Feshbach Resonances I

A tale of two potentials

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Plan of the lecture

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Interatomic potential

Effects of atom-atom elastic collisions depend on the interatomic potential. Interaction potentials having bound states consist of

- repulsive inner core,
- potential well,
- long range van der Waals.

Lennard-Jones potential is a good model

\[ V(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right], \]

\( \epsilon \) and \( \sigma \) are depth of the well and distance at which potential is zero.
Identical particles

In identical particle scattering, dominant partial waves

- bosons: s-wave,
- fermions: p-wave.

At low energies ($k \rightarrow 0$), effective form of interaction for bosons is

$$V(r) = \frac{4\pi \hbar^2 a_s}{m} \delta(r).$$

$a_s \mapsto$ s-wave scattering length. Contributes to the self-coupling in the condensate order parameter

$$\int dr_1 \int dr_2 \psi^*(r_1) \psi^*(r_2) V(r_{12}) \psi(r_1) \psi(r_2) = \frac{4\pi \hbar^2 a_s}{m} \int dr_1 |\psi(r_1)|^4.$$
Atom-atom scattering

Wavefunction in **steady-state** scattering configuration

\[ \psi(r) = e^{ikz} + f(k', k) \frac{e^{ik'r}}{r}. \]

- \( f(k', k) \) \( \leadsto \) scattering amplitude.
- Elastic scattering \( \leadsto k = k' \), so \( f(k', k) = f(k, \theta) \).
- Differential scattering Cross section \( \leadsto d\sigma = |f(k, \theta)|^2 d\Omega \).

\( \psi(r) \) should match with the **asymptotic** solution of the Schrödinger equation

\[ \left[ -\frac{\hbar^2}{m} \nabla^2 + V(r) \right] \psi(r) = E \psi(r), \]

where \( V(r) \) is the inter-atomic potential.
Phase shift

Radial Schrödinger equation for two interacting atoms

\[
-\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \frac{mV(r)}{\hbar^2} + k^2 \right] u_l(k, r) = 0.
\]

Asymptotic \((r \to \infty)\) solution is

\[
u_l(k, r) = \frac{1}{k} \sin \left( kr - \frac{l\pi}{2} \right) \to \frac{1}{k} \sin \left( kr - \frac{l\pi}{2} + \delta_l \right).
\]

Phase shift \(\delta_l\) carries all the information about the scattering potential \(V(r)\). Can we get the correct \(\delta_l\) with a simple substitution?

\[V(r) \to a\delta(r)\]

\(a\) is related to the scattering length.
Scattering length

For elastic scattering, the scattering amplitude is

\[ f(k, \theta) = \sum_l f_l(k) P_l(\cos \theta). \]

After matching the solutions in the asymptotic region

\[ f_l(k) = \frac{2l + 1}{2ik} \left[ e^{2i\delta_l(k)} - 1 \right]. \]

s-wave \((l = 0)\) scattering length is

\[ a_s = -\lim_{k \to 0} \frac{\delta_0(k)}{k}. \]

**Fermi pseudopotential** for \(k \to 0\) bosonic atom interactions is

\[ V(r) = \frac{2\pi\hbar^2}{m} a_s \delta(r). \]

E. Fermi, Ricerca Scientifica 7, 13 (1936)
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Attractive or repulsive

Depending on the form of interatomic potential, $V(r)$, scattering length $a_s$ can be

- Always repulsive $\Rightarrow$ repulsive $V(r)$.
- Repulsive or attractive $\Rightarrow$ when $v(r)$ has an attractive part.

The latter is required for Feshbach resonance.
Model potential: attractive

Consider the scattering of a beam of particles from the attractive potential

\[ V(r) = \begin{cases} -V_0 & \text{for } r \leq a, \\ 0 & \text{for } r > a, \end{cases} \]

For s-partial wave, the Schrödinger equation in the two regions are

\[ \frac{d^2 u_1}{dr^2} + k_1 u_1 = 0, \quad \text{with} \quad k_1 = \frac{2m}{\hbar^2} \sqrt{E + V_0}, \]
\[ \frac{d^2 u_2}{dr^2} + ku_2 = 0, \quad \text{with} \quad k = \frac{2m}{\hbar^2} \sqrt{E}. \]

Solutions are \( u_1 = A \sin(k_1 r) \) and \( u_2 = B \sin(kr + \delta_0) \). From the boundary conditions \( u_1(a) = u_2(a) \) and \( u_1'(a) = u_2'(a) \), we get

\[ k_1 \cot(k_1 a) = k \cot(ka + \delta_0). \]
Model potential: Phase shift

The phase shift $\delta_0$ embodies the effect of the potential. Rewrite

$$\cot(ka + \delta_0) = \frac{k_1 \cot(k_1 a)}{k}.$$ 

In the low energy limit $k \to 0$, we have

- RHS $\implies k_1 \cot(k_1 a)/k \to \infty$
- LHS $\implies \sin(ka + \delta_0) \to 0$, so $\sin(ka + \delta_0) \approx ka + \delta_0$.

Since $ka \ll 1$, this implies that $\delta_0 \ll 1$ and

$$k_1 \cot(k_1 a) \approx \frac{k}{ka + \delta_0}.$$ 

This can be rewritten as

$$\delta_0 = ka \left[ \frac{\tan(k_1 a)}{k_1 a} - 1 \right].$$
Model potential: Scattering length

From the definition of $s$-wave scattering length

$$a_s = \lim_{k \to 0} \frac{-\delta_0}{k} \rightarrow a_s = a \left[ 1 - \frac{\tan(k_1 a)}{k_1 a} \right].$$

From definition when $k \to 0$, we have $k_1 = 2m \sqrt{V_0/\hbar^2}$, so

$$a_s = a \left[ 1 - \frac{\hbar^2 \tan(2ma \sqrt{V_0/\hbar^2})}{2ma \sqrt{V_0}} \right].$$

There are $s$-wave resonances, and these happen when $V_0$ is such that $2ma \sqrt{V_0/\hbar^2} = (2n + 1)\pi/2$. Each correspond to a bound state appearance: shape resonance.
Model potential: repulsive

Consider the scattering of a beam of particles from the attractive potential

\[ V(r) = \begin{cases} V_0 & \text{for } r \leq a, \\ 0 & \text{for } r > a, \end{cases} \]

For \( s \)-partial wave, the solution in the two regions are

- \( V_0 < 0 \) case
  - \( u_1 = A \sin(k_1 r) \)
  - \( u_2 = B \sin(kr + \delta_0) \)

- \( V_0 > 0 \) case
  - \( u_1 = A \sinh(k'_1 r) \)
  - \( u_2 = B \sin(kr + \delta_0) \)

Here, \( k_1 = 2m\sqrt{E + V_0/\hbar^2} \) and \( ik'_1 = 2m\sqrt{E - V_0/\hbar^2} \) with \( E < V_0 \). Boundary conditions \( u_1(a) = u_2(a) \) and \( u'_1(a) = u'_2(a) \) imply

\[ k'_1 \coth(k'_1 a) = k \cot(ka + \delta_0). \]
Model potential: scattering length

In the limit $k \to 0$, the phase shift is

$$\delta_0 = ka \left[ \frac{\tanh(k'_1 a)}{k'_1 a} - 1 \right],$$

this implies scattering length

$$a_s = \lim_{k \to 0} \frac{-\delta_0}{k} \to a_s = a \left[ 1 - \frac{\tanh(k'_1 a)}{k'_1 a} \right] \leq a.$$

From definition when $k \to 0$, we have $ik'_1 = 2m\sqrt{-V_0/\hbar^2}$, so

$$a_s = a \left[ 1 - \frac{\hbar^2 \tanh(2ma\sqrt{V_0}/\hbar^2)}{2ma\sqrt{V_0}} \right].$$
Model potential: cross section

Recall that scattering amplitude is

\[ f(k, \theta) = \sum_{l} \frac{2l + 1}{2ik} \left[ e^{2i\delta_l(k)} - 1 \right] P_l(\cos \theta). \]

When \( T \to 0, k \to 0 \) and for bosons only \( l = 0 \) contributes

\[ f(k, \theta) \equiv f(\theta) = \frac{1}{k} e^{i\delta_0} \sin(\delta_0) \approx \frac{1}{k} e^{i\delta_0} \delta_0. \]

Cross section is

\[ \sigma = 2\pi \int_{0}^{2\pi} |f(\theta)|^2 \sin \theta d\theta = 4\pi a^2 \left[ \frac{\tanh(k'_1 a)}{k'_1 a} - 1 \right]^2. \]

As \( ik'_1 = 2m\sqrt{E - V_0/\hbar^2}, V_0 \to \infty \) implies \( k'_1 \to \infty \). Scattering potential is equivalent to hard sphere

\[ \sigma = 4\pi a^2. \]
**Key point**

**Question**: Is it possible to tune or control interatomic interaction?

**Answer**
Considering the Fermi pseudopotential form of a potential

\[ V(r) = \frac{2\pi \hbar^2}{m} a_s \delta(r), \]

Near a resonance, it is possible to tune \( V(r) \) by adjusting the appearance of a bound state by varying \( V_0 \).

How to reallyyy to do it?
Basic requirement

It is should be possible to manipulate position of a bound state.

In atoms it is not trivial to manipulate the position of the last bound state.

**Prescription:**

- Consider two manifolds corresponding to two different hyperfine states.
- Control the resonance condition through an open-close channels.
- Use external field to select the scattering length.
Molecular Hamiltonian

Electronic Hamiltonian of H₂, only electrostatic interactions

\[
H_M = -\left(\nabla^2 + \frac{1}{r_{A1}}\right) - \left(\nabla^2 + \frac{1}{r_{B2}}\right) - \frac{1}{r_{A2}} - \frac{1}{r_{B1}} + \frac{1}{r_{12}} + \frac{1}{R},
\]

\[
= H_{H}(1) + H_{H}(2) - \frac{1}{r_{A2}} - \frac{1}{r_{B1}} + \frac{1}{r_{12}} + \frac{1}{R}.
\]

Large distances \( R \rightarrow \infty \)

\[
H_M \simeq H_{H}(1) + H_{H}(2) = \sum_i H_{H}(i).
\]

Molecular state and interatomic potential \( V(R) \) are functions of atomic states.
Molecular state

Hund-Mulliken or molecular orbital method, solve

\[ H_{H}(i)\Phi_{a} = E_{A}\Phi_{a}. \]

Eigenstates of \( H_{M} \) \( \rightarrow \) antisymmetrized direct products of \( \Phi_{a} \) and spin components,

\[ \Phi_{A}(1, 2) = \Phi_{g}(1)\Phi_{g}(2)\chi_{0,0}(1, 2) \]
\[ \Phi_{B}(1, 2) = \Phi_{u}(1)\Phi_{u}(2)\chi_{0,0}(1, 2). \]

Molecular states \( \rightarrow \) linear combinations

\[ \Phi_{T} = \Phi_{A}(1, 2) + \lambda\Phi_{B}(1, 2). \]

\( \lambda \) Rayleigh-Ritz variational parameter. Interatomic potential depend on the molecular states and can be either attractive or repulsive.
Hyperfine interaction and external field

Other interaction Hamiltonians which may contribute are:

- **Hyperfine interaction** \( H_{hf} = \frac{a_{hf}}{\hbar^2} \mathbf{l} \cdot \mathbf{S} \)

- **External magnetic field** \( \mathbf{B} \) \( \mu_e \cdot \mathbf{B} - \mu_p \cdot \mathbf{B} \)

\( \mu_e \) and \( \mu_p \) are the magnetic moment of electron and proton, respectively.

Total atomic Hamiltonian is

\[
H_T = - \left( \nabla^2 + \frac{1}{r} \right) + \frac{a_{hf}}{\hbar^2} \mathbf{l} \cdot \mathbf{S} + \mu_e \cdot \mathbf{B} - \mu_p \cdot \mathbf{B}.
\]
Molecular Hamiltonian

Molecular Hamiltonian, without the hyperfine interaction, in presence of $\mathbf{B}$ is

$$H_M = \sum_i \left[ - \left( \nabla_i^2 + \frac{1}{r_i} \right) + \left( \mu_{ei} - \mu_{pi} \right) \cdot \mathbf{B} \right] + V_M(r).$$

Here, $V_M(r)$ is the interatomic potential, which depends on the electronic states of the atoms. For the alkali atoms, it is either

- **singlet** ($S = 0$) $\leftrightarrow$ electronic spins of the two atoms are opposite.
- **triplet** ($S = 1$) $\leftrightarrow$ electronic spins of the two atoms are parallel.

Corresponding potential are denoted by $V_S$ and $V_T$, respectively.
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Toy potential

Consider the interatomic toy potential for the two internal states as

\[ V_{T,S}(r) = \begin{cases} 
-V_{T,S} & \text{if } r < R, \\
0 & \text{if } r \geq R, 
\end{cases} \]

where

- Potential depth \( V_{T,S} > 0 \) and singlet states are lower in energy so \( V_S > V_T \).
- Bound state \( \Rightarrow \) assume \( V_S \) is deep enough to accommodate exactly one bound state.

Schrödinger equation of the two states are

\[
\begin{align*}
\left[-\nabla^2 + V_T(r) + \mu_T \cdot B\right] \psi_T(r) &= E_T \psi_T(r), \\
\left[-\nabla^2 + V_S(r) + \mu_S \cdot B\right] \psi_S(r) &= E_T \psi_S(r),
\end{align*}
\]
Toy interaction

With energy shift of $\mu_T \cdot B$, the Schrödinger equation is

$$\begin{pmatrix} -\nabla^2 + V_T(r) - E & 0 \\ 0 & -\nabla^2 + V_S(r) + \Delta \mu \cdot B \end{pmatrix} \begin{pmatrix} \psi_T(r) \\ \psi_S(r) \end{pmatrix} = 0.$$

Toy interaction from the electron-nucleus magnetic interaction

$$H_{\text{int}} = \begin{pmatrix} 0 & \nu_{hf} \\ \nu_{hf} & 0 \end{pmatrix},$$

such that, $0 < \nu_{hf} \ll V_T, V_S, \Delta \mu \cdot B$. The states, $\psi_T(r)$ and $\psi_S(r)$ are not the eigenstates of total Hamiltonian

$$\begin{pmatrix} -\nabla^2 + V_T(r) - E & \nu_{hf} \\ \nu_{hf} & -\nabla^2 + V_S(r) + \Delta \mu \cdot B \end{pmatrix}.$$
Toy scattering states: \( r > R \)

When \( r > R \), interatomic potential, \( V_T \) and \( V_S \), are zero. Scattering states are eigenstates of

\[
H^> = \begin{pmatrix} 0 & \nu_{hf} \\ \nu_{hf} & \Delta \mu \cdot B \end{pmatrix},
\]

defined in the basis \( \{ \psi_T, \psi_S \} \). Diagonalize \( H^> \) with transformation

\[
Q(\theta^>) = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \rightarrow QH^>Q^{-1} = \begin{pmatrix} \varepsilon_+ > & 0 \\ 0 & \varepsilon_- > \end{pmatrix},
\]

where \( \tan \theta^> = 2\nu_{hf}/\Delta \mu \cdot B \) and

\[
\varepsilon^\pm_+ = \frac{1}{2} \left[ \Delta \mu \cdot B \pm \sqrt{(\Delta \mu \cdot B)^2 + (2\nu_{hf})^2} \right],
\]

Eigenvalue equations are

\[
H^>| \uparrow\uparrow > = \varepsilon^- _+ | \uparrow\uparrow >, \text{ and } H^>| \downarrow\downarrow > = \varepsilon^+_+ | \downarrow\downarrow >.
\]
Toy channels

Since $v_{hf} \ll \Delta \mu \cdot B$, from

$$\varepsilon_{\pm} = \frac{1}{2} \left[ \Delta \mu \cdot B \pm \sqrt{(\Delta \mu \cdot B)^2 + (2V_{hf})^2} \right],$$

we get $\varepsilon_+ \approx \Delta \mu \cdot B$ and $\varepsilon_- \approx 0$.

- $r > R \implies V_T$ and $V_S$, are zero. So $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ are ideal to study atom-atom scattering.
- Channels $\implies$ as $\varepsilon_+ > \varepsilon_-$, atom-atom interactions are predominantly in $|\uparrow\uparrow\rangle$.
- Open channel $\implies$ from energy conservation, atoms in $|\uparrow\uparrow\rangle$ are not connected to $|\downarrow\downarrow\rangle$. These are open and closed channels, respectively.
Toy problem

Transforming the interatomic potential

\[ Q \left( \begin{array}{cc} V_T(r) & 0 \\ 0 & V_S(r) \end{array} \right) Q^{-1} = \left( \begin{array}{cc} V_{↑↑}(r) & V_{↑↓}(r) \\ V_{↑↓}(r) & V_{↓↓}(r) \end{array} \right). \]

Schrödinger equation in all radial ranges is

\[ \left( -\nabla^2 + V_{↑↑}(r) - E \right) \begin{pmatrix} \psi_{↑↑}(r) \\ \psi_{↓↓}(r) \end{pmatrix} = 0, \]

where, \( \delta \varepsilon = \varepsilon_+ - \varepsilon_+ \).

- Basis \( |↑↑\rangle \) and \( |↓↓\rangle \) eigenstates of Hamiltonian with hyperfine interaction.
- \( |↑↑\rangle \) and \( |↓↓\rangle \) are linear combinations of \( \psi_T(r) \) and \( \psi_S(r) \), e.g.

\[ \psi_{↑↑}(r) = C_1 \psi_T(r) + C_2 \psi_S(r), \]
To calculate phase shift, the radial Schrödinger equation is solved in two regions: $r > R$, and $r < R$. Solutions are

$$\begin{pmatrix} u_{>\uparrow\uparrow}(r) \\ u_{>\downarrow\downarrow}(r) \end{pmatrix} = \begin{pmatrix} Ce^{ikr} + De^{-ikr} \\ Fe^{-\kappa r} \end{pmatrix},$$

and

$$\begin{pmatrix} u_{<\uparrow\uparrow}(r) \\ u_{<\downarrow\downarrow}(r) \end{pmatrix} = \begin{pmatrix} A(e^{ik_{\uparrow\uparrow}r} - e^{-ik_{\uparrow\uparrow}r}) \\ B(e^{ik_{\downarrow\downarrow}r} - e^{-ik_{\downarrow\downarrow}r}) \end{pmatrix} \cdot$$

where $\kappa = \sqrt{\varepsilon^<_+ - \varepsilon^>_+ - k^2}$, $k_{\uparrow\uparrow}^<_+ = \sqrt{\varepsilon^>_+ - \varepsilon^>_+ - k^2}$, and $k_{\downarrow\downarrow}^<_+ = \sqrt{\varepsilon^>_+ - \varepsilon^>_+ - k^2}$, with

$$\varepsilon^<_\pm = \frac{\Delta \mu \cdot B - V_T - V_S}{2} \pm \frac{1}{2} \sqrt{(V_S - V_T - \Delta \mu \cdot B)^2 + (2V_{hf})^2}.$$
Toy parameters

Few observations

• $\varepsilon_\pm^\leq$ depends on $B$. Considering $V_{hf} \ll V_T, V_S$, we get $\varepsilon_+^\leq \approx -V_T$ and $\varepsilon_-^\leq \approx \Delta \mu \cdot B - V_S$.

• $\varepsilon_\pm^\geq$ from previous discussions, recall

$$\varepsilon_\pm^\geq = \frac{1}{2} \left[ \Delta \mu \cdot B \pm \sqrt{(\Delta \mu \cdot B)^2 + (2V_{hf})^2} \right],$$

we can write $\varepsilon_+^\geq \approx \Delta \mu \cdot B$ and $\varepsilon_-^\geq \approx 0$.

• $k$ and $\kappa$ from the above considerations

$$k_{\uparrow \uparrow}^\leq \approx \sqrt{V_S - \Delta \mu \cdot B - k^2}, \quad k_{\downarrow \downarrow}^\leq \approx \sqrt{V_T - k^2}$$

and

$$\kappa \approx \sqrt{\Delta \mu \cdot B - k^2}.$$

Note the dependence of the wave numbers on $B$. 
Finally: some hand waving

To obtain phase shift, we do the following

- Match the solutions $u^<$ and $u^>$ at $r = R$.
- Transform the expression from the $\{|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$ basis to $\{\psi_T, \psi_S\}$. The later is independent of $r$.
- Calculate phase shift $\delta_0$ and use the relation $a_s = \lim_{k \to 0} -\delta_0/k$ to calculate $a_s$.

The $a_s$ obtained after the calculations is of the form

$$a(B) = a_{bg} \left( 1 - \frac{\Delta B}{B - B_0} \right),$$

where, $B_0$ is the position of the Feshbach resonance.
References

- *Atom-Molecule coherence in Bose gases*,
  R. A. Duine and H. T. C. Stoof,

- *Introductory Quantum Mechanics*,

- *Bose-Einstein condensation in dilute gases*,
  C. J. Pethick and H. Smith, (2nd Ed).

- *Feshbach resonances in ultracold gases*,
  C. Chin, R. Grimm, P. Julienne and E. Tiesinga,