Quantum mechanical scattering and Feshbach resonance

Ravi Mohan
Supervised by: Prof. G. S. Singh

Indian Institute of Technology
Roorkee

April 30, 2014

Outline

Scattering

- Time independent Schrödinger equation for a free particle (eigen-vector equation)

$$(E - \hat{H}_o)|\Psi_o\rangle = 0, \tag{1}$$

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

- The solution is given by plane wave

$$\langle \vec{r}|\Psi_o\rangle = e^{i\vec{k}.\vec{r}}. \tag{2}$$

- The aim of scattering theory is to solve eigen-vector equation

$$(E - \hat{H}_o - \hat{V})|\Psi\rangle = 0, \tag{3}$$

where $E > 0$ and $\lim_{r\to\infty} \hat{V}(\vec{r}) = 0$.

- The state vector of this equation is written as linear combination

$$|\Psi\rangle = |\Psi_o\rangle + |\Psi_s\rangle. \tag{4}$$

- Then the rearrangement of Schrödinger leads to

$$|\Psi\rangle = |\Psi_o\rangle + (E - \hat{H}_o)^{-1}\hat{V}|\Psi\rangle, \tag{5}$$

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

- Define

$$\hat{G}_o = \lim_{\epsilon \to \infty} (E - \hat{H}_o + i\epsilon)^{-1}, \tag{6}$$

where $i\epsilon$ is added by hand to enforce causality.

- The *Lippman-Schwinger* equation reduces to

$$|\Psi\rangle = |\Psi_o\rangle + \hat{G}_o\hat{V}|\Psi\rangle. \tag{7}$$

- This recurrence equation is solved by following procedure

$$|\Psi_{new}\rangle = |\Psi_o\rangle + \hat{G}_o\hat{V}|\Psi_{old}\rangle, \tag{8}$$

which leads to the *Born Series*

$$|\Psi\rangle = (1 + \hat{G}_o\hat{V} + \hat{G}_o\hat{V}\hat{G}_o\hat{V} + \ldots)|\Psi_o\rangle. \tag{9}$$

- In position basis, the Born Series takes the form

$$\Psi(\vec{r}) = \underbrace{\Psi_o(\vec{r})}_{\text{(no scattering)}} + \underbrace{\int d\tau' G_o(\vec{r},\vec{r}\,')V(\vec{r}\,')\Psi_o(\vec{r}\,')}_{\text{(scattering at } \vec{r}\,')}$$
$$+ \underbrace{\int\int d\tau' d\tau'' G_o(\vec{r},\vec{r}\,')V(\vec{r}\,')G_o(\vec{r}\,',\vec{r}\,'')V(\vec{r}\,'')\Psi_o(\vec{r}\,'')}_{\text{(scattering at } \vec{r}\,'' \text{ and } \vec{r}\,')}$$
$$+ \ldots . \qquad (10)$$

where

$$G_o(\vec{r},\vec{r}\,') = \langle \vec{r}|\hat{G}_o|\vec{r}\,'\rangle. \qquad (11)$$

- The Green's operator has the form

$$\hat{G}_o = \sum_m \int_{E_c}^{\infty} dE' \frac{|E',m\rangle\langle E',m|}{E-E'+i\epsilon} + \sum_{n,m} \frac{|n,m\rangle\langle n,m|}{E-E'+i\epsilon}. \qquad (12)$$

- For non-degenerate un-bounded states with $E_c = 0$

$$\hat{G}_o = \int_0^{\infty} dE' \frac{|E'\rangle\langle E'|}{E-E'+i\epsilon}. \qquad (13)$$

- Hence

$$G_o(\vec{r},\vec{r}') = \left\langle \vec{r} \left| \int_0^\infty dE' \frac{|E'\rangle\langle E'|}{E - E' + i\epsilon} \right| \vec{r}' \right\rangle$$
$$= \int_0^\infty dE' \frac{\Psi^*_{E'}(\vec{r})\Psi_{E'}(\vec{r'})}{E - E' + i\epsilon}$$
$$= -\frac{m}{2\pi\hbar^2} \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}. \tag{14}$$

- From Born Series, we can evaluate the scattered state $|\Psi_s\rangle = |\Psi\rangle - |\Psi_o\rangle$,

$$|\Psi_s\rangle = (\hat{G}_o\hat{V} + \hat{G}_o\hat{V}\hat{G}_o\hat{V} + \hat{G}_o\hat{V}\hat{G}_o\hat{V}\hat{G}_o\hat{V} + \ldots)|\Psi_o\rangle \tag{15}$$
$$= \hat{G}_o(\hat{V} + \hat{V}\hat{G}_o\hat{V} + \hat{V}\hat{G}_o\hat{V}\hat{G}_o\hat{V} + \ldots)|\Psi_o\rangle \tag{16}$$
$$= \hat{G}_o\hat{T}|\Psi_o\rangle. \tag{17}$$

- The total wave-function can now be written using *T-matrix*

$$\Psi(\vec{r}) = \Psi_o(\vec{r}) + \int\int d\tau' d\tau'' G_o(\vec{r},\vec{r}')T(\vec{r}',\vec{r}'')\Psi_o(\vec{r}''), \tag{18}$$

where

$$T(\vec{r}',\vec{r}'') = \langle \vec{r}'|\hat{T}|\vec{r}''\rangle. \tag{19}$$

1D delta function scattering

- Consider the potential $V(x) = g\delta(x)$.
- The T-Matrix is evaluated as follows

$$
\begin{aligned}
T(x,x') &= \langle x|\hat{T}|x'\rangle && (20)\\
&= \langle x|(\hat{V} + \hat{V}\hat{G}_o\hat{V} + \hat{V}\hat{G}_o\hat{V}\hat{G}_o\hat{V} + \ldots)|x'\rangle && (21)\\
&= g\delta(x')\delta(x-x') + g\delta(x)\int dx''|x''\rangle\langle x''|\hat{G}_o \\
&\quad \int dx'''|x'''\rangle\langle x'''|x'\rangle g\delta(x') + \ldots && (22)\\
&= g\delta(x)\delta(x')\left[1 + \left(-i\frac{gm}{\hbar^2 k}\right) + \left(-i\frac{gm}{\hbar^2 k}\right)^2 + \ldots\right] && (23)\\
&= \frac{g\delta(x)\delta(x')}{1 + i\frac{gm}{\hbar^2 k}}. && (24)
\end{aligned}
$$

- The scattering wave-function can be evaluated as follows

$$\Psi_s(x) = \int dx' dx'' G_o(x,x') T(x',x'') \Psi_o(x'') \tag{25}$$

$$= -\frac{e^{ik|x|}}{1 - i\frac{\hbar^2 k}{gm}} \tag{26}$$

- At low energy

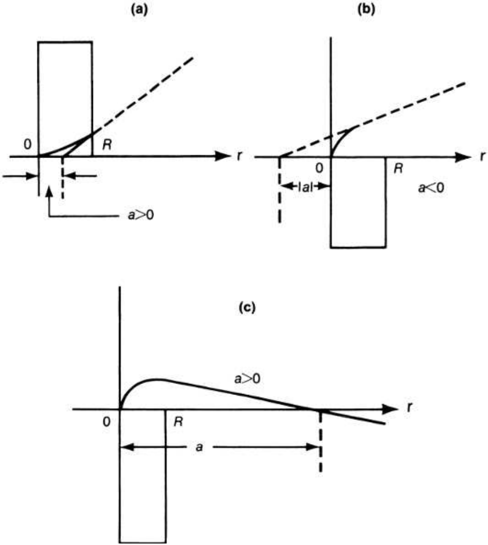
$$\lim_{k\to 0} \Psi_s(x) = \lim_{k\to 0} \left(-\left[1 + ikx + \mathcal{O}(k^2)\right] \left[1 + i\frac{\hbar^2 k}{gm} + \mathcal{O}(k^2)\right] \right)$$

$$= -\left[1 + \left(\frac{i\hbar^2}{gm} + x\right) k\right]. \tag{27}$$

- Scattering length is an intercept of scattered wave-function (outside the potential range) on real axis

$$a = \frac{\hbar^2}{mg}. \tag{28}$$

Scattering length



Feshbach Resonance

- Schrödinger for two body system

$$\left(-\frac{\hbar^2}{2m_1}\nabla^2_{r_1} - \frac{\hbar^2}{2m_2}\nabla^2_{r_2}\right)\Psi(\vec{r}_1,\vec{r}_2)+V(\vec{r}_1,\vec{r}_2)\Psi(\vec{r}_1,\vec{r}_2) = E\Psi(\vec{r}_1,\vec{r}_2). \tag{29}$$

- For central potential $V(\vec{r}_1,\vec{r}_2) = V(|\vec{r}_1 - \vec{r}_2|)$, the equation can be decoupled as shown

$$-\frac{\hbar^2}{2M}\nabla^2_R\Psi_{cm}(\vec{R}) = E_{cm}\Psi_{cm}(\vec{R}) \tag{30}$$

and

$$-\frac{\hbar^2}{2\mu}\nabla^2_r\Psi_{rel}(\vec{r}) + V(r)\Psi_{rel}(\vec{r}) = E_{rel}\Psi_{rel}(\vec{r}), \tag{31}$$

where

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

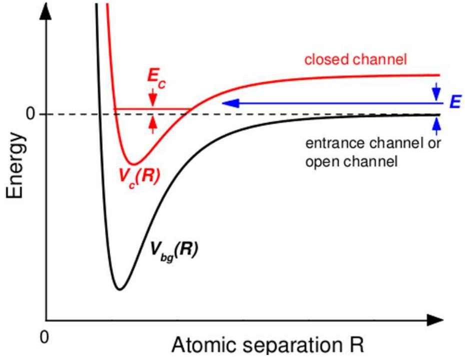
- In center of mass frame, the Schrödinger equation can be reduced to the form

$$-\frac{\hbar^2}{2\mu}\frac{d^2\phi_l(r)}{dr^2} + V_l(r)\phi_l(r) = E\phi_l(r), \tag{32}$$

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

$$\Psi(\vec{r}) = \frac{\phi_l(r)}{r} Y_{l,m_l}(\theta, \varphi). \tag{33}$$

Principle

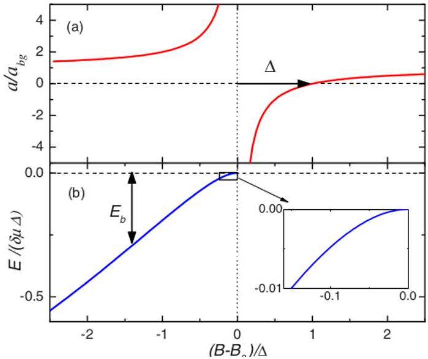


- Consider two molecular potential curves

$V_{bg}(r)$ background potential which connects to two free atoms in ultra-cold gas. For small collision energy E, it represents energetically opened channel.

$V_c(r)$ is a closed channel which supports atleast one bounded molecular state near threshold of open channel.

- A Feshbach resonance occurs when the bound molecular-state in closed channel energetically approaches the scattering state in open channel.
- The mixing of two channels becomes strong.
- E_c can be magnetically tuned. The energy difference $E_c - E$ depends on the relative difference in magnetic moment of two channels
$$\delta\mu = |\mu_{open} - \mu_{closed}|. \tag{34}$$
- For a magnetically tuned resonance, the s-wave scattering length a can be written in terms of magnetic field
$$a(B) = a_{bg}\left(1 - \frac{\Delta}{B - B_o}\right). \tag{35}$$



- Near resonance, where two channels are strongly coupled, a dressed molecular state exists with binding energy given by

$$E_b = \frac{\hbar^2}{2\mu a^2}. \tag{36}$$

- E_b depends quadratically on magnetic field.

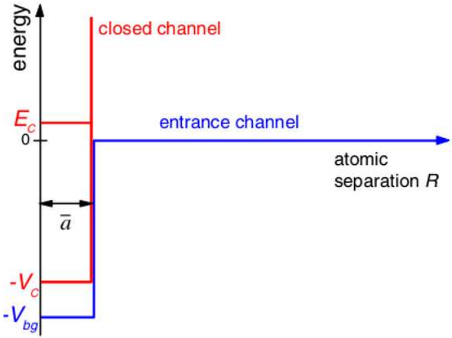
Collision channels

- Spin dependent Hamiltonian.
- A channel is defined by:
  Internal state of the two particles (spins)
  Relative partial wave with component l
- Hence, the state-vector of a channel is

$$|\alpha\rangle = |q_1, q_2\rangle |l, m_l\rangle, \tag{37}$$

  where q_1 and q_2 are spin quantum number of particles 1 and 2 respectively.

Infinite square well two channel model



- The initial state vector for a square well is given as

$$
\begin{aligned}
|\Psi\rangle =& |q_1, q_2(bg)\rangle |l, m_l(bg)\rangle |n, l(bg)\rangle + |q_1, q_2(c)\rangle |l, m_l(c)\rangle |n, l(c)\rangle \\
=& |bg\rangle |n, l(bg)\rangle + |c\rangle |n, l(c)\rangle. \qquad (38)
\end{aligned}
$$

- The Schrödinger is

$$\hat{H}|\Psi\rangle = E|\Psi\rangle, \tag{39}$$

where the Hamiltonian of the system is

$$\hat{H} = \left(\frac{\hat{p}^2}{2\mu} + \hat{V}\right). \tag{40}$$

- The potential operator has two components

$$\hat{V} = \underbrace{\hat{V}_{int} \otimes \hat{I}}_{\substack{\text{intrinsic or} \\ \text{spin-dependent part}}} + \underbrace{\hat{I} \otimes V(\hat{\vec{r}})}_{\text{spatially dependent part}} . \tag{41}$$

- On substituting the state-vector and Hamiltonian

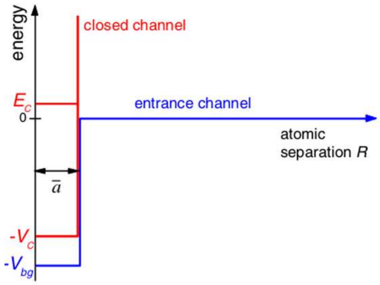
$$\left(\frac{\hat{p}^2}{2\mu} + \hat{V}\right)(|bg\rangle|n, l(bg)\rangle + |c\rangle|n, l(c)\rangle) = E(|bg\rangle|n, l(bg)\rangle + |c\rangle|n, l(c)\rangle) \tag{42}$$

- In position basis, the equation can be written in matrix form

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\begin{pmatrix} \phi_{l,bg}(r) \\ \phi_{l,c}(r) \end{pmatrix} + \mathbf{V}(r)\begin{pmatrix} \phi_{l,bg}(r) \\ \phi_{l,c}(r) \end{pmatrix} = E\begin{pmatrix} \phi_{l,bg}(r) \\ \phi_{l,c}(r) \end{pmatrix} \tag{43}$$

where

$$\mathbf{V}(r) = \begin{pmatrix} \begin{matrix} V_{bg}(r) + \frac{\hbar^2}{2\mu r^2} l_{bg}(l_{bg}+1) \\ +\langle bg|\hat{V}_{int}|bg\rangle \end{matrix} & \langle bg|\hat{V}_{int}|c\rangle \\ \\ \langle c|\hat{V}_{int}|bg\rangle & \begin{matrix} V_c(r) + \frac{\hbar^2}{2\mu r^2} l_c(lc+1) \\ +\langle c|\hat{V}_{int}|c\rangle \end{matrix} \end{pmatrix}. \tag{44}$$



- In square well example, for $r < \bar{a}$, we have the attractive potential which supports multiple bounded states.
- $\hbar\Omega$ induces Feshbach coupling between channels.
- For $r > \bar{a}$, background channel and closed channel thresholds are set to be 0 and ∞ respectively.
- Hence

$$\mathbf{V} = \begin{cases} \begin{pmatrix} -V_c & \hbar\Omega \\ \hbar\Omega & -V_{bg} \end{pmatrix} & \text{for } r < \bar{a}, \\ \begin{pmatrix} \infty & 0 \\ 0 & 0 \end{pmatrix} & \text{for } r > \bar{a}\ . \end{cases} \tag{45}$$

- The solution has the form

$$|\Psi\rangle \propto \begin{cases} \frac{\sin(q_+ r)}{r}|+\rangle + \frac{A\sin(q_- r)}{r}|-\rangle & (\text{for } r < \bar{a}), \\ \frac{\sin(kr+\eta)}{r}|bg\rangle & (\text{for } r > \bar{a}). \end{cases} \tag{46}$$

  where $\hbar^2 q_{\pm}^2/2\mu = E + \frac{1}{2}(V_e + V_c) \pm \frac{1}{2}(V_e - V_c)\sec(2\theta)$, $\tan(2\theta) = 2\hbar\Omega/(V_e - V_c)$, $|+\rangle = \cos(\theta)|bg\rangle + \sin(\theta)|c\rangle$ and $|-\rangle = -\sin(\theta)|bg\rangle + \cos(\theta)|c\rangle$.
- Using weak coupling limit ($\theta \to 0$) and continuity condition

$$\cot(k\bar{a} + \eta) = \cot(k\bar{a} + \eta_{bg}) - \frac{\Gamma/2}{k\bar{a}E_c}, \tag{47}$$

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

- Using the relation

$$a = -\lim_{k \to 0} (k \cot(\eta)^{-1}), \tag{48}$$

the scattering length can be calculated as

$$a = a_{bg} \left(1 - \frac{\Delta}{B - B_o} \right) \tag{49}$$

Harmonic oscillator: two channel model

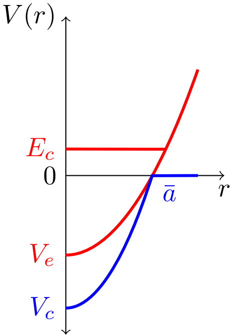


Figure : Two channel isotropic harmonic oscillator model: Red curve is the closed channel with at least one bound state E_c. The entrance channel is represented by the blue curve.

- The potential matrix of the system becomes

$$\mathbf{V}(r) = \begin{cases} \begin{pmatrix} \frac{1}{2}\mu\omega_c^2 r^2 - V_c & \hbar\Omega \\ \hbar\Omega & \frac{1}{2}\mu\omega_e^2 r^2 - V_e \end{pmatrix} & \text{for } r < \bar{a}, \\ \begin{pmatrix} \frac{1}{2}\mu\omega_c^2 r^2 - V_c & 0 \\ 0 & 0 \end{pmatrix} & \text{for } r > \bar{a}\ . \end{cases} \quad (50)$$

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

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\begin{pmatrix} \phi_c(r) \\ \phi_e(r) \end{pmatrix} + \mathbf{V}(r)\begin{pmatrix} \phi_c(r) \\ \phi_e(r) \end{pmatrix} = E\begin{pmatrix} \phi_c(r) \\ \phi_e(r) \end{pmatrix}. \quad (51)$$

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

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\phi_c(r) + \left(\frac{1}{2}\mu\omega_c^2 r^2 - V_c\right)\phi_c(r) = E\phi_c(r). \tag{52}$$

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

$$\phi_c(r) = C_1 D_{-\nu-1}(i\rho) + C_2 D_\nu(\rho), \tag{53}$$

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).

- The application of the boundary conditions imply $C_1 = 0$ with the solution

$$\phi_c(\rho) = C_2 D_\nu(\rho) \tag{54}$$

and total energy

$$E_\nu = \left(\nu + \frac{1}{2}\right)\hbar\omega_c - V_c. \tag{55}$$

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

$$\frac{d}{dr}\begin{pmatrix} \phi_c(r) \\ \phi_e(r) \\ \phi_c'(r) \\ \phi_e'(r) \end{pmatrix} = \mathbf{A}(r)\begin{pmatrix} \phi_c(r) \\ \phi_e(r) \\ \phi_c'(r) \\ \phi_e'(r) \end{pmatrix}, \tag{56}$$

- $\mathbf{A}(r)$ 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 (56) can be solved using Magnus expansion [1]. If an unknown vector $Y(r) \in \mathbb{C}^n$ with, an initial condition $Y(r_o) = Y_o$, satisfies the equation

$$\frac{d}{dr} Y(r) = A(r) Y(r), \tag{57}$$

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

$$Y(r) = \exp\left(\Omega(r, r_o)\right) Y_o, \tag{58}$$

where (with $r_o = 0$)

$$\Omega(r) = \sum_{k=1}^{\infty} \Omega_k(r). \tag{59}$$

- Each element of the summation is defined as follows

$$
\begin{aligned}
\Omega_1(r) =& \int_0^r A(r_1)\, dr_1, \\
\Omega_2(r) =& \frac{1}{2} \int_0^r dr_1 \int_0^{r_1} dr_2 \;\; [A(r_1), A(r_2)], \\
\Omega_3(r) =& \frac{1}{6} \int_0^r dr_1 \int_0^{r_1} dr_2 \int_0^{r_2} dr_3 \;\; ([A(r_1), [A(r_2), A(r_3)]] \\
& + [A(r_3), [A(r_2), A(r_1)]]), \\
\Omega_4(r) =& \frac{1}{12} \int_0^r dr_1 \int_0^{r_1} dr_2 \int_0^{r_2} dr_3 \int_0^{r_3} dr_4 \;\; ([[[A_1, A_2], A_3], A_4] \\
& + [A_1, [[A_2, A_3], A_4]] + [A_1, [A_2, [A_3, A_4]]] \\
& + [A_2, [A_3, [A_4, A_1]]]),
\end{aligned} \tag{60}
$$

where $[A, B] = AB - BA$ is the commutation of matrices A and B.

- On integration following matrices were obtained

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

$$
\Omega_2(r)=\begin{pmatrix} -\frac{2r^4\mu V_c}{3a^2\hbar^2} & 0 & 0 & 0 \\ 0 & -\frac{2r^4\mu V_e}{3a^2\hbar^2} & 0 & 0 \\ 0 & 0 & \frac{2r^4\mu V_c}{3\bar{a}^2\hbar^2} & 0 \\ 0 & 0 & 0 & \frac{2r^4\mu V_e}{3\bar{a}^2\hbar^2} \end{pmatrix} \tag{61}
$$

Scattering length

- The scattered state function $\phi_c(r) = C_2 D_\nu(r)$ for $r \ll a_{ho}$ is

$$\begin{aligned} D_\nu(r) &= D_\nu(0) + r D'_\nu(0) + \mathcal{O}(r^2) \\ &\approx D_\nu(0) \left(1 - \frac{r}{a_{ho} f(E)}\right), \end{aligned} \tag{62}$$

with

$$f(E) = \frac{\Gamma\left(\frac{1}{4} - \frac{E}{2\hbar\omega_c}\right)}{2\Gamma\left(\frac{3}{4} - \frac{E}{2\hbar\omega_c}\right)}, \tag{63}$$

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

$$\begin{aligned} a &= a_{ho} f(E) \\ &= \sqrt{\frac{\hbar}{\mu\omega_c}} \frac{\Gamma\left(\frac{1}{4} - \frac{E}{2\hbar\omega_c}\right)}{2\Gamma\left(\frac{3}{4} - \frac{E}{2\hbar\omega_c}\right)}. \end{aligned} \tag{64}$$

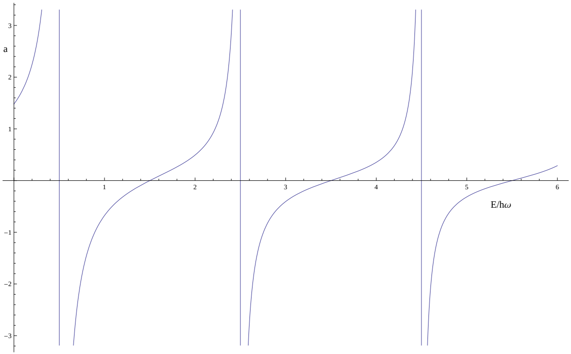


Figure : The plot of scattering length a/a_{ho} vs $E/(\hbar\omega_c)$.

References

S. Blanes, F. Casas, J. A. Oteo, and J. Ross.
The magnus expansion and some of its applications.
Rev Mod Phy, 470:151–238, 2009.

Cheng Chin, Rudolf Grimm, and Paul Julienne.
Feshbah resonances in ultracold gases.
Reviews of Modern Physics, 82:1226–1272, 2010.

P.A.M. Dirac.
The Principles of Quantum Mechanics.
Oxford University Press, 1958.

A. D. Lange, K. Pilch, A. Prantner, F. Ferlaino, B. Engeser, C. Chin, and R. Grimm.
Determination of atomic scattering lengths from measurements of molecular binding energies near feshbach resonances.
Physical Review A, 79, 2009.

M. Reed and B. Simon.
Methods of Modern Mathematical Physics, Vol.1 - Functional Analysis.
Academic Press, New York, 1980.