D where the scattering length varies greatly in magnitude: (a) small and positive due to a very repulsive potential; (b) very large and positive (intercept not seen in graph) due to a relatively large attractive potential and (3) large and negative due to a small attractive potential.

This is an important equation by which we will calculate the relation between the strength of the square potential (V_0) and the scattering length in the next section.

Physically, the value of scattering length a can vary greatly. For a repulsive interaction, scattering length is on the same order of magnitude as the range of the interaction potential r_0 ; and for a attractive interaction it can be as large as comparable to the characteristic size of the confinement, if any, which is orders of magnitude larger than r_0 . Figure 2.1 shows the cases of different scales of scattering length. Notice that by the graphical interpretation of a , it is possible for the tangent line to the radial wavefunction $u(r)$ at r_0 to be flat, i.e. $|a| = \infty$. When scattering length diverges without bound, we say the system is *at resonance*. And we will see specifically how this resonance situation is achieved in the next section.

2.3 Scattering in Free Space: 3D and 1D Cases

We now utilize equation (2.16) and by calculating the phase shift $\delta(k)$, we can obtain a relationship between scattering length a and interaction strength V_0 . Let's first consider the 3-dimensional case of two bosonic atoms interact through the square interaction defined in equation (2.9), and the problem is posed by equation (2.8) with $V_{trap} = 0$ everywhere. First let's say $V_0 \gg E_\mu > 0$ (low energy scattering states), then the differential equation from (2.8) is changed to

$$\frac{\partial^2}{\partial r^2} u(r) = \begin{cases} -\frac{2\mu E}{\hbar^2} u(r) & r > r_0 \\ \frac{2\mu(V_0 - E)}{\hbar^2} u(r) & 0 < r < r_0 \end{cases} \quad (2.17)$$

and the radial wavefunction $u(r) = r\psi(r)$ that satisfies above differential equation has form

$$u(r) \sim \begin{cases} \sin(kr - \delta) & r > r_0 \\ \sinh(\kappa r) & 0 < r < r_0 \end{cases} \quad (2.18)$$

with

$$\kappa = \frac{\sqrt{2\mu(V_0 - E)}}{\hbar} \cong \frac{\sqrt{2\mu V_0}}{\hbar}, \quad k = \frac{\sqrt{2\mu E}}{\hbar} \quad (2.19)$$

It is a hyperbolic trigonometric function inside first because the exponential decay of the wavefunction, and secondly, in 3D, the radial wavefunction has to vanish at $r = 0$ (thus it is \sinh instead of \cosh). Now we impose the boundary condition that the radial wavefunction has to be continuous and continuously differentiable at r_0 , then it is necessary to require

$$\tan(kr_0 - \delta) = \frac{k}{\kappa} \tanh(\kappa r_0) \quad (2.20)$$

but note that low energy limit corresponds to $kr_0 \ll 1$ thus left hand side is $\tan(kr_0 - \delta) \cong -\tan \delta$, then we have phase shift

$$\delta = -\arctan \left[\frac{k}{\kappa} \tanh(\kappa r_0) \right] \quad (2.21)$$

using equation (2.16), we have

$$\frac{a}{r_0} = 1 - \frac{\tanh(\kappa r_0)}{\kappa r_0} \quad (2.22)$$

This is the relation of a vs. V_0 ($\kappa = \kappa(V_0)$) for a positive V_0 . Now let's assume $V_0 < 0$ and $|V_0| \gg E_\mu > 0$, then the differential equation we want to solve becomes

$$\frac{\partial^2}{\partial r^2}u(r) = \begin{cases} -\frac{2\mu E}{\hbar^2}u(r) & r > r_0 \\ -\frac{2\mu(E-V_0)}{\hbar^2}u(r) & 0 < r < r_0 \end{cases} \quad (2.23)$$

and the solution is

$$u(r) \sim \begin{cases} \sin(kr - \delta) & r > r_0 \\ \sin(\kappa r) & 0 < r < r_0 \end{cases} \quad (2.24)$$

with again

$$\kappa = \frac{\sqrt{2\mu(E - V_0)}}{\hbar} \cong \frac{\sqrt{2\mu|V_0|}}{\hbar}, \quad k = \frac{\sqrt{2\mu E}}{\hbar} \quad (2.25)$$

so the difference from a positive V_0 is that now inside the interaction potential the radial wavefunction is a standing wave in nature, rather than an exponential decay in the repulsive case.

With the same boundary condition requirement at r_0 , we have phase shift

$$\delta = -\arctan \left[\frac{k}{\kappa} \tan(\kappa r_0) \right] \quad (2.26)$$

Putting into equation (2.16) again, we have the relation between a and V_0 for negative V_0

$$\frac{a}{r_0} = 1 - \frac{\tan(\kappa r_0)}{\kappa r_0} \quad (2.27)$$

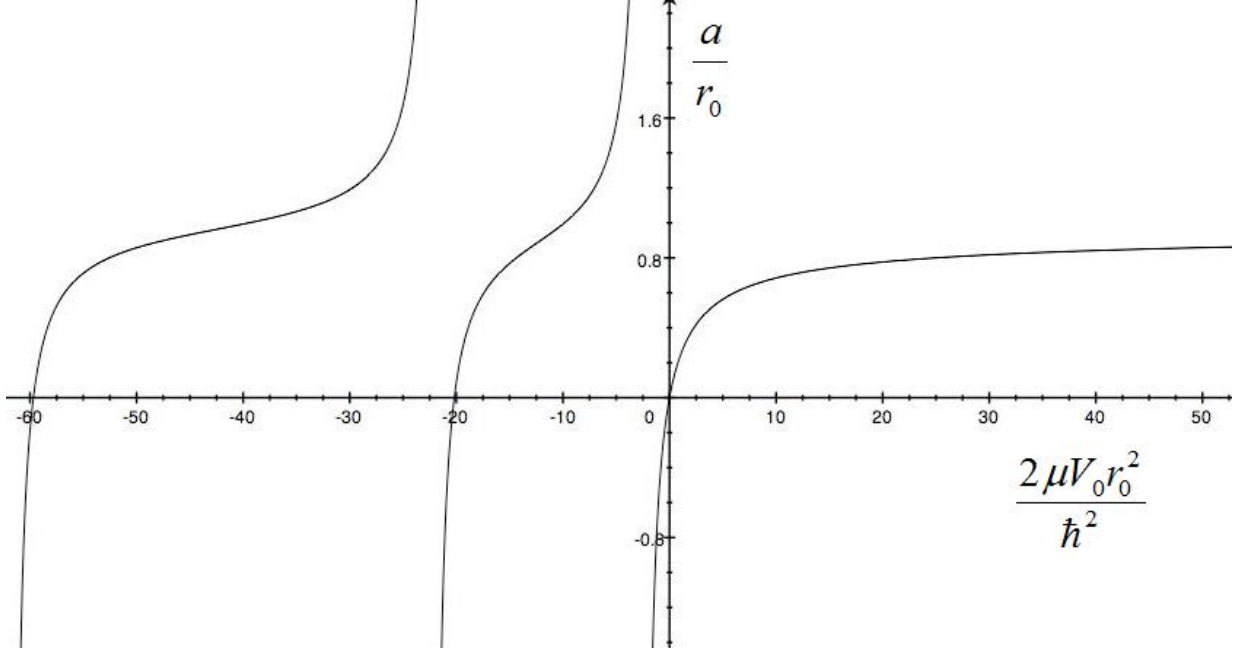
Equations (2.22) and (2.27) together give us the whole picture of a vs. V_0 , or rather, in a normalized way: a/r_0 vs. $2\mu V_0 r_0^2 / \hbar^2$. The graph is presented in Figure 2.2. Let's first note that as $V_0 \rightarrow \infty$, $\tanh(\kappa r_0) / \kappa r_0 \rightarrow 0$, and $a/r_0 \rightarrow 1$ in equation (2.22). This is the so-called Hard Sphere limit where the wavefunction is completely pushed out of the interaction potential and the scattering length is just the range of the interaction potential $a = r_0$. Near zero, i.e. $|V_0|$ is small, the relationship of a and V_0 is approximately linear, i.e.

$$\frac{a}{r_0} \cong \frac{2\mu r_0^2 V_0}{3\hbar^2} \quad (2.28)$$

which is also given by the Born Approximation at low energy [7]

$$a = -f(\theta, \phi) \cong \frac{\mu}{2\pi\hbar^2} \int V d\mathbf{r} = \frac{\mu}{2\pi\hbar^2} \frac{4}{3} \pi r_0^3 V_0 = \frac{2\mu r_0^3 V_0}{3\hbar^2} \quad (2.29)$$

Another very important feature is that $|a|$ diverges due to the $\tan(\kappa r_0)$ function and this divergence (resonance) region is repeated (although with different periods) as V_0 deepens. The resonance values of V_0 is thus $2\mu|V_0|r_0^2/\hbar^2 = (\pi/2 + n\pi)^2 = \pi^2(n + 1/2)^2$, $n = 0, 1, 2, 3, \dots$


 Figure 2.2: Scattering Length a vs. interaction strength V_0 in 3-dimensions.

Now we can repeat the above procedure to two interacting bosonic atoms in 1 dimension. The difference in the set-up of the problem includes, first of all, that there is no "s-wave" in 1D: the relative coordinate wavefunction ψ_μ has no "radial function $x\psi_\mu(x)$ "; it is simply itself. Another difference is that the interaction potential covers the spatial region from $-x_0$ to x_0 and the wavefunction does not have to vanish at $x = 0$. The Schrodinger's equation in 1D is

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + V(x) \right] \psi_\mu(x) = E \psi_\mu(x) \quad (2.30)$$

with

$$V(x) = \begin{cases} V_0 & |x| < x_0 \\ 0 & |x| > x_0 \end{cases} \quad (2.31)$$

considering the symmetry of bosonic wavefunction, we can simply solve the wavefunction inside and outside the interaction potential; let's first solve for the case where $V_0 \gg E_\mu > 0$,

$$\psi_\mu(x) \sim \begin{cases} \cosh(\kappa x) & |x| < x_0 \\ \sin(kx - \delta) & |x| > x_0 \end{cases} \quad (2.32)$$

again with

$$\kappa = \frac{\sqrt{2\mu(V_0 - E)}}{\hbar} \cong \frac{\sqrt{2\mu V_0}}{\hbar}, \quad k = \frac{\sqrt{2\mu E}}{\hbar} \quad (2.33)$$

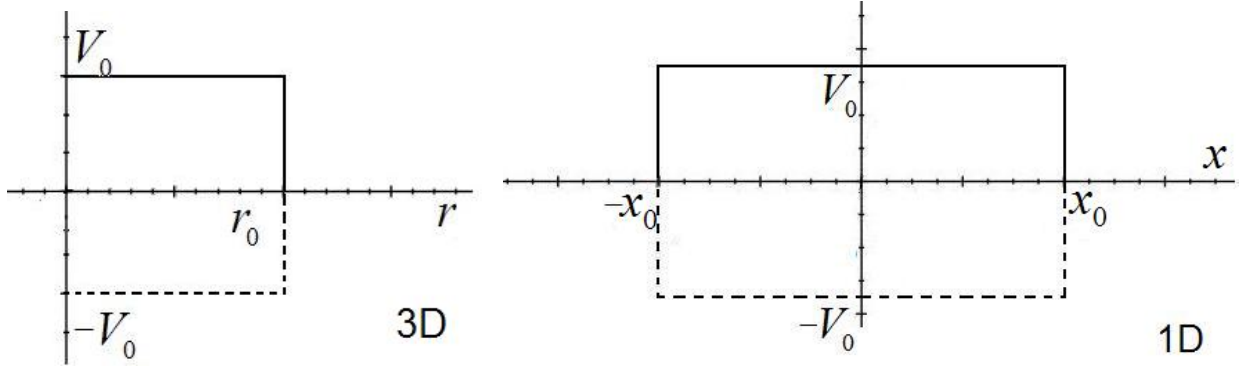


Figure 2.3: The square potentials in 3- and 1-dimensions. Solid line shows the square wall with height V_0 and dashed line shows the square well with depth V_0 . The 1-dimensional square potential is symmetric about the origin and therefore extends to negative values.

but the boundary conditions of continuity and continuous derivative at x_0 now yields

$$\tan(kx_0 - \delta) = \frac{k}{\kappa} \frac{1}{\tanh(\kappa x_0)} \quad (2.34)$$

which gives us the scattering length vs. interaction strength according to equation (2.16) ¹

$$\frac{a}{x_0} = 1 - \frac{1}{\kappa x_0 \tanh(\kappa x_0)} \quad (2.35)$$

And solve for $|V_0| \gg E_\mu > 0$ but $V_0 < 0$ case,

$$\psi_\mu(x) \sim \begin{cases} \cos(\kappa x) & |x| < x_0 \\ \sin(kx - \delta) & |x| > x_0 \end{cases} \quad (2.36)$$

the difference is again, inside the interaction potential, the wavefunction is a standing wave in essence instead of exponential decay. The boundary condition yields now

$$\tan(kx_0 - \delta) = -\frac{k}{\kappa} \frac{1}{\tan(\kappa x_0)} \quad (2.37)$$

which gives the relation of a vs V_0 for negative V_0

$$\frac{a}{x_0} = 1 + \frac{1}{\kappa x_0 \tan(\kappa x_0)} \quad (2.38)$$

¹Although equation (2.16) is obtained as a 3D example, but it is yet valid anywhere as long as phase shift exists; a more general derivation is in [6].

2.3. Scattering in Free Space: 3D and 1D Cases

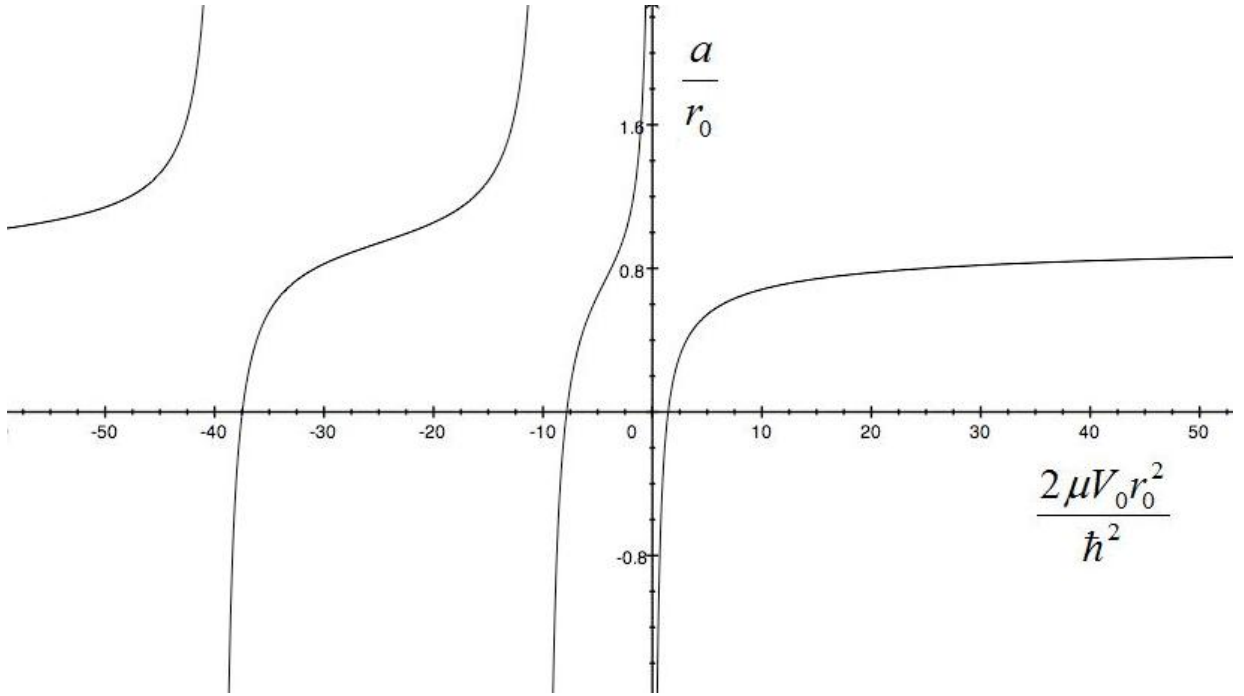


Figure 2.4: Scattering Length a vs. interaction strength V_0 in 1-dimension.

Equations (2.35) and (2.38) together gives us the whole picture of a vs V_0 in 1 dimension. We can observe there are several similarities between the a vs V_0 relations in 3D and 1D: they both have a hard sphere limit where $V_0 \rightarrow \infty$; scattering length a in each case diverges at certain finite value of V_0 : for 3D, $2\mu|V_0|r_0^2/\hbar^2 = \pi^2(n + 1/2)^2$, $n = 0, 1, 2, 3, \dots$ and for 1D, $2\mu V_0 x_0^2/\hbar^2 = (n\pi)^2$, $n = 0, 1, 2, 3, \dots$; and the resonance region appears repeatedly (again with different periods) as V_0 deepens. However, there is a significant difference between the two cases, that is, the Born Approximation limit. In 3D, scattering length is always positive for a repulsive interaction, but in 1D, very near zero, the scattering length not only diverges, but also changes sign and does not follow the Born Approximation.

The nature of this difference lies in how the system responds to perturbation in these two cases. Imagine two non-interacting atoms in a box and we turn on a square interacting potential as a small perturbation. Then perturbation theory is valid only if the ratio of the first order correction to the energy to the difference of energies between ground state and first excited state is very small, namely $E_0^{(1)}/\Delta E_{01} \ll 1$. In a 3D box with size L , the energy associated with each quantum state scales like $1/L^2$ (since momentum k scales like $1/L$), and the first order perturbation to the

energy scales like $1/L^3$ (the unit of the amplitude squared of the wavefunction in 3D is 1/volume, thus $E_0^{(1)} \sim \langle \psi | V_0 | \psi \rangle = V_0 \langle \psi | \psi \rangle$), thus $E_0^{(1)}/\Delta E_{01} \sim 1/L$, and as $L \rightarrow \infty$, perturbation theory becomes extremely accurate. However, in 1D the amplitude squared of the wavefunction scales like $1/L$, resulting that $E_0^{(1)}/\Delta E_{01} \sim L$, i.e. perturbation theory becomes invalid for $L \rightarrow \infty$. Therefore, since the energy shift is not perturbative, any small change in interaction between two atoms can result in very strong interaction between them, manifested in the divergence of the scattering length near zero.

2.4 Resonance and The Bound State

An interesting observation we have from the previous section is that V_0 has these resonance values at which $|a| \rightarrow \infty$: in 3D it is $2\mu V_0 r_0^2/\hbar^2 = -n^2\pi^2/4$ for $n = 1, 2, 3, \dots$ and in 1D it is $2\mu V_0 x_0^2/\hbar^2 = -(n-1)^2\pi^2$ for $n = 1, 2, 3, \dots$. Across these values of V_0 the scattering length first diverges to negative infinity, then comes back from positive infinity and then slowly comes to zero and repeat the whole process again. This is reflected in the graphical interpretation of the concept of scattering length, which is the intercept of the tangent line to the radial wavefunction at range r_0 (back in Figure 2.1, this process is partly shown): as most part of the radial wavefunction, $u(r)$, is outside the range r_0 , the slope of $u(r)$ at r_0 is positive and small, then as the body of $u(r)$ moves towards the interaction potential, this slope becomes more and more flat; when it is eventually flat, the intercept of the tangent line to the spatial axis can be thought of as being at positive and negative infinity, but as the tangent line keeps rotating, its slope becomes negative and intercepts the spatial axis at positive side, signally that most part of $u(r)$ is now inside the range r_0 . And as this whole resonance process happens when $V_0 < 0$, one may wonder what happens to the bound states, if any.

Now let's continue from the free space scattering situation in previous section and try to solve the problem of negative eigen-energy and look for possible bound states for $V_0 < 0$. Let's consider the 3D situation first and let $E < 0$ (and $|V_0| \gg |E|$), in order to satisfy radial equation, the radial wavefunction has the form

$$u(r) \sim \begin{cases} \sin(\kappa r) & 0 < r < r_0 \\ e^{-\kappa r} & r > r_0 \end{cases} \quad (2.39)$$

with

$$\kappa = \frac{\sqrt{2\mu(E - V_0)}}{\hbar} \cong \frac{\sqrt{2\mu|V_0|}}{\hbar}, \quad k = \frac{\sqrt{2\mu|E|}}{\hbar} \quad (2.40)$$

contrasting with equation (2.18) that the outside wavefunction is exponential decay instead of free sinusoidal wave, i.e. the very essence of a bound state. Posing again the continuity and continuous derivative boundary condition at range r_0 , we have the following quantization condition

$$\tan(\kappa r_0) = -\frac{\kappa}{k} \quad (2.41)$$

and if we express κ in terms of V_0 using equation (2.40) above, we have

$$\tan \sqrt{\frac{2\mu|V_0|r_0^2}{\hbar^2}} = \frac{\sqrt{\frac{2\mu|V_0|r_0^2}{\hbar^2}}}{-kr_0} \quad \text{or} \quad kr_0 = -\frac{\sqrt{2\mu|V_0|r_0^2/\hbar^2}}{\tan \sqrt{2\mu|V_0|r_0^2/\hbar^2}} \quad (2.42)$$

which gives us the value of the bound state energy for a given value of V_0 : notice that for $2\mu|V_0|r_0^2/\hbar^2$ in the range from zero to $\pi^2/4$, the value of k is negative, i.e. there is no bound state; when $2\mu|V_0|r_0^2/\hbar^2 = \pi^2/4$, k is zero and a bound state is "born" (notice that above equation reproduces the resonance values of V_0 where scattering length diverges, as predicted by equation (2.27), bottom of page 10); lastly for $2\mu|V_0|r_0^2/\hbar^2$ slightly larger than $\pi^2/4$, k is positive. So let's expand the above expression around $2\mu|V_0|r_0^2/\hbar^2 = \pi^2/4$, say $2\mu|V_0|r_0^2/\hbar^2 = \pi^2/4 + \epsilon$

$$\begin{aligned} \tan \sqrt{\frac{\pi^2}{4} + \epsilon} &= \frac{\sqrt{\frac{\pi^2}{4} + \epsilon}}{-kr_0} \Rightarrow \tan\left(\frac{\pi}{2} + \frac{\epsilon}{\pi}\right) \cong \frac{\frac{\pi}{2} + \frac{\epsilon}{\pi}}{-kr_0} \\ &\Rightarrow -\cot \frac{\epsilon}{\pi} \cong \frac{\frac{\pi}{2} + \frac{\epsilon}{\pi}}{-kr_0} \\ &\Rightarrow kr_0 \cong \frac{\epsilon}{2} \end{aligned} \quad (2.43)$$

Now on the other hand, recall equation (2.27) gives the a vs. V_0 relation, we can now expand a around $2\mu|V_0|r_0^2/\hbar^2 = \pi^2/4 + \epsilon$, then

$$\frac{a}{r_0} = 1 - \frac{\tan \sqrt{\frac{\pi^2}{4} + \epsilon}}{\sqrt{\frac{\pi^2}{4} + \epsilon}} \cong 1 - \frac{\tan(\frac{\pi}{2} + \frac{\epsilon}{\pi})}{\frac{\pi}{2} + \frac{\epsilon}{\pi}} \cong 1 + \frac{\cot \frac{\epsilon}{\pi}}{\pi/2} \cong 1 + \frac{2}{\epsilon} \cong \frac{2}{\epsilon} \quad (2.44)$$

and combining (2.43) and (2.44), we have

$$k \cong \frac{1}{a} \quad (2.45)$$

in other words, the bound state energy is effectively

$$E \cong \frac{\hbar^2}{2\mu} \frac{1}{a^2} \quad (2.46)$$

Physically, the significance of $k \cong 1/a$ is that the radial wavefunction outside becomes $u(r) \sim e^{-r/a}$, which describes a *diatomic molecule*, or a dimer: two atoms separated over long distance in a weakly bounded state, and its momentum (thus energy) is dominantly described by the inverse of the scattering length alone.

We can apply the above procedure to the 1-dimensional case as well. For $E < 0$ and $|V_0| \gg |E|$, the wavefunction is

$$\psi(x) \sim \begin{cases} \cos(\kappa x) & -x_0 < x < x_0 \\ e^{-kx} & x > x_0 \\ e^{kx} & x < -x_0 \end{cases} \quad (2.47)$$

with

$$\kappa = \frac{\sqrt{2\mu(E - V_0)}}{\hbar} \cong \frac{\sqrt{2\mu|V_0|}}{\hbar}, \quad k = \frac{\sqrt{2\mu|E|}}{\hbar} \quad (2.48)$$

a patching boundary condition gives a similar quantization to (2.41)

$$k = \kappa \tan(\kappa x_0) \quad (2.49)$$

and again we expand around the resonance value $2\mu|V_0|x_0^2/\hbar^2 = 0$ and let $2\mu|V_0|x_0^2/\hbar^2 = \epsilon$, then above equation becomes

$$kx_0 = \epsilon \tan \epsilon \cong \epsilon^2 \quad (2.50)$$

and use (2.38) to get a in this expansion

$$\frac{a}{x_0} = 1 + \frac{1}{\epsilon \tan \epsilon} \cong 1 + \frac{1}{\epsilon^2} \cong \frac{1}{\epsilon^2} \quad (2.51)$$

combining (2.50) and (2.51)

$$k \cong \frac{1}{a} \quad (2.52)$$

thus again we recovered this relation similarly found in (2.45). So the 1-dimensional dimer molecule near the resonance also has this binding energy large dependent on scattering length alone

$$E \cong \frac{\hbar^2}{2\mu} \frac{1}{a^2} \quad (2.53)$$

Chapter 3

Energy Spectrum for Harmonic Confinement

3.1 The Schrodinger's Equation

Now we consider a 3-dimensional isotropic harmonic well as a confinement of the two interacting atoms. The motivation for this set-up is that it is a very good model to the modern laser traps. Thus this chapter is devoted to an effective model to the realistic experimental situation of trapped interacting ultracold bosonic atoms in optical lattices, and through Feshbach resonance scattering, their interaction is tunable. We consider the trapped atomic gas is so dilute that there are no more than two atoms per cell, hence our set-up of two interacting ultracold atoms in a isotropic 3-dimensional harmonic well.

Since all the assumptions summarized in Section 2.1 are met, our main task is then to solve equation (2.8). The relative coordinate trapping potential is found first by looking at

$$V_{trap} = \frac{1}{2}m_1\omega^2r_1^2 + \frac{1}{2}m_2\omega^2r_2^2 \quad (3.1)$$

then after centre-of-mass transformation,

$$V_{trap} = \frac{1}{2}M\omega^2R^2 + \frac{1}{2}\mu\omega^2r^2 \quad (3.2)$$

therefore, the $V_{trap}(r)$ term in equation (2.8) is

$$V_{trap}(r) = \frac{1}{2}\mu\omega^2r^2 \quad (3.3)$$

rewriting (2.8) as follows

$$\left[-\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} + \frac{1}{2}\mu\omega^2r^2 + V_{12}(r) \right] u(r) = E_\mu u(r) \quad (3.4)$$

3.2. Boundary Conditions

where recall $u(r) = r\psi(r)$ is the radial wavefunction, and V_{12} is again the square interaction defined as equation (2.9). Employing the convention of harmonic oscillator units, namely letting new spatial variable $x = r/(\sqrt{\hbar/\mu\omega})$ and energy $\eta = 2E_\mu/\hbar\omega$, then equation (3.4) readily changes to

$$\left[-\frac{d^2}{dx^2} + x^2 + V_{12}(x) \right] u(x) = \eta u(x) \quad (3.5)$$

with square interaction

$$V_{12}(x) = \begin{cases} 2V_0/\hbar\omega & \text{for } 0 < x < x_0 \\ 0 & \text{for } x > x_0 \end{cases} \quad (3.6)$$

where $x_0 = r_0/(\sqrt{\hbar/\mu\omega})$.

3.2 Boundary Conditions

To tackle the problem posed by equation (3.5), we first see that for a general solution satisfying differential equation (3.5), boundary conditions are needed in order to obtain exact quantization of energy. So aside from the usual normalization boundary condition that wavefunction has to vanish at infinite distances, there is also some boundary condition set by the interaction potential V_{12} near zero, and the whole existence of this V_{12} term is to impose that condition.

An immediate idea that follows is that, since we devoted Chapter 2 on the relation between the s -wave scattering length and the interaction potential, we can somehow relate the interaction potential here with the scattering length. And that is, the very definition of scattering length from equation (2.15) (in new variable x)

$$\lim_{k \rightarrow 0} \frac{u'(0)}{u(0)} = -\frac{1}{a} \quad (3.7)$$

which is precisely a (mixed) boundary condition for solution $u(x)$ set by interaction potential V_{12} (since a sets V_{12}).

Another way of looking at how we can obtain this boundary condition is the δ -pseudo-potential method where we replace V_{12} by an effective potential involving a regularized Dirac- δ function [8]. Physically to justify the effectiveness of the δ potential (also known as a zero-range or contact

3.2. Boundary Conditions

potential), we firstly have the low energy limit where large de Broglie wavelengths result in poor resolution, therefore the object atoms scatter off are essentially point-like. Furthermore, we can see the interaction range r_0 is much smaller than the harmonic oscillator length $\sqrt{\hbar/\mu\omega}$ (or equivalently $x_0 \ll 1$) for our experimental setting: the cold atom interaction is dominated by van der Waals potentials with range on the order of angstroms, whereas the smallest optical traps have frequencies on the order of 100 kHz, corresponding to a harmonic oscillator length on the order of 100 nm. And the "strength" of the δ potential is represented by a factor in front of the δ -function.

So mathematically, we recall the original Schrodinger's equation in relative coordinate (equation (2.5))

$$\left[-\frac{\hbar^2}{2\mu}\nabla_r^2 + \frac{1}{2}\mu\omega^2 r^2 + V_{12}(r) \right] \psi(r) = E_\mu \psi(r) \quad (3.8)$$

and we replace the interaction potential by the effective potential

$$V_{12}(x) \rightarrow \frac{2\pi a \hbar^2}{\mu} \delta^3(r) \frac{\partial}{\partial r} r \quad (3.9)$$

where $\delta^3(r)$ is the 3-dimensional Dirac- δ function and the $\frac{\partial}{\partial r} r$ term is there to make the Hamiltonian self-adjoint, thus the term "regularized" [8]. Then what we can do to the new differential equation

$$\left[-\frac{\hbar^2}{2\mu}\nabla_r^2 + \frac{1}{2}\mu\omega^2 r^2 + \frac{2\pi a \hbar^2}{\mu} \delta^3(r) \frac{\partial}{\partial r} r \right] \psi(r) = E_\mu \psi(r) \quad (3.10)$$

is to integrate both sides over a small sphere in space with radius going to the limit of zero, upon which the right hand side of the equation and the $\frac{1}{2}\mu\omega^2 r^2$ term on the left go to zero, and we are left with is

$$\int \nabla \cdot \nabla \psi(r) d^3 \mathbf{r} = 4\pi a \int \delta^3(r) \frac{\partial}{\partial r} (r\psi(r)) d^3 \mathbf{r} \quad (3.11)$$

by divergence law from calculus we have

$$\oint \nabla \psi(r) \cdot d\mathbf{A} = 4\pi a \frac{\partial}{\partial r} (r\psi(r))_{r=0} = 4\pi a u'(0) \quad (3.12)$$

and as the radius goes to zero, the closed integral over the surface of the sphere becomes

$$\oint \nabla \psi(r) \cdot d\mathbf{A} = \oint \frac{\partial}{\partial r} \psi(r) dA = \oint \left(-\frac{u(r)}{r^2} + \frac{u'(r)}{r} \right) dA = 4\pi r^2 \left(-\frac{u(0)}{r^2} \right) = -4\pi u(0) \quad (3.13)$$

equating to the right hand side of (3.12) gives us

$$\frac{u'(0)}{u(0)} = -\frac{1}{a} \quad (3.14)$$

Therefore, the δ -pseudo-potential is a good effective potential to our square interaction as long as the range of the interaction is much smaller than the harmonic oscillator length and the scattering is kept at low energy, then the effective potential reproduces the same boundary condition (3.7) as the definition of the scattering length.

3.3 Energy Spectrum

So continuing from previous section, we have had two boundary conditions for the solution to the differential equation (3.5), namely $u(x) \rightarrow 0$ as $x \rightarrow \infty$ and the mixed one in equation (3.7). Now let's look at what general solution we have for (3.5) outside the interaction range x_0 . Outside x_0 , we want to solve for $u(x)$ in

$$\left[-\frac{d^2}{dx^2} + x^2 \right] u(x) = \eta u(x) \quad (3.15)$$

Motivated by the classical textbook problem on solving harmonic oscillator eigenstates, we factor out a Gaussian term from $u(x)$ and let $u(x) = e^{-x^2/2} w(x)$, then we have a new equation for $w(x)$

$$\left[-\frac{d^2}{dx^2} + 2x \frac{d}{dx} + 1 \right] w(x) = \eta w(x) \quad (3.16)$$

and changing variable $y = x^2$, thus letting $d/dx = (dy/dx)(d/dy)$ changes above equation to the so-called confluent hypergeometric equation (or sometimes called Kummer's equation) [9]

$$y \frac{d^2 w}{dy^2} + \left(\frac{1}{2} - y \right) \frac{dw}{dy} - \frac{1-\eta}{4} w = 0 \quad (3.17)$$

with parameters $c = \frac{1}{2}$ and $b = \frac{1-\eta}{4}$. The solutions of the confluent hypergeometric equation are given by two linearly independent confluent hypergeometric functions [9],

3.3. Energy Spectrum

$$F(b, c; y) = \sum_{n=0}^{\infty} \frac{(b)_n y^n}{(c)_n n!} \quad \text{and} \quad G(b, c; y) = y^{1-c} F(b - c + 1, 2 - c; y) \quad (3.18)$$

where $(b)_n$ denotes the forward factorial $(b)_n := b(b+1)(b+2)\dots(b+n-1)$ with $(b)_0 = 1 \forall b$. And G is a solution only when parameter c is not an integer [9](which is true our case, $c = 1/2$). So writing out the solution for $w(y(x))$ in linear combinations of F and G

$$\begin{aligned} w(x) &= C_1 F\left(\frac{1-\eta}{4}, \frac{1}{2}; x^2\right) + C_2 (x^2)^{1-\frac{1}{2}} F\left(\frac{1-\eta}{4} - \frac{1}{2} + 1, 2 - \frac{1}{2}; x^2\right) \\ &= C_1 F\left(\frac{1-\eta}{4}, \frac{1}{2}; x^2\right) + C_2 x F\left(\frac{3-\eta}{4}, \frac{3}{2}; x^2\right) \end{aligned} \quad (3.19)$$

so

$$u(x) = e^{\frac{-x^2}{2}} \left[C_1 F\left(\frac{1-\eta}{4}, \frac{1}{2}; x^2\right) + C_2 x F\left(\frac{3-\eta}{4}, \frac{3}{2}; x^2\right) \right] \quad (3.20)$$

Applying the boundary condition in (3.7) immediately gives us a relation between constants C_1 and C_2

$$-\frac{1}{a} = \frac{u'(x=0)}{u(x=0)} = \frac{C_2 F\left(\frac{3-\eta}{4}, \frac{3}{2}; 0\right) \frac{dx}{dr}}{C_1} = \frac{C_2}{C_1} \frac{1}{\sqrt{\hbar/\mu\omega}} \quad (3.21)$$

where $F(b, c, 0) = 1 \forall b, c$ by the definition of F in (3.18). Whereas the condition to require $u \rightarrow 0$ as $x \rightarrow \infty$ is bit complicated: we look at the asymptotic behaviour of $F(b, c; y)$ for large y

$$F(b, c; y) \sim \frac{\Gamma(c)}{\Gamma(b)} y^{b-c} e^y \quad (3.22)$$

with the usual Γ -function. By this, we see at large x ,

$$\begin{aligned} u(x) &\sim e^{x^2 - \frac{x^2}{2}} \left[C_1 \frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{1-\eta}{4})} (x^2)^{\frac{1-\eta}{4} - \frac{1}{2}} + C_2 x \frac{\Gamma(\frac{3}{2})}{\Gamma(\frac{3-\eta}{4})} (x^2)^{\frac{3-\eta}{4} - \frac{3}{2}} \right] \\ &= e^{\frac{x^2}{2}} x^{\frac{-1-\eta}{2}} \left[C_1 \frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{1-\eta}{4})} + C_2 \frac{\Gamma(\frac{3}{2})}{\Gamma(\frac{3-\eta}{4})} \right] \rightarrow 0 \end{aligned} \quad (3.23)$$

only if

$$C_1 \frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{1-\eta}{4})} + C_2 \frac{\Gamma(\frac{3}{2})}{\Gamma(\frac{3-\eta}{4})} = 0 \quad (3.24)$$

or

$$\frac{C_1}{C_2} = -\frac{\Gamma(\frac{3-\eta}{4})\Gamma(\frac{1}{2})}{\Gamma(\frac{1-\eta}{4})\Gamma(\frac{3}{2})} = -\frac{\Gamma(\frac{3-\eta}{4})\sqrt{\pi}}{\Gamma(\frac{1-\eta}{4})\sqrt{\pi}/2} = -2 \frac{\Gamma((3-\eta)/4)}{\Gamma((1-\eta)/4)} \quad (3.25)$$

3.3. Energy Spectrum

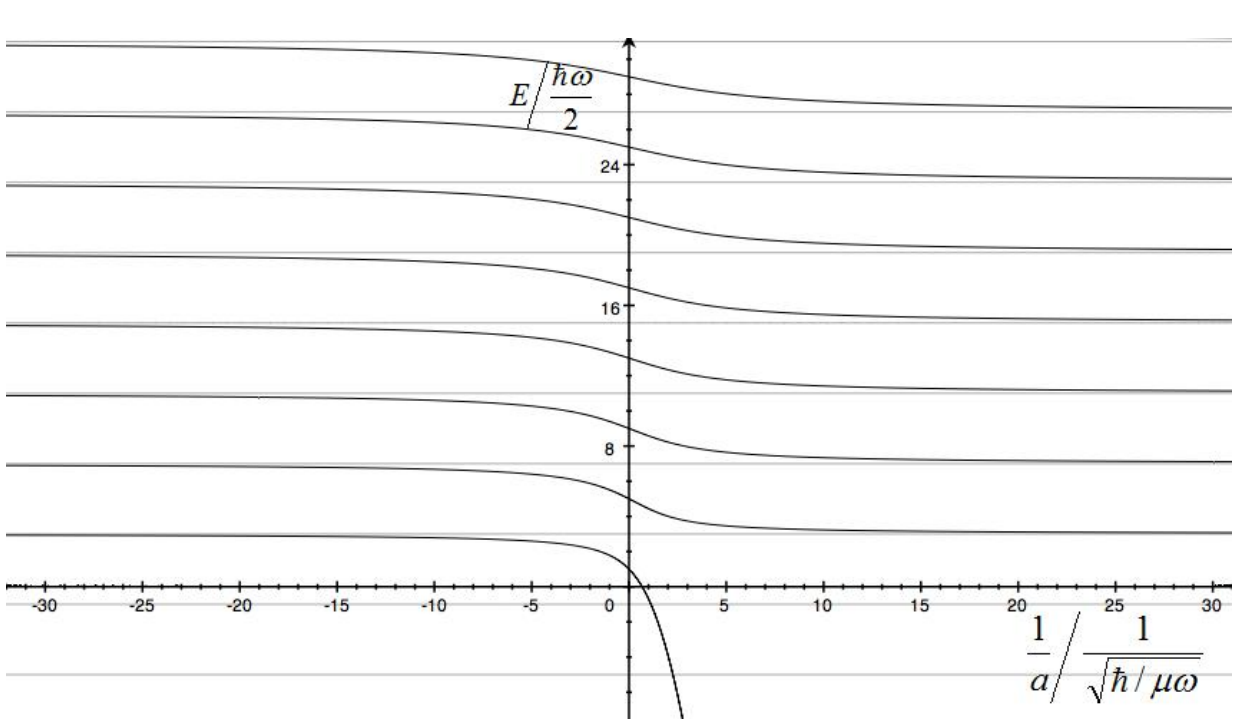


Figure 3.1: The s -state energies of two bosonic atoms interacting through a square potential with scattering length a , inside a 3-dimensional isotropic harmonic well with frequency ω . The darker lines are the energy levels in the harmonic oscillator energy unit vs. the inverse of the scattering length in the unit of the inverse of the harmonic oscillator length; shadowed lines are asymptotic values $E = (\frac{1}{2} + n)\frac{\hbar\omega}{2}$, $n = 1, 3, 5, 7, \dots$

Combining (3.25) above with (3.21), we have

$$\frac{\sqrt{\hbar/\mu\omega}}{a} = 2 \frac{\Gamma((3-\eta)/4)}{\Gamma((1-\eta)/4)} \quad (3.26)$$

or more clearly,

$$\frac{\sqrt{\hbar/\mu\omega}}{a} = 2 \frac{\Gamma((3 - \frac{2E}{\hbar\omega})/4)}{\Gamma((1 - \frac{2E}{\hbar\omega})/4)} \quad (3.27)$$

which is the quantization of energy (and is also theoretically obtained by some previous papers [8], [10], [11]). In Figure 3.1, the s -state energy levels are plotted according to equation (3.27) in the harmonic oscillator energy unit ($\hbar\omega/2$) against the inverse of the scattering length in the unit of the inverse of the harmonic oscillator length ($1/\sqrt{\hbar/\mu\omega}$). This is the most important graph for this Chapter, and it has several interesting features:

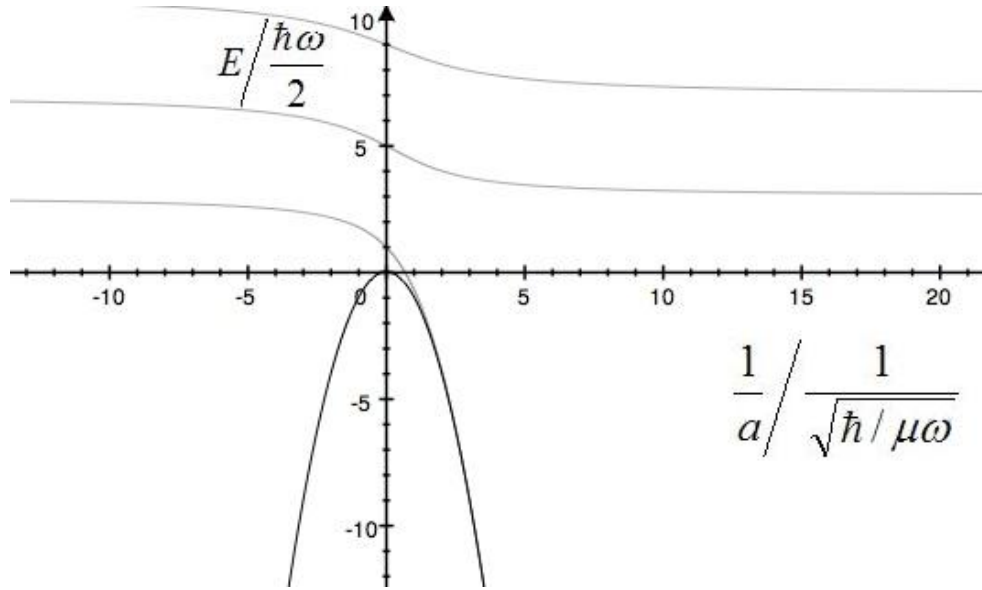


Figure 3.2: The scaling property of the bound state energy (negative in sign), comparing to the function of quadratic dependence in the graph units (darker curve).

- Universality: the energy spectrum is dependent on the inverse of the scattering length alone. The details of the interaction potential is not concerned.
- Equally spaced energy levels at resonance ($1/a = 0$): a special feature of energy spectrum to the harmonic oscillator. The energies are calculated by the zeros of equation (3.27), which is equivalent to solving $\Gamma((1 - \frac{2E}{\hbar\omega})/4) = 0$. Since the zeros of the Γ -function are negative integers, say $-m$, $m = 1, 2, 3, \dots$, then we have energies $E = (4n + 1)\frac{\hbar\omega}{2}$, $n = 0, 1, 2, 3, \dots$. This equally spaced spectrum implies the system is still harmonic at resonance even though there is a strong interaction between the two atoms.
- Forming of a bound state and the binding energy: reproduced as shown in Section 2.4. As the scattering length a is positive and very large, corresponding to $1/a$ is small and positive, there is bound state with energy scaling like $1/a^2$, shown in Figure 3.2, where the parabolic function is $E = \frac{\hbar^2}{2\mu} \frac{1}{a^2}$. This also reconfirms what we saw in Section 2.4, that as we increase the well depth V_0 across each resonance value, $1/a$ goes across the origin from negative to positive values, and a bound state forms.

3.3. Energy Spectrum

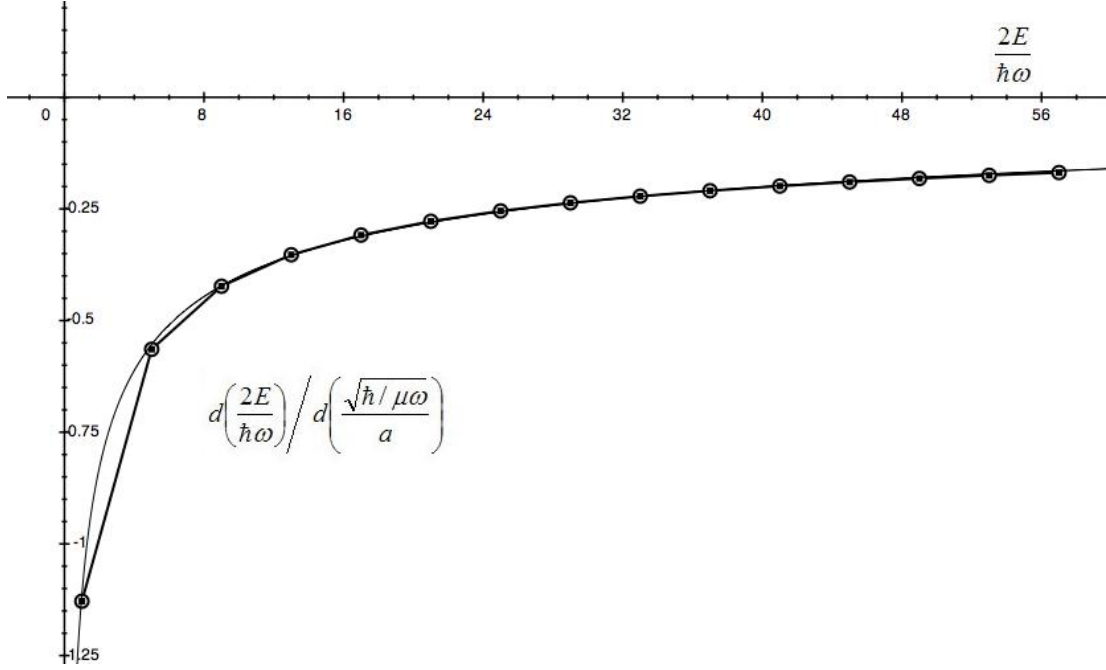


Figure 3.3: The numerical values of the derivatives of each energy level in harmonic oscillator unit with respect to $1/a$ at resonance $1/a = 0$; graph shows first 15 levels.

- Energy shifts from $a = 0$ to $a = \infty$: in both cases the energy levels are equally spaced. At $a = 0$, there is no interaction, the energy spectrum is merely the one for the harmonic oscillator but with only half of the spatial axis (r can't be negative), which corresponds to the well known harmonic oscillator spectrum with only odd quantum numbers, namely, $E = (\frac{1}{2} + n)\frac{\hbar\omega}{2}$, $n = 1, 3, 5, 7, \dots$. When $a = \infty$, the energies are $E = (4n + 1)\frac{\hbar\omega}{2}$, $n = 0, 1, 2, 3, \dots$, thus giving the uniform energy shifts for each state, with value $\hbar\omega$.
- Anharmonicity: the interaction introduces anharmonicities slightly away from resonance shown by the first derivative of the energy with respect to $1/a$ at $1/a = 0$ (Figure 3.3). A computer interpolation shows the derivatives approach zero at a rate of $(2E/\hbar\omega)^{-0.4065}$ as $(2E/\hbar\omega)$ takes discrete values 1, 5, 9, .. in Figure 3.1. The derivatives of each energy level with respect to $1/a$ at resonance ($1/a = 0$) are not equal, thus when $1/a$ is slightly away from zero the energy spectrum is no longer harmonic (equally spaced). The anharmonicities imply an analog to the classical damping to the quantum harmonic motion: for a coherent

quantum state, at resonance, oscillating in time between these equally spaced energy levels, when we slightly shift the scattering length away from resonance, the energy levels are no longer equally spaced and thus causes the coherent quantum state to dephase, resulting in the coherent state finally collapsing to one energy state (decoherence) after certain dephasing time. The decay rate of the derivatives in Figure 3.3 may be of future use to determine the change in this dephasing time for higher energy levels, since their change in energy with respect to inverse of the scattering length slightly away from zero is small (and asymptotically approaching zero).

Finally, we look back to the assumption we made to solve this energy spectrum in order to verify the validity range to which the spectrum is effectively correct. The short range (comparing to harmonic oscillator length) of the interaction has already been justified by order-of-magnitude comparison with actual experimental facts (Section 3.2). As of the low energy limit, where we required the de Broglie wavelength $(2\pi)/k \gg r_0$, we can estimate an appropriate bound for k : say $r_0 = 1$ nm (since r_0 is on the order of angstroms), then our result is valid for $2E/\hbar\omega \ll 10^4$, which is much larger than the top of our graph in Figure 3.1, where $2E/\hbar\omega$ is only around 30.

3.4 Harmonic Well in 1D

Here we briefly look at the case of the same scenario as previous sections but in a harmonic confinement in 1-dimension. The Schrodinger's equation in 1D is

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dx^2} + \frac{1}{2}\mu\omega^2 x^2 + V_{12}(x) \right] \psi_\mu(x) = E_\mu \psi_\mu(x) \quad (3.28)$$

which is exactly in the same form as equation (3.4), but with the relative coordinate wavefunction here instead of the radial wavefunction, and with variable x instead of r (here x is the 1D spatial variable, not the same as the r dressed in harmonic oscillator unit in previous sections). The square interaction $V_{12}(x)$ is now extended to 1D as Figure 2.3 showed.

3.4. Harmonic Well in 1D

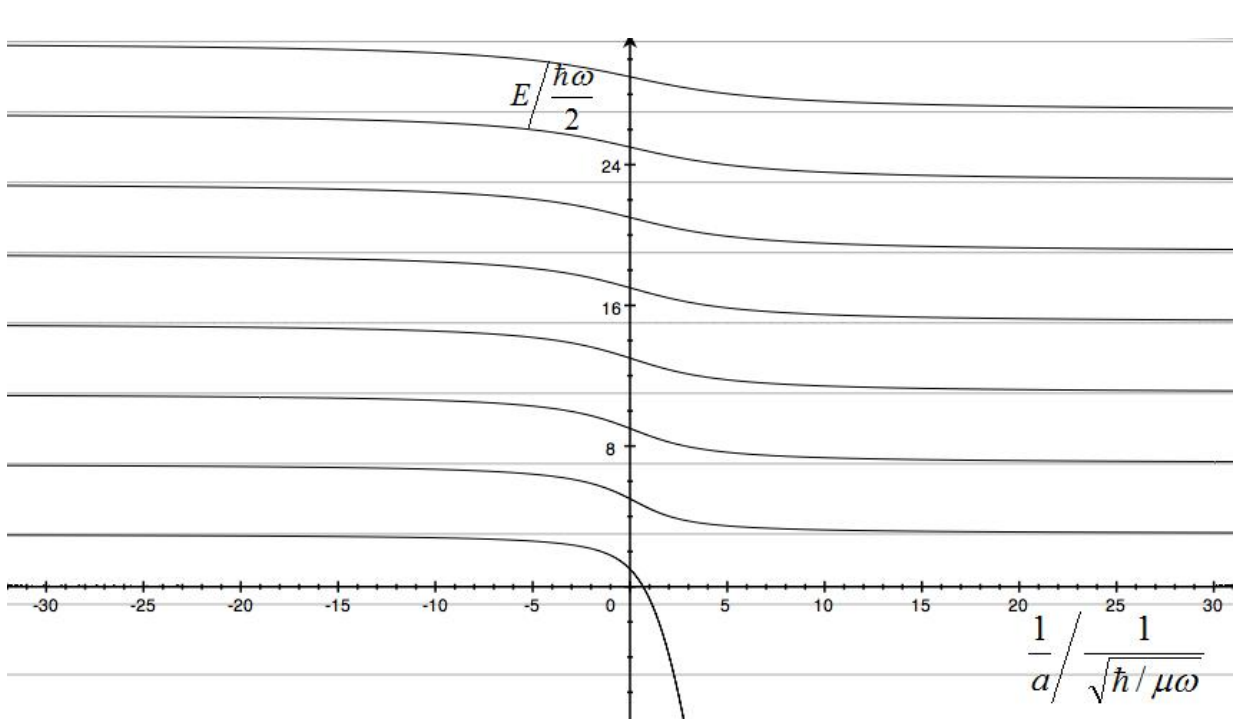


Figure 3.4: The energies of two bosonic atoms interacting through a square potential with scattering length a , inside a 1-dimensional harmonic well with frequency ω .

Now notice that we still have the boundary condition relating to the scattering length specified by equation (3.7). The general solution to the Schrodinger's equation (in harmonic oscillator units again) again involves the linear combination of confluent hypergeometric function (equation (3.20) but for $\psi_\mu(x)$ instead of $u(x)$). Now to require normalization condition for $\psi_\mu(x)$, we need it to go to zero at both ∞ and $-\infty$. However, since we are looking at bosonic atoms, the relative coordinate wavefunction is of even parity (also reflected in the solution involving the confluent hypergeometric functions of x^2). Thus, the negative side normalization is naturally taken care of by the requirement on the positive side. Apply the same procedure in Section 3.3 to the Schrodinger's equation in this 1D case, and we then have exactly the same quantization of energy condition as equation (3.27) and same plot (Figure 3.4).

However, even with the same energy spectrum, the 3D and 1D systems have very different behaviours near the non-interacting point (i.e. the point when we first turn on a non-zero interaction between the two atoms), because with no interaction ($V_0 = 0$), the 1D case is already at resonance (i.e. $1/a = 0$) but the 3D case is not. The scaling for the correction to the energy

3.4. Harmonic Well in 1D

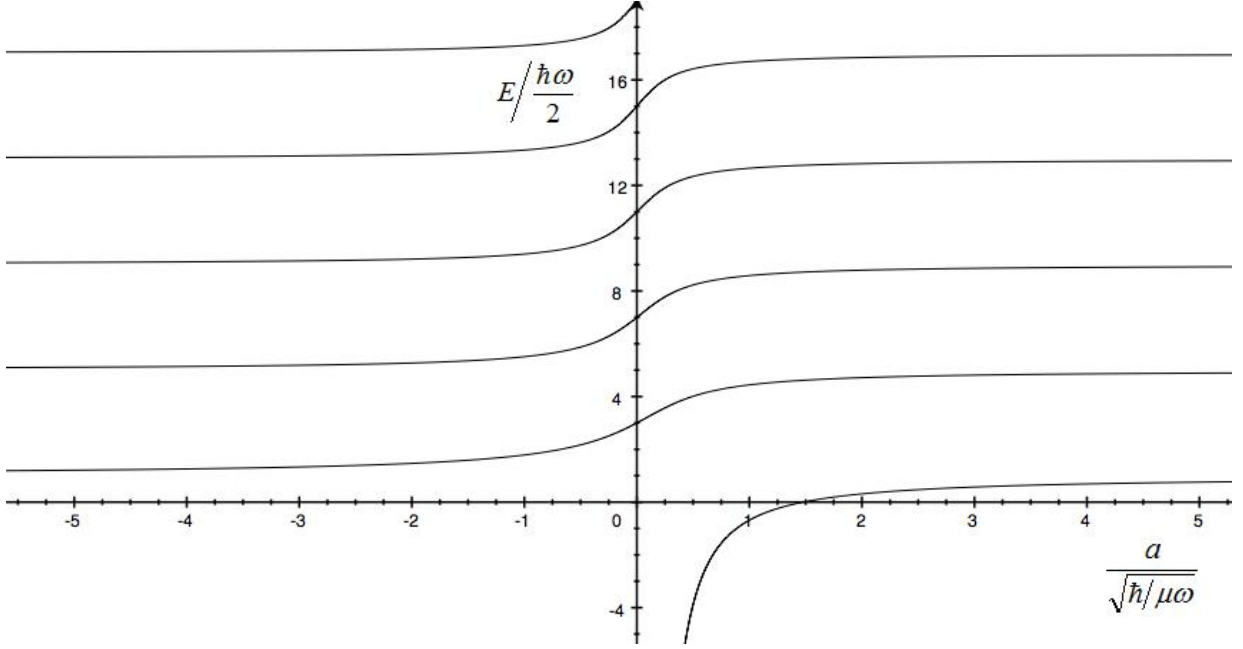


Figure 3.5: The s -state energies of two bosonic atoms interacting through a square potential with scattering length a , inside a 3-dimensional isotropic harmonic well with frequency ω . The energies are plotted against a .

in 1D is like $\langle \psi_n | V_0 | \psi_n \rangle_{1D} \sim V_0 \sim -1/a$ where $V_0 \sim -1/a$ as Figure 2.4 showed. So near the non-interacting point where $V_0 = 0$, i.e. $1/a = 0$, the derivative of the energy with respect to $1/a$ is negative, which is consistent with Figure 3.4. In 3D, the energy correction scaling behaviour near non-interacting point is different: the correction is proportional to a , specifically, $\langle \psi_n | V_0 | \psi_n \rangle_{3D} \sim V_0 \sim a$, where $V_0 \sim a$ as in Born approximation; thus when $V_0 = 0$, $a = 0$, so the scaling of the correction energy is an expansion around $a = 0$. This is directly seen if we re-plot Figure 3.1 with E vs. a (Figure 3.5): the derivative of the energy with respect to scattering length a at $a = 0$ is positive.

Chapter 4

Conclusion

In conclusion, let's summarize the main points discussed in this research project. We started out by looking at the 3-dimensional two-body quantum mechanical problem of interacting atoms in the context of ultracold limit, where we pose the Schrodinger's equation for their eigen-energies. We use the low energy scattering limit and approximate the interaction of the ultracold atoms by an isotropic square potential with finite range and a variable strength which can be either repulsive or attractive. By the classic change of reference frame transformation to the centre of mass coordinate and relative coordinate, the two-body problem is effectively reduced to a one-body quantum scattering problem with the interaction potential as the scattering centre.

We then turn to the scattering of the two atoms in free space without any confinement, where of course the reduced one-body scattering problem applies. In this context the concept of *s*-wave scattering length is introduced and several properties, such as its sign and scale, are discussed. Then by solving the Schrodinger's equation and apply patching boundary conditions at the range of interaction, we obtain the relation between the scattering length and the interaction strength; the results in 3-dimensions and 1-dimension are compared and contrasted. An interesting feature of a bound state, also known as the di-atomic molecular state, that comes into existence near resonance, is presented, and its binding energy in terms of the scattering length is calculated.

Then we looked at a specific confinement for the two interacting atoms, namely a 3-dimensional isotropic harmonic well. We discussed in detail the boundary conditions for the problem and solved its *s*-state energy spectrum, which is effectively the complete spectrum in the ultracold limit, in terms of the scattering length as a parameter alone. The universal energy spectrum has several interesting properties including the harmonicity at resonance, the anharmonicity away but near resonance, and the forming of the bound state and its scaling property in terms of scattering length near resonance as shown in previous sections.

Continuing from the results of this project, the future work may include several aspects of the dynamics of the system near resonance, which may be explored by considering the anharmonicity when the system is slightly away from the resonance, causing the classical analogue of damping. When some parameter varies with time, interesting dynamical properties can also be derived; for example the harmonic oscillator frequency ω may vary with time, with applications to the situation where the harmonic trap is turned off slowly in time such that $\omega(t) \rightarrow 0$ as time goes on [12]. Similar discussions may also apply to fermionic atoms where the universal properties should also apply; technical differences include the partial wave approximation and the requirement on the symmetry of two-body wavefunctions, where the complete energy spectrum may apply to bosonic atoms occupying the energy states with even-parity wavefunctions, and fermionic atoms occupying the states with odd-parity wavefunctions.

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