Elements of the scattering theory
Elastic scattering
Two colliding (interacting) particles

Particles with masses $m_1$ and $m_2$, interacting with potential $V(r_1 - r_2)$

$$\mathbf{r} = r_1 - r_2$$

Coordinate of the center of mass

$$\mathbf{R}_{\text{cm}} = (m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2) / (m_1 + m_2)$$

In the centre-of-mass frame of reference, the coordinates of the two particles are

$$\mathbf{r}_1^{(\text{cm})} = \frac{m_2}{m_1 + m_2} \mathbf{r}, \quad \mathbf{r}_2^{(\text{cm})} = -\frac{m_1}{m_1 + m_2} \mathbf{r}$$

If one introduces the reduced mass $\mu$

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

The Hamilton function becomes

$$H(p, r) = \frac{\mathbf{p}^2}{2\mu} + V(r) \quad \text{with} \quad \mathbf{p} = \mu \frac{d\mathbf{r}}{dt}$$

Then, the Hamiltonian operator is

$$H = \frac{\mathbf{p}^2}{2\mu} + V(r) \quad \text{with} \quad \mathbf{p} = -\hbar \nabla_r$$
Scattering Amplitude

Schrödinger equation

\[
\left[-\frac{\hbar^2}{2\mu} \Delta + V(\mathbf{r})\right] \psi(\mathbf{r}) = E \psi(\mathbf{r})
\]

\[ E = \frac{\hbar^2 k^2}{2\mu} \]

Boundary conditions for a solution

\[
\psi(\mathbf{r}) \xrightarrow{r \to \infty} e^{i k z} + f(\theta, \phi) \frac{e^{i k r}}{r}
\]

Now, we assume that the potential falls off faster than \(1/r^2\):

\[
r^2 V(\mathbf{r}) \xrightarrow{r \to \infty} 0
\]
Current density

The amplitude $f(\theta, \phi)$ depends on the current density, $j(r)$. 

Classically, $j(r) = \mathbf{v} n$ is the product of particle density and velocity.

Quantum-mechanical expression is:

$$j(r) = \mathcal{R} \left[ \psi^*(r) \hat{p} \psi(r) \right] = \frac{\hbar}{2i\mu} \psi^*(r) \nabla \psi(r) + \text{cc}$$

Its value depends on normalization of the incident wave. For example, for

$$\psi(r) \xrightarrow{r \to \infty} e^{ikz} + f(\theta, \phi) \frac{e^{ikr}}{r}$$

the current density in the incident wave is $j_{\text{in}} = \hat{e}_z \hbar k / \mu$

But $j$ in the outgoing wave is

$$j_{\text{out}}(r) = \frac{\hbar k}{\mu} |f(\theta, \phi)|^2 \frac{\hat{e}_r}{r} + O\left(\frac{1}{r^3}\right)$$
Cross Section

Number of particles crossing area $ds$ at large $r$ per unit time in the outgoing wave:

$$\lim_{r \to \infty} j_{\text{out}}(r) \cdot ds$$

with

$$ds = \hat{e}_r r^2 d\Omega \quad d\Omega = \sin \theta d\theta d\phi$$

I.e. the current density in the outgoing wave is

$$(\hbar k/\mu) |f(\theta, \phi)|^2 d\Omega$$

If one normalizes with respect to the current density $|j_{\text{in}}| = \hbar k / \mu$

$$d\sigma = |f(\theta, \phi)|^2 d\Omega \quad \frac{d\sigma}{d\Omega} = |f(\theta, \phi)|^2$$

It is the differential elastic cross section. The integrated elastic cross section is

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^{2\pi} d\phi \int_0^\pi \sin \theta d\theta |f(\theta, \phi)|^2.$$
Cross Section

$$d\sigma = |f(\theta, \phi)|^2 d\Omega$$

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^{2\pi} d\phi \int_0^\pi \sin \theta d\theta \left| f(\theta, \phi) \right|^2$$
The differential Schrödinger equation

\[ \left( E + \frac{\hbar^2}{2\mu} \Delta \right) \psi(\mathbf{r}) = V(\mathbf{r}) \psi(\mathbf{r}) \]

is transformed into an integral equation using the free-particle Green's function

\[ \left( E + \frac{\hbar^2}{2\mu} \Delta_{\mathbf{r}} \right) \mathcal{G}(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \]

\[ \mathcal{G}(\mathbf{r}, \mathbf{r}') = -\frac{\mu}{2\pi \hbar^2} \frac{e^{ik|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} \]

The wave function obeying

\[ \psi(\mathbf{r}) = e^{ikz} + \int \mathcal{G}(\mathbf{r}, \mathbf{r}') V(\mathbf{r}') \psi(\mathbf{r}') d\mathbf{r}' \quad (1) \]

is also a solution of

\[ \left( E + \frac{\hbar^2}{2\mu} \Delta \right) \psi(\mathbf{r}) = V(\mathbf{r}) \psi(\mathbf{r}) \]

The \( e^{ikz} \) in (1) can be replaced by any solution of the homogeneous equation

\[ [E + (\hbar^2/(2\mu)) \Delta] \psi(\mathbf{r}) = 0 \]
Born Approximation

When \(|r| \gg |r'|\) the Green's function is approximated by

\[
G(r, r') = -\frac{\mu}{2\pi \hbar^2} \frac{e^{ik|r-r'|}}{|r-r'|} \left[ e^{-ikr} + O\left(\frac{r'}{r}\right) \right].
\]

plugging it in

\[
\psi(r) = e^{ikz} + \int G(r, r') V(r')\psi(r')dr'.
\]

\[
f(\theta, \phi) = -\frac{\mu}{2\pi \hbar^2} \int e^{-ikr} V(r')\psi(r')dr'.
\]

It is an exact solution if it converges. It converges if \(V(r)\) is less singular than \(1/r^2\) at the origin and

\[
r^2 V(r) \to 0 \quad r \to \infty
\]
Born Approximation

Inserting

\[ \psi(r) = e^{ikz} + \int G(r, r') V(r') \psi(r') dr' \]

in

\[ f(\theta, \phi) = -\frac{\mu}{2\pi \hbar^2} \int e^{-ikr \cdot r'} V(r') \psi(r') dr' \]

We obtain

\[ f(\theta, \phi) = -\frac{\mu}{2\pi \hbar^2} \left[ \int dr' e^{-ikr \cdot r'} V(r') e^{ikz'} ight. \\
+ \int dr' e^{-ikr \cdot r'} V(r') \int dr'' G(r', r'') V(r'') \psi(r'') \] 

Retaining only the first term gives the Born approximation.

\[ f^{\text{Born}}(\theta, \phi) = -\frac{\mu}{2\pi \hbar^2} \int dr' e^{-ikr \cdot r'} V(r') e^{ikz'} = -\frac{\mu}{2\pi \hbar^2} \int dr' e^{-i q \cdot r'} V(r') \]

\[ q = k(\hat{e}_r - \hat{e}_z) \]

\[ q = 2k \sin(\theta/2) \]
Angular Momentum: summary

Definition\[ \hat{\mathbf{L}} = \mathbf{r} \times \hat{\mathbf{p}} \]\n
properties

\[ [\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z \]

Eigenstates and eigenvalues

\[ \hat{\mathbf{L}}^2 Y_{l,m}(\theta, \phi) = l(l + 1)\hbar^2 Y_{l,m}(\theta, \phi), \quad l = 0, 1, 2, \ldots; \]

\[ \hat{L}_z Y_{l,m}(\theta, \phi) = m\hbar Y_{l,m}(\theta, \phi), \quad m = -l, -l + 1, \ldots, l - 1, l. \]

Spherical harmonics \( Y_{lm}(\theta, \phi) \)

\[
Y_{l,m}(\theta, \phi) = e^{im\phi} \sin^{|m|}(\theta) \text{Pol}_{l-|m|}(\cos \theta) \\
\int Y_{l,m}(\Omega)^* Y_{l',m'}(\Omega) d\Omega = \int_0^{2\pi} d\phi \int_{-1}^{+1} d\cos \theta Y_{l,m}(\theta, \phi)^* Y_{l',m'}(\theta, \phi) \\
= \delta_{l,l'} \delta_{m,m'},
\]

\[ Y_{l,m}(\theta - \pi, \phi + \pi) = Y_{l,-m}(\theta, \phi) = (-1)^l Y_{l,m}(\theta, \phi) \]

for two vectors \( \mathbf{a}, \mathbf{b}, \) with \( |\mathbf{a}| \leq |\mathbf{b}| \)

\[ Y_{l,m=0}(\theta) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos \theta) \]

\[ \int_{-1}^{1} P_l(x) P_{l'}(x) dx = \frac{2}{2l+1} \delta_{l,l'} \]

\[ \frac{1}{|\mathbf{a} - \mathbf{b}|} = \sum_{l=0}^{\infty} \frac{|\mathbf{a}|^l}{|\mathbf{b}|^{l+1}} P_l(\cos \theta) \]
Partial-Waves Expansion

The solution with boundary conditions

$$\psi(r) \sim r \rightarrow \infty e^{ikz} + f(\theta, \phi) \frac{e^{ikr}}{r}$$

is usually represented as an expansion over states with a definite angular momentum, so-called partial waves.

$$\psi(r, \theta) = \sum_{l=0}^{\infty} \frac{u_l(r)}{r} P_l(\cos \theta)$$

From the Schrödinger equation in spherical coordinates

$$-\frac{\hbar^2}{2\mu} \Delta = -\frac{\hbar^2}{2\mu} \left( \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{\hat{L}^2}{2\mu r^2}$$

one obtains the radial Schrödinger equation

$$\left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r) \right] u_l(r) = E u_l(r)$$

$$\langle u_l | \tilde{u}_l \rangle = \int_0^\infty u_l(r)^* \tilde{u}_l(r) dr$$
Scattering Phase Shifts

For free motion, $V(r) = 0$, the solutions of

$$\left[-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r)\right] u_l(r) = E u_l(r)$$

are obtained from spherical Bessel functions

$$u_l^{(s)}(kr) = kr j_l(kr), \quad u_l^{(c)}(kr) = -kr y_l(kr),$$

$$u_l^{(s)}(kr) \underset{kr \to \infty}{\approx} \sin\left(kr - l \frac{\pi}{2}\right) + O\left(\frac{1}{kr}\right),$$

$$u_l^{(c)}(kr) \underset{kr \to \infty}{\approx} \cos\left(kr - l \frac{\pi}{2}\right) + O\left(\frac{1}{kr}\right),$$

$$u_l^{(s)}(kr) \underset{kr \to 0}{\sim} \frac{\sqrt{\pi}(kr)^{l+1}}{2^{l+1} \Gamma(l + \frac{3}{2})} \left[1 - \frac{(kr)^2}{4l + 6}\right]$$

$u_l^{(s)}$ is a physical or regular solution

$$u_l^{(c)}(kr) \underset{kr \to 0}{\sim} \frac{2^l \Gamma(l + \frac{1}{2})}{\sqrt{\pi}(kr)^l} \left[1 + \frac{(kr)^2}{4l - 2}\right]$$

$u_l^{(c)}$ is an unphysical or irregular solution
Scattering Phase Shifts

When $V(r) \neq 0$, the solutions of

$$\left[ -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r) \right] u_l(r) = Eu_l(r)$$

at large distances are superpositions

$$u_l(r) \propto \lim_{r \to \infty} A u_l^{(s)}(kr) + B u_l^{(c)}(kr) \quad \lim_{r \to \infty} \sin \left( kr - l \frac{\pi}{2} + \delta_l \right)$$

$\delta_l$ is scattering phase shifts

$$\tan \delta_l = \frac{B}{A}$$

The partial-wave expansion

$$\psi(r) = \psi(r, \theta) = \sum_{l=0}^{\infty} \frac{u_l(r)}{r} P_l(\cos \theta)$$

In

$$\psi(r) \sim e^{ikz} + f(\theta, \phi) \frac{e^{ikr}}{r}$$

the $e^{ikz}$ term is

$$e^{ikz} = \sum_{l=0}^{\infty} (2l+1)i^l j_l(kr) P_l(\cos \theta)$$
Scattering Phase Shifts

In the second term could be written as

$$\psi(\mathbf{r}) \xrightarrow{r \to \infty} e^{ikz} + f(\theta, \phi) \frac{e^{ikr}}{r}$$

where $f_l$ are called partial-wave scattering amplitudes.

$$f(\theta) = \sum_{l=0}^{\infty} f_l P_l(\cos \theta)$$

$$\psi(\mathbf{r}) = \psi(r, \theta) = \sum_{l=0}^{\infty} \frac{u_l(r)}{r} P_l(\cos \theta).$$

$$e^{ikz} = \sum_{l=0}^{\infty} (2l + 1) i^l j_l(kr) P_l(\cos \theta)$$

$$u_l(r) \xrightarrow{r \to \infty} i^l \left[ \frac{2l + 1}{k} \sin \left( kr - l \frac{\pi}{2} \right) + f_l e^{i(kr-l\pi/2)} \right]$$

$$= i^l \left[ \left( \frac{2l + 1}{k} + i f_l \right) \sin \left( kr - l \frac{\pi}{2} \right) + f_l \cos \left( kr - l \frac{\pi}{2} \right) \right]$$
Scattering Phase Shifts

\[ u_l(r) \xrightarrow{r \to \infty} A u_l^{(s)}(kr) + B u_l^{(c)}(kr) \xrightarrow{r \to \infty} \sin \left( kr - l \frac{\pi}{2} + \delta_l \right) \]
\[ \tan \delta_l = B/A \]

\[ u_l(r) \xrightarrow{r \to \infty} i^l \left[ \frac{2l + 1}{k} \sin \left( kr - l \frac{\pi}{2} \right) + f_l e^{i(kr - l\pi/2)} \right] \]
\[ = i^l \left[ \left( \frac{2l + 1}{k} + i f_l \right) \sin \left( kr - l \frac{\pi}{2} \right) + f_l \cos \left( kr - l \frac{\pi}{2} \right) \right] \]

\[ \cot \delta_l = \frac{A}{B} \equiv \frac{2l + 1}{kf_l} + i \]
\[ f_l = \frac{2l + 1}{k} e^{i\delta_l} \sin \delta_l = \frac{2l + 1}{2ik} \left( e^{2i\delta_l} - 1 \right) \]

\[ u_l(r) \xrightarrow{r \to \infty} \frac{2l + 1}{k} i^l e^{i\delta_l} \sin \left( kr - l \frac{\pi}{2} + \delta_l \right) \]

\[ \psi(r) \xrightarrow{r \to \infty} \sum_{l=0}^{\infty} \frac{2l + 1}{kr} i^l e^{i\delta_l} \sin \left( kr - l \frac{\pi}{2} + \delta_l \right) P_l(\cos \theta) \]
Cross section

Using

\[
\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^{2\pi} d\phi \int_0^\pi \sin \theta d\theta |f(\theta, \phi)|^2
\]

\[
\psi(r) \sim \sum_{l=0}^\infty \frac{2l + 1}{k r} i^l e^{i\delta_l} \sin \left( kr - l \frac{\pi}{2} + \delta_l \right) P_l(\cos \theta)
\]

\[
\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{1}{k^2} \sum_{l,l'} e^{i(\delta_l - \delta_{l'})} (2l + 1) \sin \delta_l (2l' + 1) \sin \delta_{l'} P_l(\cos \theta) P_{l'}(\cos \theta)
\]

\[
\int_{-1}^1 P_l(x) P_{l'}(x) dx = \frac{2}{2l + 1} \delta_{l,l'}
\]

\[
\sigma = \sum_{l=0}^\infty \frac{4\pi}{2l + 1} |f_l|^2 = \frac{4\pi}{k^2} \sum_{l=0}^\infty (2l + 1) \sin^2 \delta_l = \frac{\pi}{k^2} \sum_{l=0}^\infty (2l + 1) |e^{2i\delta_l} - 1|^2
\]

\[
\sigma = \sum_{l=0}^\infty \sigma_{[l]}, \quad \sigma_{[l]} = \frac{4\pi}{k^2} (2l + 1) \sin^2 \delta_l
\]

Maximum possible cross section, the unitarity limit:

\[
(\sigma_{[l]})_{\text{max}} = \frac{4\pi}{k^2} (2l + 1)
\]
Normalization

For a bound state
\[
\langle u_b | u_b \rangle = \int_0^\infty u_b(r)^* u_b(r) \, dr = 1
\]

For a continuum state (regular solution of the Schrödinger equation):
\[
\langle u^{(k)}_l | u^{(k')}_l \rangle \propto \delta(k - k')
\]

To find the normalization coefficient, one uses the property:
\[
\langle u^{(k)}_s | u^{(k')}_s \rangle = \int_0^\infty \sin(kr) \sin(k'r) \, dr = \frac{\pi}{2} \delta(k - k')
\]

Therefore, the regular solution should be normalized as
\[
\lim_{r \to \infty} u^{(k)}_l(r) \sim \sqrt{\frac{2}{\pi}} \sin\left( kr - l \frac{\pi}{2} + \delta_l \right) \quad \Rightarrow \quad \langle u^{(k)}_l | u^{(k')}_l \rangle = \delta(k - k')
\]

Energy normalization:
\[
\lim_{r \to \infty} \tilde{u}^{(E)}_l(r) \sim \sqrt{\frac{2\mu}{\pi \hbar^2 k}} \sin\left( kr - l \frac{\pi}{2} + \delta_l \right) \quad \Rightarrow \quad \langle \tilde{u}^{(E)}_l | \tilde{u}^{(E')}_l \rangle = \delta(E - E')
\]
We derived
\[ u_l(r) \to_{r \to \infty} \frac{2l + 1}{k} i^l e^{i\delta_l} \sin \left( kr - l \frac{\pi}{2} + \delta_l \right) \]

It can be written as
\[ u_l(r) \sim \frac{2l + 1}{2k} i^{l+1} \left[ e^{-i(kr-l\pi/2)} - e^{2i\delta_l}e^{i(kr-l\pi/2)} \right] \]
\[ = \frac{2l + 1}{2k} i^{2l+1} \left[ e^{-ikr} - (-1)^l e^{2i\delta_l}e^{ikr} \right]. \]

The quantity \( S_l = e^{2i\delta_l} \) is the scattering matrix.
Example: scattering from a hard sphere

A hard sphere of radius \( R \)

For \( r < R \) the solution \( u_l(r) = 0 \).

For \( r > R \) the solution is

\[
Au_l^{(s)}(kr) + Bu_l^{(c)}(kr)
\]

At the boundary:

\[
Au_l^{(s)}(kR) + Bu_l^{(c)}(kR) = 0
\]

\[
\frac{B}{A} = -\frac{u_l^{(s)}(kR)}{u_l^{(c)}(kR)} = \frac{j_l(kR)}{y_l(kR)}
\]

\[
\delta_l = \arctan \left( \frac{j_l(kR)}{y_l(kR)} \right)
\]

\[
\tan \delta_l = \frac{B}{A}
\]

\[
\delta_{l=0} = -kR
\]

for \( l > 0 \):

\[
\delta_l \underset{kR \to 0}{\sim} -\frac{\pi}{\Gamma(l + \frac{3}{2})\Gamma(l + \frac{1}{2})} \left( \frac{kR}{2} \right)^{2l+1} \left[ 1 - \left( \frac{kR}{2} \right)^2 \left( \frac{1}{l - \frac{1}{2}} + \frac{1}{l + \frac{3}{2}} \right) \right]
\]

\[
\delta_l \underset{kR \to \infty}{\sim} -kR + l \frac{\pi}{2}
\]
Scattering phase shifts for the hard sphere

\[ \delta_{l=0} = -kR \]

\[ \delta_l \xrightarrow{kR \to 0} -\frac{\pi}{\Gamma(l + \frac{3}{2})\Gamma(l + \frac{1}{2})} \left( \frac{kR}{2} \right)^{2l+1} \left[ 1 - \left( \frac{kR}{2} \right)^2 \left( \frac{1}{l - \frac{1}{2}} + \frac{1}{l + \frac{3}{2}} \right) \right] \]

\[ \delta_l \xrightarrow{kR \to \infty} -kR + l \frac{\pi}{2} \]
Low-energy collisions

For small energies, the wave function near the origin is

$$u_l(r) \propto u_l^{(s)}(kr) + \tan \delta_l u_l^{(c)}(kr)$$

$$\sim \frac{\sqrt{\pi k^{l+1}}}{2^{l+1} \Gamma(l + \frac{3}{2})} \left[ r^{l+1} + \tan \delta_l \frac{2^{2l+1} \Gamma(l + \frac{1}{2}) \Gamma(l + \frac{3}{2})}{\pi k^{2l+1} r^l} \right]$$

But for small $k$, the solution $u_l(r)$ should be just $A u_l^{(s)}(r)$, i.e. expression in the parenthesis should not depend on $k$. It means that

$$\tan \delta_l \sim -\frac{\pi}{\Gamma(l + \frac{1}{2}) \Gamma(l + \frac{3}{2})} \left( \frac{a_l k}{2} \right)^{2l+1}$$

$a_l$ are some constants depending on details of the interaction $V(r)$. They are called scattering lengths.

At $E \to 0$ ($k \to 0$), the equation gives Wigner’s threshold law for various processes.

$$\lim_{k \to 0} \frac{d\sigma}{d\Omega} = a^2 \quad \text{and} \quad \lim_{k \to 0} \sigma = 4\pi a^2$$

For elastic scattering
When $k \to 0$, the wave function at large $r$ is ($kr$ is small but finite)

$$u_l(r) \propto \tan \delta_l u_l^{(c)}(kr) + \frac{\sqrt{\pi} k^{l+1}}{2^{l+1} \Gamma(l + \frac{3}{2})} \left[ r^{l+1} + \frac{\tan \delta_l 2^{l+1} \Gamma(l + \frac{1}{2}) \Gamma(l + \frac{3}{2})}{\pi k^{2l+1} r^l} \right]$$

When $a_l = 0$, $u_l^{(0)}(r)$ is just the regular solution of the radial Schrödinger equation with $V=0$.

When $a_l = \to \infty$, $u_l^{(0)}(r) \sim r^{-l}$, i.e. for $l>0$ it can be normalized to 1, i.e. it corresponds to a bound state exactly at the threshold.

For the $s$-wave

$$u_l=0 \propto \frac{r}{\sqrt{a}} \sim 1 - \frac{r}{a}$$
Example: square potential well

\[ V(r) = \begin{cases} -V_s & \text{for } r \leq L, \\ 0 & \text{for } r > L, \end{cases} \quad V_s = \frac{\hbar^2 K_s^2}{2\mu} \]

Bound state with \( E=0 \) when \( K_S L = \pi/2 \) and \( V_s \) is

\[ E_0 = (\frac{\pi}{2} \hbar)^2 / (2\mu L^2) \]

For this solution, \( u_{l=0} (r) \rightarrow = \) constant at \( r > L \).

For a slightly larger \( V_s \), a bound state with \( E < 0 \) appears.
Scattering length for the square potential well

For $V_S > E_0$, $a_0 > 0$
For $V_S < E_0$, $a_0 < 0$
For $V_S = E_0$, $a = \infty$
For $V_S = 0$, $a = 0$

$V(r) = V_0$ for $r < L$
$V(r) = 0$ for $r \geq L$

$u_{l=0}^{(0)} \propto r \to \infty$ $r - a \propto 1 - \frac{r}{a}$

$a = L - \frac{\tan(K_S L)}{K_S}$

$\kappa L = \frac{3\pi}{2}$
Scattering length and weakly-bound states

A weakly-bound state

\[ E_b = -\frac{\hbar^2\kappa_b^2}{2\mu} \]

\[ u_{l=0}^{(\kappa_b)}(r) \propto 1 - r \left[ \kappa_b + O(\kappa_b^2) \right] \quad (\kappa_b > 0) \]

\[ u_{l=0}^{(0)} \propto r \to \infty \quad r - a \propto 1 - \frac{r}{a} \]

\[ \frac{1}{a} \sim \kappa_b + O(\kappa_b^2) \]

\[ E_b = -\frac{\hbar^2\kappa_b^2}{2\mu} \sim -\frac{\hbar^2}{2\mu a^2} + O\left(\frac{1}{a^3}\right) \]

It corresponds to a large positive scattering length \( a \).
Example: Ultracold cesium gas

**FIG. 3:** (color online). Binding energy of cesium molecules near three Feshbach resonances as a function of the magnetic field. Zero energy corresponds to two Cs atoms in the absolute hyperfine ground-state sublevel $|F = 3, m_F = 3\rangle$. The measurements are shown as open circles. The fit (solid line) is based on Eq. (13), see text. The inset shows an expanded view in the region of the two $d$- and $g$-wave narrow resonances. The error bars refer to the statistical uncertainties.

**FIG. 4:** (color online) Scattering length of $|F = 3, m_F = 3\rangle$ cesium atoms in the magnetic field range where three Feshbach resonances overlap. The solid curve shows the result of this work while the dashed curve represents the prediction from a previous multi-channel calculation [17].

\[
E_b = -\frac{\hbar^2 k_b^2}{2\mu} a \to \infty - \frac{\hbar^2}{2\mu a^2} + O\left(\frac{1}{a^3}\right)
\]
Consider a solution of the Schrödinger equation, which behaves asymptotically

\[ u_l(r) \xrightarrow{r \to \infty} e^{-i(kr - l\pi/2)} - e^{2i\delta_l} e^{i(kr - l\pi/2)} \]

Consider the time-dependent Schrödinger equation. Its solution is

\[ u^{(k)}(r, t) = u(r) e^{-i\omega t} \]

where

\[ \omega(k) = \frac{\hbar k^2}{2\mu} \]

Consider now a wave packet (a superposition) of solutions of the stationary equation

\[ u(r, t) = \int_0^\infty u^{(k)}(r, t) \phi(k) dk \]

\[ \phi(k) \] is a narrow function of \( k \) such that

\[ \omega(k) \approx \bar{\omega} + \bar{\nu}(k - \bar{k}), \quad \bar{\omega} = \omega(\bar{k}), \quad \bar{\nu} = \frac{d\omega}{dk} \bigg|_{\bar{k}} = \frac{\hbar \bar{k}}{\mu} \]
Potential (shape) Resonances

\[ \omega(k) \approx \tilde{\omega} + \bar{\nu}(k - \bar{k}), \quad \tilde{\omega} = \omega(\bar{k}), \quad \bar{\nu} = \left. \frac{d\omega}{dk} \right|_{\bar{k}} = \frac{\hbar \bar{k}}{\mu} \]

The lower limit of the integral can be extended to \(-\infty\). The first term in

\[ u(r, t) = \int_{0}^{\infty} u^{(k)}(r, t) \phi(k) dk \]

can be written as

\[ u^{\text{in}}(r, t) = \int_{-\infty}^{\infty} e^{-i(kr + \omega t - l\pi/2)} \phi(k) dk \]

\[ \approx e^{-ikr - i\tilde{\omega}t} l \int_{-\infty}^{\infty} e^{-i(k-\bar{k})(r+\bar{\nu}t)} \tilde{\phi}(k - \bar{k}) d(k - \bar{k}) \]

or in the form

\[ u^{\text{in}}(r, t) = e^{-ikr - i\tilde{\omega}t} \Psi(r + \bar{\nu}t) \]

For example:

\[ \tilde{\phi}(q) \propto e^{-B^2 q^2/2} \quad \Rightarrow \quad \Psi(x) \propto e^{-x^2/(2B^2)} \]
Potential (shape) Resonances

For the outgoing wave in the small interval of $k$

$$u_l(r) \sim \int_{-\infty}^{\infty} e^{-i(kr-l\pi/2)} - e^{2i\delta_l} e^{i(kr-l\pi/2)}$$

the integral

$$\delta_l(k) \approx \delta_l(\bar{k}) + (k - \bar{k}) \frac{d\delta_l}{dk} \bigg|_{\bar{k}}$$

is approximated

$$u(r, t) = \int_0^\infty u^{(k)}(r, t) \phi(k) dk$$

$$u^{\text{out}}(r, t) = -\int_{-\infty}^{\infty} e^{i(kr-o\omega t-l\pi/2)} e^{2i\delta_l} \phi(k) dk$$

$$\approx -e^{i\bar{k}r-i\bar{\omega}t} e^{2i\delta_l(\bar{k})} (-i)^l \int_{-\infty}^{\infty} e^{-i(k-\bar{k})[-(r-\bar{\omega}t+\Delta r)]} \tilde{\phi}(k-\bar{k}) d(k-\bar{k})$$

$\Delta r = 2 \frac{d\delta_l}{dk} \bigg|_{\bar{k}}$

The integral can be expressed in terms of the same function $\Psi$

$$u^{\text{out}}(r, t) = e^{i\bar{k}r-i\bar{\omega}t} e^{2i\delta_l(\bar{k})} (-1)^l \Psi[-(r-\bar{\omega}t+\Delta r)]$$
Wigner time-delay

Incoming wave in
\[ u^{\text{in}}(r, t) = e^{-ikr - i\omega t} \psi (r + \bar{v}t) \]

Outgoing wave
\[ u^{\text{out}}(r, t) = e^{ikr - i\omega t} e^{2i\delta_l(\bar{k})} (-1)^l \psi \left[ -(r - \bar{v}t + \Delta r) \right] \]

For a free wave (scattering with \( V=0 \), \( \Delta r = 0 \).

Therefore, \( \Delta r \) is the space delay due to the potential.

The time delay is
\[ \Delta t = \frac{\Delta r}{\bar{v}} = 2 \frac{\mu}{\hbar k} \frac{d\delta_l}{dk} \bigg|_{\bar{k}} = 2\hbar \frac{d\delta_l}{dE} \bigg|_{\tilde{E}} \quad \tilde{E} = 4\mu \bar{k}^2 

Time delay could be positive, zero, or negative.

For example, for the hard sphere:
\[ \delta_{l=0} = -kR \]

\[ \delta_l \xrightarrow{kR \to \infty} -kR + \frac{l\pi}{2} \]

\[ \Delta r = -2R \text{ for } l = 0 \]

\[ \Delta r \xrightarrow{kR \to \infty} -2R \text{ for } l > 0 \]
Resonances and phase shifts

If at certain energy $E$ time delay becomes large, one calls this situation a resonance at energy $E_r$.

A resonance is characterized by its energy $E_r$ and time delay $\Delta t_r$ or its widths $\Gamma = 4\hbar / \Delta t_r$.

A resonance could also be viewed as a (almost) bound state, which decays with time.

**FIG. 3.** Potentials of Li$_2$ ($2p+2s$). Full line: $B^1\Pi_u$ (Ref. [9]); dashed line: $1^1\Pi_g$ (Ref. [15]).

**FIG. 4.** The wave function (real part) of the $v' = 16, J' = 1$ level of $^6$Li$^7$Li. The dissociation rate is $k = 8670 \times 10^6$ s$^{-1}$, corresponding to a lifetime $\tau = 115$ ps. The inset shows the long-range part responsible for the decay due to tunneling through the barrier.
The asymptotic behavior of a solution of TISE is
\[ u_l(r) \approx 0 \frac{2l + 1}{2k} i^{l+1} \left[ e^{-i(kr-l\pi/2)} - e^{2i\delta_l} e^{i(kr-l\pi/2)} \right] \]

The formula can be used to obtain energies of bound states \((k\text{ would be imaginary}).\) For a bound state with \(E<0: \]
\[ e^{-i\delta_l(E)} = 0. \]

Now, we apply the same idea for positive energies (analytical continuation). If there is a solution of
\[ e^{-i\delta_l(E)} = 0. \]

Then the energy \(E\) is a complex number \(E = E_{re} + iE_{im}\) with negative \(E_{im}\), such that the norm of the wave function decays with time as
\[ |u_l|^2 \propto e^{2E_{im}t/\hbar} \]

Near \(E\)
\[ e^{-i\delta_l(E)} \approx C(E - E) \]
because \(\delta_l(E)\) is an analytical function near \(E\)

For real \(E\)
\[ e^{i\delta_l(E)} = \left[e^{-i\delta_l(E)}\right]^* \approx C^*(E - E)^* \]

\[ e^{-i\delta_l(E)} = 0. \]
Time-dependent vs time-independent picture

\[ e^{-i\delta_l(E)} \approx C(E - \mathcal{E}) \]

\[ e^{+i\delta_l(E)} = \left[ e^{-i\delta_l(E)} \right]^* \approx C^*(E - \mathcal{E}^*) \]

\[ S_l = e^{+i\delta_l(E)} / e^{-i\delta_l(E)} \]

\[ S_l = \frac{C^*}{C} \frac{E - E_{re} + iE_{im}}{E - E_{re} - iE_{im}} \]

\[ 2\delta_l = -2 \arg(C) + 2 \arctan \left( \frac{E_{im}}{E - E_{re}} \right) \]

\[ \tau_R = \frac{\hbar}{\Gamma} |u_l|^2 \propto e^{2E_{im}t/\hbar} \text{ electron energy (eV)} \]
Breit-Wigner formula

The $l$-wave cross section

$$\sigma[l] = \frac{4\pi}{k^2} (2l + 1) \sin^2 \delta_l = \frac{4\pi}{k^2} \frac{2l + 1}{1 + \cot^2 \delta_l} = \frac{4\pi}{k^2} \frac{(2l + 1)(\Gamma/2)^2}{(E - E_R)^2 + (\Gamma/2)^2}$$

$$2\delta_l = -2 \arg(C) + 2 \arctan\left(\frac{E_{im}}{E - E_{re}}\right)$$

It is Breit-Wigner formula for the cross section near a resonance.

For the Wigner time delay near a resonance

$$\Delta t = 2\hbar \frac{d\delta_l}{dE} = \frac{\hbar \Gamma}{(E - E_R)^2 + (\Gamma/2)^2}$$
$C_3N + e^- \text{ example}$

$$\sigma_{[l]} = \frac{4\pi}{k^2} (2l + 1) \sin^2 \delta_l = \frac{4\pi}{k^2} \frac{2l + 1}{1 + \cot^2 \delta_l} = \frac{4\pi}{k^2} \frac{(2l + 1)(\Gamma/2)^2}{(E - E_R)^2 + (\Gamma/2)^2}$$
Inelastic scattering
Several internal states of colliding particles

In the two particles after a collision could be in states different than their states before the collision, the total wave function should be written as

$$\Psi (r, \xi) = \sum_j \psi_j (r) \gamma_j (\xi)$$

$\xi$ refers to all internal degrees of freedom of projectile and target.

$$\hat{H}_\xi \gamma_i (\xi) = E_i \gamma_i (\xi)$$

The internal states $\gamma_i$ define **channels** for the scattering process. Wave functions $\psi_i (r)$ are channel wave functions.

The Schrödinger equation

$$\left[ -\frac{\hbar^2}{2\mu} \Delta + \hat{H}_\xi + \hat{W} (r, \xi) \right] \Psi (r, \xi) = E \Psi (r, \xi)$$

$$-\frac{\hbar^2}{2\mu} \Delta \psi_i (r) + \sum_j V_{i,j} \psi_j (r) = (E - E_i) \psi_i (r).$$

$$V_{i,j} = \langle \gamma_i | \hat{W} | \gamma_j \rangle \xi$$
Scattering amplitude

Open and closed channels, channel thresholds $E_j$

$$\Psi(r, \xi) = \sum_j \psi_j(r) \gamma_j(\xi)$$

The description of a scattering process starts with

$$\Psi(r, \xi) \xrightarrow{r \to \infty} \sum_{j \text{ open}} f_{i,j}(\theta, \phi) \frac{e^{ik_j r}}{r} \gamma_j(\xi)$$

Total energy $E$ is conserved, kinetic energy $E - E_j$ changes if the internal state changes (inelastic scattering)

**Open channel**

$$E - E_j = \frac{\hbar^2 k_j^2}{2\mu} > 0, \quad k_j = \frac{1}{\hbar} \sqrt{2\mu(E - E_j)}.$$

**Closed channel**

$$E - E_j = -\frac{\hbar^2 \kappa_j^2}{2\mu} < 0, \quad \kappa_j = \frac{1}{\hbar} \sqrt{2\mu(E_j - E)}.$$
Coupled-channel equations

\[ \Psi (r, \xi) \underset{r \to \infty}{\sim} e^{ikz} \gamma_i(\xi) + \sum_{j \text{ open}} f_{i,j}(\theta, \phi) \frac{e^{ikjr}}{r} \gamma_j(\xi) \]

\[ \psi_j(r) \underset{r \to \infty}{\sim} e^{ikz} \delta_{i,j} + f_{i,j}(\theta, \phi) \frac{e^{ikjr}}{r} \]

Current density in channel \( j \)

\[ j_j(r) = \frac{\hbar k_j}{\mu} |f_{i,j}(\theta, \phi)|^2 \hat{e}_r \frac{2}{r^2} + O\left( \frac{1}{r^3} \right) \]

The incoming current density is \( |j_i| = \hbar k_i / \mu \).

The differential cross section for scattering from the incident channel \( i \) to the outgoing channel \( j \) is

\[ \frac{d\sigma_{i \to j}}{d\Omega} = \frac{k_j}{k_i} |f_{i,j}(\theta, \phi)|^2 \]

Integrated cross section is

\[ \sigma = \sum_{j \text{ open}} \sigma_{i \to j}, \quad \sigma_{i \to j} = \int \frac{d\sigma_{i \to j}}{d\Omega} d\Omega = \frac{k_j}{k_i} \int |f_{i,j}(\theta, \phi)|^2 d\Omega \]
\textbf{Multichannel Green's function}

\textbf{Multi-channel Schrödinger equation}

\[-\frac{\hbar^2}{2\mu} \Delta \psi_i (\mathbf{r}) + \sum_i V_{i,j} \psi_j (\mathbf{r}) = (E - E_i) \psi_i (\mathbf{r}).\]

in a vector form

\[
\left( \hat{E} + \frac{\hbar^2}{2\mu} \Delta \right) \psi = \hat{V} \psi
\]

\textbf{Multi-channel Green's function}

\[
\begin{bmatrix}
\hat{E} + \frac{\hbar^2}{2\mu} \Delta \\
E - E_j + \frac{\hbar^2}{2\mu} \Delta
\end{bmatrix} \mathcal{G}_{j,j} (\mathbf{r}, \mathbf{r}') = \delta (\mathbf{r} - \mathbf{r}')
\]

\textbf{If } \Psi \text{ is a solution then it satisfies}

\[
\Psi = \Psi^{\text{hom}} + \hat{G} \hat{V} \Psi, \quad [\hat{E} + \frac{\hbar^2}{2\mu} \Delta] \Psi^{\text{hom}} = 0
\]

\textbf{Free-particle Green's function is}

\[
\mathcal{G}_{j,j} (\mathbf{r}, \mathbf{r}') = -\frac{\mu}{2\pi \hbar^2} \frac{e^{ik_j |\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} \quad |\mathbf{r}||\mathbf{r}'| - \frac{\mu}{2\pi \hbar^2} \frac{e^{ik_j |\mathbf{r}|}}{r} e^{-ik_j \cdot \mathbf{r}'}
\]

\[k_j = k_j \hat{e}_r\]
Multi-channel Lippmann-Schwinger equation

\[ \Psi = \psi_{\text{hom}} + \hat{G} \hat{V} \psi \]

Accounting for boundary conditions in

\[ \Psi(r, \xi) \sim \sum_{j \text{ open}} f_{i, j}(\theta, \phi) \frac{e^{ikjr}}{r} \gamma_j(\xi) \]

\[ \psi_{i, \text{hom}}(r) = e^{ik_ir}, \quad \psi_{j, \text{hom}}(r) \equiv 0 \quad \text{for } j \neq i \]

Lippmann-Schwinger equation becomes

\[ \psi_j(r) = e^{ik_jz} \delta_{i,j} + \int G_{j, j}(r, r') \sum_n V_{j, n} \psi_n(r') \, dr' \]
Multichannel Scattering amplitude

Asymptotically, the equation

$$\psi_j(r) = e^{ik_i z} \delta_{i,j} + \int G_{j,j}(r, r') \sum_n V_{j,n} \psi_n(r') \, dr'$$

could be written as

$$\psi_j(r) \overset{r \to \infty}{\to} e^{ik_i z} \delta_{i,j} - \frac{\mu}{2\pi \hbar^2} \frac{e^{ik_j r}}{r} \sum_n \int e^{-ik_j \cdot r'} V_{j,n} \psi_n(r') \, dr'$$

Comparing with

$$\Psi(r, \xi) \overset{r \to \infty}{\to} e^{ik_i z} \gamma_i(\xi) + \sum_{j \text{ open}} f_{i,j}(\theta, \phi) \frac{e^{ik_j r}}{r} \gamma_j(\xi)$$

the amplitudes can be written as

$$f_{i,j}(\theta, \phi) = -\frac{\mu}{2\pi \hbar^2} \sum_n \int e^{-ik_j \cdot r'} V_{j,n}(r') \psi_n(r') \, dr'.$$
If one substitutes $\Psi^{\text{hom}}$ instead of $\Psi^n$ in the incoming wave, one obtains the amplitude in the Born approximation:

$$f_{i,j}^{\text{Born}}(\theta, \phi) = -\frac{\mu}{2\pi \hbar^2} \sum_n \int e^{-i\mathbf{k}_j \cdot \mathbf{r}'} V_{j,n}(\mathbf{r}') \psi_n(\mathbf{r}') \, d\mathbf{r}'$$

It looks as a Fourier transform of $V_{j,i}$.

The Born scattering amplitude is a function of momentum transfer:

$$\mathbf{q} = \mathbf{k}_j - \mathbf{k}_i \hat{e}_z = k_j \hat{e}_r - k_i \hat{e}_z$$
Feshbach resonances

A shape resonance is trapped by a potential barrier.

Feshbach resonance is trapped by a closed channel

\[-\frac{\hbar^2}{2\mu} \Delta \psi_i(\mathbf{r}) + \sum_i V_{i,j} \psi_j(\mathbf{r}) = (E - E_i) \psi_i(\mathbf{r}) V(\mathbf{r})\]

\[
\begin{bmatrix}
-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V_1(r) \\
-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V_2(r)
\end{bmatrix}
\begin{bmatrix}
u_1(r) \\
u_2(r)
\end{bmatrix}
+ V_{1,2} u_2(r) = Eu_1(r)
\]

\[
\begin{bmatrix}
u_1(r) \\
u_2(r)
\end{bmatrix}
+ V_{2,1} u_1(r) = Eu_2(r)
\]
Feshbach resonances

If there is no coupling between the channels, \( V_{1,2} = V_{2,1} = 0 \)

\[
\begin{bmatrix}
-\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + V_2(r)
\end{bmatrix} u_0(r) = E_0 u_0(r), \quad \langle u_0 | u_0 \rangle = 1, \quad E_1 < E_0 < E_2
\]

If there is a weak coupling, \( u_0(r) \) would not be modified significantly.

The two component solution can then be written as

\[
U \equiv \begin{pmatrix}
    u_1(r) \\
    A u_0(r)
\end{pmatrix}
\]

From the second equation we

\[
V_{2,1}(r) u_1(r) = A (E - E_0) u_0(r)
\]

or

\[
A (E - E_0) = \langle u_0 | V_{2,1} | u_1 \rangle
\]
Feshbach resonances

The first equation is

$$\left[ E + \frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} - V_1(r) \right] u_1(r) = AV_{1,2}u_0(r).$$

Again, a Green's function is introduced

$$\left[ E + \frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} - V_1(r) \right] \mathcal{G}(r, r') = \delta(r - r').$$

$$\mathcal{G}(r, r') = -\pi \tilde{u}_1^{(\text{reg})}(r_<) \tilde{u}_1^{(\text{irr})}(r_>)$$

$$\tilde{u}_1^{(\text{reg})}(r) \xrightarrow{r \to \infty} \sqrt{\frac{2\mu}{\pi \hbar^2 k}} \sin(kr + \delta_{bg})$$

$$\tilde{u}_1^{(\text{irr})}(r) \xrightarrow{r \to \infty} \sqrt{\frac{2\mu}{\pi \hbar^2 k}} \cos(kr + \delta_{bg})$$
Feshbach resonances

From the Green's function and the first equation

\[
\begin{bmatrix}
E + \frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} - V_1(r)
\end{bmatrix} \mathcal{G}(r, r') = \delta(r - r')
\]

we obtain

\[\psi = \psi_{\text{hom}} + \hat{G} \hat{V} \psi\]

\[
\begin{align*}
\psi_1(r) &= \tilde{u}_1^{(\text{reg})}(r) + A \int_0^\infty \mathcal{G}(r, r') V_{1,2}(r') u_0(r') dr' \\
&\to \infty \quad \tilde{u}_1^{(\text{reg})}(r) - \pi A \langle \tilde{u}_1^{(\text{reg})} | V_{1,2} | u_0 \rangle \tilde{u}_1^{(\text{irr})}(r).
\end{align*}
\]

\[
\mathcal{G}(r, r') = -\pi \tilde{u}_1^{(\text{reg})}(r_<) \tilde{u}_1^{(\text{irr})}(r_>)
\]

introducing \(\delta_{\text{res}}\) as

\[-\pi A \langle \tilde{u}_1^{(\text{reg})} | V_{1,2} | u_0 \rangle = \tan \delta_{\text{res}}\]

\[
u_1(r) \to \infty \quad \sqrt{\frac{2\mu}{\pi \hbar^2 k}} \left[ \sin(kr + \delta_{bg}) + \tan \delta_{\text{res}} \cos(kr + \delta_{bg}) \right]
\]

\[= \frac{1}{\cos(\delta_{\text{res}})} \sqrt{\frac{2\mu}{\pi \hbar^2 k}} \sin(kr + \delta_{bg} + \delta_{\text{res}}).\]
Feshbach resonances

We had

\[ A(E - E_0) = \langle u_0 | V_{2,1} | u_1 \rangle \]

\[
\begin{align*}
    u_1(r) &= \bar{u}_1^{\text{reg}}(r) + A \int_0^\infty G(r, r') V_{1,2}(r') u_0(r') \, dr' \\
    &\quad \overset{r \to \infty}{\sim} \bar{u}_1^{\text{reg}}(r) - \pi A \langle \bar{u}_1^{\text{reg}} | V_{1,2} | u_0 \rangle \bar{u}_1^{\text{irr}}(r) .
\end{align*}
\]

we obtain

\[
A(E - E_0) = \langle u_0 | V_{2,1} | \bar{u}_1^{\text{reg}} \rangle + A \langle u_0 | V_{2,1} \hat{G} V_{1,2} | u_0 \rangle
\]

\[
\implies A = \frac{\langle u_0 | V_{2,1} | \bar{u}_1^{\text{reg}} \rangle}{E - E_0 - \langle u_0 | V_{2,1} \hat{G} V_{1,2} | u_0 \rangle} .
\]

For \( \delta_{\text{res}} \) we had

\[
-\pi A \langle \bar{u}_1^{\text{reg}} | V_{1,2} | u_0 \rangle = \tan \delta_{\text{res}}
\]

\[
\tan \delta_{\text{res}} = -\frac{\pi |\langle u_0 | V_{2,1} | \bar{u}_1^{\text{reg}} \rangle|^2}{E - E_0 - \langle u_0 | V_{2,1} \hat{G} V_{1,2} | u_0 \rangle}
\]
Feshbach resonances

We had

\[ \tan \delta_{\text{res}} = -\frac{\pi |\langle u_0 | V_{2,1} | \tilde{u}_1^{(\text{reg})} \rangle|^2}{E - E_0 - \langle u_0 | V_{2,1} \hat{G} V_{1,2} | u_0 \rangle} \]

Introducing notations:

\[ E_R = E_0 + \langle u_0 | V_{2,1} \hat{G} V_{1,2} | u_0 \rangle \]

position of the resonance

\[ \Gamma = 2\pi |\langle u_0 | V_{2,1} | \tilde{u}_1^{(\text{reg})} \rangle|^2 \]

width of the resonance

The tangent can be written as

\[ \tan \delta_{\text{res}} = -\frac{\Gamma/2}{E - E_R} \]

It is useful to compare \( \Gamma \) with the Fermi golden rule

\[ P_{\text{in} \rightarrow \text{fin}} = \frac{2\pi}{\hbar} |\langle \psi_{\text{in}} | \hat{W} | \psi_{\text{fin}} \rangle|^2 \rho_{\text{fin}}(E) \]
Landau-Zener model
Non-adiabatic coupling

The time dependent Schrödinger equation for a diatomic molecule

\[ i\hbar \frac{\partial \Psi}{\partial t} = H \Psi = \left[ \sum_{\alpha} T_{\alpha} + H_{\text{cl}} \right] \Psi \]

Adiabatic electronic functions

\[ H_{\text{cl}} (r, R) \varphi_l (r, R) = E_l (R) \varphi_l (r, R) \]

and adiabatic basis set

\[ \Phi_{ln} (r, R, t) = \varphi_l (r, R) \chi_{ln} (R) \exp \left( - \frac{i}{\hbar} E_{ln} t \right) \]

The Schrödinger equation takes the form

\[ \left[ \sum_{\alpha} T_{\alpha} + E_l (R) \right] \chi_{ln} (R) = E_{ln} \chi_{ln} (R) \]

For a truncated adiabatic basis set, the system of equations could be solved numerically.
Semi-classical treatment

For nuclei, we introduce a trajectory $R = R(t)$

$$H_{el}(r, R) \Psi(r, t) = i \hbar \frac{\partial \Psi(r, t)}{\partial t}$$

$H_{el}(r, R)$ depends on time $t$ because of $R(t)$.

The solution $\Psi$ is now represented as

$$\Psi = \sum_{l} a_l(t) \varphi_l(r, R(t)) \exp \left[ - \frac{i}{\hbar} \int E_l(R) \, dt \right]$$

Inserting into the Schrödinger equation

$$i \hbar \dot{a}_l = \sum_{l'} a_{l'} \langle \varphi_l^* \left( - i \hbar \frac{\partial}{\partial t} \right) \varphi_{l'} \rangle \exp \left[ - \frac{i}{\hbar} \int (E_{l'} - E_l) \, dt \right]$$
Semi-classical treatment

Comparing with the formula for transition amplitudes in the time-dependent perturbation theory

\[ i \hbar \dot{a}_l = \sum_{l'} a_{l'} \langle \varphi_{l'}^* \left( -i \hbar \frac{\partial}{\partial t} \right) \varphi_{l'} \rangle \exp \left[ -\frac{i}{\hbar} \int^{t} (E_{l'} - E_l) \, dt \right] \]

We conclude that

\[ W = -i \hbar \frac{\partial}{\partial t} \]

\[ W_{l' r} = \left( -i \hbar \frac{\partial}{\partial t} \right)_{l' r} = -i \hbar v \langle \varphi_{l'}^* \frac{\partial \varphi_{l'}}{\partial R} \rangle \]

Let us call \( |\langle \varphi_{l'}^* \frac{\partial \varphi_{l'}}{\partial R} \rangle|^{-1} \) as \( \delta R \) (characteristic length)

\[ W_{l' r} \approx \hbar v |\delta R| \]

The applicability condition of the perturbation approach

\[ |W_{l' r}| \ll |E_l - E_{l'}| = \Delta E_{l' r} \quad \text{or} \quad \Delta E_{l' r} \cdot \delta R / \hbar v \gg 1 \]
Two-state approximation

Adiabatic functions $\varphi_1$ and $\varphi_2$.

They correspond to solid potential curves.

In the basis of $\varphi_1$ and $\varphi_2$,

$$
H_{el}(\varphi) = \begin{pmatrix} E_1(R) & 0 \\ 0 & E_2(R) \end{pmatrix}
$$
Diabatic basis

Another pair $\varphi_1^0$ and $\varphi_2^0$ of electronic functions is introduced as a linear combination:

$$\varphi_1 = \varphi_1^0 \cos \chi + \varphi_2^0 \sin \chi$$
$$\varphi_2 = -\varphi_1^0 \sin \chi + \varphi_2^0 \cos \chi$$

In the basis of $\varphi_1^0$ and $\varphi_2^0$

$$H_{\text{el}}(\varphi) = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$$

$H_{12}$ and $H_{21}$ as well as $\varphi_1^0$ and $\varphi_2^0$ depend weakly on $R$. 
Two-state approximation

\[
H_{\text{cl}}(\varphi) = \begin{pmatrix} E_1(R) & 0 \\ 0 & E_2(R) \end{pmatrix}
\]

\[
H_{\text{cl}}(\varphi^0) = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}
\]

We want that \( \varphi_{1,2} = \varphi^0_{1,2} \) far from the region of the strong coupling

\[
\frac{H_{12}(R)}{[H_{11}(R) - H_{22}(R)]} \to 0
\]

We use approximation

\[
H_{12}(R) = H_{12}(R_p) + H'_{12}(R_p)(R - R_p) + \cdots,
\]

\[
H_{11} - H_{22} = \Delta H(R) = \Delta H(R_p) + \Delta H'(R_p)(R - R_p) + \cdots
\]

where \( R_p \) is defined as

\[
\Delta H(R_p) = 0
\]
Two-state approximation

$$H_{el}(\varphi) = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \approx \begin{pmatrix} E_0 + k_1 x & a \\ a & E_0 + k_2 x \end{pmatrix} =$$

$$\begin{pmatrix} E_0 + \frac{(k_1 + k_2)}{2} x + \frac{(k_1 - k_2)}{2} x & a \\ a & E_0 + \frac{(k_1 + k_2)}{2} x - \frac{(k_1 - k_2)}{2} x \end{pmatrix} =$$

$$\begin{pmatrix} E_0 + F x + \frac{\Delta F}{2} x & a \\ a & E_0 + F x - \frac{\Delta F}{2} x \end{pmatrix}$$

$$E_0 = H_{11}(R_p) = H_{22}(R_p), a = H_{12}(R_p) \text{ and } \Delta F = -\frac{\partial}{\partial R} (H_{11} - H_{22}) \bigg|_{R = R_p}$$

Eigenvalues are

$$E_{1,2} = E_0 + F x \pm \frac{1}{2} \sqrt{(\Delta F x)^2 + 4a^2}$$

$$\varphi_{1,2} = \varphi^0_{1,2} \text{ far from the region of the strong coupling}$$
Non-adiabatic functions

Two-component wave function $\Psi(t)$ is

$$\Psi(t) = a_1(t) \varphi_1 \exp \left[ -\frac{i}{\hbar} \int E_1 dt \right] + a_2(t) \varphi_2 \exp \left[ -\frac{i}{\hbar} \int E_2 dt \right]$$

$$\Psi(t) = b_1(t) \varphi_1^0 \exp \left[ -\frac{i}{\hbar} \int H_{11} dt \right] + b_2(t) \varphi_2^0 \exp \left[ -\frac{i}{\hbar} \int H_{22} dt \right]$$

$$\dot{a}_1 = i \chi \exp \left[ -\frac{i}{\hbar} \int (E_2 - E_1) dt \right] a_2$$

$$\dot{a}_2 = -i \chi \exp \left[ \frac{i}{\hbar} \int (E_2 - E_1) dt \right] a_1$$

$$\hbar \dot{b}_1 = a \exp \left[ -\frac{i}{\hbar} \int (H_{22} - H_{11}) dt \right] b_1$$

$$\hbar \dot{b}_2 = a \exp \left[ \frac{i}{\hbar} \int (H_{22} - H_{11}) dt \right] b_1$$

In the region of interaction ($R$ within $\delta R$) we have either

(a) adiabatic non-crossing potentials $E_1$ and $E_2$ plus non-adiabatic coupling

(b) crossing zero-order potentials $H_{11}$ and $H_{22}$ plus adiabatic coupling
Transition probability

We assume $a$ to be small and start with $t=-\infty$ and $R$ far from $R_p$ and end up with $t=\infty$ and $R$ again far from $R_p$.

\[
\begin{align*}
\dot{b}_1 b_1 &= a \exp \left[ -\frac{i}{\hbar} \int \left( H_{22} - H_{11} \right) dt \right] b_1 \\
\dot{b}_2 b_2 &= a \exp \left[ \frac{i}{\hbar} \int \left( H_{22} - H_{11} \right) dt \right] b_1 
\end{align*}
\]

Initially, the system is in state $\varphi_1^0$ 

\[ b_1(-\infty) = 1, \quad b_2(-\infty) = 0 \]

At the end $|b_2(\infty)|^2$ give the probability $P_{12}^0$ of transition from state $\varphi_1^0$ to $\varphi_1^0$.

\[
b_2(+\infty) = \int_{-\infty}^{\infty} \frac{a}{i\hbar} \exp \left[ -\frac{i}{\hbar} \frac{\Delta F v^2}{2} \right] dt = \frac{a}{i\hbar} \left[ \pi \sqrt{-\frac{i\Delta F v}{2\hbar}} \right]^{1/2}
\]

Therefore, 

\[ P_{12}^0 = 2\pi a^2 |\Delta F \hbar v|, \quad \text{if } P_{12}^0 \ll 1 \]
Landau-Zener probability

When \( a \) is large the treatment is not good, \( P_{12}^0 \) could be become comparable or larger than 1.

\[
i \hat{a}_1 = i \chi \exp \left[ - \frac{i}{\hbar} \int (E_2 - E_1) \, dt \right] a_2
\]
\[
i \hat{a}_2 = -i \chi \exp \left[ \frac{i}{\hbar} \int (E_2 - E_1) \, dt \right] a_1
\]

Solving the system of equations, one obtains

\[
P_{12} = \exp \left[ - \frac{2 \pi a^2}{\Delta F \hbar v} \right] = 1 - P_{12}^0
\]

In atomic collisions nuclei go through the coupling region twice. Then the total probability for transition from 1 to 2 would be

\[
P = 2 P_{12} (1 - P_{12}) = 2 (1 - P_{12}^0) P_{12}^0
\]

\[
P = 2 \exp \left( - \frac{2 \pi a^2}{\Delta F \hbar v} \right) \left[ 1 - \exp \left( - \frac{2 \pi a^2}{\Delta F \hbar v} \right) \right]
\]
Few-body bound and scattering states at low energies (near dissociation)
3-body collisions

- Quantum-mechanical description of three interacting particles
- Nuclear physics
- Chemical reactions A+B+C → AB + C at low energies
- Many experiments observing three-body (and few-body) quantum effects (Efimov states)
- Symmetry of particles should be accounted for if only a few quantum states are populated.
Hyper-spherical coordinates

Three inter-particle distances are represented by two hyperangles and the hyper-radius.

Changing hyper-radius

(θ, φ)=const
Jacobi coordinates

* Three different arrangements: three sets of coordinates
Mass-weighted Jacobi coordinates

\[ \vec{R}_{CM} = \vec{R}_{CM,0} \]
\[ \vec{r}^k = d_k^{-1} \vec{r}_0^k \]
\[ \vec{R}^k = d_k \vec{R}_0^k \]

\[ M = \sum_{i=1}^{3} m_i \]
\[ \mu = \sqrt{\frac{\prod_{i=1}^{3} m_i}{M}} \]
\[ d_k = \sqrt{\frac{m_k}{\mu} \left(1 - \frac{m_k}{M}\right)} \]

Arrangement \( j \)
Arrangement \( i \)
Arrangement \( k \)

Space-fixed "SF"
Hyperspherical coordinates

\[
\vec{R}_{CM} = \vec{R}_{CM,0} \quad \vec{r}^k = d_k^{-1} \vec{r}_0^k \quad \vec{R}^k = d_k \vec{R}_0^k
\]

\[
\rho^2 = (r_X^k)^2 + (r_Y^k)^2 + (r_Z^k)^2 + (R_X^k)^2 + (R_Y^k)^2 + (R_Z^k)^2
\]

\[
r_1(\rho, \theta, \phi) = \frac{d_1 \rho}{\sqrt{2}} \sqrt{1 + \sin \theta \sin(\phi + \epsilon_1)}
\]

\[
r_2(\rho, \theta, \phi) = \frac{d_2 \rho}{\sqrt{2}} \sqrt{1 + \sin \theta \sin(\phi + \epsilon_2)}
\]

\[
r_3(\rho, \theta, \phi) = \frac{d_3 \rho}{\sqrt{2}} \sqrt{1 + \sin \theta \sin(\phi + \epsilon_3)}
\]

\[
0 \leq \rho < \infty, \quad 0 \leq \theta \leq \frac{\pi}{2} \quad \text{et} \quad 0 \leq \phi < 2\pi
\]

\[
\epsilon_3 = 2 \arctan \left( \frac{m_2}{\mu} \right)
\]

\[
\epsilon_2 = -2 \arctan \left( \frac{m_3}{\mu} \right)
\]
If two or three particles are identical, one has to account for bosonic or fermionic nature of the particles.

Hyperspherical coordinates are well adapted for it.
$C_{3v} / D_3 / S_3$ symmetry group

* Group of permutation of three identical particles, $S_3$:

$$S_3 = \{E, (12), (23), (13), (123), (132)\}$$

* $S_3$ is isomorphic to the group of rotations of a triangular prism

$$D_3 = \{E, C_{2a}, C_{2b}, C_{2c}, C_{3d}, C_{3d}^2\}$$

* and to the molecular point group $C_{3v}$ of

$$C_{3v} = \{E, C_3, C_3^2, 3\sigma_v\}$$
Types of wave functions
Irreducible representations

* $A_1$ is a totally symmetric wave function

* $A_2$ changes sign under any binary permutation

* $E$ is a 2-dimensional irrep.

\[(123) E'_\pm = e^{i\omega} E'_\pm\]

\[(12) E'_\pm = E'_{\mp}, \quad \omega = 2\pi/3\]
**A\(_1\), A\(_2\), and E states**

- **A\(_1\)** is totally symmetric wave function.
- **A\(_2\)** changes sign under any binary permutation.
- **E** is a 2-dimensional irrep.
Schrödinger equation in hyperspherical coordinates

\* Hamiltonian

\[ H = T_\rho + H_{\text{ad}} \]

\[ T_\rho = -\frac{1}{2\mu} \frac{\partial^2}{\partial \rho^2} \]

\[ H_{\text{ad}} = \frac{\Lambda^2 + 15/4}{2\mu \rho^2} + V \]

\[ \Lambda^2 = -\frac{4}{\sin(2\theta)} \frac{\partial}{\partial \theta} \sin(2\theta) \frac{\partial}{\partial \theta} - \frac{4}{\sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} + \frac{2J_x^2}{1 - \sin \theta} \]

\[ + \frac{2J_Z^2}{1 + \sin \theta} + \frac{J_Y^2}{\sin^2 \theta} + \frac{4i \cos \theta J_Y}{\sin^2 \theta} \frac{\partial}{\partial \phi}, \]
How to solve it

* Adiabatic separation of the hyper-radius and hyperangles

\[ H = T_\rho + H_{\text{ad}} \]

\[ H_{\text{ad}}^{\rho=\rho_j} \varphi_{a,j}(\omega) = U_a(\rho_j) \varphi_{a,j}(\omega) \]

\[ H_{\text{ad}} = \frac{\Lambda^2 + 15/4}{2\mu \rho^2} + V \]

* An idea similar to the Born-Oppenheimer separation of electronic and nuclear coordinates

\[ [\hat{T}(\rho) + U_a(\rho)]\psi_{a,n}(\rho) = E_n^{\text{vib}} \psi_{a,n}(\rho) \]
$H_3^-$
Hyperspherical adiabatic approximation is inaccurate

- Non-adiabatic couplings between \( U_a(\phi_a) \) should be accounted for.

- The vibrational wave function \( \psi(\rho,\theta,\phi) \) as the expansion

\[
\psi(\rho,\theta,\phi) = \sum_k y_k(\rho,\theta,\phi) c_k
\]

- in the basis of non-orthogonal basis functions

\[
y_k(\rho,\theta,\phi) = \pi_j(\rho) \varphi_{a,j}(\theta,\phi)
\]

\[
k \equiv \{ a, j \}
\]

- where \( \pi_j(\rho) \) are some convenient basis functions and \( \varphi_{a,j}(\theta,\phi) \) are hyperspherical adiabatic states calculated at fixed hyper-radii \( \rho_j \), with the corresponding eigenvalue \( U_a(\rho_j) \); \( V(\rho,\theta,\phi) \) is the molecular (three-body) potential.

\[
\sum_{i',a'} \left[ \langle \pi_i | \hat{T}(\rho) | \pi_{i'} \rangle \mathcal{O}_{i,a,i',a'} + \langle \pi_i | U_a(\rho) | \pi_{i'} \rangle \delta_{a,a'} \right] c_{i',a'}
\]

\[
= E \sum_{i',a'} \langle \pi_i | \pi_{i'} \rangle \mathcal{O}_{i,a,i',a'} c_{i',a'},
\]

\( \mathcal{O}_{i,a,i',a'} = \langle \varphi_a(\rho_i;\theta,\phi) | \varphi_{a'}(\rho_{i'};\theta,\phi) \rangle \)
H$_2$D$^-$ and D$_2$H$^-$
H+H+H $\rightarrow$ H$_2$+H recombination

Diabatic 2-channel 3-body potential for H$_3$.

$$V_{H_3}(\rho, \theta, \phi) = \begin{pmatrix} A & C e^{i\phi} \\ C e^{-i\phi} & A \end{pmatrix}$$

$$A(\rho, \theta, \phi) = [V_1(\rho, \theta, \phi) + V_2(\rho, \theta, \phi)]/2$$

$$C(\rho, \theta, \phi) = [V_1(\rho, \theta, \phi) - V_2(\rho, \theta, \phi)]/2$$

Obtained from ab initio calculation of 1$^2$A' ($V_1$) and 2$^2$A'($V_2$) electronic states of H$_3$. Hyperspherical adiabatic energies obtained for the uncoupled and coupled H$_3$ two-channel potential. Crossings in the above figure turn into avoided crossings below.
$\text{H}_3$ resonances

<table>
<thead>
<tr>
<th>${\nu_1, \nu_2^l}$</th>
<th>$E_r$, $\tau$; this work</th>
<th>$E_r$, $\tau$; Ref. [8]</th>
<th>$E_r$, $\tau$; Ref. [9]</th>
</tr>
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<tbody>
<tr>
<td>${0, 0^0}$</td>
<td>$-3.85$, 13</td>
<td>…</td>
<td>$-3.79$, $\sim 3$</td>
</tr>
<tr>
<td>${1, 0^0}$</td>
<td>$-3.11$, 13</td>
<td>…</td>
<td>$-3.05$, $\sim 3$</td>
</tr>
<tr>
<td>${2, 0^0}$</td>
<td>$-2.4$, 14</td>
<td>…</td>
<td>$-2.37$, …</td>
</tr>
<tr>
<td>${3, 0^0}$</td>
<td>$-1.8$, 14</td>
<td>…</td>
<td>$-1.75$, …</td>
</tr>
<tr>
<td>${4, 0^0}$</td>
<td>$-1.2$, 16</td>
<td>$-1.24$, $\sim 15$</td>
<td>$-1.19$, …</td>
</tr>
<tr>
<td>${5, 0^0}$</td>
<td>$-0.7$, 18</td>
<td>$-0.47$, $\sim 17$</td>
<td>$-0.70$, …</td>
</tr>
<tr>
<td>${0, 2^0}$</td>
<td>$-0.2$, 130</td>
<td>…</td>
<td>$-0.26$, $\sim 4.5$</td>
</tr>
</tbody>
</table>
On Efimov states (1970)

\[ \tan \delta \sim \frac{k \to 0}{\frac{\pi}{\Gamma(l + \frac{1}{2}) \Gamma(l + \frac{3}{2})} \left( \frac{a l k}{2} \right)^{2l+1}} \]

\[ k / \tan (\delta_0) = -\frac{1}{a} + r_0 k^2 / 2 \]

- \( r_0 \) – effective range of 2-body potential, \( a \)- 2-body scattering length. If \( r_0 \ll a \), the wave function in the region \( r_0 \ll r \ll a \) does not depend on \( r_0 \) or \( a \).

- Effective 3-body potential in the region is \( \sim 1/r^2 \). Thus, 3-body bound states may exist even if there is no 2-body bound states. When \( a \to +\infty \), the number of 3-body bound states \( \to \infty \).
When \( a=\infty \), the hyper-radial equation is

\[
\left( -\frac{d^2}{dR^2} - \frac{1}{R} \frac{d}{dR} + \frac{s_i^2}{R^2} \right) F_{s_i}(R) = EF_{s_i}(R)
\]

\( s_i \) is a transcendental constant. The lowest \( s \) is \( s_0 = 1.00624i \).

Spectrum for \( s_0 \) is

\[
E_N = -\frac{1}{R_0^2} e^{-2\pi N_1 |s_0|} \exp \frac{2}{|s_0|} \left[ \arccos \frac{\Lambda R_0}{|s_0|} - \Delta \right]
\]

When \( a \neq \infty \), the spectrum:

\( g \) is the interaction parameter, such that at

\( g=1, \ a=\infty \)
Observation of Efimov states

No direct observation. Kramer et al. see the increase of the 3-body recombination rate very close to 3-body dissociation limit as predicted by theory (Esry, Greene). This is an indirect evidence for Efimov states.
Observation of Efimov states:

Theory

Experiment
Collisions between Tunable Halo Dimers: Exploring an Elementary Four-Body Process with Identical Bosons

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(Received 28 March 2008; published 9 July 2008)

We study inelastic collisions in a pure, trapped sample of Feshbach molecules made of bosonic cesium atoms in the quantum halo regime. We measure the relaxation rate coefficient for decay to lower-lying molecular states and study the dependence on scattering length and temperature. We identify a pronounced loss minimum with varying scattering length along with a further suppression of loss with decreasing temperature. Our observations provide insight into the physics of a few-body quantum system that consists of four identical bosons at large values of the two-body scattering length.
Another example

Complex absorbing potential is placed at large hyper-radius to absorb the dissociating outgoing wave flux.

\[ U_a(\rho) \rightarrow U_a(\rho) - iA(\rho - \rho_i)^2 \]