Elements of the scattering theory

Elastic scattering

Two colliding (interacting) particles

Particles with masses m_1 and m_2. interacting with potential V($\boldsymbol{r}_1$-$\boldsymbol{r}_2$)

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$$

Coordinate of the center of mass

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

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

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

If one introduces the reduced mass μ

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

The Hamilton function becomes

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

Then, the Hamiltonian operator is

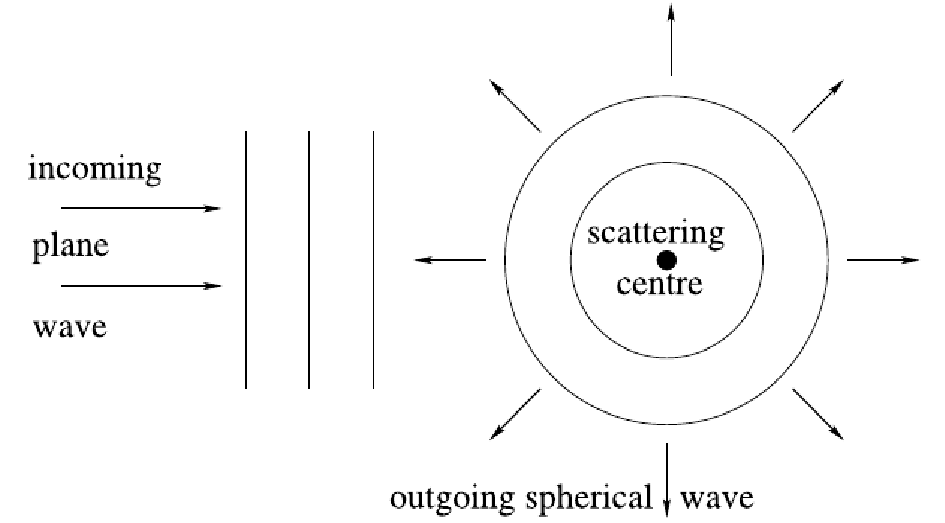
$$H = \frac{\vec{p}^2}{2\mu} + V(r) \quad with \quad \vec{p} = -\hbar\vec{\nabla}_r$$

Scattering Amplitude

Schrödinger equation

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

Boundary conditions for a solution



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

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, $\boldsymbol{j}(\boldsymbol{r})$.

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

Quantum-mechanical expression is:

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

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

$$\psi(\mathbf{r}) \overset{r\to\infty}{\sim} \mathrm{e}^{\mathrm{i}kz} + f(\theta,\phi)\frac{\mathrm{e}^{\mathrm{i}kr}}{r}$$

the current density in the incident wave is $\mathbf{j}_{\mathrm{in}} = \hat{\mathbf{e}}_z\hbar k/\mu$

But $\boldsymbol{j}$ in the outgoing wave is $\mathbf{j}_{\mathrm{out}}(\mathbf{r}) = \frac{\hbar k}{\mu}\left|f(\theta,\phi)\right|^2\frac{\hat{\mathbf{e}}_{\mathbf{r}}}{r^2} + O\left(\frac{1}{r^3}\right)$

Cross Section

Number of particles crossing area $d\mathbf{s}$ at large r per unit time in the outgoing wave:

$$\lim_{r\to\infty} \mathbf{j}_{\text{out}}(\mathbf{r}) \cdot \mathrm{d}\mathbf{s}$$

with $\mathrm{d}\mathbf{s} = \hat{\mathbf{e}}_{\mathbf{r}} r^2 \mathrm{d}\Omega$ $\quad \mathrm{d}\Omega = \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$

I.e. the current density in the outgoing wave is $(\hbar k/\mu)|f(\theta,\phi)|^2 \mathrm{d}\Omega$

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

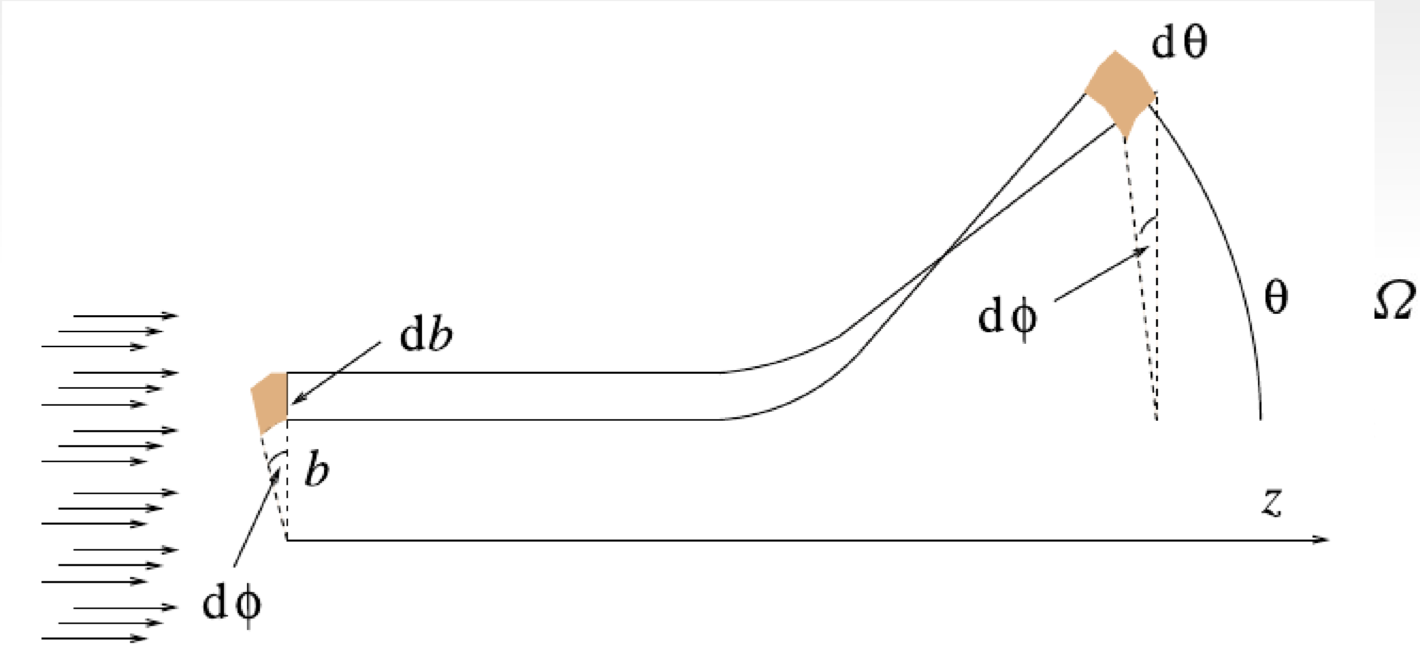
$$\mathrm{d}\sigma = \left|f(\theta,\phi)\right|^2 \mathrm{d}\Omega \qquad \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left|f(\theta,\phi)\right|^2$$

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

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

Cross Section

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



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

Lippmann–Schwinger Equation

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

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

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

The wave function obeying

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

Lippmann–Schwinger equation

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 $|\mathbf{r}| \gg |\mathbf{r}'|$ the Green's function $\mathscr{G}(\mathbf{r}, \mathbf{r}') = -\frac{\mu}{2\pi\hbar^2} \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}$

is approximated by

$$\mathscr{G}(\mathbf{r}, \mathbf{r}') = -\frac{\mu}{2\pi\hbar^2} \frac{e^{ikr}}{r} \left[e^{-i\mathbf{k_r}\cdot\mathbf{r}'} + O\left(\frac{r'}{r}\right) \right].$$

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

plugging it in

$$\psi(\mathbf{r}) = e^{ikz} + \int \mathscr{G}(\mathbf{r}, \mathbf{r}') V(\mathbf{r}') \psi(\mathbf{r}') d\mathbf{r}'$$

$$f(\theta, \phi) = -\frac{\mu}{2\pi\hbar^2} \int e^{-i\mathbf{k_r}\cdot\mathbf{r}'} V(\mathbf{r}') \psi(\mathbf{r}') d\mathbf{r}'.$$

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

$$r^2 V(\mathbf{r}) \overset{r\to\infty}{\longrightarrow} 0.$$

Born Approximation

Inserting

$$\psi(\mathbf{r}) = \mathrm{e}^{\mathrm{i}kz} + \int \mathscr{G}(\mathbf{r}, \mathbf{r}')V(\mathbf{r}')\psi(\mathbf{r}')\mathrm{d}\mathbf{r}'$$

in

$$f(\theta, \phi) = -\frac{\mu}{2\pi\hbar^2}\int \mathrm{e}^{-\mathrm{i}\mathbf{k}_\mathbf{r}\cdot\mathbf{r}'}V(\mathbf{r}')\psi(\mathbf{r}')\mathrm{d}\mathbf{r}'.$$

We obtain

$$f(\theta, \phi) = -\frac{\mu}{2\pi\hbar^2}\Big[\int \mathrm{d}\mathbf{r}'\mathrm{e}^{-\mathrm{i}\mathbf{k}_\mathbf{r}\cdot\mathbf{r}'}V(\mathbf{r}')\mathrm{e}^{\mathrm{i}kz'}$$

$$+\int \mathrm{d}\mathbf{r}'\mathrm{e}^{-\mathrm{i}\mathbf{k}_\mathbf{r}\cdot\mathbf{r}'}V(\mathbf{r}')\int \mathrm{d}\mathbf{r}''\mathscr{G}(\mathbf{r}', \mathbf{r}'')V(\mathbf{r}'')\psi(\mathbf{r}'')\Big]$$

Retaining only the first term gives the Born approximation.

$$f^{\mathrm{Born}}(\theta, \phi) = -\frac{\mu}{2\pi\hbar^2}\int \mathrm{d}\mathbf{r}'\mathrm{e}^{-\mathrm{i}\mathbf{k}_\mathbf{r}\cdot\mathbf{r}'}V(\mathbf{r}')\mathrm{e}^{\mathrm{i}kz'} = -\frac{\mu}{2\pi\hbar^2}\int \mathrm{d}\mathbf{r}'\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{r}'}V(\mathbf{r}')$$

$$\mathbf{q} = k(\hat{\mathbf{e}}_\mathbf{r} - \hat{\mathbf{e}}_z) \qquad q = 2k\sin(\theta/2)$$

Angular Momentum: summary

Definition $\hat{\mathbf{L}} = \mathbf{r} \times \hat{\mathbf{p}}$ 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 $Y_{lm}(\theta,\phi)$

$$Y_{l,m}(\theta,\phi) = \mathrm{e}^{im\phi} \sin^{|m|}(\theta) \mathrm{Pol}_{l-|m|}(\cos\theta)$$

$$\int Y_{l,m}(\Omega)^* Y_{l',m'}(\Omega) \mathrm{d}\Omega = \int_0^{2\pi} \mathrm{d}\phi \int_{-1}^{+1} \mathrm{d}\cos\theta\, Y_{l,m}(\theta,\phi)^* Y_{l',m'}(\theta,\phi)$$
$$= \delta_{l,l'} \delta_{m,m'},$$

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

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

$$\int_{-1}^{1} P_l(x) P_{l'}(x) \mathrm{d}x = \frac{2}{2l+1} \delta_{l,l'}$$

for two vectors **a**, **b**, with $|\mathbf{a}| \le |\mathbf{b}|$

$$\frac{1}{|\mathbf{a} - \mathbf{b}|} = \sum_{l=0}^{\infty} \frac{|\mathbf{a}|^l}{|\mathbf{b}|^{l+1}} P_l(\cos\theta)$$

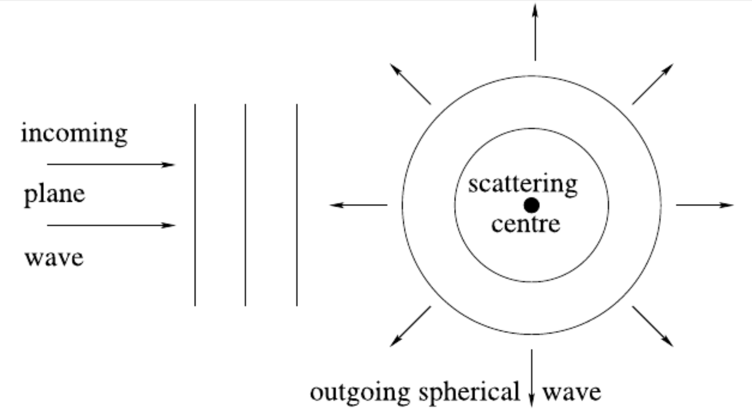
Partial-Waves Expansion

The solution with boundary conditions

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

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

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



From the Schrödinger equation in spherical coordinates

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

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

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

are obtained from spherical Bessel functions

$$u_l^{(s)}(kr)=krj_l(kr), \qquad u_l^{(c)}(kr)=-kry_l(kr),$$

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

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

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

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

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

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

Scattering Phase Shifts

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

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

at large distances are superpositions

$$u_l(r) \overset{r\to\infty}{\propto} Au_l^{(\mathrm{s})}(kr) + Bu_l^{(\mathrm{c})}(kr) \overset{r\to\infty}{\propto} \sin\left(kr - l\frac{\pi}{2} + \delta_l\right)$$

δ_l is scattering phase shifts

$$\tan\delta_l = B/A$$

The partial-wave expansion

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

In $\psi(\mathbf{r}) \overset{r\to\infty}{\sim} \mathrm{e}^{ikz} + f(\theta,\phi)\frac{\mathrm{e}^{ikr}}{r}$ the e^{ikz} term is

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

Scattering Phase Shifts

In $\psi(\mathbf{r}) \overset{r\to\infty}{\sim} \mathrm{e}^{\mathrm{i}kz} + f(\theta,\phi)\frac{\mathrm{e}^{\mathrm{i}kr}}{r}$ the second term could be written as

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

where f_l are called partial-wave scattering amplitudes.

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

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

$$\begin{aligned} u_l(r) &\overset{r\to\infty}{\sim} \mathrm{i}^l\left[\frac{2l+1}{k}\sin\left(kr - l\frac{\pi}{2}\right) + f_l \mathrm{e}^{\mathrm{i}(kr - l\pi/2)}\right] \\ &= \mathrm{i}^l\left[\left(\frac{2l+1}{k} + \mathrm{i} f_l\right)\sin\left(kr - l\frac{\pi}{2}\right) + f_l\cos\left(kr - l\frac{\pi}{2}\right)\right] \end{aligned}$$

Scattering Phase Shifts

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

$$\tan\delta_l = B/A$$

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

$$\cot\delta_l = \frac{A}{B} \equiv \frac{2l+1}{kf_l} + \mathrm{i}$$

$$f_l = \frac{2l+1}{k}\mathrm{e}^{\mathrm{i}\delta_l}\sin\delta_l = \frac{2l+1}{2\mathrm{i}k}\left(\mathrm{e}^{2\mathrm{i}\delta_l} - 1\right)$$

$$u_l(r) \overset{r\to\infty}{\sim} \frac{2l+1}{k}\mathrm{i}^l\mathrm{e}^{\mathrm{i}\delta_l}\sin\left(kr - l\frac{\pi}{2} + \delta_l\right)$$

$$\psi(\mathbf{r}) \overset{r\to\infty}{\sim} \sum_{l=0}^{\infty}\frac{2l+1}{kr}\mathrm{i}^l\mathrm{e}^{\mathrm{i}\delta_l}\sin\left(kr - l\frac{\pi}{2} + \delta_l\right)P_l(\cos\theta)$$

Cross section

Using

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

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

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

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

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

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

Maximum possible cross section, the unitarity limit:

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

Normalization

For a bound state

$$\langle u_b | u_b \rangle = \int_0^\infty u_b(r)^* u_b(r) \mathrm{d}r = 1$$

For a continuum state (regular solution of the Schrödinger equation):

$$\langle u_l^{(k)} | u_l^{(k')} \rangle \propto \delta(k - k')$$

To find the normalization coefficient, one uses the property:

$$\langle u_s^{(k)} | u_s^{(k')} \rangle = \int_0^\infty \sin(kr) \sin(k'r) \mathrm{d}r = \frac{\pi}{2} \delta(k - k')$$

Therefore, the regular solution should be normalized as

$$u_l^{(k)}(r) \overset{r\to\infty}{\sim} \sqrt{\frac{2}{\pi}} \sin\left(kr - l\frac{\pi}{2} + \delta_l\right) \quad \Longrightarrow \quad \langle u_l^{(k)} | u_l^{(k')} \rangle = \delta(k - k')$$

Energy normalization:

$$\bar{u}_l^{(E)}(r) \overset{r\to\infty}{\sim} \sqrt{\frac{2\mu}{\pi \hbar^2 k}} \sin\left(kr - l\frac{\pi}{2} + \delta_l\right) \qquad \langle \bar{u}_l^{(E)} | \bar{u}_l^{(E')} \rangle = \delta(E - E')$$

S-Matrix

We derived $$u_l(r) \overset{r\to\infty}{\sim} \frac{2l+1}{k} \mathrm{i}^l \mathrm{e}^{\mathrm{i}\delta_l} \sin\left(kr - l\frac{\pi}{2} + \delta_l\right)$$

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

The quantity $S_l = \mathrm{e}^{2\mathrm{i}\delta_l}$ 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 $$A u_l^{(s)}(kr) + B u_l^{(c)}(kr)$$

At the boundary: $$A u_l^{(s)}(kR) + B u_l^{(c)}(kR) = 0$$

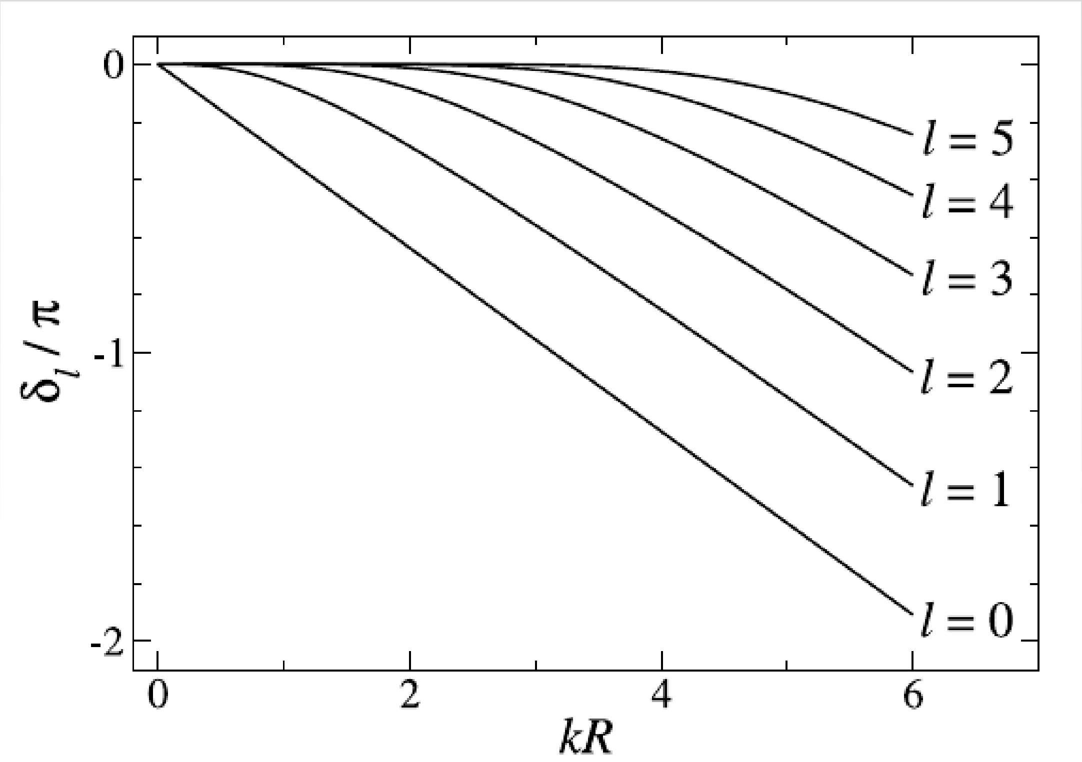
$$\frac{B}{A} = -\frac{u_l^{(s)}(kR)}{u_l^{(c)}(kR)} = \frac{j_l(kR)}{y_l(kR)} \qquad \delta_l = \arctan\left(\frac{j_l(kR)}{y_l(kR)}\right) \qquad \tan\delta_l = B/A$$

$$\delta_{l=0} = -kR$$

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

$$\delta_l \overset{kR\to\infty}{\sim} -kR + l\frac{\pi}{2}$$

Scattering phase shifts for the hard sphere



$$\delta_{l=0} = -kR$$

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

$$\delta_l \overset{kR\to\infty}{\sim} -kR + l\frac{\pi}{2}$$

Low-energy collisions

For small energies, the wave function near the origin is

$$u_l(r) \overset{kr\to 0}{\propto} u_l^{(s)}(kr) + \tan\delta_l u_l^{(c)}(kr)$$
$$\sim \frac{\sqrt{\pi}k^{l+1}}{2^{l+1}\Gamma(l+\frac{3}{2})}\left[r^{l+1} + \tan\delta_l \frac{2^{2l+1}\Gamma(l+\frac{1}{2})\Gamma(l+\frac{3}{2})}{\pi k^{2l+1} r^l}\right]$$

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

$$\tan\delta_l \overset{k\to 0}{\sim} -\frac{\pi}{\Gamma(l+\frac{1}{2})\Gamma(l+\frac{3}{2})}\left(\frac{a_l k}{2}\right)^{2l+1}$$

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

Scattering length

$$u_l(r) \overset{kr\to 0}{\propto} u_l^{(s)}(kr) + \tan\delta_l u_l^{(c)}(kr)$$
$$\sim \frac{\sqrt{\pi}k^{l+1}}{2^{l+1}\Gamma(l+\frac{3}{2})}\left[r^{l+1} + \tan\delta_l \frac{2^{2l+1}\Gamma(l+\frac{1}{2})\Gamma(l+\frac{3}{2})}{\pi k^{2l+1} r^l}\right]$$

$$\tan\delta_l \overset{k\to 0}{\sim} -\frac{\pi}{\Gamma(l+\frac{1}{2})\Gamma(l+\frac{3}{2})}\left(\frac{a_l k}{2}\right)^{2l+1}$$

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

$$u_l^{(0)}(r) \overset{r\to\infty}{\propto} r^{l+1} - \frac{a_l^{2l+1}}{r^l}$$

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

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

Example: square potential well

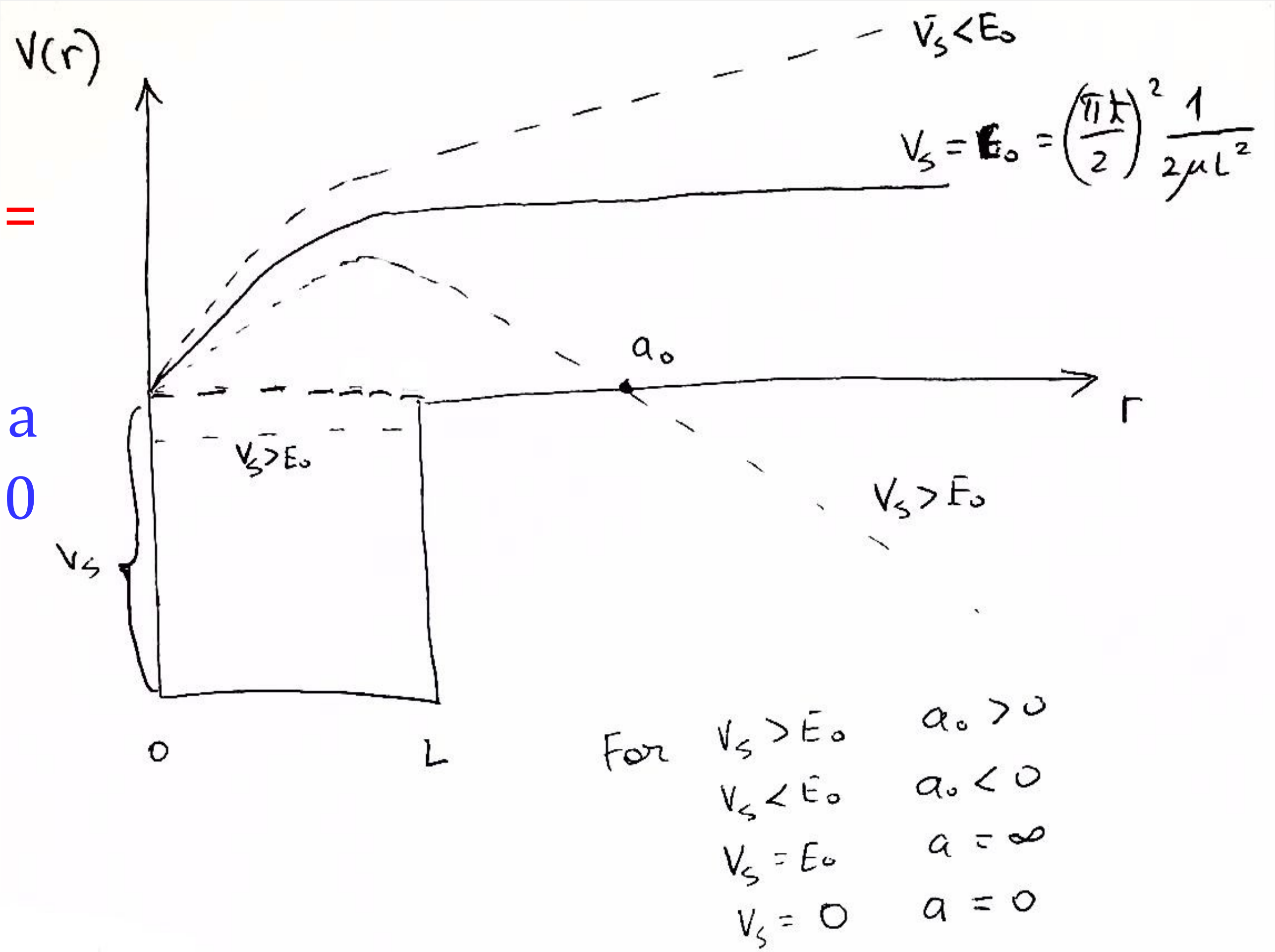
$$V(r) = \begin{cases} -V_S & \text{for } r \le L, \\ 0 & \text{for } r > L, \end{cases} \qquad V_S = \frac{\hbar^2 K_S^2}{2\mu}$$

Bound state with E=0 when $K_S L=\pi/2$ and V_S is

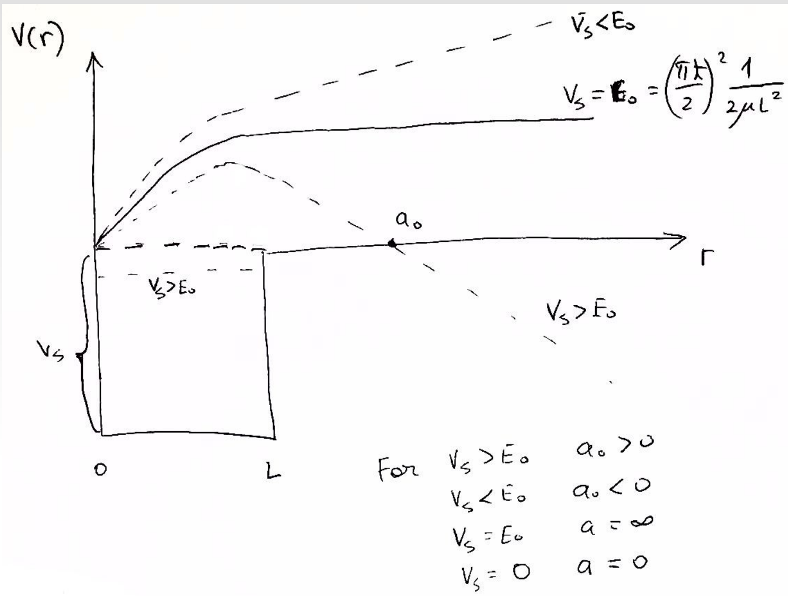
$$E_0 = (\tfrac{\pi}{2}\hbar)^2/(2\mu L^2)$$

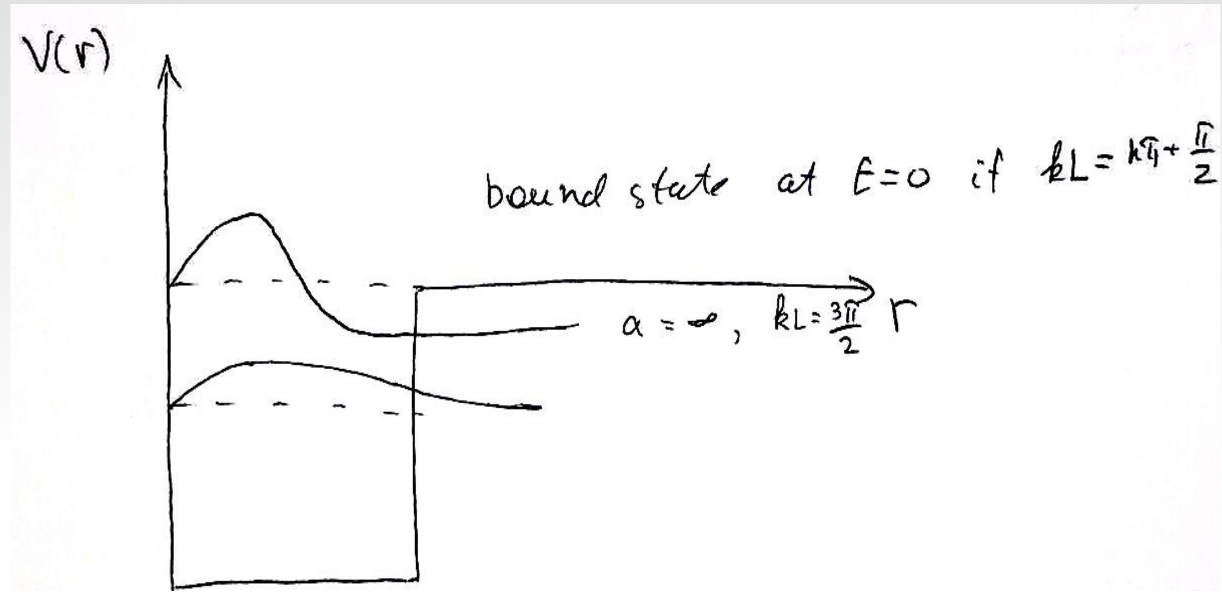
For this solution, $u_{l=0}(r) \to$ = constant at $r>L$.

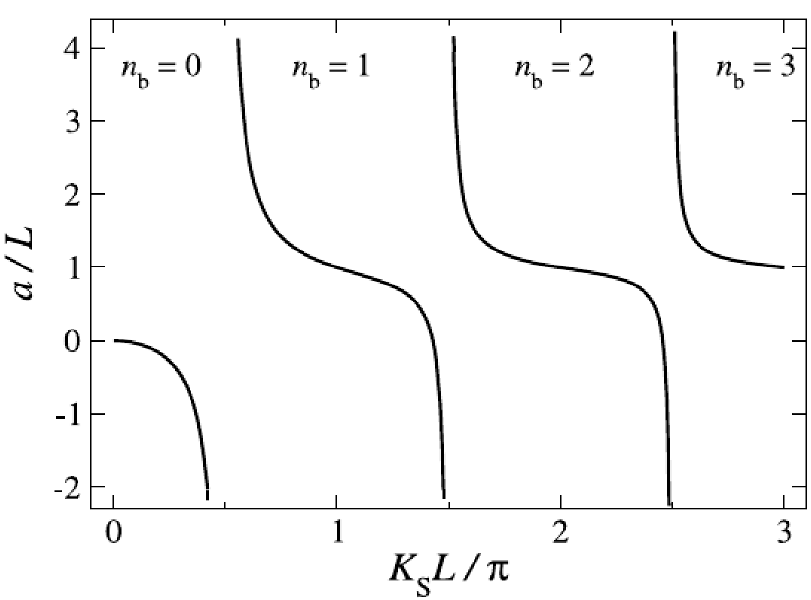
For a slightly larger V_S, a bound state with $E<0$ appears.



Scattering length for the square potential well



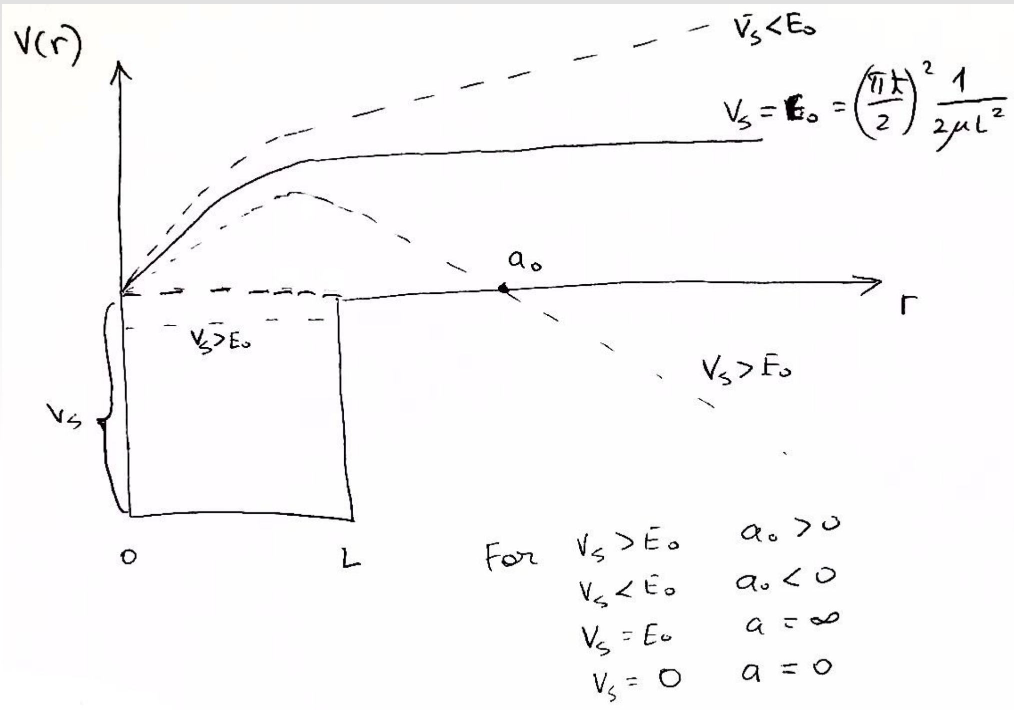




$$u_{l=0}^{(0)} \overset{r\to\infty}{\propto} r - a \propto 1 - \frac{r}{a}$$

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

Scattering length and weakly-bound states



A weakly-bound state

$$E_\mathrm{b} = -\hbar^2\kappa_\mathrm{b}^2/(2\mu)$$

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

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

$$\frac{1}{a} \overset{\kappa_\mathrm{b}\to 0}{\sim} \kappa_\mathrm{b} + O\left(\kappa_\mathrm{b}^2\right)$$

$$E_\mathrm{b} = -\frac{\hbar^2\kappa_\mathrm{b}^2}{2\mu} \overset{a\to\infty}{\sim} -\frac{\hbar^2}{2\mu a^2} + O\left(\frac{1}{a^3}\right)$$

It corresponds to a large positive scattering length *a*.

Example: Ultracold cesium gas

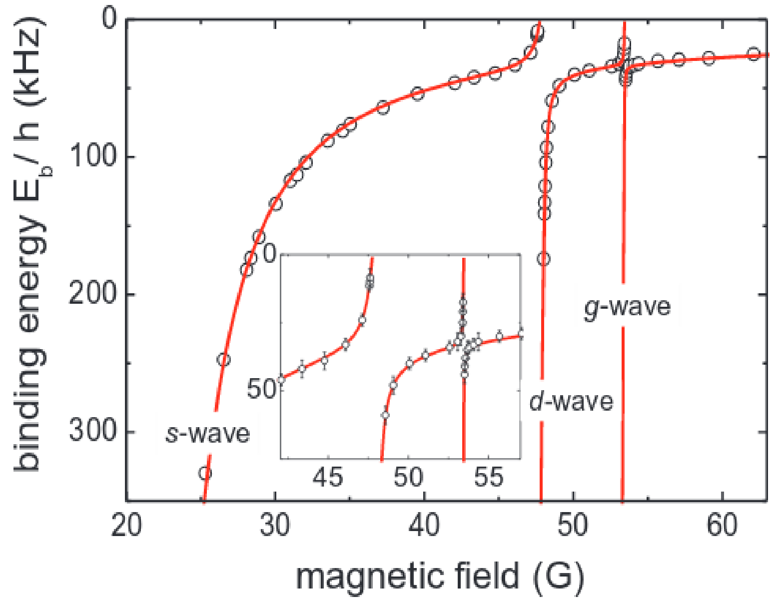


FIG. 3: (color online). Binding energy of cesium molecules near three Feshbach resonances as a function of the magnetic field. Zero energy corresponds to two Cs atoms in the absolute hyperfine ground-state sublevel $|F=3, m_F=3\rangle$. The measurements are shown as open circles. The fit (solid line) 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.

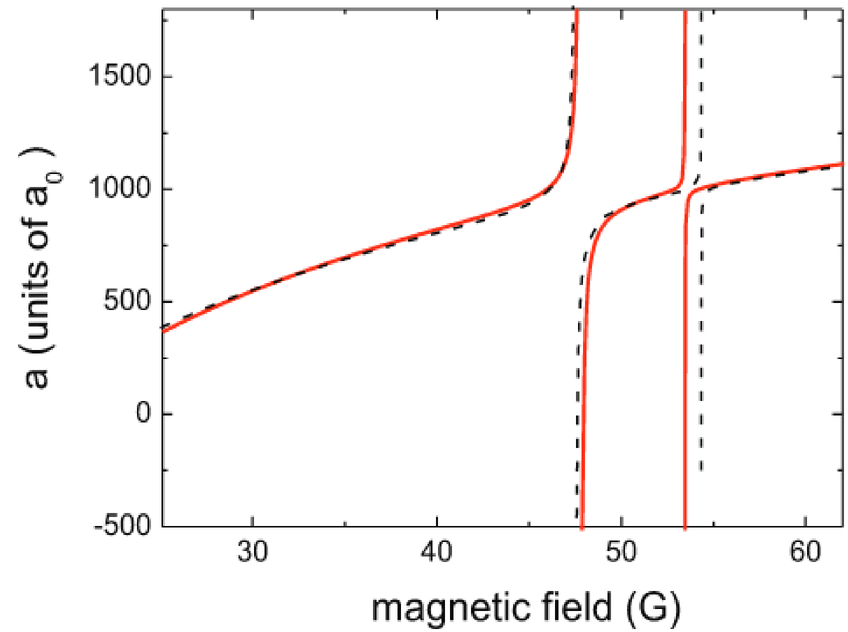


FIG. 4: (color online) Scattering length of $|F=3, m_F=3\rangle$ cesium atoms in the magnetic field range where three Feshbach resonances overlap. The solid curve shows the result of this work while the dashed curve represents the prediction from a previous multi-channel calculation [17].

$$E_\mathrm{b} = -\frac{\hbar^2 \kappa_\mathrm{b}^2}{2\mu} \overset{a\to\infty}{\sim} -\frac{\hbar^2}{2\mu a^2} + O\left(\frac{1}{a^3}\right)$$

Potential (shape) Resonances

Consider a solution of the Schrödinger equation, which behaves asymptotically

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

Consider the time-dependent Schrödinger equation. Its solution is

$$u^{(k)}(r,t) = u(r)\mathrm{e}^{-\mathrm{i}\omega t} \qquad \omega(k) = \frac{\hbar k^2}{2\mu}$$

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

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

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

$$\omega(k) \approx \bar{\omega} + \bar{\upsilon}(k-\bar{k}), \quad \bar{\omega} = \omega(\bar{k}),\ \bar{\upsilon} = \left.\frac{\mathrm{d}\omega}{\mathrm{d}k}\right|_{\bar{k}} = \frac{\hbar\bar{k}}{\mu}$$

Potential (shape) Resonances

$$\omega(k) \approx \bar{\omega} + \bar{\upsilon}(k - \bar{k}), \quad \bar{\omega} = \omega(\bar{k}),\ \bar{\upsilon} = \left.\frac{\mathrm{d}\omega}{\mathrm{d}k}\right|_{\bar{k}} = \frac{\hbar\bar{k}}{\mu}$$

The lower limit of the integral can be extended to -∞. The first term in

$$u(r,t) = \int_0^\infty u^{(k)}(r,t)\phi(k)\mathrm{d}k \qquad u_l(r) \overset{r\to\infty}{\sim} \mathrm{e}^{-\mathrm{i}(kr - l\pi/2)} - \mathrm{e}^{2\mathrm{i}\delta_l}\mathrm{e}^{+\mathrm{i}(kr - l\pi/2)}$$

can be written as

$$u^{\mathrm{in}}(r,t) = \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}(kr+\omega t - l\pi/2)}\phi(k)\mathrm{d}k$$

$$\approx \mathrm{e}^{-\mathrm{i}\bar{k}r - \mathrm{i}\bar{\omega}t}\,\mathrm{i}^l \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}(k-\bar{k})(r+\bar{\upsilon}t)}\tilde{\phi}(k-\bar{k})\mathrm{d}(k-\bar{k})$$

or in the form

$$u^{\mathrm{in}}(r,t) = \mathrm{e}^{-\mathrm{i}\bar{k}r - \mathrm{i}\bar{\omega}t}\Psi(r + \bar{\upsilon}t)$$

For example:

$$\tilde{\phi}(q) \propto \mathrm{e}^{-B^2q^2/2} \quad \Longrightarrow \quad \Psi(x) \propto \mathrm{e}^{-x^2/(2B^2)}$$

Potential (shape) Resonances

For the outgoing wave in $u_l(r) \overset{r\to\infty}{\sim} \mathrm{e}^{-\mathrm{i}(kr-l\pi/2)} - \mathrm{e}^{2\mathrm{i}\delta_l}\mathrm{e}^{+\mathrm{i}(kr-l\pi/2)}$

in the small interval of k $\delta_l(k) \approx \delta_l(\bar{k}) + (k-\bar{k})\left.\frac{\mathrm{d}\delta_l}{\mathrm{d}k}\right|_{\bar{k}}$

the integral $u(r,t) = \int_0^\infty u^{(k)}(r,t)\phi(k)\mathrm{d}k$

is approximated

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

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

$$\Delta r = 2\left.\frac{\mathrm{d}\delta_l}{\mathrm{d}k}\right|_{\bar{k}}$$

The integral can be expressed in terms of the same function Ψ

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

Wigner time-delay

Incoming wave in $u^{\text{in}}(r,t) = e^{-i\bar{k}r - i\bar{\omega}t}\Psi(r+\bar{v}t)$

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

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

For a free wave (scattering with V=0), Δr=0 .

Therefore, Δr is the space delay due to the potential.

The time delay is $\Delta t = \frac{\Delta r}{\bar{v}} = 2\frac{\mu}{\hbar\bar{k}}\frac{d\delta_l}{dk}\bigg|_{\bar{k}} = 2\hbar\frac{d\delta_l}{dE}\bigg|_{\bar{E}}$, $\bar{E} = \hbar^2\bar{k}^2/(2\mu)$

Time delay could be positive, zero, or negative.

For example, for the hard sphere:

$$\delta_{l=0} = -kR$$

$$\delta_l \overset{kR\to\infty}{\sim} -kR + l\frac{\pi}{2}$$

$\Delta r = -2R$ for $l = 0$ $\qquad$ $\Delta r \overset{kR\to\infty}{\sim} -2R$ for $l > 0$

Resonances ans 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 Δt_r or its widths $\Gamma=4\hbar/\Delta t_r$.

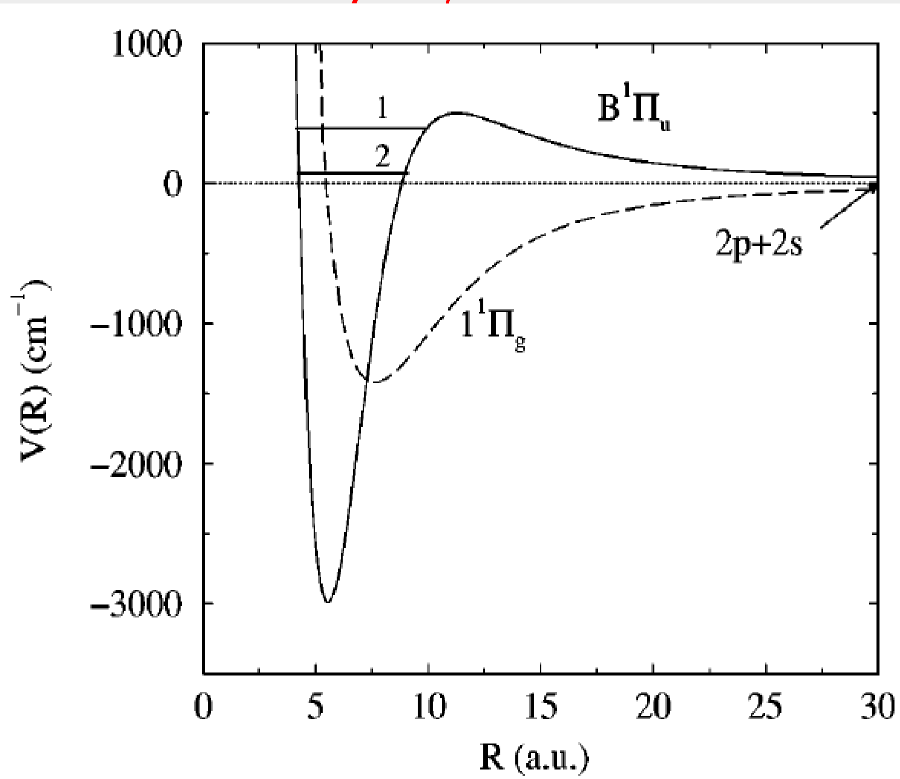


FIG. 3. Potentials of Li_2 $(2p+2s)$. Full line: $B\ ^1\Pi_u$ (Ref. [9]); dashed line: $1\ ^1\Pi_g$ (Ref. [15]).

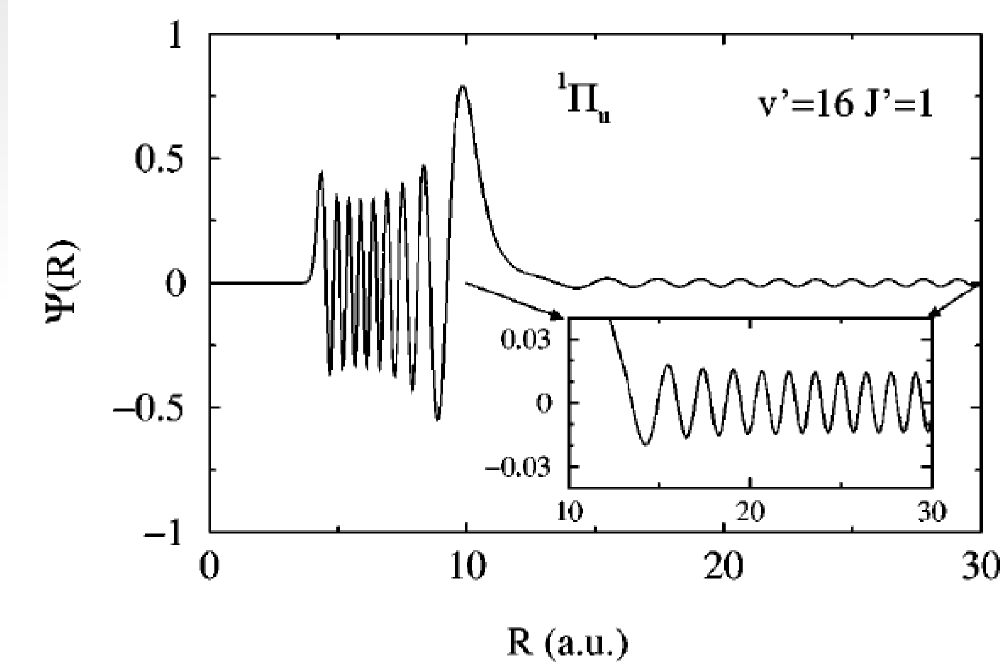


FIG. 4. The wave function (real part) of the $v'=16$, $J'=1$ level of $^6Li^7Li$. The dissociation rate is $k=8670\times10^6\ s^{-1}$, corresponding to a lifetime $\tau=115$ ps. The inset shows the long-range part responsible for the decay due to tunneling through the barrier.

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

Time-dependent vs time-independent picture

The asymptotic behavior of a solution of TISE is

$$u_l(r) \overset{r\to 0}{\sim} \frac{2l+1}{2k} \mathrm{i}^{l+1}[\mathrm{e}^{-\mathrm{i}(kr-l\pi/2)} - \mathrm{e}^{2\mathrm{i}\delta_l}\mathrm{e}^{+\mathrm{i}(kr-l\pi/2)}]$$

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

Now, we apply the same idea for positive energies (analytical continuation). If there is a solution of

$$\mathrm{e}^{-\mathrm{i}\delta_l(\mathscr{E})} = 0.$$

Then the energy $\mathscr{E}$ is a complex number $\mathscr{E} = E_{\mathrm{re}} + \mathrm{i}E_{\mathrm{im}}$ with negative $\mathscr{E}_{\mathrm{im}}$, such that the norm of the wave function decays with time as

$$|u_l|^2 \propto \mathrm{e}^{2E_{\mathrm{im}}t/\hbar}$$

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

$$\mathrm{e}^{-\mathrm{i}\delta_l(\mathscr{E})} = 0.$$

For real E $\mathrm{e}^{+\mathrm{i}\delta_l(E)} = [\mathrm{e}^{-\mathrm{i}\delta_l(E)}]^* \approx C^*(E-\mathscr{E}^*)$

Time-dependent vs time-independent picture

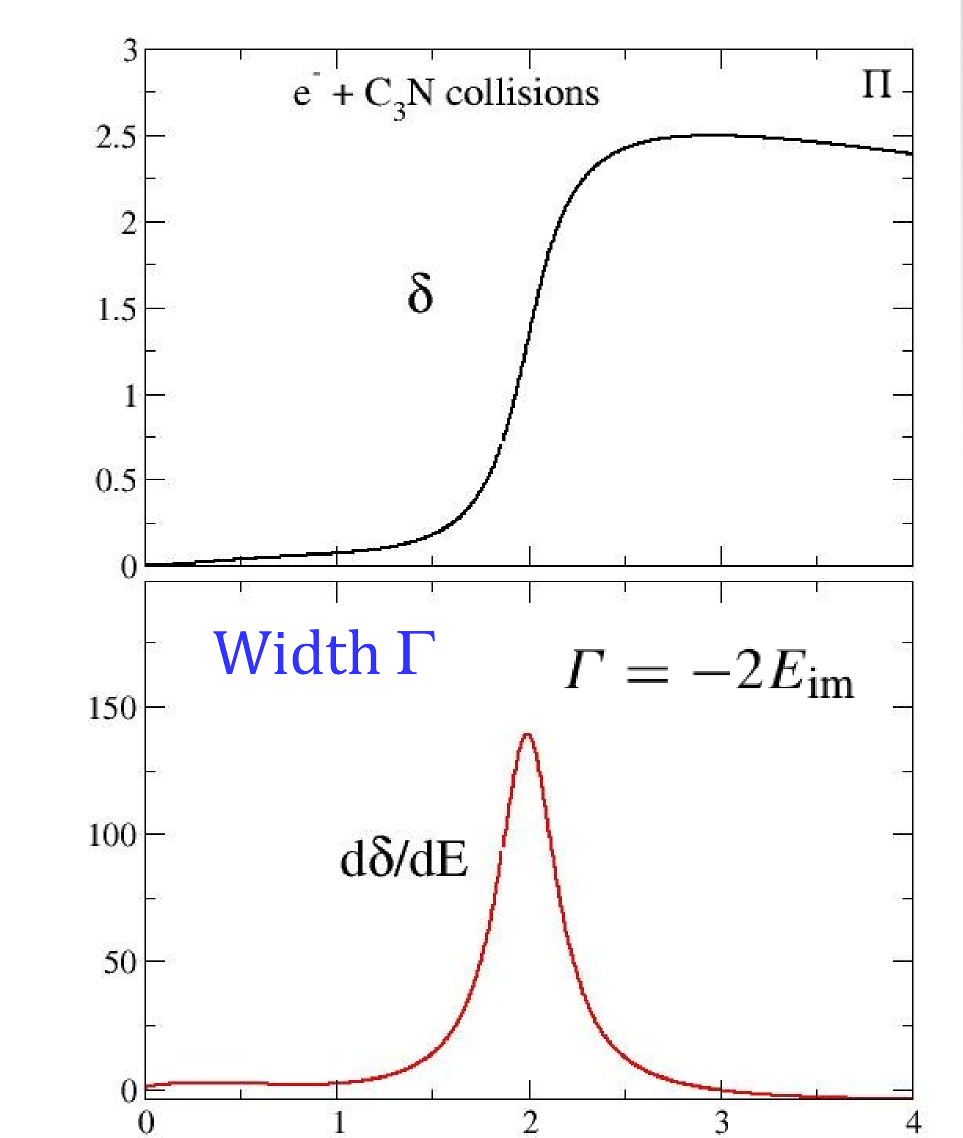
$$\mathrm{e}^{-\mathrm{i}\delta_l(E)} \approx C(E - \mathscr{E})$$

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

$$S_l = \mathrm{e}^{+\mathrm{i}\delta_l(E)} / \mathrm{e}^{-\mathrm{i}\delta_l(E)}$$

$$S_l = \frac{C^*}{C} \frac{E - E_{\mathrm{re}} + \mathrm{i}E_{\mathrm{im}}}{E - E_{\mathrm{re}} - \mathrm{i}E_{\mathrm{im}}}$$

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



$$\tau_{\mathrm{R}} = \frac{\hbar}{\Gamma} \quad |u_l|^2 \propto \mathrm{e}^{2E_{\mathrm{im}}t/\hbar}$$

Breit-Wigner formula

The *l*-wave cross section

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

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

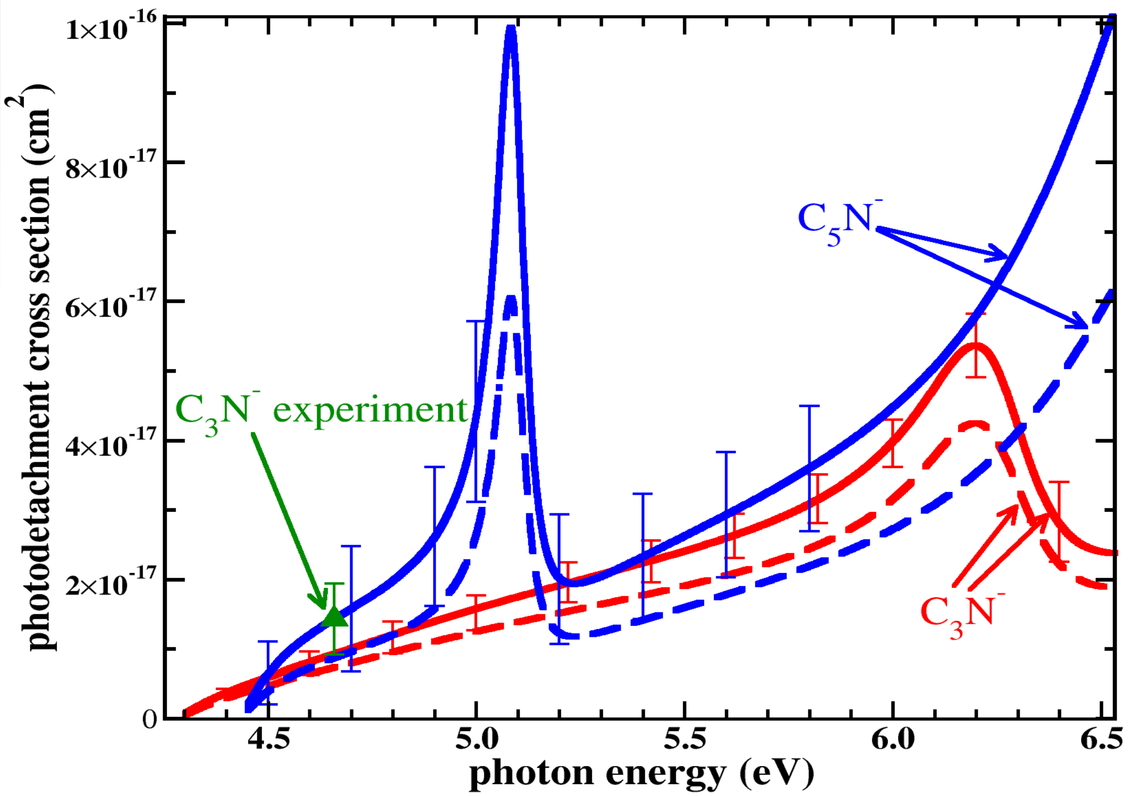
It is Breit-Wigner formula for the cross section near a resonance.

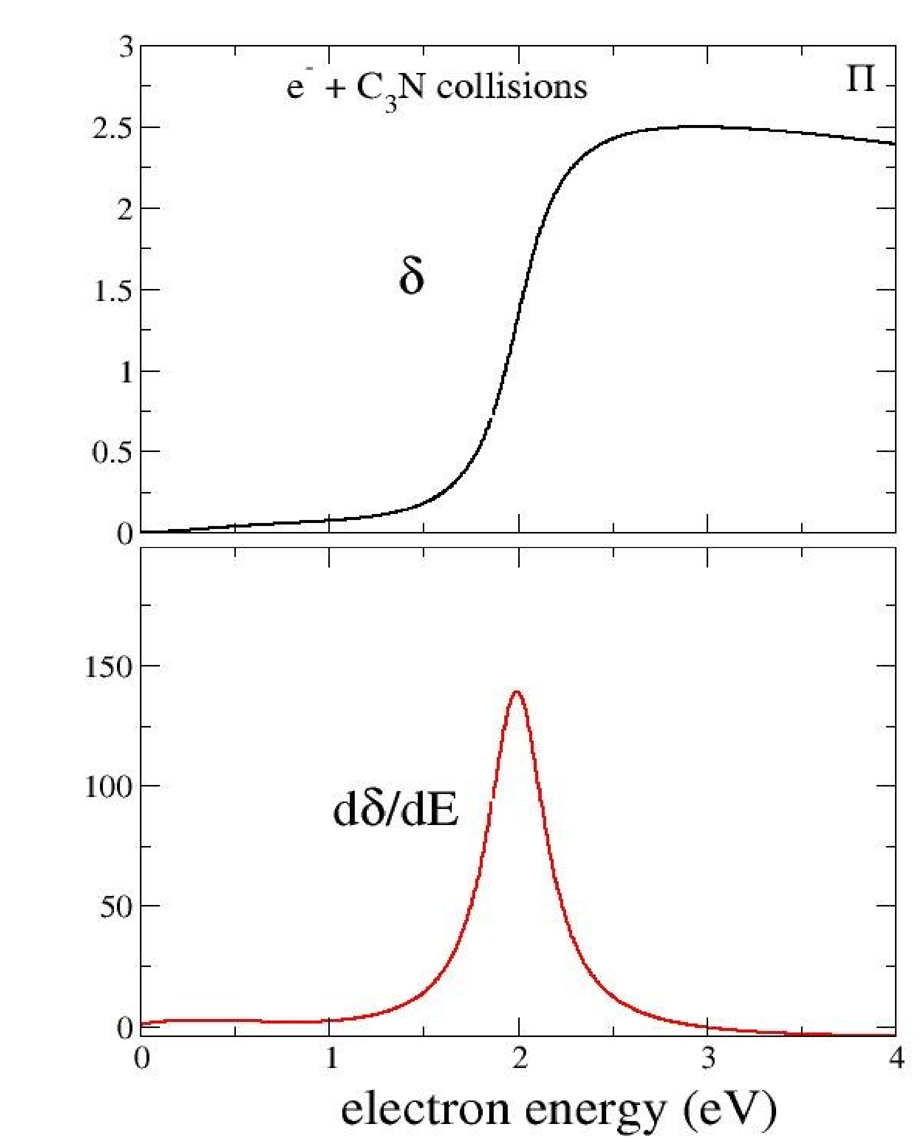
For the Wigner time delay near a resonance

$$\Delta t = 2\hbar\frac{\mathrm{d}\delta_l}{\mathrm{d}E} = \frac{\hbar\Gamma}{(E-E_{\mathrm{R}})^2+(\Gamma/2)^2}$$

$C_3N + e^-$ 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

$$\boldsymbol{\Psi}(\mathbf{r},\xi) = \sum_j \psi_j(\mathbf{r})\Upsilon_j(\xi)$$

ξ refers to all internal degrees of freedom of projectile and target.

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

The internal states Υ_i define ***channels*** for the scattering process.
Wave functions ψ_i (*r*) are channel wave functions.
The Schrödinger equation

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

$$-\frac{\hbar^2}{2\mu}\Delta\psi_i(\mathbf{r}) + \sum_j V_{i,j}\psi_j(\mathbf{r}) = (E - E_i)\psi_i(\mathbf{r}) \qquad V_{i,j} = \langle \Upsilon_i|\hat{W}|\Upsilon_j\rangle_\xi$$

Scattering amplitude

Open and closed channels, channel thresholds E_j

$$\boldsymbol{\Psi}(\mathbf{r},\xi)=\sum_j \psi_j(\mathbf{r})\Upsilon_j(\xi)$$

The description of a scattering process starts with

$$\boldsymbol{\Psi}(\mathbf{r},\xi) \overset{r\to\infty}{\sim} \mathrm{e}^{\mathrm{i}k_i z}\Upsilon_i(\xi)+\sum_{j\ \mathrm{open}} f_{i,j}(\theta,\phi)\frac{\mathrm{e}^{\mathrm{i}k_j r}}{r}\Upsilon_j(\xi)$$

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

$$\boldsymbol{\Psi}(\mathbf{r},\xi) \overset{r\to\infty}{\sim} \mathrm{e}^{\mathrm{i}k_i z}\Upsilon_i(\xi) + \sum_{j\ \text{open}} f_{i,j}(\theta,\phi)\frac{\mathrm{e}^{\mathrm{i}k_j r}}{r}\Upsilon_j(\xi)$$

$$\psi_j(\mathbf{r}) \overset{r\to\infty}{\sim} \mathrm{e}^{\mathrm{i}k_i z}\delta_{i,j} + f_{i,j}(\theta,\phi)\frac{\mathrm{e}^{\mathrm{i}k_j r}}{r}$$

Current density in channel *j*

$$\mathbf{j}_j(\mathbf{r}) = \frac{\hbar k_j}{\mu}\left|f_{i,j}(\theta,\phi)\right|^2\frac{\hat{\mathbf{e}}_\mathbf{r}}{r^2} + O\left(\frac{1}{r^3}\right)$$

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

$$\frac{\mathrm{d}\sigma_{i\to j}}{\mathrm{d}\Omega} = \frac{k_j}{k_i}\left|f_{i,j}(\theta,\phi)\right|^2$$

Integrated cross section is

$$\sigma = \sum_{j\ \text{open}} \sigma_{i\to j}, \quad \sigma_{i\to j} = \int \frac{\mathrm{d}\sigma_{i\to j}}{\mathrm{d}\Omega}\mathrm{d}\Omega = \frac{k_j}{k_i}\int \left|f_{i,j}(\theta,\phi)\right|^2\mathrm{d}\Omega$$

Multichannel Green's function

Multi-channel Schrödinger equation

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

in a vector form

$$\left(\hat{E}+\frac{\hbar^2}{2\mu}\Delta\right)\Psi=\hat{V}\Psi$$

Multi-channel Green's function

$$\left[\hat{E}+\frac{\hbar^2}{2\mu}\Delta\right]\hat{G}=\mathbf{1}$$

$$\left[E-E_j+\frac{\hbar^2}{2\mu}\Delta\right]\mathscr{G}_{j,j}(\mathbf{r},\mathbf{r}')=\delta(\mathbf{r}-\mathbf{r}')$$

If Ψ is a solution then it satisfies $\Psi=\Psi^{\text{hom}}+\hat{G}\hat{V}\Psi,$ $[\hat{E}+\frac{\hbar^2}{2\mu}\Delta]\Psi^{\text{hom}}=0$

Free-particle Green's function is

$$\mathscr{G}_{j,j}(\mathbf{r},\mathbf{r}')=-\frac{\mu}{2\pi\hbar^2}\frac{\mathrm{e}^{ik_j|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}\overset{|\mathbf{r}|\gg|\mathbf{r}'|}{\sim}-\frac{\mu}{2\pi\hbar^2}\frac{\mathrm{e}^{ik_jr}}{r}\mathrm{e}^{-\mathrm{i}\mathbf{k}_j\cdot\mathbf{r}'}$$

$$\mathbf{k}_j=k_j\hat{\mathbf{e}}_{\mathbf{r}}$$

Multichannel Lippmann-Schwinger equation

Multi-channel Lippmann-Schwinger equation

$$\Psi = \Psi^{\text{hom}} + \hat{G}\hat{V}\Psi.$$

Accounting for boundary conditions in

$$\boldsymbol{\Psi}(\mathbf{r},\xi) \overset{r\to\infty}{\sim} \mathrm{e}^{\mathrm{i}k_i z}\Upsilon_i(\xi) + \sum_{j\text{ open}} f_{i,j}(\theta,\phi)\frac{\mathrm{e}^{\mathrm{i}k_j r}}{r}\Upsilon_j(\xi)$$

$$\psi_i^{\text{hom}}(\mathbf{r}) = \mathrm{e}^{\mathrm{i}k_i z}, \qquad \psi_j^{\text{hom}}(\mathbf{r}) \equiv 0 \quad \text{for } j \neq i$$

Lippmann-Schwinger equation becomes

$$\psi_j(\mathbf{r}) = \mathrm{e}^{\mathrm{i}k_i z}\delta_{i,j} + \int \mathscr{G}_{j,j}(\mathbf{r},\mathbf{r}')\sum_n V_{j,n}\psi_n(\mathbf{r}')\,\mathrm{d}\mathbf{r}'$$

Multichannel Scattering amplitude

Asymptotically, the equation

$$\psi_j(\mathbf{r}) = \mathrm{e}^{\mathrm{i}k_i z}\delta_{i,j} + \int \mathscr{G}_{j,j}(\mathbf{r},\mathbf{r}')\sum_n V_{j,n}\psi_n(\mathbf{r}')\,\mathrm{d}\mathbf{r}'$$

could be written as

$$\mathscr{G}_{j,j}(\mathbf{r},\mathbf{r}') = -\frac{\mu}{2\pi\hbar^2}\frac{\mathrm{e}^{\mathrm{i}k_j|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \overset{|\mathbf{r}|\gg|\mathbf{r}'|}{\sim} -\frac{\mu}{2\pi\hbar^2}\frac{\mathrm{e}^{\mathrm{i}k_j r}}{r}\mathrm{e}^{-\mathrm{i}\mathbf{k}_j\cdot\mathbf{r}'}$$

$$\psi_j(\mathbf{r}) \overset{r\to\infty}{\sim} \mathrm{e}^{\mathrm{i}k_i z}\delta_{i,j} - \frac{\mu}{2\pi\hbar^2}\frac{\mathrm{e}^{\mathrm{i}k_j r}}{r}\sum_n \int \mathrm{e}^{-\mathrm{i}\mathbf{k}_j\cdot\mathbf{r}'} V_{j,n}\psi_n(\mathbf{r}')\,\mathrm{d}\mathbf{r}'$$

Comparing with

$$\boldsymbol{\Psi}(\mathbf{r},\xi) \overset{r\to\infty}{\sim} \mathrm{e}^{\mathrm{i}k_i z}\Upsilon_i(\xi) + \sum_{j\ \text{open}} f_{i,j}(\theta,\phi)\frac{\mathrm{e}^{\mathrm{i}k_j r}}{r}\Upsilon_j(\xi)$$

the amplitudes can be written as

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

Multichannel Born approximation

If one substitutes Ψ^{hom} instead of ψ_n in the incoming wave

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

one obtains the amplitude in the Born approximation

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

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

The Born scattering amplitude is a function of momentum transfer:

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

Feshbach resonances

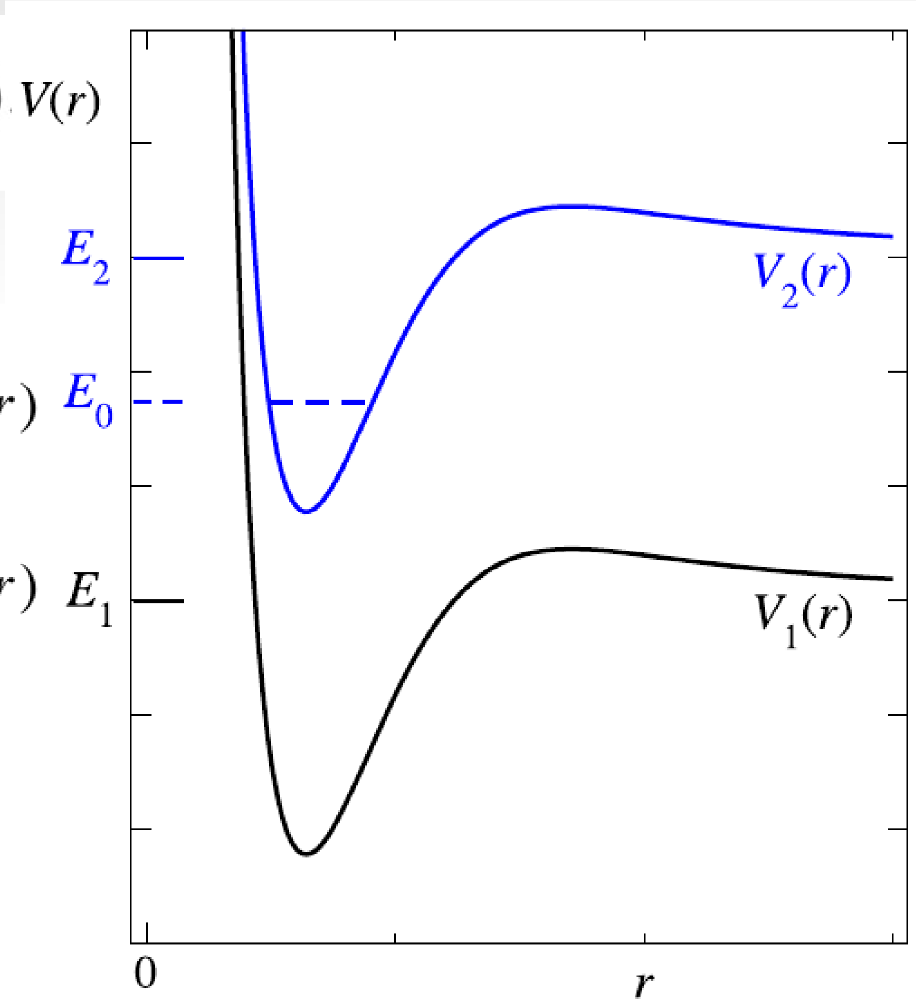
A shape resonance is trapped by a potential barrier.

Feshbach resonance is trapped by a closed channel

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

$$\left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_1(r)\right]u_1(r) + V_{1,2}u_2(r) = Eu_1(r)$$

$$\left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_2(r)\right]u_2(r) + V_{2,1}u_1(r) = Eu_2(r)$$



Feshbach resonances

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

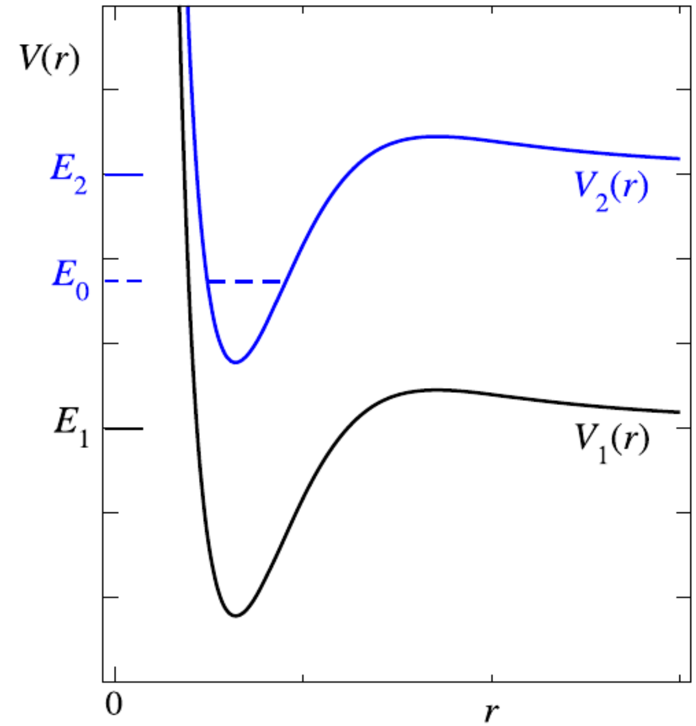
$$\left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2}+V_2(r)\right]u_0(r)=E_0u_0(r),\quad \langle u_0|u_0\rangle=1,\ E_1<E_0<E_2$$

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

$$\left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2}+V_1(r)\right]u_1(r)+V_{1,2}u_2(r)=Eu_1(r)$$
$$\left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2}+V_2(r)\right]u_2(r)+V_{2,1}u_1(r)=Eu_2(r)$$

The two component solution can then be written as

$$U\equiv\begin{pmatrix}u_1(r)\\ Au_0(r)\end{pmatrix}$$



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

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

$$\left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_1(r)\right]u_1(r) + V_{1,2}u_2(r) = Eu_1(r)$$

$$\left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_2(r)\right]u_2(r) + V_{2,1}u_1(r) = Eu_2(r)$$

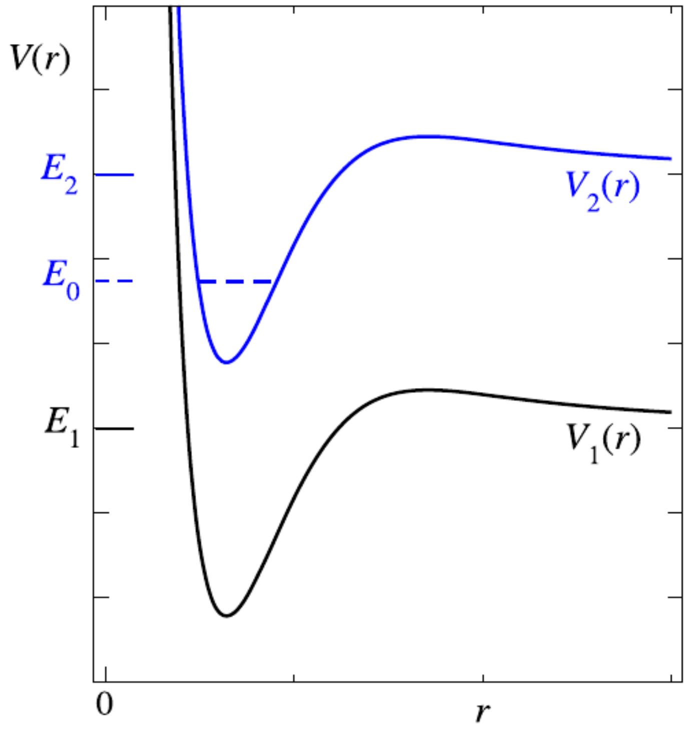
Again, a Green's function is introduced

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

$$\mathscr{G}(r,r') = -\pi\bar{\mathrm{u}}_1^{(\mathrm{reg})}(r_<)\bar{\mathrm{u}}_1^{(\mathrm{irr})}(r_>)$$

$$\bar{\mathrm{u}}_1^{(\mathrm{reg})}(r) \overset{r\to\infty}{\sim} \sqrt{\frac{2\mu}{\pi\hbar^2 k}}\sin(kr+\delta_{\mathrm{bg}})$$

$$\bar{\mathrm{u}}_1^{(\mathrm{irr})}(r) \overset{r\to\infty}{\sim} \sqrt{\frac{2\mu}{\pi\hbar^2 k}}\cos(kr+\delta_{\mathrm{bg}}).$$



Feshbach resonances

From the Green's function and the first equation

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

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

we obtain $\Psi = \Psi^{\text{hom}} + \hat{G}\hat{V}\Psi.$

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

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

introducing δ_{res} as $-\pi A\langle\bar{u}_1^{(\text{reg})}|V_{1,2}|u_0\rangle = \tan\delta_{\text{res}}$

$$\begin{aligned} u_1(r) &\overset{r\to\infty}{\sim} \sqrt{\frac{2\mu}{\pi\hbar^2 k}}\left[\sin(kr+\delta_{\text{bg}}) + \tan\delta_{\text{res}}\cos(kr+\delta_{\text{bg}})\right] \\ &= \frac{1}{\cos(\delta_{\text{res}})}\sqrt{\frac{2\mu}{\pi\hbar^2 k}}\sin(kr+\delta_{\text{bg}}+\delta_{\text{res}}). \end{aligned}$$

Feshbach resonances

We had $A(E-E_0) = \langle u_0 | V_{2,1} | u_1 \rangle$

$$\begin{aligned} u_1(r) &= \bar{u}_1^{(\mathrm{reg})}(r) + A \int_0^\infty \mathscr{G}(r,r') V_{1,2}(r') u_0(r') \, \mathrm{d}r' \\ &\overset{r\to\infty}{\sim} \bar{u}_1^{(\mathrm{reg})}(r) - \pi A \langle \bar{u}_1^{(\mathrm{reg})} | V_{1,2} | u_0 \rangle \bar{u}_1^{(\mathrm{irr})}(r). \end{aligned}$$

we obtain

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

$$\Longrightarrow \quad A = \frac{\langle u_0 | V_{2,1} | \bar{u}_1^{(\mathrm{reg})} \rangle}{E - E_0 - \langle u_0 | V_{2,1} \hat{G} V_{1,2} | u_0 \rangle}.$$

For δ_{res} we had

$$-\pi A \langle \bar{u}_1^{(\mathrm{reg})} | V_{1,2} | u_0 \rangle = \tan \delta_{\mathrm{res}}$$

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

Feshbach resonances

We had

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

Introducing notations:

$$E_{\text{R}} = E_0 + \langle u_0|V_{2,1}\hat{G}V_{1,2}|u_0\rangle$$

position of the resonance

$$\Gamma = 2\pi\left|\langle u_0\right|V_{2,1}\left|\bar{\text{u}}_1^{(\text{reg})}\rangle\right|^2$$

width of the resonance

The tangent can be written as

$$\tan\delta_{\text{res}} = -\frac{\Gamma/2}{E - E_{\text{R}}}$$

It is useful to compare Γ with the Fermi golden rule

$$P_{\text{in}\to\text{fin}} = \frac{2\pi}{\hbar}\left|\langle\Psi_{\text{in}}|\hat{W}|\Psi_{\text{fin}}\rangle\right|^2\rho_{\text{fin}}(E)$$

Landau-Zener model

Non-adiabatic coupling

The time dependent Schrödinger equation for a diatomic molecule

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

Adiabatic electronic functions

$$H_{el}(\mathbf{r},\mathbf{R})\varphi_l(\mathbf{r},\mathbf{R}) = E_l(\mathbf{R})\varphi_l(\mathbf{r},\mathbf{R})$$

and adiabatic basis set

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

The Schrödinger equation takes the form

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

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*)

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

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

The solution Ψ is now represented as

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

Inserting into the Schrödinger equation

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

Semi-classical treatment

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

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

$$\Psi_n = \sum_k a_{kn}(t)\, \Psi_k^{(0)}$$

$$a_{kn}^{(1)} = -\frac{i}{\hbar}\int W_{kn} e^{i\omega_{kn}t}\, dt$$

$$\omega_{mk} = \frac{E_m^{(0)} - E_k^{(0)}}{\hbar}$$

We conclude that

$$W = -i\hbar\frac{\partial}{\partial t}$$

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

Let us call $|\langle \varphi_l^* \frac{\partial \varphi_{l'}}{\partial R} \rangle|^{-1}$ as δR (characteristic length) $\quad W_{ll'} \approx \hbar v / \delta R$

The applicability condition of the perturbation approach

$$|W_{ll'}| \ll |E_l - E_{l'}| = \Delta E_{ll'}$$

or

$$\Delta E_{ll'} \cdot \delta R / \hbar v \gg 1$$

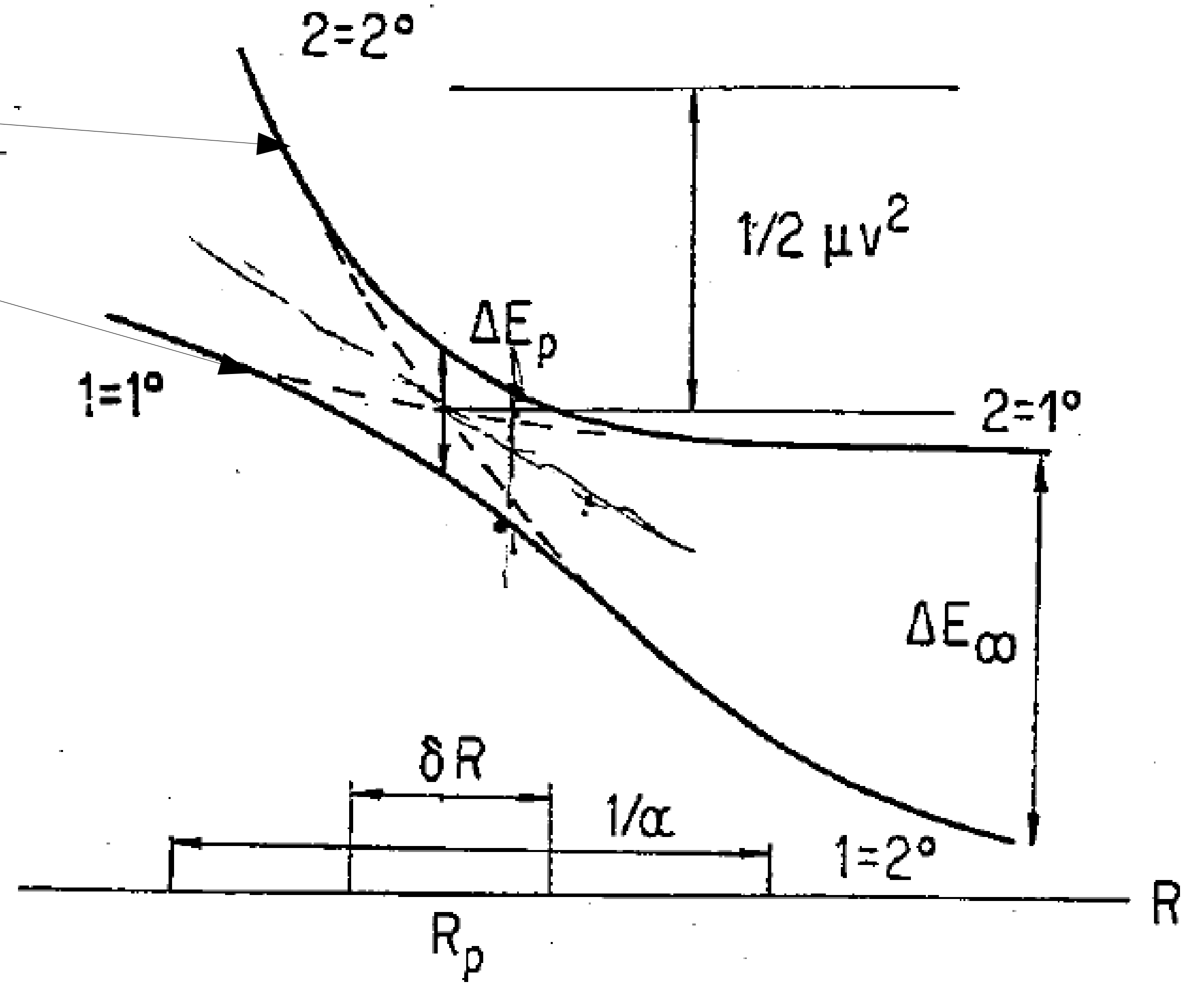
Two-state approximation

Adiabatic functions φ_1 and φ_2 .

They correspond to solid potential curves.

In the basis of φ_1 and φ_2

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



Diabatic basis

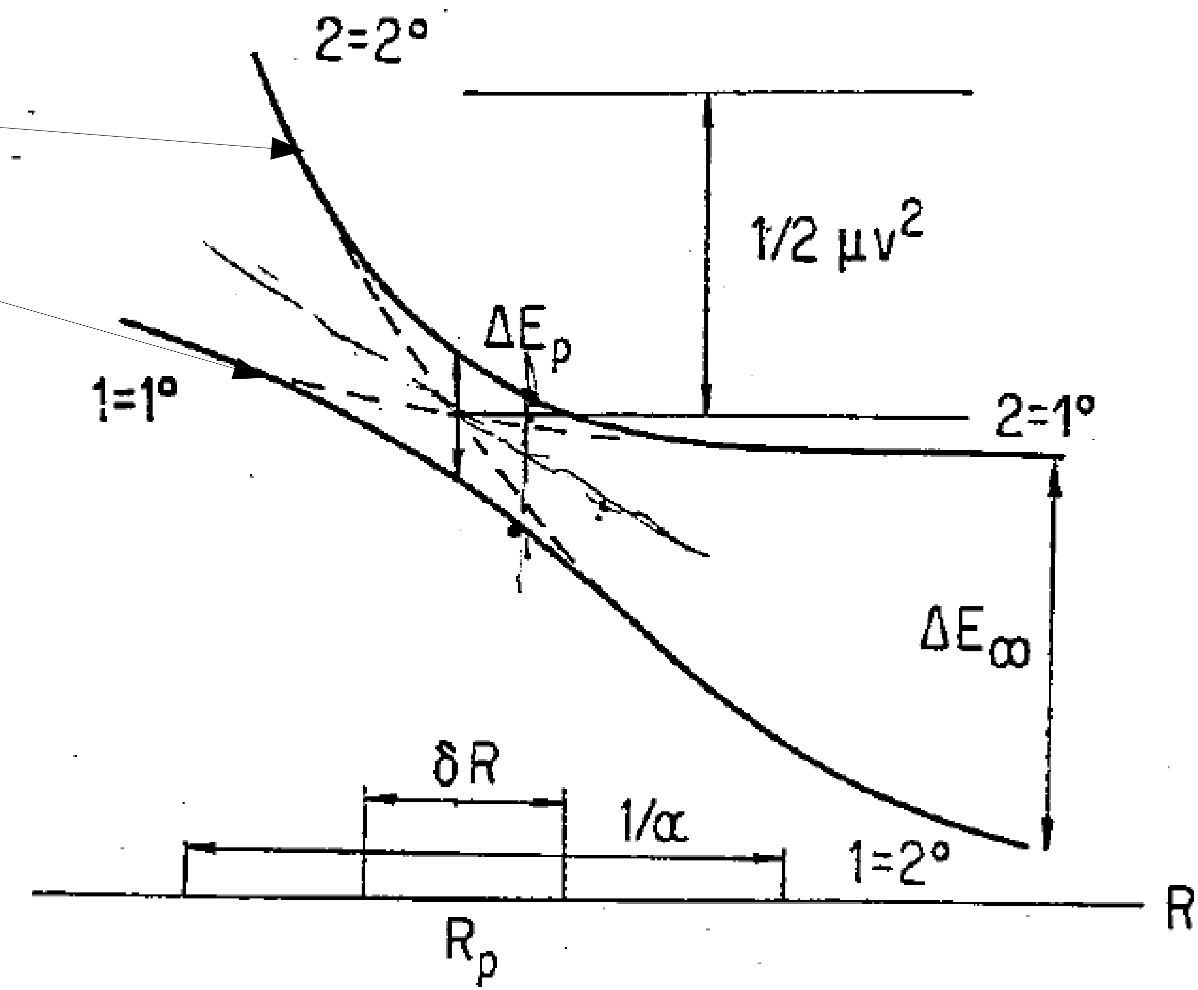
$$H_{el}(\varphi) = \begin{pmatrix} E_1(R) & 0 \\ 0 & E_2(R) \end{pmatrix}$$

Another pair φ^0_1 and φ^0_2 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 φ^0_1 and φ^0_2

$$H_{el}(\varphi^0) = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$$



H_{12} and H_{21} as well as φ^0_1 and φ^0_2 depend weakly on R.

Two-state approximation

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

$$H_{el}(\varphi^0) = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$$

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

$$H_{12}(R)/[H_{11}(R) - H_{22}(R)] \rightarrow 0$$

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

$$x = R - R_p$$

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

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

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

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

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

$$\chi=\frac{1}{2}\operatorname{arctg}\frac{2a}{\Delta F x}$$

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

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

Non-adiabatic functions

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

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

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

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

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

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

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

In the region of interaction (R withing δR) 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=-∞ and R far from R_p and end up with t=∞ and R again far from R_p.

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

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

Initially, the system is in state φ^0_1 $\quad b_1(-\infty)=1,\ b_2(-\infty)=0$

At the end $|b_2(+\infty)|^2$ give the probability P^0_{12} of transition from state φ^0_1 to φ^0_1.

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

Therefore, $\quad P^0_{12}=2\pi a^2/\Delta F\hbar v,\ \ if\ P^0_{12}\ll 1$

Landau-Zener probability

When a is large the treatment is not good, P^0_{12} could be become comparable or larger than 1.

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

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

Solving the system of equations, one obtains $P_{12} = \exp\left[-\frac{2\pi a^2}{\Delta F \hbar v}\right] = 1 - P^0_{12}$

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

$$P = 2P_{12}(1 - P_{12}) = 2(1 - P^0_{12})P^0_{12}$$

$$P = 2\exp\left(-\frac{2\pi a^2}{\Delta F \hbar v}\right)\left[1 - \exp\left(-\frac{2\pi a^2}{\Delta F \hbar v}\right)\right]$$

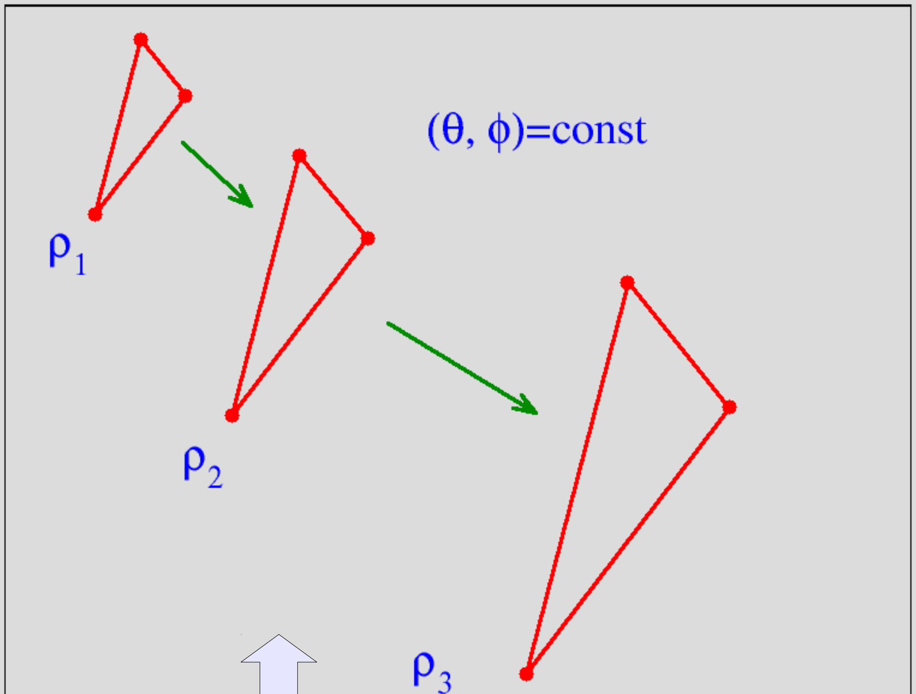
Few-body bound and scattering states at low energies (near dissociation)

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-boby) quantum effects (Efimov states)
* Symmetry of particles should be accounted for if only a few quantum states are populated.

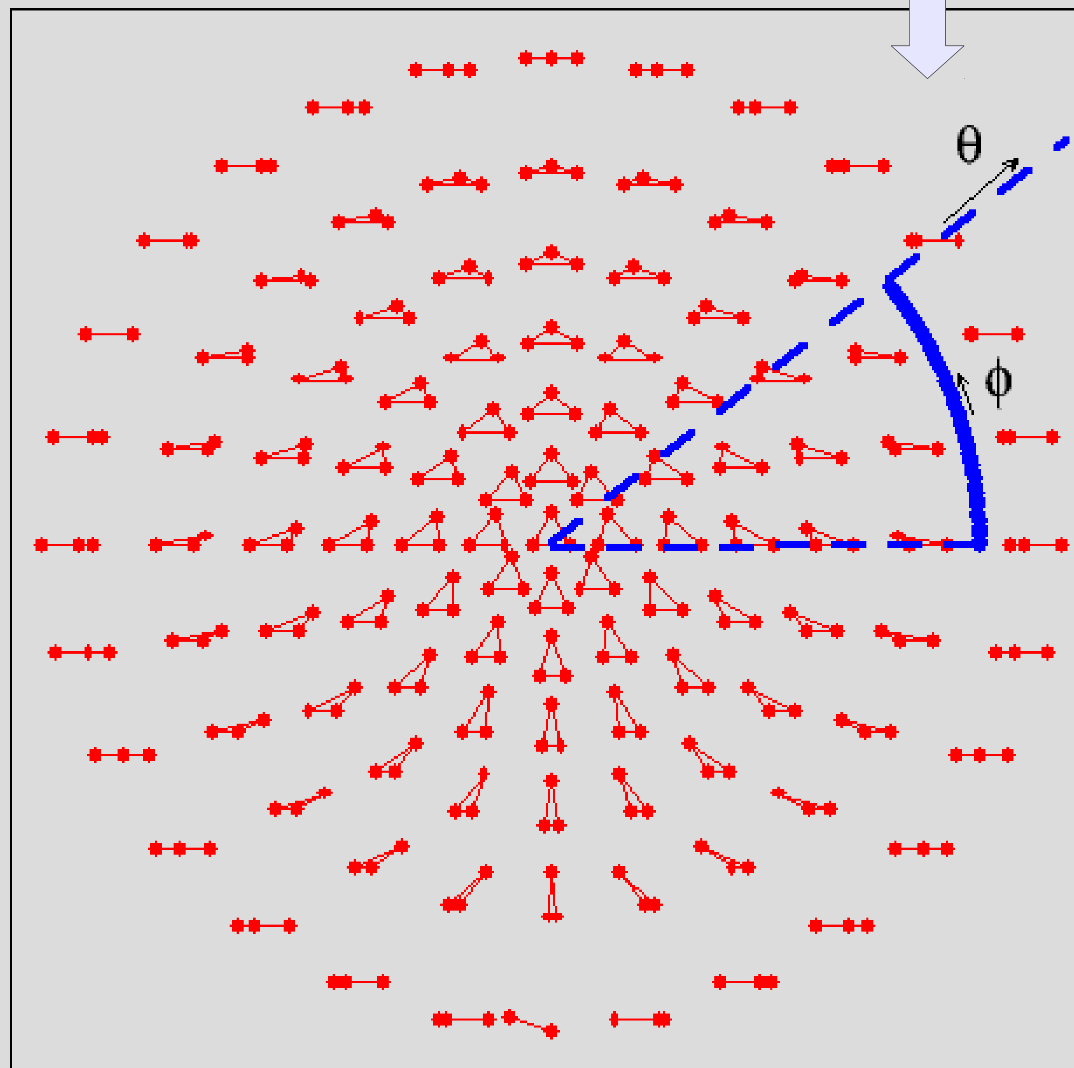
Hyper-spherical coordinates

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



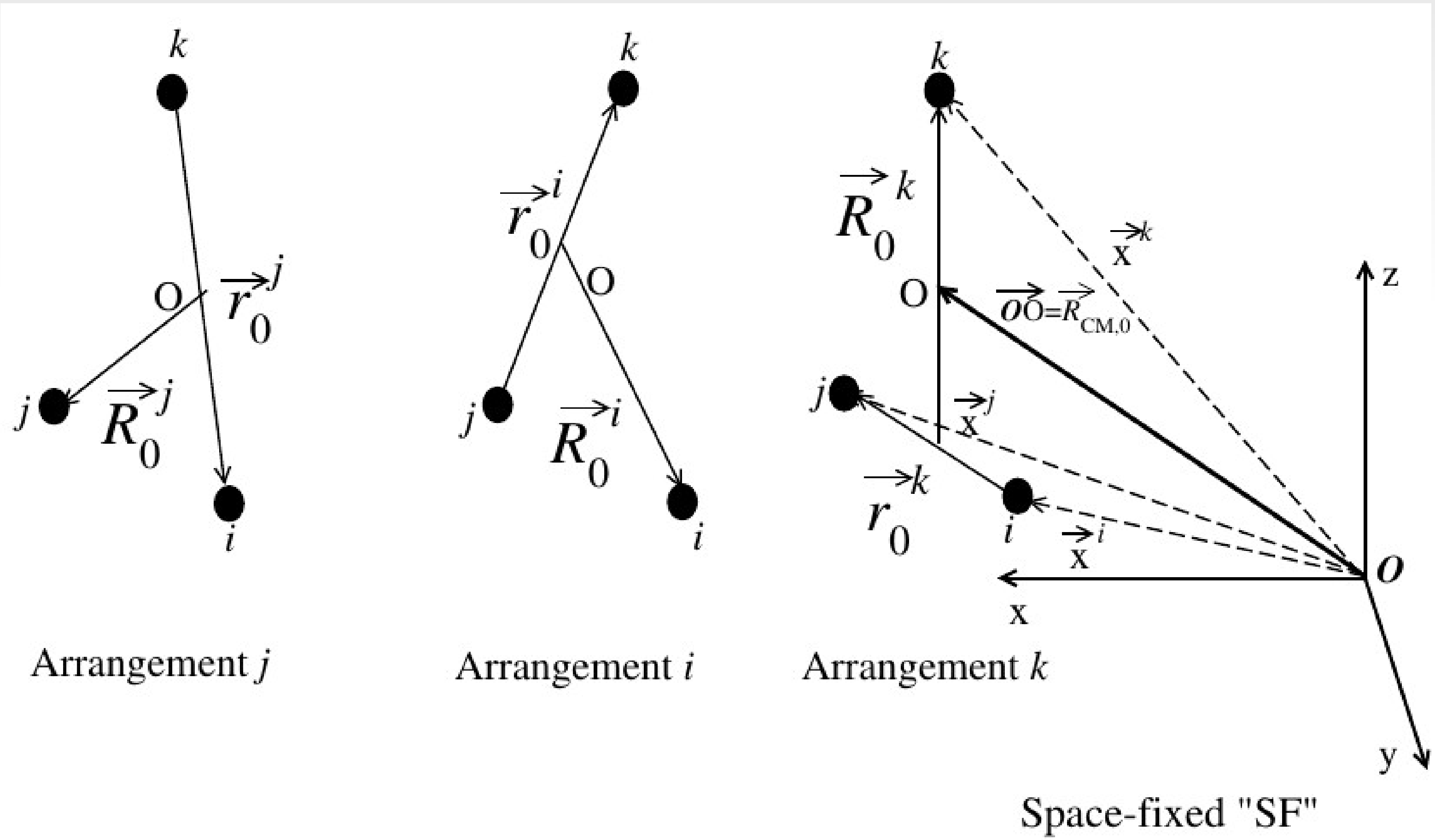
Changing hyper-radius

Changing hyperangles



Jacobi coordinates

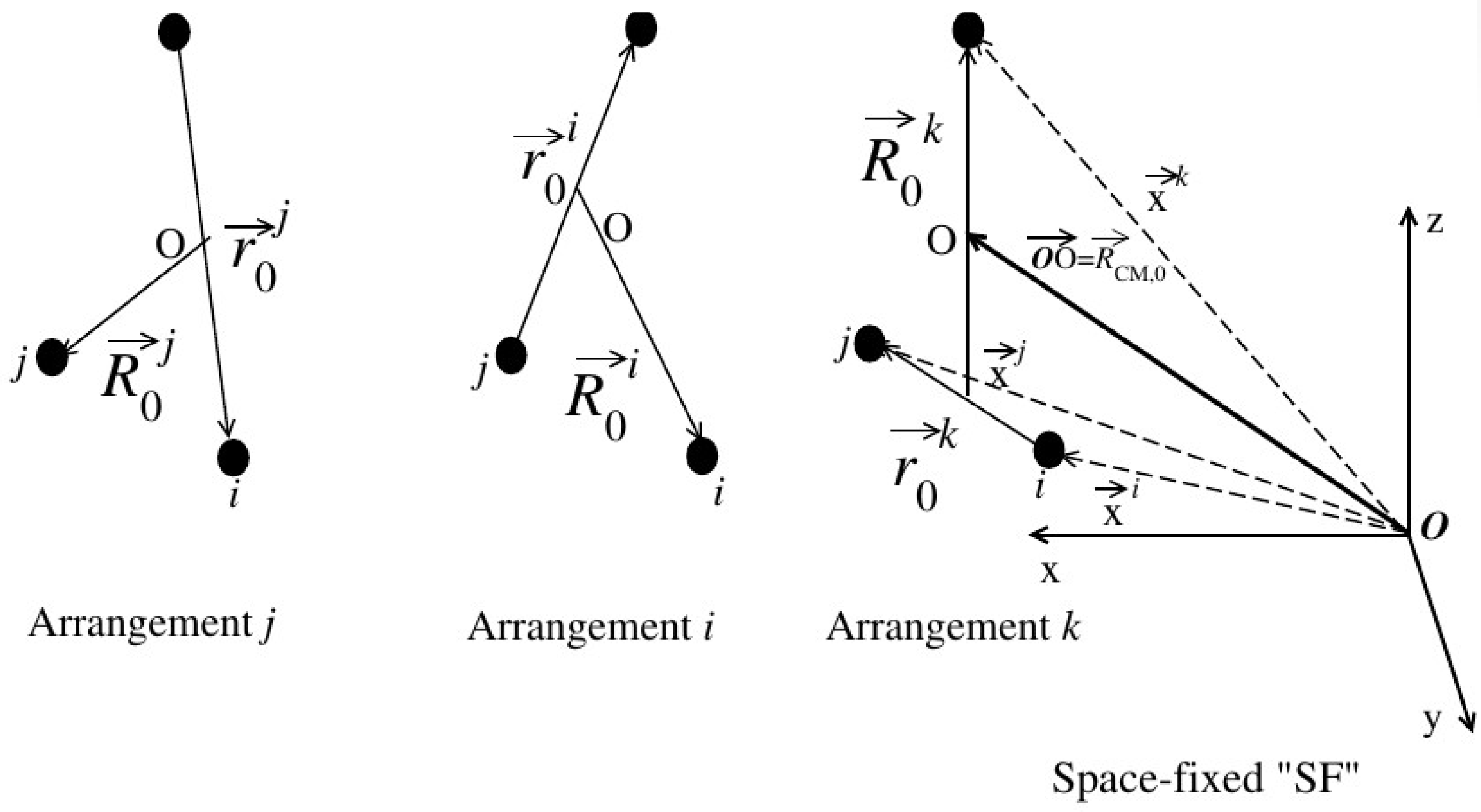
* Three different arrangements: three sets of coordinates



Mass-weighted Jacobi coordinates

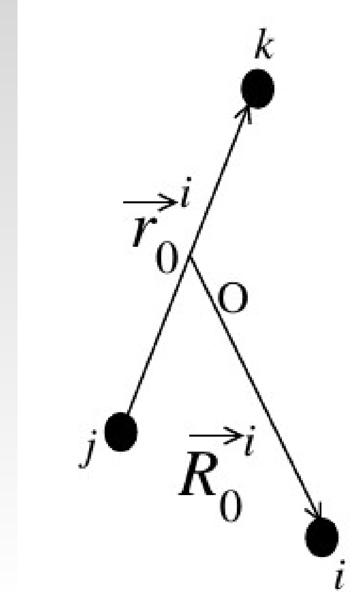
$$\vec{R}_{CM} = \vec{R}_{CM,0} \qquad \vec{r}^k = d_k^{-1}\vec{r}_0^k \qquad \vec{R}^k = d_k \vec{R}_0^k$$

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



Hyperspherical coordinates

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



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

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

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

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

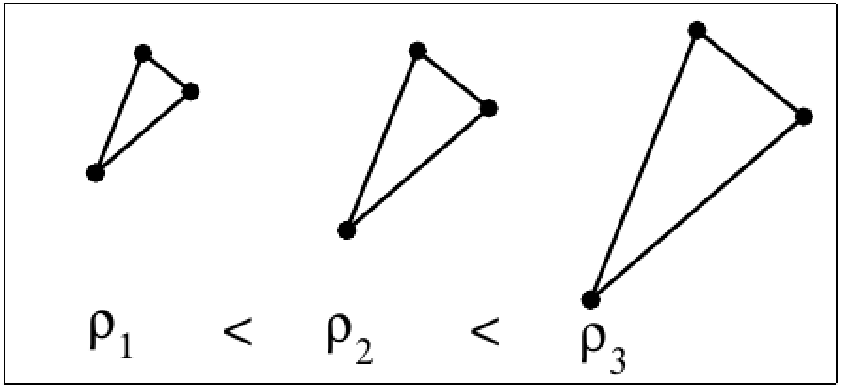
$$0 \le \rho < \infty, \qquad 0 \le \theta \le \frac{\pi}{2} \qquad \text{et} \qquad 0 \le \phi < 2\pi$$

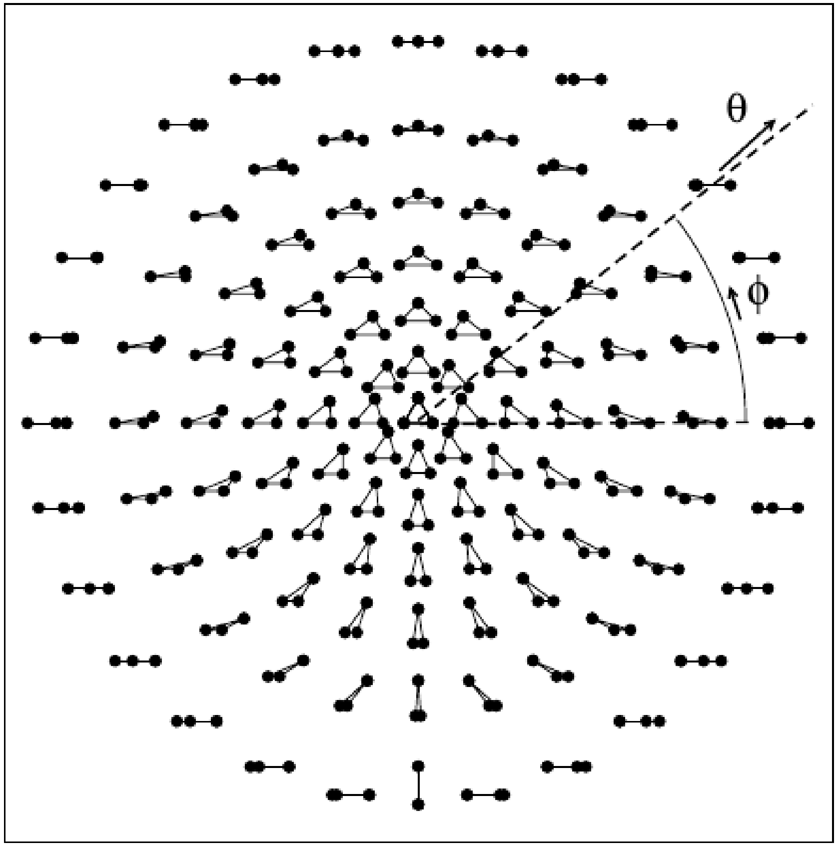
$$\epsilon_3 = 2\arctan\left(\frac{m_2}{\mu}\right)$$

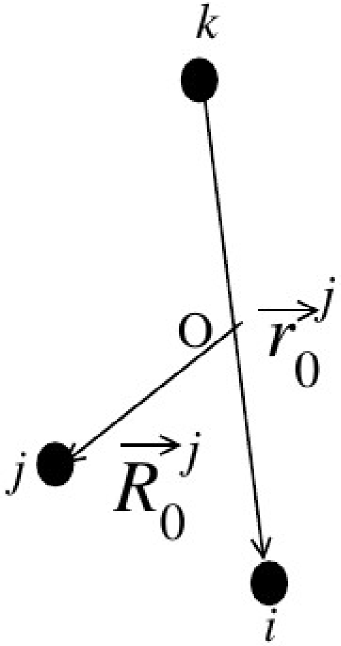
$$\epsilon_2 = -2\arctan\left(\frac{m_3}{\mu}\right)$$

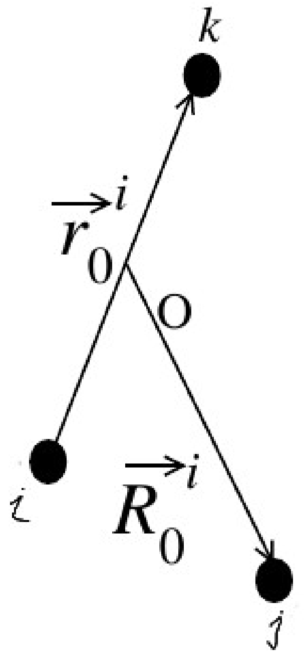
Symmetry

* 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.







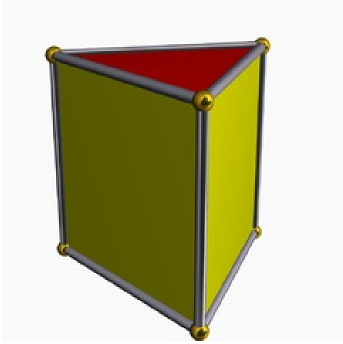


C_{3v} /D_3/ S_3 symmetry group

- Group of permutation of three identical particles, S_3:

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

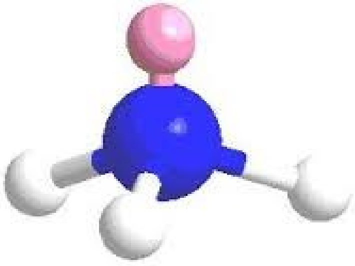
- S_3 is isomorphic to the group of rotations of a triangular prism



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

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

- $C_{3v} = \{E, C_3, C_3^{\,2}, 3\sigma_v\}$



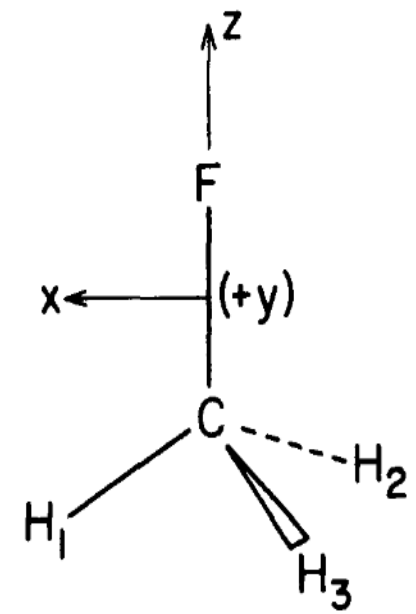
Types of wave functions
Irreducible representations

- A_1 is a totally symmetric wave function
- A_2 changes sign under any binary permutation
- E is a 2-dimensional irrep.

C_{3v}	D_3	E / E	$2C_3$ / $2C_3$	$3\sigma_v$ / $3U_2$
A_1; z	A_1	1	1	1
A_2	A_2; z	1	1	-1
E; x, y	E; x, y	2	-1	0

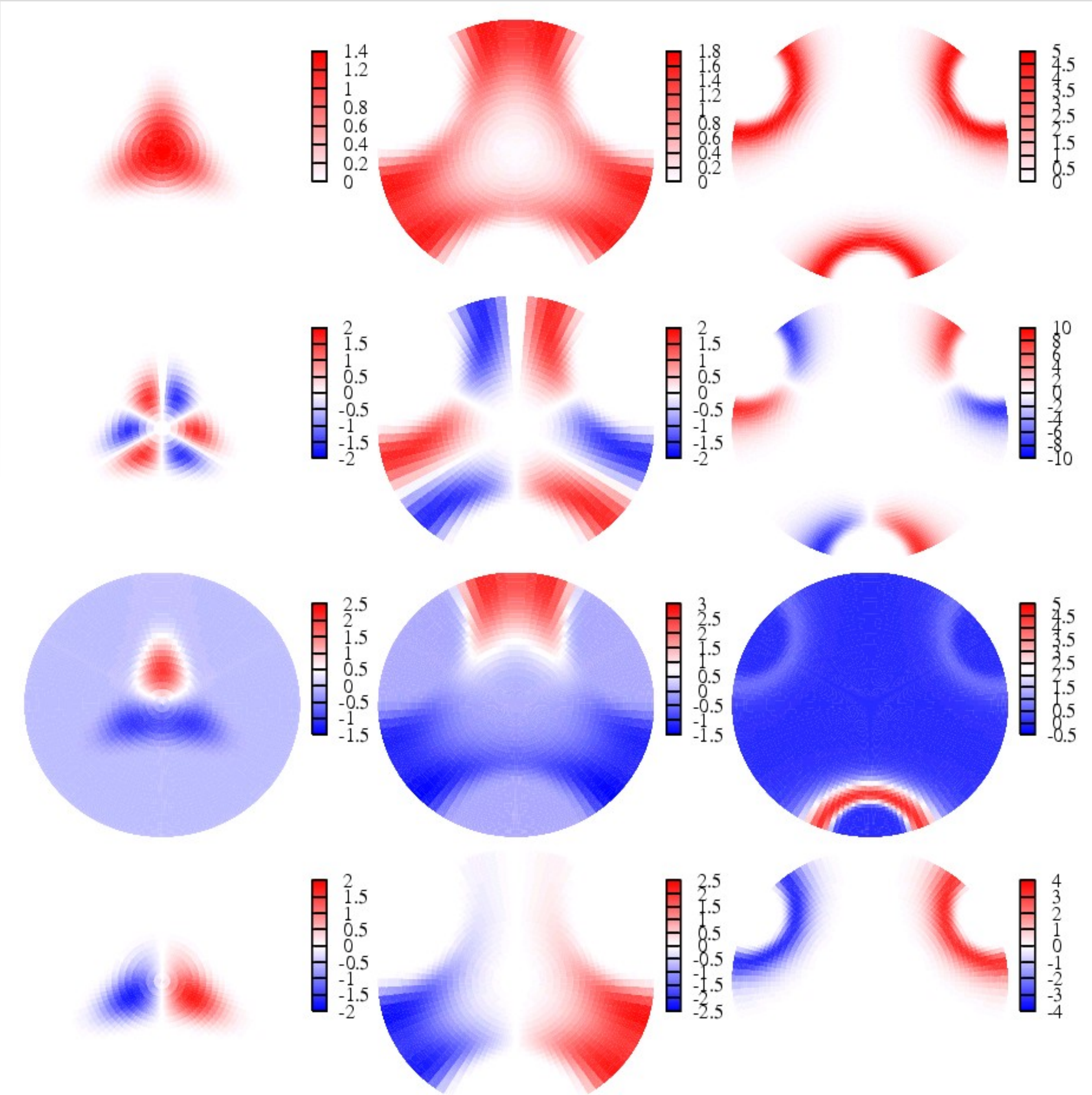
$$(\mathbf{123})E'_{\pm} = e^{i\omega} E'_{\pm}$$

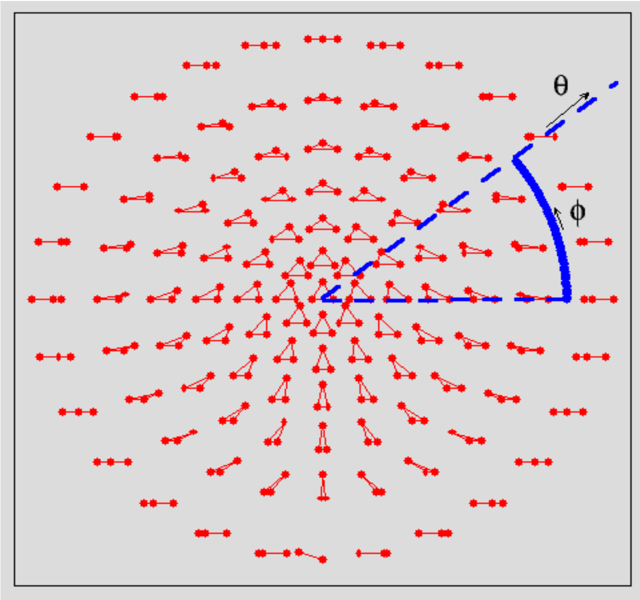
$$(\mathbf{12})E'_{\pm} = E'_{\mp}, \qquad \omega = 2\pi/3$$



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

$$H = T_\rho + H_{\rm ad}$$

$$T_\rho = -\frac{1}{2\mu}\frac{\partial^2}{\partial\rho^2} \qquad H_{\rm ad} = \frac{\Lambda^2 + 15/4}{2\mu\rho^2} + V$$

$$\Lambda^2 = -\frac{4}{\sin(2\theta)}\frac{\partial}{\partial\theta}\sin(2\theta)\frac{\partial}{\partial\theta} - \frac{4}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2} + \frac{2J_X^2}{1-\sin\,\theta} + \frac{2J_Z^2}{1+\sin\,\theta} + \frac{J_Y^2}{\sin^2\,\theta} + \frac{4i\cos\,\theta J_Y}{\sin^2\,\theta}\frac{\partial}{\partial\phi},$$

How to solve it

* Adiabatic separation of the hyper-radius and hyperangles

$$H = T_\rho + H_{\text{ad}}$$

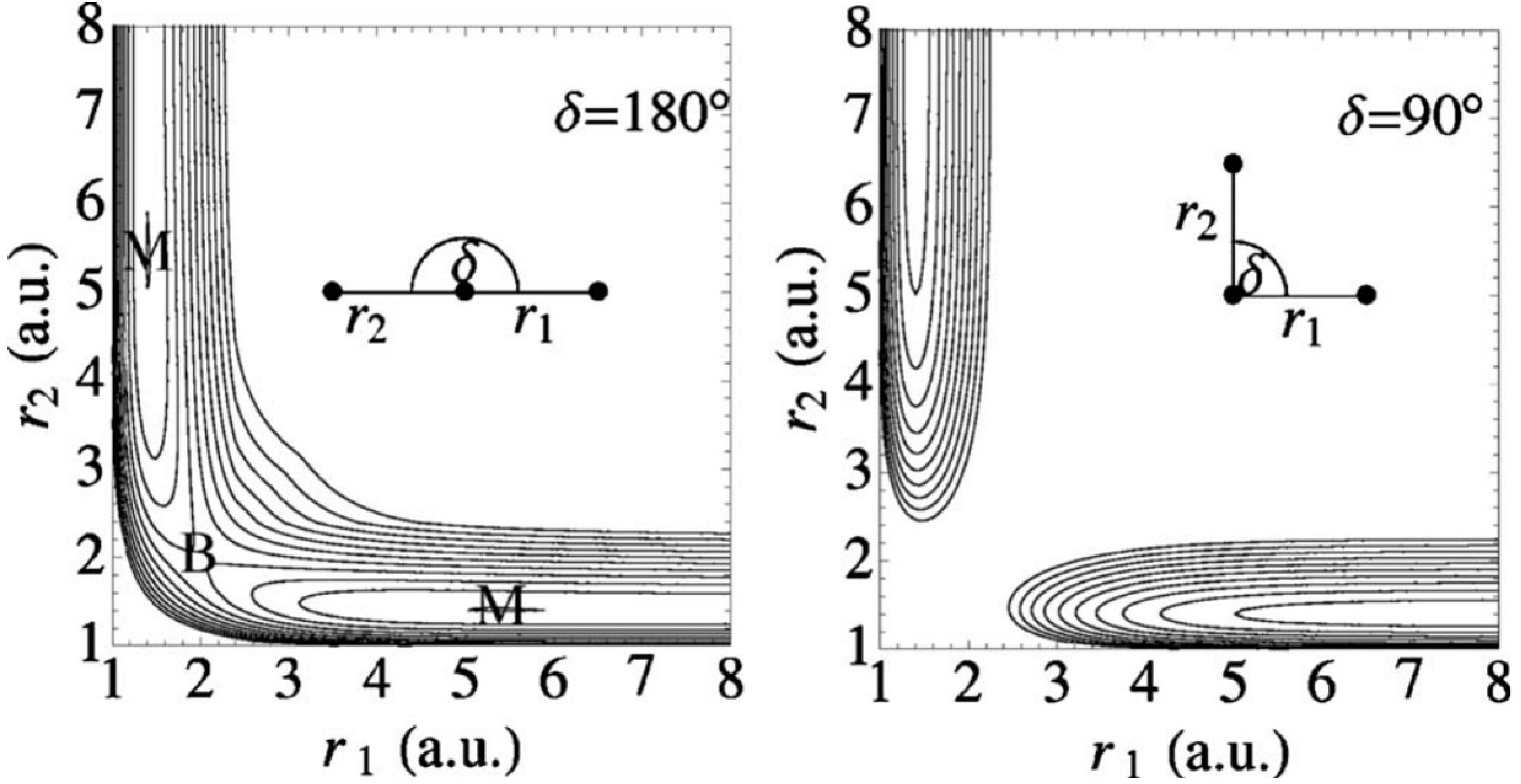
$$H_{\text{ad}}^{\rho=\rho_j}\varphi_{a,j}(\omega) = U_a(\rho_j)\varphi_{a,j}(\omega)$$

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

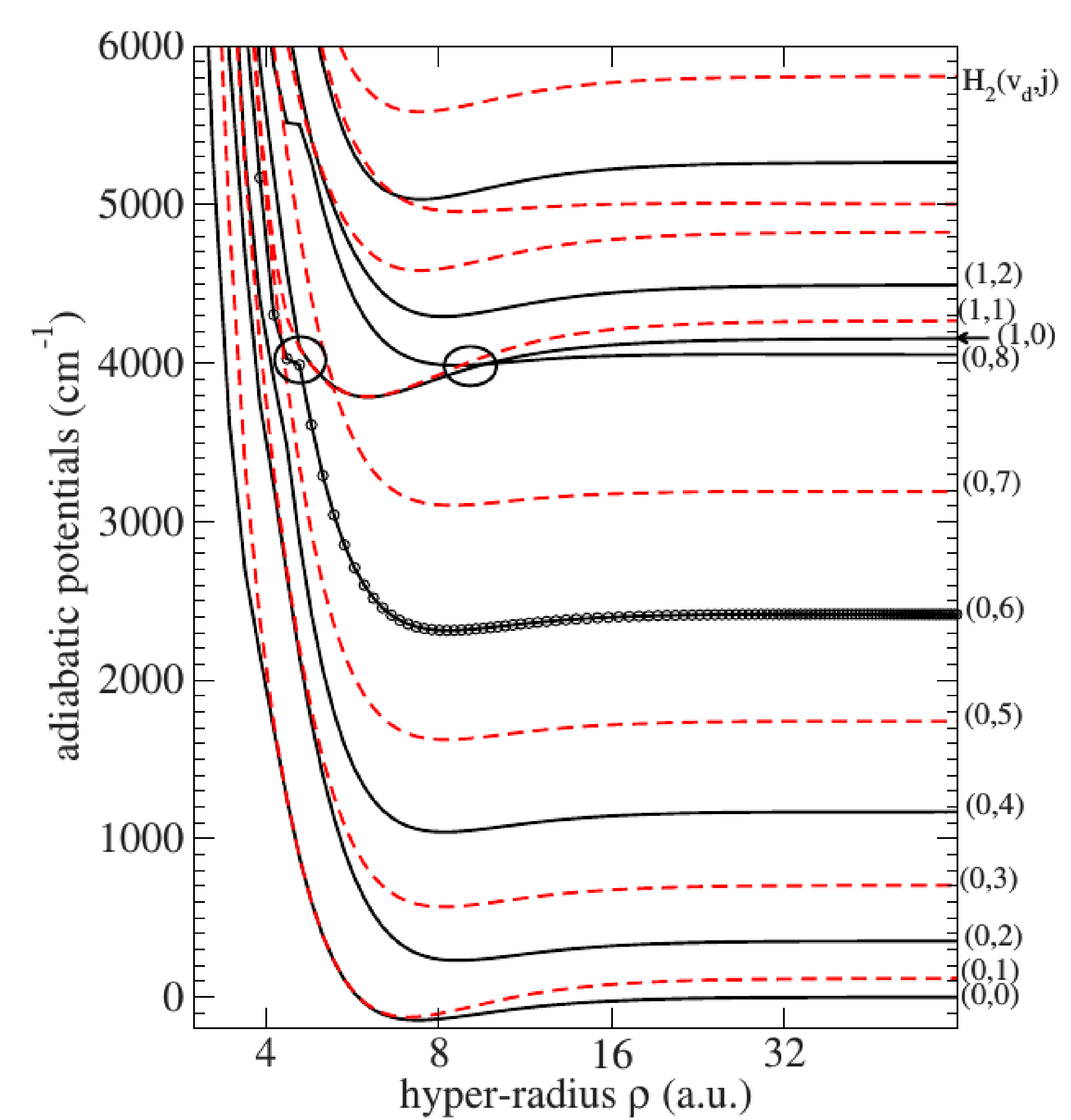
* An idea similar to the Born-Oppenheimer separation of electronic and nuclear coordinates

$$[\hat{T}(\rho) + U_a(\rho)]\psi_{a,n}(\rho) = E_n^{vib}\psi_{a,n}(\rho)$$

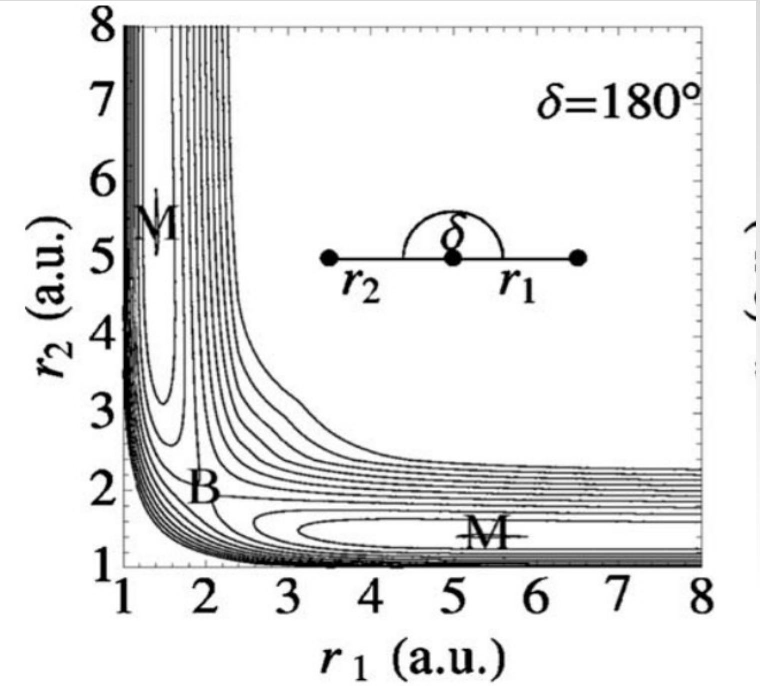
H_3^-



H_3^-



6000
5000
4000
3000
2000
1000
0
adiabatic potentials (cm-1)
4
8
16
32
hyper-radius ρ (a.u.)
H2(vd,j)
(1,2)
(1,1)
(1,0)
(0,8)
(0,7)
(0,6)
(0,5)
(0,4)
(0,3)
(0,2)
(0,1)
(0,0)



δ=180°
δ
r2
r1
M
B
M
r2 (a.u.)
r1 (a.u.)
1
2
3
4
5
6
7
8

Hyperspherical adiabatic approximation is inaccurate

- Non-adiabatic couplings between U_a (φ_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

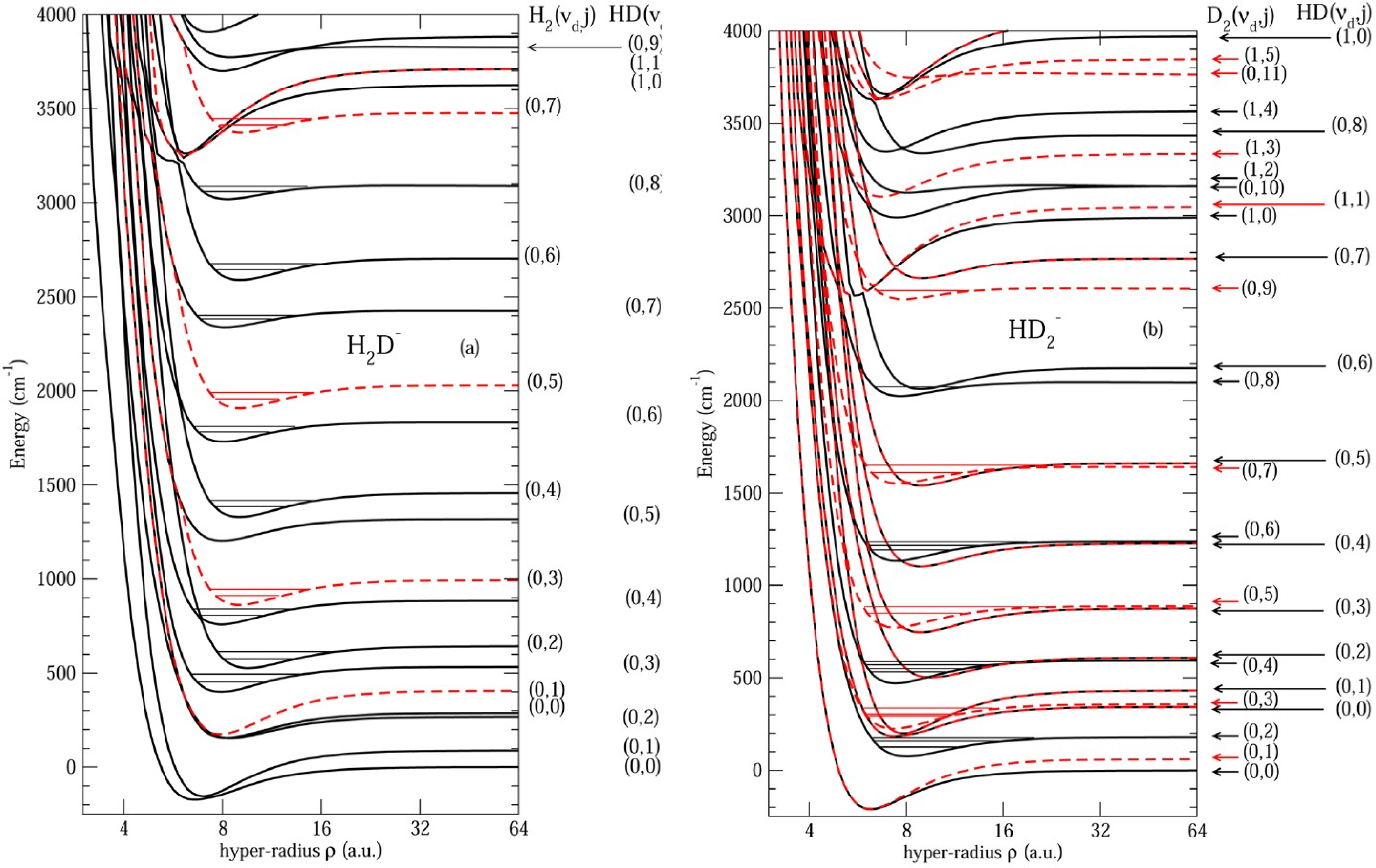
$$y_k(\rho,\theta,\phi)=\pi_j(\rho)\varphi_{a,j}(\theta,\phi)$$
$$k\equiv\{a,j\}$$

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

$$\sum_{i',a'}[\langle\pi_i|\hat{T}(\rho)|\pi_{i'}\rangle\mathcal{O}_{ia,i'a'}+\langle\pi_i|U_a(\rho)|\pi_{i'}\rangle\delta_{aa'}]c_{i'a'}$$
$$=E\sum_{i',a'}\langle\pi_i|\pi_{i'}\rangle\mathcal{O}_{ia,i'a'}c_{i'a'},$$

$$\mathcal{O}_{ia,i'a'}=\langle\varphi_a(\rho_i;\theta,\phi)|\varphi_{a'}(\rho_{i'};\theta,\phi)\rangle$$

H_2D^- and D_2H^-



(a)
H_2D^-
$H_2(v_d,j)$
HD(v
Energy (cm^{-1})
hyper-radius ρ (a.u.)
(b)
HD_2^-
$D_2(v_d,j)$
$HD(v_d,j)$
Energy (cm^{-1})
hyper-radius ρ (a.u.)

H+H+H → H_2+H recombination

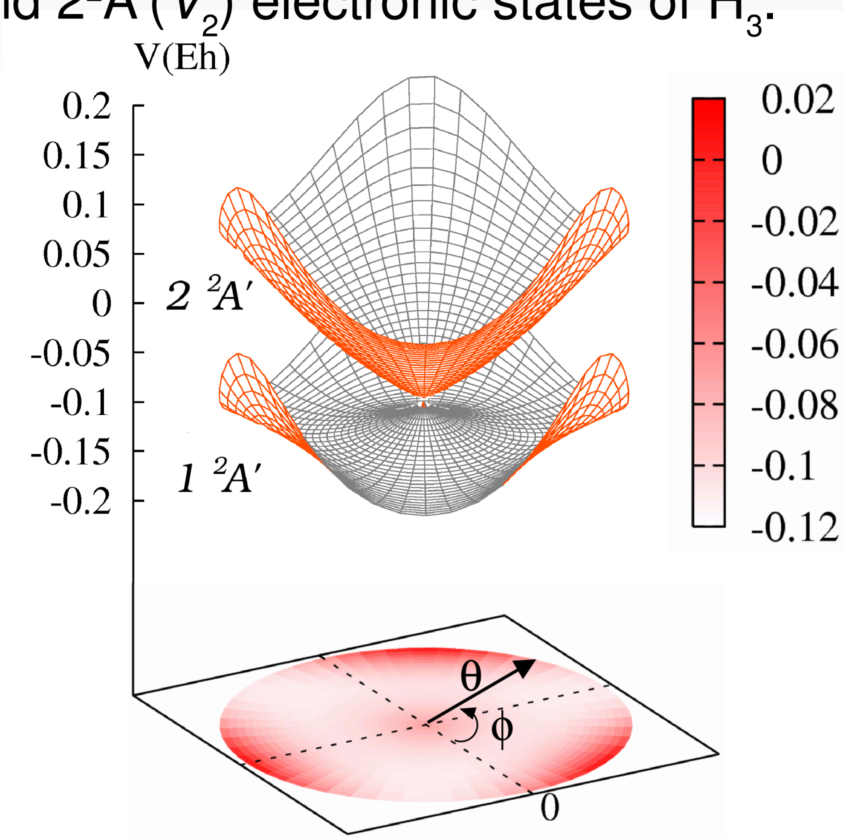
Diabatic 2-channel 3-body potential for H_3.

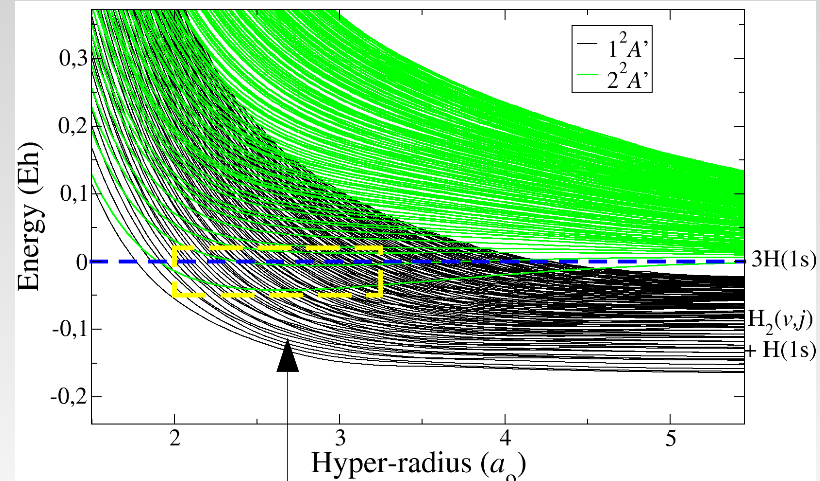
$$V_{H_3}(\rho,\theta,\phi)=\begin{pmatrix} A & C\,e^{if} \\ C\,e^{-if} & A \end{pmatrix}$$

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

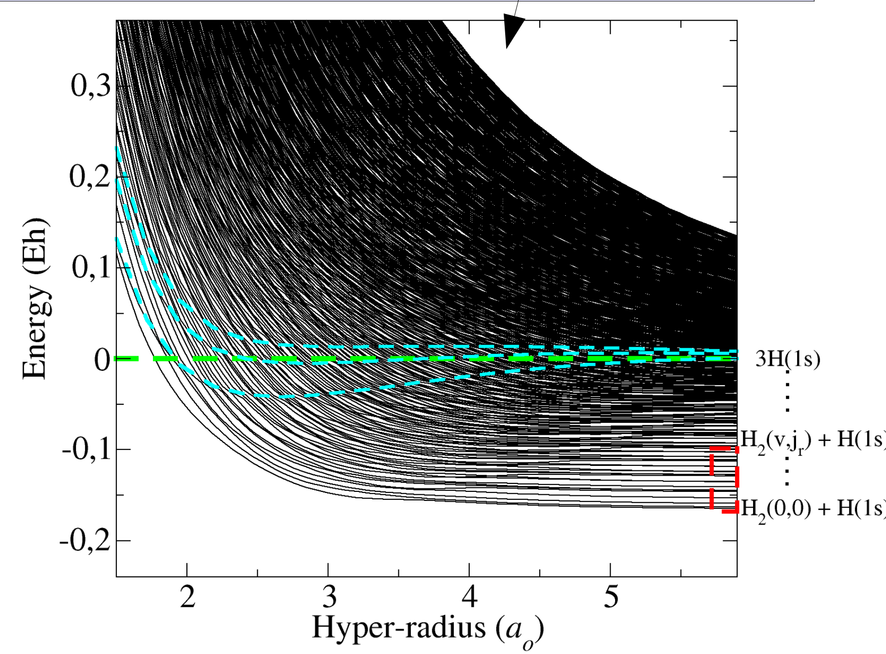
$$C(\rho,\theta,\phi)=\left[V_1(\rho,\theta,\phi)-V_2(\rho,\theta,\phi)\right]/2$$

Obtained from *ab initio* calculation of 1^2A' (V_1) and 2^2A'(V_2) electronic states of H_3.

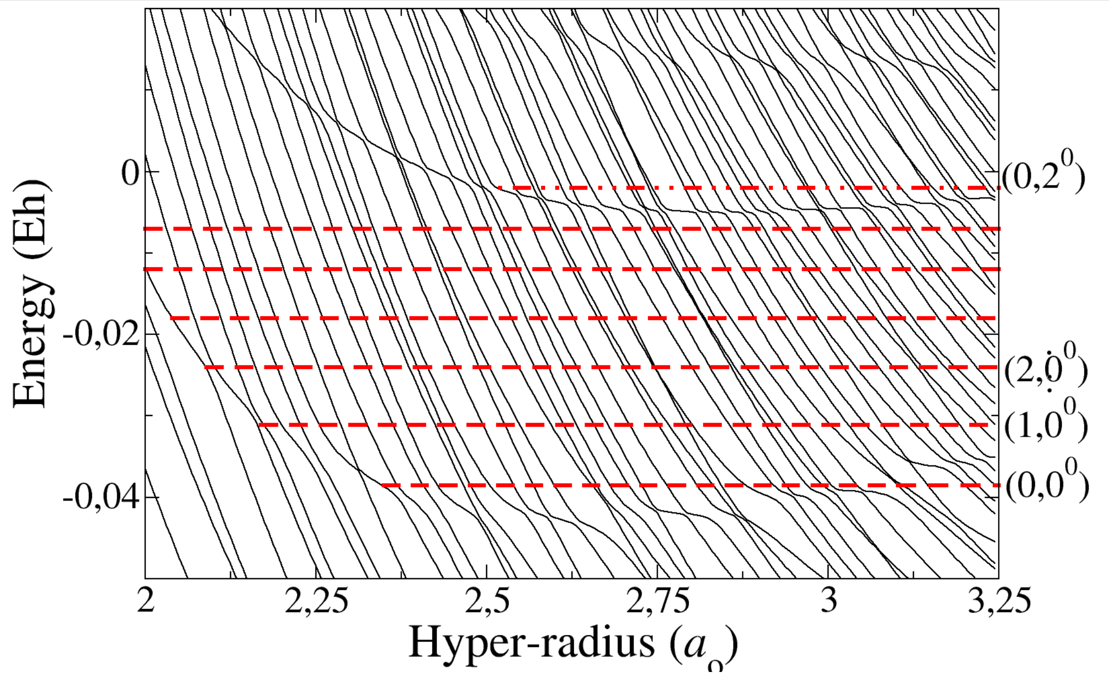


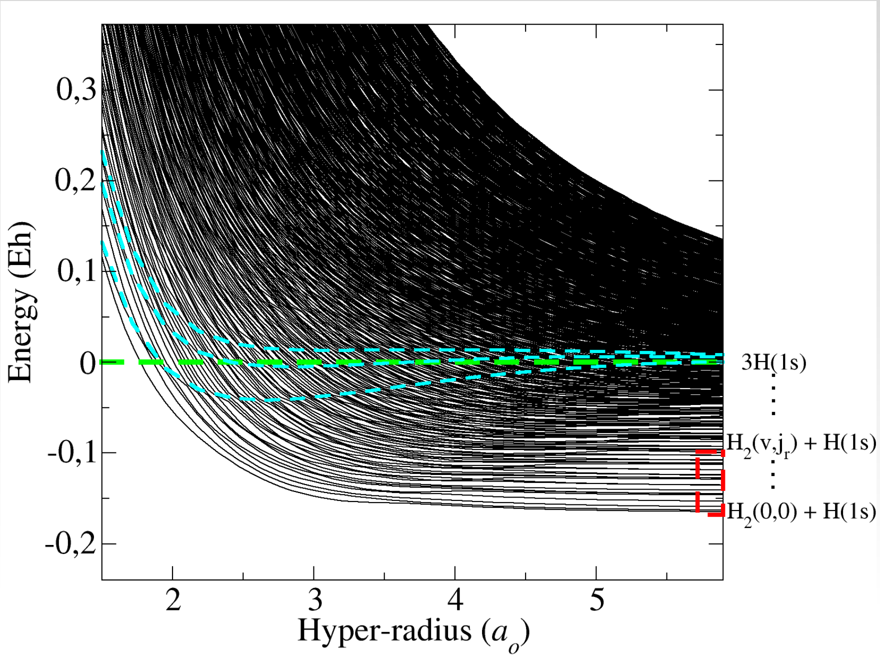


Hyperspherical adiabatic energies obtained for the uncoupled and coupled H_3 two-channel potential. Crossings in the above figure turn into avoided crossings below.



H_3 resonances





$\{v_1, v_2^{l_2}\}$	E_r, τ; this work	E_r, τ; Ref. [8]	E_r, τ; Ref. [9]
$\{0, 0^0\}$	-3.85, 13	...	-3.79, ~ 3
$\{1, 0^0\}$	-3.11, 13	...	-3.05, ~ 3
$\{2, 0^0\}$	-2.4, 14	...	-2.37, ...
$\{3, 0^0\}$	-1.8, 14	...	-1.75, ...
$\{4, 0^0\}$	-1.2, 16	-1.24, ~ 15	-1.19, ...
$\{5, 0^0\}$	-0.7, 18	-0.47, ~ 17	-0.70, ...
$\{0, 2^0\}$	-0.2, 130	...	-0.26, ~ 4.5

On Efimov states (1970)

$$\tan\delta_l \overset{k\to 0}{\sim} -\frac{\pi}{\Gamma(l+\frac{1}{2})\Gamma(l+\frac{3}{2})}\left(\frac{a_l k}{2}\right)^{2l+1}$$

$$k/\tan(\delta_0) = -1/a + r_0 k^2/2$$

ЯДЕРНАЯ ФИЗИКА
JOURNAL OF NUCLEAR PHYSICS
т. 12, вып. 5, 1970

СЛАБОСВЯЗАННЫЕ СОСТОЯНИЯ ТРЕХ РЕЗОНАНСНО ВЗАИМОДЕЙСТВУЮЩИХ ЧАСТИЦ

В. Й. ЕФИМОВ

ФИЗИКО-ТЕХНИЧЕСКИЙ ИНСТИТУТ им. А. Ф. ИОФФЕ АКАДЕМИИ НАУК СССР

(*Поступила в редакцию 16 февраля 1970 г.*)

* 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 $\to \infty$

On Efimov states (1970)

When $a=\infty$, the hyper-radial equation is

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

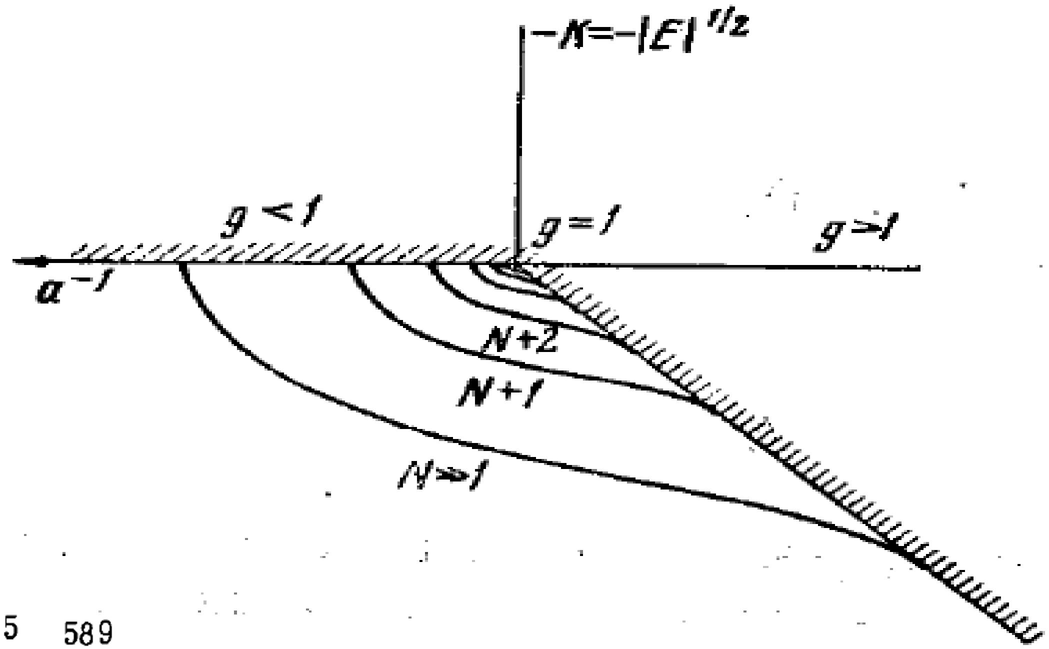
s_i is a transcendental constant. The lowest s_i is $s_0=1.00624i$.

Spectrum for s_0 is

$$E_N=-\frac{1}{R_0^2}e^{-2\pi N/|s_0|}\exp\frac{2}{|s_0|}\left[\operatorname{arcctg}\frac{\Lambda R_0}{|s_0|}-\Delta\right]$$

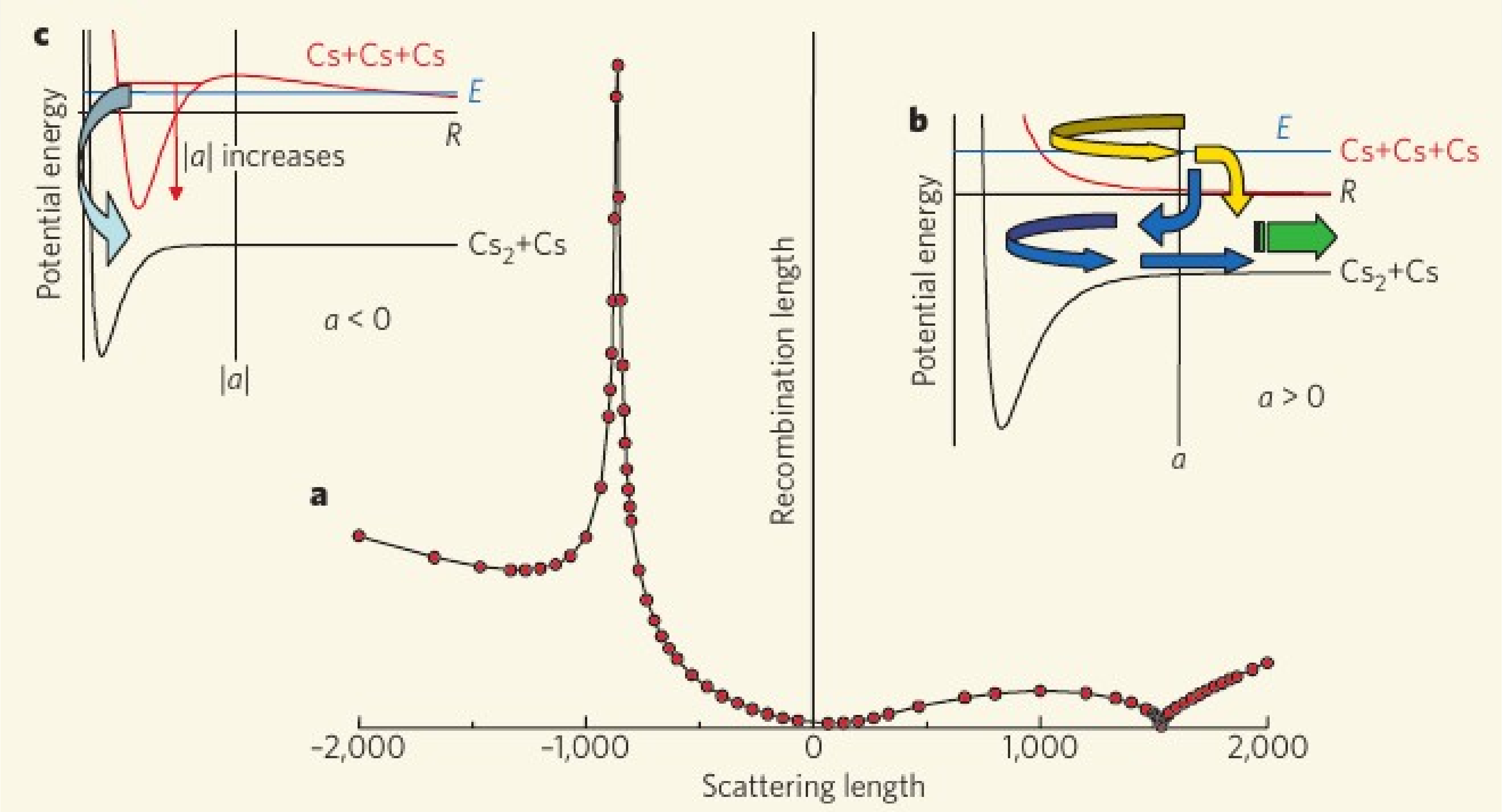
When $a\neq\infty$, the spectrum:

g is the interaction parameter, such that at $g=1$, $a=\infty$



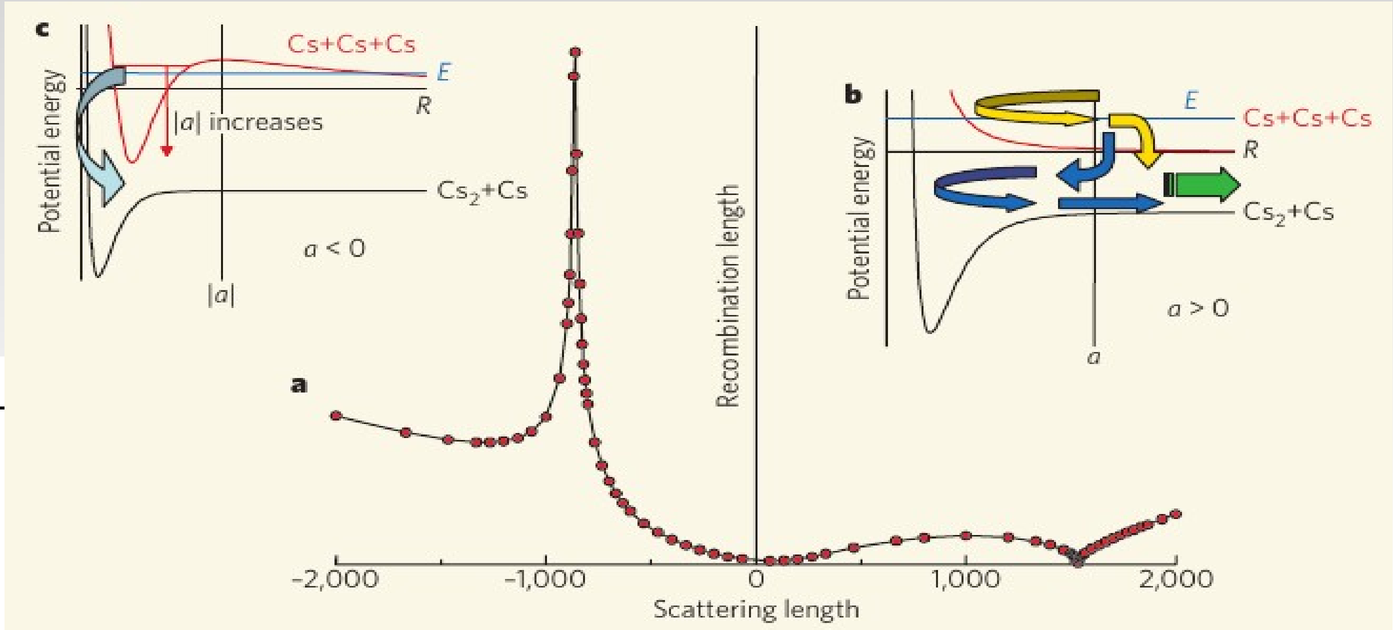
Observation of Efimov states

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.

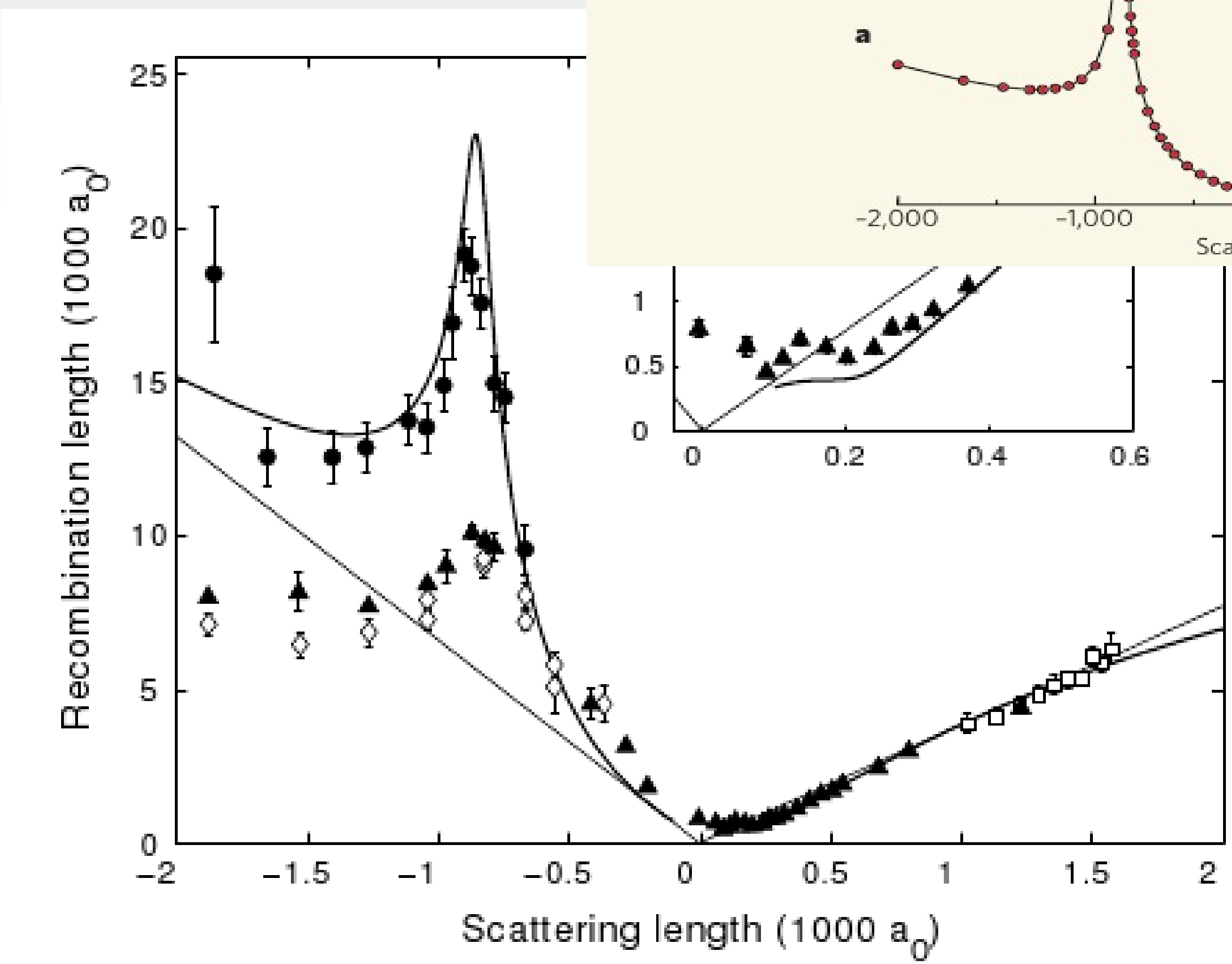


Observation of Efimov states:

Theory

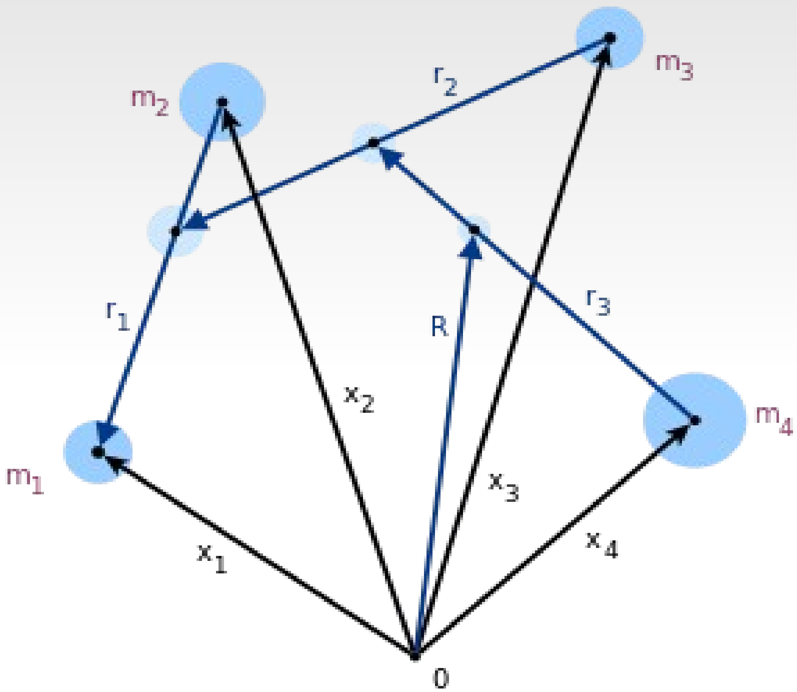


Experiment



More than three particles

Jacobi coordinates for four particles → hyperspherical coordinates



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

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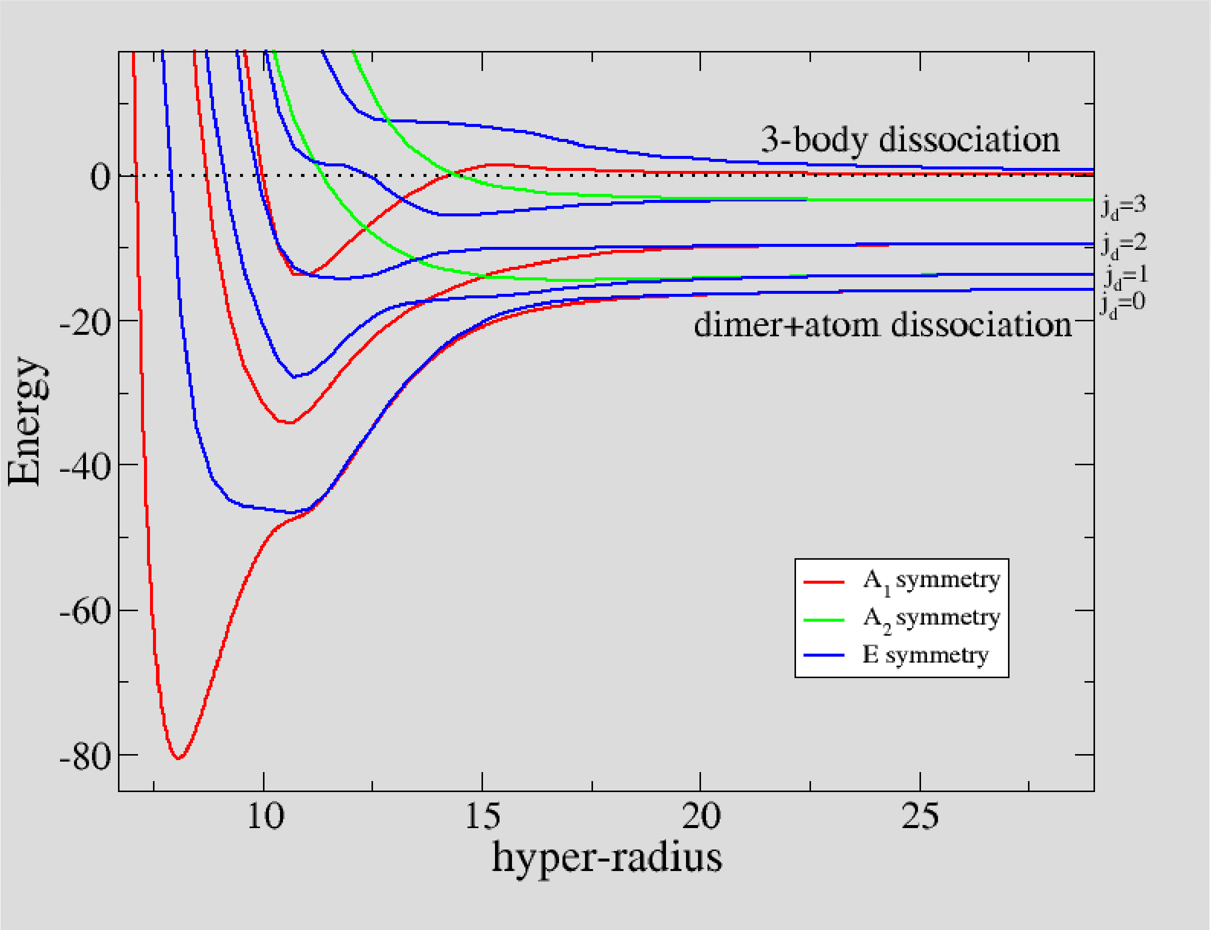
We study inelastic collisions in a pure, trapped sample of Feshbach molecules made of bosonic cesium atoms in the quantum halo regime. We measure the relaxation rate coefficient for decay to lower-lying molecular states and study the dependence on scattering length and temperature. We identify a pronounced 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.



$$U_a(\rho) \rightarrow U_a(\rho) - iA(\rho - \rho_l)^2$$