Quantum Mechanical Scattering and Feshbach Resonance

by

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Declaration

This dissertation entitled "Quantum Mechanical Scattering and Feshbach Resonsnce" has been prepared by Mr. Ravi Mohan in partial fulfilment for the award of the degree of Integrated Master of Science in Physics from IIT Roorkee

The dissertation is composed of original research work. Wherever contributions of others are involved, every effort is made to indicate this clearly, with due reference to the literature, and acknowledgement of collaborative research and discussions.

The work was done under the guidance of Professor G. S. Singh, at Indian Institute of Technology Roorkee, Roorkee.

(Ravi Mohan)

Place: Roorkee
Date: April 30, 2014

In my capacity as supervisor of the candidate's thesis, I certify that the above statements are true to the best of my knowledge.

(G. S. Singh)

Place: Roorkee
Date: April 30, 2014

Certificate

This is to certify that the project report entitled "Quantum Mechanical Scattering and Feshbach Resonsnce", prepared by Mr. Ravi Mohan, in partial fulfilment for the award of degree of Integrated Master of Science in Physics from IIT Roorkee is a record of his own work carried out under my advice and guidance.

(G. S. Singh)

Place: Roorkee
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Abstract

Feshbach resonances are the essential tool to control the interaction between atoms in ultracold quantum gases. They have found numerous experimental applications, opening up the way to important breakthroughs and facilitating the study of quantum mechanical phenomena.

This dissertation reports the analytical investigation of magnetically tuned Feshbach resonance with two coupled channels in harmonic oscillator potential.

Chapter 1

Introduction

In the field of physics, a Feshbach resonance, named after Herman Feshbach, is a feature of many-body systems in which a bound state is achieved if the coupling(s) between at least one internal degree of freedom and the reaction coordinates which lead to dissociation vanish. The opposite situation, when a bound state is not formed, is a shape resonance.

The impact of ultracold atomic and molecular quantum gases on present-day physics is linked to the extraordinary degree of control that such systems offer to investigate the fundamental behavior of quantum matter under various conditions. The interest goes beyond atomic and molecular physics, reaching far into other fields, such as condensed matter and few- and many-body physics. In all these applications, Feshbach resonances represent the essential tool to control the interaction between the atoms, which has been the key to many breakthroughs [6].

Chapter 2

Time-independent Scattering

The time evolution of a state vector $|\Psi(t)\rangle$ is given by the Schrödinger equation

$$i\hbar \frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle, \tag{2.1}$$

where $\hat{H}$ is the Hamiltonian of the system. According to the spectral theorem[3], the state vector $|\Psi(t)\rangle$ can be expanded in the energy basis (eigen-vectors of the Hamiltonian operator)

$$|\Psi(t)\rangle = \sum_n C_n(t)|\mathit{\Psi}_n\rangle + \int_E f(E)|E\rangle dE, \tag{2.2}$$

where $C_n(t) = \langle \mathit{\Psi}_n|\Psi(t)\rangle$ and $f(E) = \langle E|\Psi(t)\rangle$. Here we are working in Schröndinger picture. The energy eigen-vectors satisfy the eigen-equations

$$\hat{H}|\mathit{\Psi}_n\rangle = E_n|\mathit{\Psi}_n\rangle, \hat{H}|E\rangle = E|E\rangle. \tag{2.3}$$

These are also known as time independent Schrödinger equations.

For a free particle, the Hamiltonian of the system is

$$\hat{H}_o = \frac{\hat{p}^2}{2m}. \tag{2.4}$$

Thus, the time independent Schrödinger equation becomes

$$\hat{H}_o|\mathit{\Psi}_{(o)n}\rangle = E|\mathit{\Psi}_{(o)n}\rangle. \tag{2.5}$$

In position basis the equation becomes (from now on, the quantum number 'n' will be suppressed)

$$\begin{aligned}
\langle \vec{r}|E|\mathit{\Psi}_o\rangle &= \langle \vec{r}|\hat{H}_o|\mathit{\Psi}_o\rangle \\
&= \left\langle \vec{r}\left|\frac{\hat{p}^2}{2m}\right|\mathit{\Psi}_o\right\rangle \\
&= -\frac{\hbar^2}{2m}\nabla^2\langle \vec{r}|\mathit{\Psi}_o\rangle.
\end{aligned} \tag{2.6}$$

The solution of equation (2.6) is a plane wave given by

$$\langle \vec{r}|\Psi_o\rangle = e^{i\vec{k}.\vec{r}}, \tag{2.7}$$

where $E = \frac{\hbar^2 k^2}{2m}$.

In presence of a potential, the Schrödinger equation becomes

$$(E - \hat{H}_o - \hat{V})|\Psi\rangle = 0, \tag{2.8}$$

where $E > 0$ and $\lim_{r\to\infty} \hat{V}(\vec{r}) = 0$. The aim of the scattering theory is to solve the eigen-equation (2.8) and find the energy eigen-states.

2.1 T-matrix approach

The state-vector $|\Psi\rangle$ is expressed as linear super position of scattered state-vector and free particle state-vector

$$|\Psi\rangle = |\Psi_s\rangle + |\Psi_o\rangle. \tag{2.9}$$

Using equation (2.9), the equation (2.8) can be re-arranged as follows

$$|\Psi\rangle = |\Psi_o\rangle + (E - \hat{H}_o)^{-1}\hat{V}|\Psi\rangle, \tag{2.10}$$

which is known as the *Lippman-Schwinger* equation.

We define Green's operator

$$\hat{G}_o = \lim_{\epsilon\to 0^+} (E - \hat{H}_o + i\epsilon)^{-1}, \tag{2.11}$$

where $i\epsilon$ is added by hand to enforce out-going waves, as explained in section (2.1.1). Now the Lippman-Schwinger equation takes the form

$$|\Psi\rangle = |\Psi_o\rangle + \hat{G}_o\hat{V}|\Psi\rangle. \tag{2.12}$$

Equation (2.12) is a recursion relation which is solved by the successive substitution of the state vector as shown

$$|\Psi_{new}\rangle = |\Psi_o\rangle + \hat{G}_o\hat{V}|\Psi_{old}\rangle. \tag{2.13}$$

It leads to an infinite series known as *Born series*

$$|\Psi\rangle = (1 + \hat{G}_o\hat{V} + \hat{G}_o\hat{V}\hat{G}_o\hat{V} + \ldots)|\Psi_o\rangle. \tag{2.14}$$

In position basis, the Born series takes the form

$$\begin{aligned}\Psi(\vec{r}) = &\underbrace{\Psi_o(\vec{r})}_{\text{(no scattering)}} + \underbrace{\int d\tau' G_o(\vec{r},\vec{r}\,')V(\vec{r}\,')\Psi_o(\vec{r}\,')}_{\text{(scattering at } \vec{r}\,')} \\ &+ \underbrace{\int\int d\tau' d\tau'' G_o(\vec{r},\vec{r}\,')V(\vec{r}\,')G_o(\vec{r}\,',\vec{r}\,'')V(\vec{r}\,'')\Psi_o(\vec{r}\,'')}_{\text{(scattering at } \vec{r}\,'' \text{ and } \vec{r}\,')} \\ &+ \ldots. \end{aligned} \tag{2.15}$$

Equation (2.15) can be understood intuitively by reading from left to right. If we place a detector at $\vec{r}$, then the state function $\Psi(\vec{r}) = \langle \vec{r}|\Psi\rangle$ is the total amplitude of the particle to get detected at position $\vec{r}$. This amplitude is equal to the sum of infinite amplitudes at R.H.S of equation (2.15).

The first term is the state-function of a free particle at position $\vec{r}$. It is an amplitude of the particle, which reaches the position $\vec{r}$ without undergoing the scattering from the potential $V(\vec{r})$. The state-function $\Psi_o(\vec{r}\,')$ in second term is the amplitude of free particle which scatters at the position $\vec{r}\,'$ and gains the factor of $V(\vec{r}\,')$. The Green's function $G_o(\vec{r},\vec{r}\,') = \langle \vec{r}|\hat{G}_o|\vec{r}\,'\rangle$, then, propagates the particle from the position $\vec{r}$ (state $|\vec{r}\rangle$) to $\vec{r}\,'$ (state $|\vec{r}\,'\rangle$). The integration over the volume $d\tau'$ is the sum of all such *one-point scattering* events.

Similarly, the third term is the sum of all the two-point scattering events :

- scattering at the position $\vec{r}\,''$
- propagation via $G_o(\vec{r}\,',\vec{r}\,'')$ to the position $\vec{r}\,'$
- scattering at the position $\vec{r}\,'$
- propagation via $G_o(\vec{r},\vec{r}\,')$ to the detector positioned at $\vec{r}$.

2.1.1 Green's function

Green's operator has been defined in equation (2.11). It can be easily checked that the Hamiltonian commutes with the Green's operator. Therefore, they share a complete set of eigenvectors[4]. One can write the explicit form of Green's operator in energy basis

$$\hat{G}_o = \lim_{\epsilon\to 0^+}\left(\sum_m \int_{E_c}^{\infty} dE' \frac{|E',m\rangle\langle E',m|}{E-E'+i\epsilon} + \sum_{n,m}\frac{|n,m\rangle\langle n,m|}{E-E'+i\epsilon}\right). \tag{2.16}$$

We are chiefly interested in the non-degenerate scattered states in which the threshold energy is set to 0. The Green's operator, then, reduces to

$$\hat{G}_o = \lim_{\epsilon\to 0^+}\left(\int_0^{\infty} dE' \frac{|E'\rangle\langle E'|}{E-E'+i\epsilon}\right). \tag{2.17}$$

Green's function is the Green's operator sandwiched between position basis. One can evaluate the Green's function as shown

$$\begin{aligned} G_o(\vec{r},\vec{r}\,') &= \lim_{\epsilon\to 0^+}\left(\left\langle \vec{r}\left|\int_0^{\infty} dE' \frac{|E'\rangle\langle E'|}{E-E'+i\epsilon}\right|\vec{r}\,'\right\rangle\right) \\ &= \lim_{\epsilon\to 0^+}\left(\int_0^{\infty} dE' \frac{\Psi^*_{E'}(\vec{r})\Psi_{E'}(\vec{r}\,')}{E-E'+i\epsilon}\right). \end{aligned} \tag{2.18}$$

Here $\Psi_{E'}$ is a free particle energy eigen-function.

$$\begin{aligned} G_o(\vec{r},\vec{r}\,') &= \lim_{\epsilon\to 0^+}\left(\int_0^{\infty} dE' \frac{e^{-i\vec{k}'.\vec{r}}e^{i\vec{k}'.\vec{r}\,'}}{\frac{\hbar^2k^2}{2m}-\frac{\hbar^2k'^2}{2m}+i\epsilon}\right) \\ &= \lim_{\epsilon\to 0^+}\frac{2m}{\hbar^2}\left(\int_0^{\infty} dE' \frac{e^{i\vec{k}'.(\vec{r}\,'-\vec{r})}}{k^2-k'^2+i\epsilon\frac{2m}{\hbar^2}}\right) \\ &= -\frac{m}{2\pi\hbar^2}\frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}. \end{aligned} \tag{2.19}$$

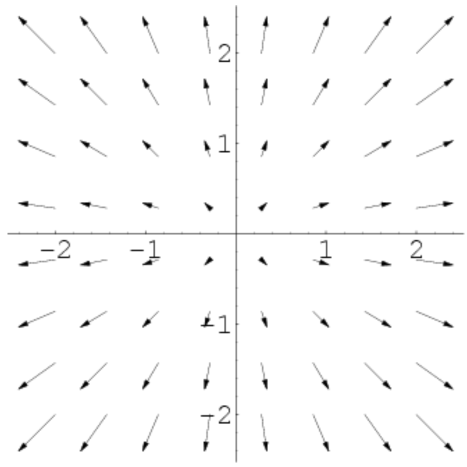

Figure 2.1: A diverging field from $\vec{r}' = 0$[1].

Detailed calculations have been done in APPENDIX A.

One can calculate the probability current associated with this function from the equation

$$\vec{j}(\vec{r}) = \frac{i\hbar}{2m}\left(G_o(\vec{r},\vec{r}')\vec{\nabla}_{\vec{r}}G_o^*(\vec{r},\vec{r}') - G_o^*(\vec{r},\vec{r}')\vec{\nabla}_{\vec{r}}G_o(\vec{r},\vec{r}')\right). \tag{2.20}$$

The probability current turns out to be

$$\vec{j}(\vec{r}) = \frac{k}{4\pi^2\hbar^3|\vec{r}-\vec{r}'|^3}(\vec{r}-\vec{r}'). \tag{2.21}$$

It is easy to see that this is a vector field going outwards from a point $\vec{r}'$ in all the directions (as shown in Figure (2.1)). This result depends on the definition of Green's operator, equation (2.11), where the term $+i\epsilon$ is added by hand. For $-i\epsilon$ we get a vector field converging towards the point $\vec{r}'$.

2.1.2 T matrix

The scattered state vector of the particle, $|\Psi_s\rangle = |\Psi\rangle - |\Psi_o\rangle$, can be calculated from the Born series

$$\begin{aligned}|\Psi_s\rangle &= (\hat{G}_o\hat{V} + \hat{G}_o\hat{V}\hat{G}_o\hat{V} + \hat{G}_o\hat{V}\hat{G}_o\hat{V}\hat{G}_o\hat{V} + \ldots)|\Psi_o\rangle \\ &= \underbrace{\hat{G}_o}_{\substack{\text{final propagation}\\ \text{to the detector}}}\underbrace{(\hat{V} + \hat{V}\hat{G}_o\hat{V} + \hat{V}\hat{G}_o\hat{V}\hat{G}_o\hat{V} + \ldots)}_{\substack{\text{series of scattering}\\ \text{operations and propagations}}}|\Psi_o\rangle \\ &= \hat{G}_o\hat{T}|\Psi_o\rangle. \end{aligned} \tag{2.22}$$

The point scattering and the propagation to other points can be combined and represented by a single operator known as the *T-matrix*. The Green's operator, then, propagates the particle to the final position where the detector is situated.

The total state-function can now written in terms of the T-matrix

$$\Psi(\vec{r}) = \Psi_o(\vec{r}) + \int\int d\tau' d\tau'' G_o(\vec{r},\vec{r}')T(\vec{r}',\vec{r}'')\Psi_o(\vec{r}''), \tag{2.23}$$

where

$$T(\vec{r}', \vec{r}'') = \langle \vec{r}' | \hat{T} | \vec{r}'' \rangle. \tag{2.24}$$

2.2 1-d Dirac delta potential

The T-matrix contains the information of the scattering potential. The computation of the T-matrix facilitates the calculation of the scattered state. Let us consider an example of the potential given by

$$V(x) = g\delta(x), \tag{2.25}$$

where g is the strength of the delta potential.

The T-matrix can be computed as follows

$$\begin{aligned}
T(x, x') =& \langle x | \hat{T} | x' \rangle & (2.26)\\
=& \langle x | (\hat{V} + \hat{V}\hat{G}_o\hat{V} + \hat{V}\hat{G}_o\hat{V}\hat{G}_o\hat{V} + \ldots) | x' \rangle & (2.27)\\
=& g\delta(x')\delta(x - x') + g\delta(x) \int dx'' |x''\rangle\langle x''| \hat{G}_o \\
& \int dx''' |x'''\rangle\langle x''' | x' \rangle g\delta(x') + \ldots & (2.28)\\
=& g\delta(x)\delta(x') \left[1 + \left(-i\frac{gm}{\hbar^2 k} \right) + \left(-i\frac{gm}{\hbar^2 k} \right)^2 + \ldots \right] & (2.29)\\
=& \frac{g\delta(x)\delta(x')}{1 + i\frac{gm}{\hbar^2 k}}. & (2.30)
\end{aligned}$$

The scattering state-function is

$$\begin{aligned}
\Psi_s(x) =& \int dx' dx'' G_o(x, x') T(x', x'') \Psi_o(x'') & (2.31)\\
=& -\frac{e^{ik|x|}}{1 - i\frac{\hbar^2 k}{gm}}. & (2.32)
\end{aligned}$$

2.2.1 Low energy regime

In the low energy regime ($k \to 0$), the scattered state-function takes the form (for $x > 0$)

$$\begin{aligned}
\Psi_s(x) =& -\left[1 + ikx + \mathcal{O}(k^2)\right] \left[1 + i\frac{\hbar^2 k}{gm} + \mathcal{O}(k^2) \right] \\
\approx& -\left[1 + \left(\frac{i\hbar^2}{gm} + x \right) k \right]. & (2.33)
\end{aligned}$$

The scattered state-function makes an intercept $a = \frac{\hbar^2}{mg}$ with the real axis. This intercept is known as the scattering length of the scattering process.

2.2.2 Scattering length

Physically, the scattering length is the measure of the scatterer length-scale, that an incoming particle feels at low energy. In 3-dimensional coordinate space,

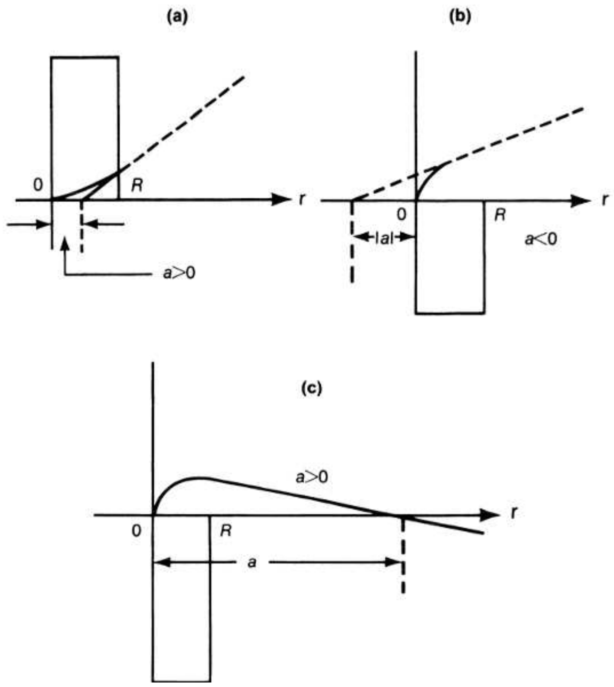

Figure 2.2: (a) for repulsive potential $a > 0$, (b) for attractive potential $a < 0$ and (c) large a for bound state[5]

incoming particle significantly scatters if it goes through the cross-sectional area of $4\pi a^2$.

The scattering length of a scattering process depends on the scattering potential. Figure (2.2) elicits the intuitive dependence. Conversely if we control the scattering length, we control the scattering process. This concept is extensively used to achieve the Feshbach resonance.

Chapter 3

Feshbach resonance

3.1 Collision prerequisites

The time-independent Schrödinger equation for a system of two bodies is

$$\left(-\frac{\hbar^2}{2m_1}\nabla^2_{r_1} - \frac{\hbar^2}{2m_2}\nabla^2_{r_2}\right)\Psi(\vec{r}_1,\vec{r}_2) + V(\vec{r}_1,\vec{r}_2)\Psi(\vec{r}_1,\vec{r}_2) = E\Psi(\vec{r}_1,\vec{r}_2). \quad (3.1)$$

For a central potential ($V(\vec{r}_1,\vec{r}_2) = V(|\vec{r}_1 - \vec{r}_2|)$), equation (3.1) can be decoupled in two equations

$$-\frac{\hbar^2}{2M}\nabla^2_R \Psi_{cm}(\vec{R}) = E_{cm}\Psi_{cm}(\vec{R}) \quad (3.2)$$

and

$$-\frac{\hbar^2}{2\mu}\nabla^2_r \Psi_{rel}(\vec{r}) + V(r)\Psi_{rel}(\vec{r}) = E_{rel}\Psi_{rel}(\vec{r}), \quad (3.3)$$

where

$$M = m_1 + m_1\ ,\ \mu = \frac{m_1 m_2}{m_1 + m_2} \text{ and } \vec{r} = \vec{r}_1 - \vec{r}_2\ ,\ \vec{R} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1 + m_2}.$$

Here, the two sets of coordinates ($\vec{r}_1$ and $\vec{r}_2$), associated with each mass, have been replaced by the coordinates of relative separation ($\vec{r}$) between the two masses and center of mass coordinate ($\vec{R}$).

Physically, we can understand the decoupling of the equation (3.1). The interaction potential is of central nature which makes it dependent on the relative separation between the two masses. Therefore, the Schrödinger equation of the center of mass (equation (3.2)) should be independent of the interaction. The effect of potential $V(r)$ is felt by the two masses. This physics can be replicated by a single mass μ, moving in the potential $V(r)$ (equation (3.3)).

The spherical symmetry allows the separation of variables which leads to the following second order differential equation

$$-\frac{\hbar^2}{2\mu}\frac{d^2\phi_l(r)}{dr^2} + V_l(r)\phi_l(r) = E\phi_l(r), \quad (3.4)$$

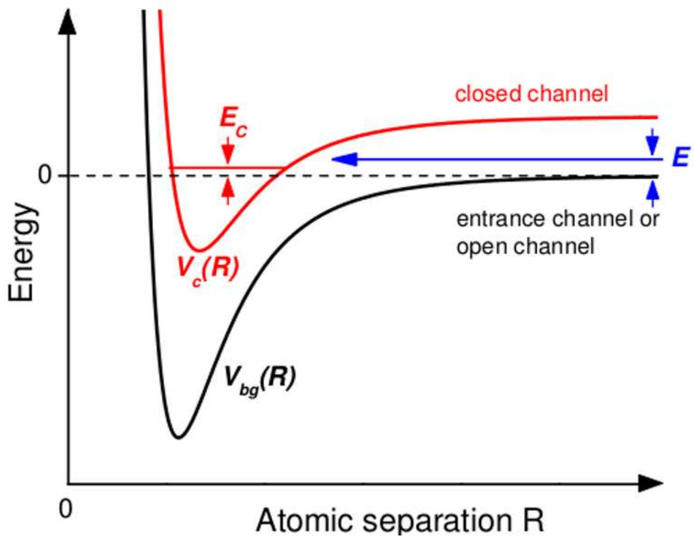

Figure 3.1: Basic two-channel model for a Feshbach resonance. The phenomenon occurs when two atoms colliding at energy E in the entrance channel resonantly couple to a molecular bound state with energy E_c supported by the closed channel potential. In the ultracold domain, collisions take place near zero energy, $E \to 0$. Resonant coupling is then conveniently realized by magnetically tuning E_c near 0 if the magnetic moments of the closed and open channels differ[6].

where $V_l(r) = V(r) + \frac{\hbar^2}{2\mu r^2} l(l+1)$ such that

$$\Psi(\vec{r}) = \frac{\phi_l(r)}{r} Y_{l,m_l}(\theta, \varphi). \tag{3.5}$$

In the proceeding sections, we will consider the physics in center of mass frame and use the notions of reduced mass and relative separation.

3.2 Collision channel

A channel is the state of the colliding masses in the center of mass frame. It includes both spatial and intrinsic degrees of freedom. Mathematically, the state-vector of a collision channel is defined by

$$|\alpha\rangle = |q_1, q_2\rangle |l, m_l\rangle, \tag{3.6}$$

where q_1 and q_2 are spin quantum number of particles 1 and 2 respectively. The angular momentum and magnetic quantum numbers of the partial waves in center of mass frame are denoted by l and m_l respectively.

3.3 Principle of Feshbach resonance

Figure (3.3) shows the two potential curves as function of the inter atomic separation. The addition of the atomic spins results in singlet (anti symmetric)

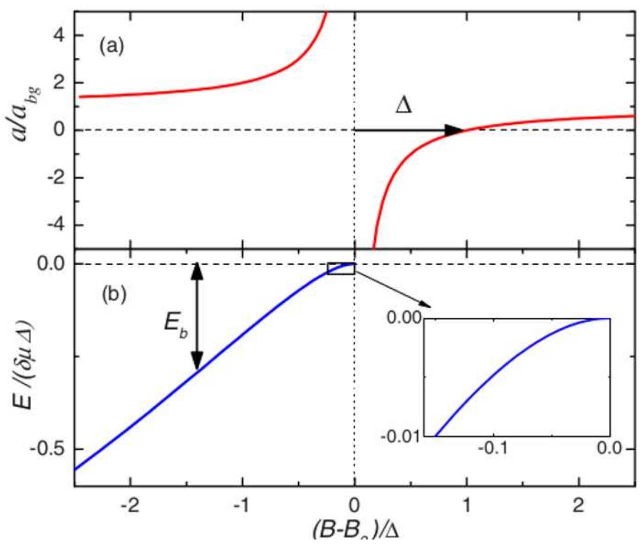

Figure 3.2: Feshbach resonance properties. (a) Scattering length a and (b) molecular state energy E near a magnetically tuned Feshbach resonance. The binding energy is defined to be positive, $E_b = E$. The inset shows the universal regime near the point of resonance where a is very large and positive[6].

and triplet (symmetric) states. Fermions follow Pauli's exclusion principle which forbids their existence in the same quantum state. Consequently, the fermions with same spin projections experience greater repulsive force than the fermions with opposite spin projections, at closer distances. On the other hand, the bosons with same spin projections experience greater attractive force at closer distances.

The fermionic triplet states result in the closed channel potential (red curve) and singlet states result in open channel potential (black curve). For bosons the triplet states result in open channel and singlet state results in closed channel.

A Feshbach resonance occurs when the bound molecular state in the closed channel energetically approaches the scattering state in the open channel (or entrance channel). Then even weak coupling can lead to strong mixing between the two channels. The energy difference can be controlled via a magnetic field when the corresponding magnetic moments are different. This leads to a magnetically tuned Feshbach resonance. For a magnetically tuned resonance, the s-wave scattering length a can be written in terms of magnetic field (figure (3.3))

$$a(B) = a_{bg}\left(1 - \frac{\Delta}{B - B_o}\right). \tag{3.7}$$

This result has been derived for the two channel infinite square well model in section (3.4).

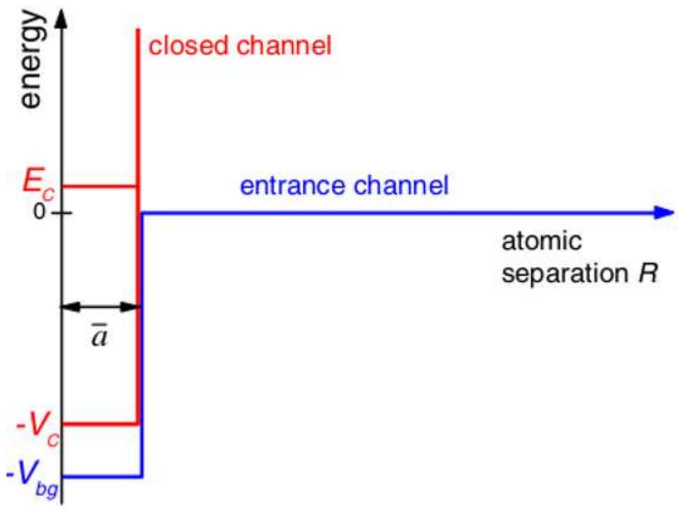

Figure 3.3: Two channel square well[2]

3.4 Infinite square well: two channel model

Figure (3.4) shows the potential curves for three dimensional, two channel square well. The closed channel potential supports at least one bound state with energy E_c. The state vector of the system is written as superposition of the two channels

$$\begin{aligned}|\Psi\rangle =& \underbrace{|q_1, q_2(e)\rangle|l, m_l(e)\rangle}_{\text{entrance channel}}|n, l(e)\rangle + \underbrace{|q_1, q_2(c)\rangle|l, m_l(c)\rangle}_{\text{closed channel}}|n, l(c)\rangle\\ =& |e\rangle|n, l(e)\rangle + |c\rangle|n, l(c)\rangle. \end{aligned} \tag{3.8}$$

A linear vector can be obtained by taking inner-product of $|\Psi\rangle$ with the radial degree of freedom $|r\rangle$. Thus $\langle r|\Psi\rangle = |\Psi(r, E)\rangle$

In exact sense this is not a proper way to take the inner product. The inner product with $|\text{radial}\rangle \otimes |\text{intrinsic}\rangle$ should be taken to obtain a scalar function. Here a "partial" inner product is taken with the radial basis to obtain a hybrid of function and abstract linear vector.

$$|\Psi(r, E)\rangle = |e\rangle\frac{\phi_e(r, E)}{r} + |c\rangle\frac{\phi_c(r, E)}{r}. \tag{3.9}$$

Equation (3.9) is widely used in the literature. We will work with equation (3.8) and obtain same results using much lucid calculations.

The time independent Schrödinger equation is

$$\hat{H}|\Psi\rangle = E|\Psi\rangle, \tag{3.10}$$

where the Hamiltonian of the system is

$$\hat{H} = \left(\frac{\hat{p}^2}{2\mu} + \hat{V}\right). \tag{3.11}$$

The potential operator has two components

$$\hat{V} = \underbrace{\hat{V}_{int} \otimes \hat{I}}_{\text{intrinsic or spin-dependent part}} + \underbrace{\hat{I} \otimes V(\hat{\vec{r}})}_{\text{spatially dependent part}} . \quad (3.12)$$

On substituting the state-vector and Hamiltonian of the system in equation (3.10) we get

$$\left(\frac{\hat{p}^2}{2\mu} + \hat{V}\right)(|e\rangle|n,l(e)\rangle + |c\rangle|n,l(c)\rangle) = E(|e\rangle|n,l(e)\rangle + |c\rangle|n,l(c)\rangle). \quad (3.13)$$

We take the inner product (with respect to the channel state vectors) on both sides of the equation (3.13) and obtain two coupled differential equations

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\begin{pmatrix} \phi_{l,c}(r) \\ \phi_{l,e}(r) \end{pmatrix} + \mathbf{V}\begin{pmatrix} \phi_{l,c}(r) \\ \phi_{l,e}(r) \end{pmatrix} = E\begin{pmatrix} \phi_{l,c}(r) \\ \phi_{l,e}(r) \end{pmatrix} \quad (3.14)$$

where

$$\mathbf{V} = \begin{pmatrix} V_c(r) + \frac{\hbar^2}{2\mu r^2} l_c(l_c+1) + \langle c|\hat{V}_{int}|c\rangle & \langle e|\hat{V}_{int}|c\rangle \\ \langle c|\hat{V}_{int}|e\rangle & V_e(r) + \frac{\hbar^2}{2\mu r^2} l_e(l_e+1) + \langle e|\hat{V}_{int}|e\rangle \end{pmatrix}. \quad (3.15)$$

The off diagonal terms of $\mathbf{V}$ represent the coupling between two channels. Detailed calculations have been done in APPENDIX B.

In the square well example, we have the attractive potential for $r < \bar{a}$. For $r > \bar{a}$, entrance channel and closed channel thresholds are set to be 0 and ∞ respectively. Therefore the potential matrix for this problem is (with $l = 0$)

$$\mathbf{V} = \begin{cases} \begin{pmatrix} -V_c & \hbar\Omega \\ \hbar\Omega & -V_e \end{pmatrix} & \text{for } r < \bar{a}, \\ \begin{pmatrix} \infty & 0 \\ 0 & 0 \end{pmatrix} & \text{for } r > \bar{a} . \end{cases} \quad (3.16)$$

The solution has the form

$$|\Psi\rangle \propto \begin{cases} \frac{\sin(q_+ r)}{r}|+\rangle + \frac{A\sin(q_- r)}{r}|-\rangle & (\text{for } r < \bar{a}), \\ \frac{\sin(kr+\eta)}{r}|e\rangle & (\text{for } r > \bar{a}). \end{cases} \quad (3.17)$$

where $\hbar^2 q_{\pm}^2/2\mu = E + \frac{1}{2}(V_e + V_c) \pm \frac{1}{2}(V_e - V_c)\sec(2\theta)$, $\tan(2\theta) = 2\hbar\Omega/(V_e - V_c)$, $|+\rangle = \cos(\theta)|e\rangle + \sin(\theta)|c\rangle$ and $|-\rangle = -\sin(\theta)|e\rangle + \cos(\theta)|c\rangle$. Detailed calculations have been done in APPENDIX C.

The scattering phase shift η can be computed from the continuity condition of the statefunction at $r = \bar{a}$, which gives

$$\frac{k}{\tan(k\bar{a} + \eta)} = \frac{q_+ \cos^2\theta}{\tan(q_+\bar{a})} + \frac{q_- \sin^2\theta}{\tan(q_-\bar{a})}. \quad (3.18)$$

In weak coupling limit $\theta \to 0$

$$\frac{q_+}{\tan(q_+\bar{a})} = \frac{k}{\tan(k\bar{a} + \eta_{bg})}, \quad (3.19)$$

also the boundary condition of the infinite square well imply

$$\sin\left(\frac{\sqrt{2m_r(E_c+V_c)}\bar{a}}{\hbar}\right)=0 \tag{3.20}$$

Assuming that there is only one bound state near the continuum $|E_C| < \sqrt{V_c E_{vdW}}$, we get

$$cot(k\bar{a}+\eta)=\cot(k\bar{a}+\eta_{bg})-\frac{\Gamma/2}{k\bar{a}E_c}, \tag{3.21}$$

where $\Gamma/2 = 2\theta^2 V_e$ is a Feshbach coupling strength.

Scattering lengths can be derived from the threshold relation $a_{bg} = -\lim_{k\to 0}(k\cot\eta_{bg})^{-1}$. Thus equation (3.21) reduces to

$$\frac{1}{a-\bar{a}}=\frac{1}{a_{bg}-\bar{a}}+\frac{\Gamma/2}{k\bar{a}E_c}. \tag{3.22}$$

The magnetic tunability of Feshbach resonances can be modeled by linear Zeeman shift of bare bound state as $E_c = \delta\mu(B - B_c)$, where B is the magnetic field, $\delta\mu$ is the relative magnetic moment of two channels and B_c is the magnetic field that tunes the bare state to entrance-channel threshold. Thus we get

$$a = a_{bg}\left(1-\frac{\Delta}{B-B_o}\right). \tag{3.23}$$

Chapter 4

Harmonic oscillator potential

In this chapter we will develop and investigate the two channel model of the Feshbach resonance in isotropic harmonic oscillator potential illustrated in figure (4.1).

4.1 Coupled channel state function

The coupled state function of the system is

$$|\Psi(r,E)\rangle = |e\rangle\frac{\phi_e(r,E)}{r} + |c\rangle\frac{\phi_c(r,E)}{r}. \tag{4.1}$$

In the ultra cold regime, only the s-wave component of the state function becomes appreciable. Therefore, we set $l = 0$ in the following equations. The potential matrix (given by equation (3.15)) of the system becomes

$$\mathbf{V} = \begin{cases} \begin{pmatrix} \frac{1}{2}\mu\omega_c^2 r^2 - V_c & \hbar\Omega \\ \hbar\Omega & \frac{1}{2}\mu\omega_e^2 r^2 - V_e \end{pmatrix} & \text{for } r < \bar{a}, \\ \begin{pmatrix} \frac{1}{2}\mu\omega_c^2 r^2 - V_c & 0 \\ 0 & 0 \end{pmatrix} & \text{for } r > \bar{a}\ . \end{cases} \tag{4.2}$$

Here $\omega_{c,e} = \frac{1}{\bar{a}}\sqrt{\frac{2V_{c,e}}{\mu}}$. We are now required to solve the following coupled differential equation of the system

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\begin{pmatrix} \phi_c(r) \\ \phi_e(r) \end{pmatrix} + \mathbf{V}\begin{pmatrix} \phi_c(r) \\ \phi_e(r) \end{pmatrix} = E\begin{pmatrix} \phi_c(r) \\ \phi_e(r) \end{pmatrix}. \tag{4.3}$$

For $r > \bar{a}$, the system of coupled differential equation reduces to

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\phi_c(r) + \left(\frac{1}{2}\mu\omega_c^2 r^2 - V_c\right)\phi_c(r) = E\phi_c(r). \tag{4.4}$$

The general solution is a linear combination of the parabolic cylinder functions given by

$$\phi_c(r) = C_1 D_{-\nu-1}(i\rho) + C_2 D_\nu(\rho), \tag{4.5}$$

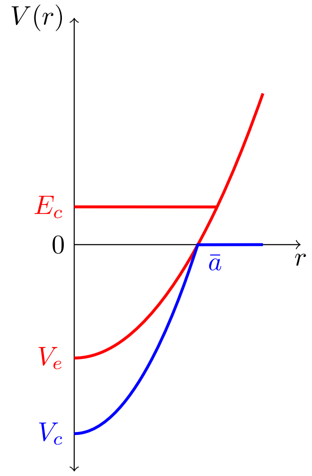

Figure 4.1: Two channel isotropic harmonic oscillator model: Red curve is the closed channel with at least one bound state E_c. The entrance channel is represented by the blue curve.

where $a_{ho} = \sqrt{\frac{\hbar}{\mu\omega_c}}$, $\rho = \sqrt{2}\frac{r}{a_{ho}}$ and $\nu = \frac{E+V_c}{\hbar\omega_c} - \frac{1}{2}$ (for ν as non negative integer we obtain Hermite polynomials[7]). The application of the boundary conditions imply $C_1 = 0$ with the solution

$$\phi_c(\rho) = C_2 D_\nu(\rho) \tag{4.6}$$

and total energy

$$E_\nu = \left(\nu + \frac{1}{2}\right)\hbar\omega_c - V_c. \tag{4.7}$$

For $r < \bar{a}$, we have a system of second ordered coupled equations which can be transformed into system of first ordered differential equations

$$\frac{d}{dr}\begin{pmatrix}\phi_c(r)\\ \phi_e(r)\\ \phi_c'(r)\\ \phi_e'(r)\end{pmatrix} = \mathbf{A}\begin{pmatrix}\phi_c(r)\\ \phi_e(r)\\ \phi_c'(r)\\ \phi_e'(r)\end{pmatrix}, \tag{4.8}$$

where $\mathbf{A}$ is

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\\ \frac{2\mu}{\hbar^2}\left(\frac{1}{2}\mu\omega_c^2 r^2 - (V_c + E)\right) & \frac{2\mu}{\hbar^2}\hbar\Omega & 0 & 0\\ \frac{2\mu}{\hbar^2}\hbar\Omega & \frac{2\mu}{\hbar^2}\left(\frac{1}{2}\mu\omega_e^2 r^2 - (V_e + E)\right) & 0 & 0 \end{pmatrix}.$$

Equation (4.8) can be solved using Magnus expansion[8]. If an unknown vector $Y(r) \in \mathbb{C}^n$ with, an initial condition $Y(r_o) = Y_o$, satisfies the equation

$$\frac{d}{dr}Y(r) = A(r)Y(r), \tag{4.9}$$

where $A(r) \in \mathbb{C}^{n\times n}$, then the solution is

$$Y(r) = \exp\left(\Omega(r, r_o)\right) Y_o, \tag{4.10}$$

where (with $r_o = 0$)

$$\Omega(r) = \sum_{k=1}^{\infty} \Omega_k(r). \tag{4.11}$$

Each element of the above summation is defined as follows

$$\begin{aligned}
\Omega_1(r) =& \int_0^r A(r_1)\, dr_1, \\
\Omega_2(r) =& \frac{1}{2}\int_0^r dr_1 \int_0^{r_1} dr_2 \ \left[A(r_1), A(r_2)\right], \\
\Omega_3(r) =& \frac{1}{6}\int_0^r dr_1 \int_0^{r_1} dt_r \int_0^{r_2} dr_3 \ \left([A(r_1),[A(r_2),A(r_3)]] + [A(r_3),[A(r_2),A(r_1)]]\right), \\
\Omega_4(r) =& \frac{1}{12}\int_0^r dr_1 \int_0^{r_1} dr_2 \int_0^{r_2} dr_3 \int_0^{r_3} dr_4 \ \left([[[A_1,A_2],A_3],A_4] + [A_1,[[A_2,A_3],A_4]] \right. \\
& \left. + [A_1,[A_2,[A_3,A_4]]] + [A_2,[A_3,[A_4,A_1]]]\right),
\end{aligned} \tag{4.12}$$

where $[A, B] = AB - BA$ is the commutation of matrices A and B. Sufficient condition for the series to converge is

$$\int_0^r \|A(s)\| ds < \pi, \tag{4.13}$$

where $\|.\|$ represents the matrix norm.

On integration, the following matrices can be obtained

$$\Omega_1(r) = \begin{pmatrix} 0 & 0 & r & 0 \\ 0 & 0 & 0 & r \\ \frac{8\mu V_c r^3}{3a^2\hbar^2} - \frac{2E\mu r}{\hbar^2} - \frac{2\mu V_c r}{\hbar^2} & \frac{2r\mu\Omega}{h} & 0 & 0 \\ \frac{2r\mu\Omega}{\hbar} & \frac{8\mu V_e r^3}{3a^2\hbar^2} - \frac{2E\mu r}{\hbar^2} - \frac{2\mu V_e r}{h^2} & 0 & 0 \end{pmatrix}$$

$$\Omega_2(r) = \begin{pmatrix} -\frac{2r^4\mu V_c}{3a^2\hbar^2} & 0 & 0 & 0 \\ 0 & -\frac{2r^4\mu V_e}{3a^2\hbar^2} & 0 & 0 \\ 0 & 0 & \frac{2r^4\mu V_c}{3\bar{a}^2\hbar^2} & 0 \\ 0 & 0 & 0 & \frac{2r^4\mu V_e}{3\bar{a}^2\hbar^2} \end{pmatrix}$$

$$\Omega_3(r) = \begin{pmatrix} 0 & 0 & -\frac{2r^5\mu V_c}{45\bar{a}^2\hbar^2} & 0 \\ 0 & 0 & 0 & -\frac{2r^5\mu V_e}{45\bar{a}^2\hbar^2} \\ -\frac{4r^5\mu^2 V_c\left(21E\bar{a}^2 + \left(21\bar{a}^2 + 100r^2\right)V_c\right)}{945\bar{a}^4\hbar^4} & \frac{2r^5\mu^2\Omega(V_c+V_e)}{45\bar{a}^2\hbar^3} & 0 & 0 \\ \frac{2r^5\mu^2\Omega(V_c+V_e)}{45\bar{a}^2\hbar^3} & -\frac{4r^5\mu^2 V_e\left(21E\bar{a}^2 + \left(21\bar{a}^2 + 100r^2\right)V_e\right)}{945\bar{a}^4\hbar^4} & 0 & 0 \end{pmatrix}.$$

4.2 Scattering length

As noted in the section (2.2.2), the scattering length is the intercept of the scattered state function on the real axis. The scattered state function $\phi_c(r) = C_2 D_\nu(r)$ for $r \ll a_{ho}$ is

$$\begin{aligned}
D_\nu(r) =& D_\nu(0) + r D'_\nu(0) + \mathcal{O}(r^2) \\
\approx& D_\nu(0)\left(1 - \frac{r}{a_{ho} f(E)}\right),
\end{aligned} \tag{4.14}$$

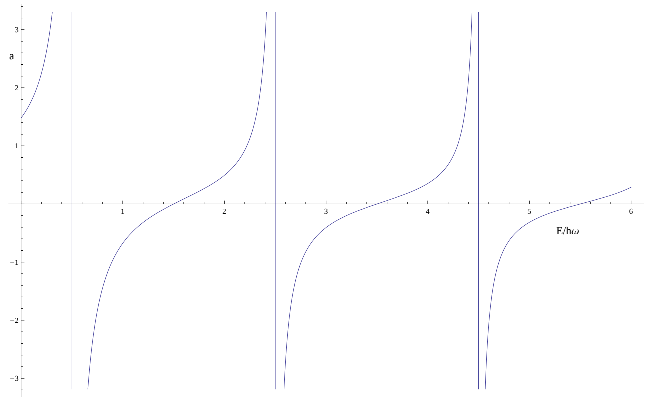

Figure 4.2: The plot of scattering length a/a_{ho} vs $E/(\hbar\omega_c)$.

with

$$f(E) = \frac{\Gamma\left(\frac{1}{4} - \frac{E}{2\hbar\omega_c}\right)}{2\Gamma\left(\frac{3}{4} - \frac{E}{2\hbar\omega_c}\right)}, \tag{4.15}$$

where $\Gamma(x)$ is the Gamma function.

The scattering length for the energy E is given by equating D_ν to 0. Consequently we get

$$\begin{aligned} a =& a_{ho} f(E) \\ =& \sqrt{\frac{\hbar}{\mu\omega_c}} \frac{\Gamma\left(\frac{1}{4} - \frac{E}{2\hbar\omega_c}\right)}{2\Gamma\left(\frac{3}{4} - \frac{E}{2\hbar\omega_c}\right)}. \end{aligned} \tag{4.16}$$

Figure (4.2) shows the variation of the scattering length with the energy of atoms in center of mass frame.

Chapter 5

Discussions and further possible research

The coupled two channel harmonic oscillator model of magnetically tuned Feshbash resonance has been analytically investigated. The dependence of the scattering length a on the energy E of the atoms in center of mass frame has been established. The range of scattering length is found to be $(-\infty, \infty)$, where infinities represent the Feshbach resonances.

As we have seen in figure (2.2), the nature of interaction affects the value of scattering length. Consequently the plot of the scattering length in figure (4.2) shows the variation of mutual interaction of the colliding atoms from attractive to repulsive. The infinities of the scattering length show the occurrence of Feshbach resonance.

We have calculated the matrices of the Magnus expansion. The radial wavefunction of the coupled channel system can be evaluated for specific examples like for colliding alkali-atoms. Numerical methods[8] can be employed to truncate the expansion and compute the expressions by using the convergence relation 4.13.

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Appendix A

Green's function

The Green's function corresponding to Green's operator $\hat{G}_o = \lim_{\epsilon\to 0^+}(E - \hat{H}_o + i\epsilon)^{-1}$ is

$$G_o(\vec{r},\vec{r}\,')= \lim_{\epsilon\to 0^+}\left(\int_0^\infty dE' \frac{e^{-i\vec{k}'.\vec{r}}e^{i\vec{k}'.\vec{r}\,'}}{\frac{\hbar^2 k^2}{2m} - \frac{\hbar^2 k'^2}{2m} + i\epsilon}\right)$$
$$= \lim_{\epsilon\to 0^+}\frac{2m}{\hbar^2}\left(\int_0^\infty dE' \frac{e^{i\vec{k}'.(\vec{r}\,'-\vec{r})}}{k^2 - k'^2 + i\epsilon\frac{2m}{\hbar^2}}\right). \tag{A.1}$$

Now $E' = \frac{\hbar^2 k'^2}{2m}$ implies that $dE' = \frac{\hbar^2 k'}{m}dk'$ and $\Psi_{E'}(\vec{r}\,') = \exp(-i\vec{k}'.\vec{r}\,')$. Therefore

$$G_o(\vec{r},\vec{r}\,')= \lim_{\epsilon\to 0^+} -\frac{2m}{(2\pi)^3\hbar^2}\left(\int d^3k' \frac{e^{i\vec{k}'.(\vec{r}\,'-\vec{r})}}{k'^2 - k^2 - i\epsilon\frac{2m}{\hbar^2}}\right) \tag{A.2}$$

Now $k'^2 - k^2 - i\epsilon\frac{2m}{\hbar^2} = (k' - \sqrt{k^2+i\epsilon})(k' + \sqrt{k^2+i\epsilon})$ (since ϵ is positive infinitesimal). Thus

$$G_o(\vec{r},\vec{r}\,')= \lim_{\epsilon\to 0^+} -\frac{2m}{(2\pi)^3\hbar^2}\left(\int d^3k' \frac{e^{i\vec{k}'.(\vec{r}\,'-\vec{r})}}{(k' - \sqrt{k^2+i\epsilon})(k' + \sqrt{k^2+i\epsilon})}\right)$$
$$= \lim_{\epsilon\to 0^+} -\frac{2m}{(2\pi)^3\hbar^2}\left(\int_0^\infty k'^2 dk' \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\varphi \frac{e^{i\vec{k}'.(\vec{r}\,'-\vec{r})}}{(k' - \sqrt{k^2+i\epsilon})(k' + \sqrt{k^2+i\epsilon})}\right)$$
$$= \lim_{\epsilon\to 0^+} -\frac{2m}{(2\pi)^2\hbar^2}\left(\int_0^\infty k'^2 dk' \int_0^\pi \sin\theta d\theta \frac{e^{i\vec{k}'.(\vec{r}\,'-\vec{r})}}{(k' - \sqrt{k^2+i\epsilon})(k' + \sqrt{k^2+i\epsilon})}\right) \tag{A.3}$$

Align $\hat{a}_z$ axis (of momentum space) along $\vec{r} - \vec{r}\,'$,

$$G_o(\vec{r},\vec{r}\,')= \lim_{\epsilon\to 0^+} -\frac{2m}{(2\pi)^2\hbar^2}\left(\int_0^\infty k'^2 dk' \int_0^\pi \sin\theta d\theta \frac{e^{ik'|\vec{r}\,'-\vec{r}|\cos(\theta)}}{(k' - \sqrt{k^2+i\epsilon})(k' + \sqrt{k^2+i\epsilon})}\right)$$
$$= \lim_{\epsilon\to 0^+} -\frac{2m}{(2\pi)^2\hbar^2}\left(\int_0^\infty k' dk' \frac{e^{ik'|\vec{r}\,'-\vec{r}|} - e^{-ik'|\vec{r}\,'-\vec{r}|}}{(k' - \sqrt{k^2+i\epsilon})(k' + \sqrt{k^2+i\epsilon})|\vec{r} - \vec{r}\,'|}\right)$$
$$= \lim_{\epsilon\to 0^+} -\frac{2m}{(2\pi)^2\hbar^2}\left(\int_{-\infty}^\infty k' dk' \frac{e^{ik'|\vec{r}\,'-\vec{r}|}}{(k' - \sqrt{k^2+i\epsilon})(k' + \sqrt{k^2+i\epsilon})|\vec{r} - \vec{r}\,'|i}\right)$$

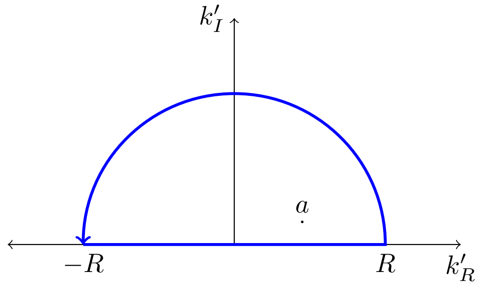

Figure A.1: Argand plane with a contour.

The integration can be solved by method of residues. In this approach, $k' = k'_R + ik'_I$ (k'_R is real and k'_I is imaginary part of the complex number k') is considered as a complex number and the integration is performed on the complex plane (also known as argand plane).

Let us consider an integration along the semicircle in the figure (A.1)

$$\begin{aligned} I(R) &= \oint_C dk' f(k') \\ &= \underbrace{\int_{-R}^{R} dk'_R f(k'_R)}_{\text{on real line}} + \underbrace{\int_0^{\pi} Rd\theta f(k')}_{\text{on the semicircle}} . \end{aligned} \tag{A.4}$$

Let $f(k') = \frac{k' e^{i\alpha k'}}{(k'-a)(k'+a)}$ where $a \in \mathbb{C}$ is the pole enclosed in the contour and $\alpha \in \mathbb{R}$ is some constant. In our example, $a = \sqrt{k^2 + i\epsilon}$ is in the first quadrant and $\alpha > 0$.

The integration takes the form

$$I(R) = \int_{-R}^{R} dk'_R \frac{k'_R e^{i\alpha k'_R}}{(k'-a)(k'+a)} + \int_0^{\pi} Rd\theta \frac{Re^{i\alpha(k'_R + ik'_I)}}{(k'-a)(k'+a)} \tag{A.5}$$

Now the modulus of second term decreases exponentially with R

$$\begin{aligned} \left| \int_0^{\pi} Rd\theta \frac{Re^{i\alpha(k'_R+ik'_I)}}{(k'-a)(k'+a)} \right| &\le \int_0^{\pi} R^2 d\theta \left| \frac{e^{i\alpha(k'_R+ik'_I)}}{(k'-a)(k'+a)} \right| \\ &= \int_0^{\pi} e^{-\alpha R\cos\theta} R^2 \left| \frac{1}{k'^2 - a^2} \right| \end{aligned} \tag{A.6}$$

In the limit $R \to \infty$, the second term in the equation (A.5) vanishes and we are left with

$$\lim_{R\to\infty} I(R) = \int_{-\infty}^{\infty} dk'_R \frac{k'_R e^{i\alpha k'_R}}{(k'-a)(k'+a)} \tag{A.7}$$

But according to calculus of residues, $I(R)$ is

$$\begin{aligned} I(R) =& \oint_C dk' f(k') \\ =& 2\pi i (\text{sum of residues}) \\ =& 2\pi i \lim_{k' \to a} (k' - a) f(a) \\ =& 2\pi i \frac{a e^{i\alpha a}}{2a} \\ =& \pi i e^{i\alpha a} \end{aligned} \tag{A.8}$$

Thus the Green's function can be written as

$$\begin{aligned} G_o(\vec{r}, \vec{r}\,') =& \lim_{\epsilon \to 0^+} -\frac{2m}{(2\pi)^2 \hbar^2} \left(\int_{-\infty}^{\infty} k' dk' \frac{e^{ik'|\vec{r}\,' - \vec{r}|}}{(k' - \sqrt{k^2 + i\epsilon})(k' + \sqrt{k^2 + i\epsilon})|\vec{r} - \vec{r}\,'|i} \right) \\ =& \lim_{\epsilon \to 0^+} -\frac{2m}{(2\pi)^2 \hbar^2} \left(\pi i \frac{e^{i\sqrt{k^2 + i\epsilon}|\vec{r}\,' - \vec{r}|}}{|\vec{r} - \vec{r}\,'|i} \right) \\ =& -\frac{m}{2\pi \hbar^2} \frac{e^{ik|\vec{r}\,' - \vec{r}|}}{|\vec{r}\,' - \vec{r}|} \end{aligned} \tag{A.9}$$

Appendix B

Two-channel coupling

We start with equation

$$\left(\frac{\hat{p}^2}{2\mu}+\hat{V}\right)(|e\rangle|n,l(e)\rangle+|c\rangle|n,l(c)\rangle)=E(|e\rangle|n,l(e)\rangle+|c\rangle|n,l(c)\rangle),$$

$$\left(\frac{\hat{p}^2}{2\mu}+\hat{V}_{int}\otimes\hat{I}+\hat{I}\otimes V(\hat{\vec{r}})\right)(|e\rangle|n,l(e)\rangle+|c\rangle|n,l(c)\rangle)=E(|e\rangle|n,l(e)\rangle+|c\rangle|n,l(c)\rangle).$$

Take a "partial" inner-product with the position basis $|\vec{r}\rangle$ on both sides of the equation

$$\langle\vec{r}|\left(\frac{\hat{p}^2}{2\mu}+\hat{V}_{int}\otimes\hat{I}+\hat{I}\otimes V(\hat{\vec{r}})\right)(|e\rangle|n,l(e)\rangle+|c\rangle|n,l(c)\rangle)=\langle\vec{r}|E(|e\rangle|n,l(e)\rangle+|c\rangle|n,l(c)\rangle).$$

Let us evaluate each term of the above equation. The L.H.S with entrance channel consists of three terms

1. The first term is

$$\left\langle\vec{r}\left|\frac{\hat{p}^2}{2\mu}\right|e,n\right\rangle=|q_1,q_2(e)\rangle\left\langle\vec{r}\left|\frac{\hat{p}^2}{2\mu}\right|n,l,m_l(e)\right\rangle \tag{B.1}$$

2. Second term is

$$\langle\vec{r}|\hat{V}_{int}\otimes\hat{I}|q_1,q_2(e)\rangle|n,l,m_l(e)\rangle=\hat{V}_{int}|q_1,q_2(e)\rangle\langle\vec{r}|n,l,m_l(e)\rangle \tag{B.2}$$

3. Third term is

$$\begin{aligned}\langle\vec{r}|\hat{I}\otimes V(\hat{\vec{r}})|q_1,q_2(e)\rangle|n,l,m_l(e)\rangle&=|q_1,q_2(e)\rangle\langle\vec{r}|V(\hat{\vec{r}})|n,l,m_l(e)\rangle\\&=|q_1,q_2(e)\rangle V(\vec{r})\langle\vec{r}|n,l,m_l(e)\rangle\end{aligned} \tag{B.3}$$

R.H.S terms consists of one with entrance channel

$$\langle\vec{r}|E|e\rangle|n,l(e)\rangle=E|q_1,q_2(e)\rangle\langle\vec{r}|n,l,m_l(e)\rangle \tag{B.4}$$

Now, on taking the full inner-product with the vector $|q_1, q_2(e)\rangle$, we get (using orthonormality)

$$\begin{aligned}E\langle\vec{r}|n,l,m_l(e)\rangle = &\left\langle \vec{r}\left|\frac{\hat{p}^2}{2\mu}\right|n,l,m_l(e)\right\rangle + \langle q_1,q_2(e)|\hat{V}_{int}|q_1,q_2(e)\rangle\langle\vec{r}|n,l,m_l(e)\rangle \\ &+V(\vec{r})\langle\vec{r}|n,l,m_l(e)\rangle + \langle q_1,q_2(e)|\hat{V}_{int}|q_1,q_2(c)\rangle\langle\vec{r}|n,l,m_l(c)\rangle \\ =&-\frac{\hbar^2}{2\mu}\nabla^2\Psi_{n,l,m_l(e)}(\vec{r}) + \langle q_1,q_2(e)|\hat{V}_{int}|q_1,q_2(e)\rangle\Psi_{n,l,m_l(e)}(\vec{r}) \\ &+V(\vec{r})\Psi_{n,l,m_l(e)}(\vec{r}) + \langle q_1,q_2(e)|\hat{V}_{int}|q_1,q_2(c)\rangle\Psi_{n,l,m_l(e)}(\vec{r})\end{aligned}$$

Since there is a spherical symmetry, the equation can further be written as

$$\begin{aligned}E\phi_{l(e)}(r) = &-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\phi_{l(e)}(r) + \frac{\hbar^2}{2\mu r^2}l_e(l_e+1)\phi_{l(e)}(r) + \langle q_1,q_2(e)|\hat{V}_{int}|q_1,q_2(c)\rangle\phi_{l(e)}(r) \\ &+\langle q_1,q_2(e)|\hat{V}_{int}|q_1,q_2(e)\rangle\phi_{l(e)}(r). \qquad \text{(B.5)}\end{aligned}$$

On taking inner-product with closed channel, we get

$$\begin{aligned}E\phi_{l(c)}(r) = &-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\phi_{l(c)}(r) + \frac{\hbar^2}{2\mu r^2}l_c(l_c+1)\phi_{l(c)}(r) + \langle q_1,q_2(c)|\hat{V}_{int}|q_1,q_2(e)\rangle\phi_{l(c)}(r) \\ &+\langle q_1,q_2(c)|\hat{V}_{int}|q_1,q_2(c)\rangle\phi_{l(e)}(r). \qquad \text{(B.6)}\end{aligned}$$

On combining equation (B.5) and equation (B.6), we get

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\begin{pmatrix}\phi_{l,c}(r)\\ \phi_{l,e}(r)\end{pmatrix} + \mathbf{V}\begin{pmatrix}\phi_{l,c}(r)\\ \phi_{l,e}(r)\end{pmatrix} = E\begin{pmatrix}\phi_{l,c}(r)\\ \phi_{l,e}(r)\end{pmatrix} \qquad \text{(B.7)}$$

where

$$\mathbf{V} = \begin{pmatrix} V_c(r) + \frac{\hbar^2}{2\mu r^2}l_c(l_c+1) + \langle c|\hat{V}_{int}|c\rangle & \langle e|\hat{V}_{int}|c\rangle \\ \langle c|\hat{V}_{int}|e\rangle & V_e(r) + \frac{\hbar^2}{2\mu r^2}l_e(l_e+1) + \langle e|\hat{V}_{int}|e\rangle \end{pmatrix}. \qquad \text{(B.8)}$$

Appendix C

Square-well potential

The potential matrix for the infinite square-well is

$$\mathbf{V} = \begin{cases} \begin{pmatrix} -V_c(r) & \frac{V_e - V_c}{2}\tan 2\theta \\ \frac{V_e - V_c}{2}\tan 2\theta & -V_e \end{pmatrix} & \text{for } r < \bar{a}, \\ \begin{pmatrix} \infty & 0 \\ 0 & 0 \end{pmatrix} & \text{for } r > \bar{a}\ . \end{cases} \tag{C.1}$$

Where $\hbar\Omega = \frac{V_e - V_c}{2}\tan 2\theta$. The coupled differential equation that we need to solve is

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\begin{pmatrix} \phi_{l,c}(r) \\ \phi_{l,e}(r) \end{pmatrix} = \begin{pmatrix} E + V_c & \frac{V_e - V_c}{2}\tan 2\theta \\ \frac{V_e - V_c}{2}\tan 2\theta & E + V_e \end{pmatrix}\begin{pmatrix} \phi_{l,c}(r) \\ \phi_{l,e}(r) \end{pmatrix} \tag{C.2}$$

The column vector in the above equation belongs to $\mathbb{C}^2$ space. Let $\mathbf{e_1}$ and $\mathbf{e_2}$ be the eigen-vectors of $\mathbf{V} = \begin{pmatrix} E + V_c & \frac{V_e - V_c}{2}\tan 2\theta \\ \frac{V_e - V_c}{2}\tan 2\theta & E + V_e \end{pmatrix}$ such that

$$\mathbf{V}\mathbf{e_1} = \lambda_1 \mathbf{e_1} \tag{C.3}$$

and

$$\mathbf{V}\mathbf{e_2} = \lambda_2 \mathbf{e_2}. \tag{C.4}$$

Then $\mathbf{e_1}$ and $\mathbf{e_2}$ form the basis of the Hilbert space $\mathbb{C}^2$($\mathbf{V}$ is a self-adjoint matrix). One can find the eigen-vectors and eigen-values to be

$$\mathbf{e_1} = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}, \ \mathbf{e_2} = \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}. \tag{C.5}$$

and

$$\lambda_{1,2} = \frac{2\mu}{\hbar^2}\left(E + \frac{V_e - V_c}{2}(+,-)\frac{V_e - V_c}{2}\sec 2\theta\right). \tag{C.6}$$

Now

$$\begin{pmatrix} \phi_{l,c}(r) \\ \phi_{l,e}(r) \end{pmatrix} = C_1(r)\mathbf{e_1} + C_2(r)\mathbf{e_2}. \tag{C.7}$$

Substitute this in equation (C.2) and obtain

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\left(C_1(r)\mathbf{e_1}+C_2(r)\mathbf{e_2}\right)=\begin{pmatrix} E+V_c & \frac{V_e-V_c}{2}\tan 2\theta \\ \frac{V_e-V_c}{2}\tan 2\theta & E+V_e \end{pmatrix}\left(C_1(r)\mathbf{e_1}+C_2(r)\mathbf{e_2}\right)$$
$$=(\lambda_1 C_1(r)\mathbf{e_1}+\lambda_2 C_2(r)\mathbf{e_2}) \tag{C.8}$$

Now we have a set of decoupled equations

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}C_1(r)=\lambda_1 C_1(r) \tag{C.9}$$

and

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}C_2(r)=\lambda_2 C_2(r). \tag{C.10}$$

Once $C_1(r)$ and $C_2(r)$ are known, we can plug the values in equation (C.7) to get the final solution.

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