2015 原子分子與光學物理暑期學校

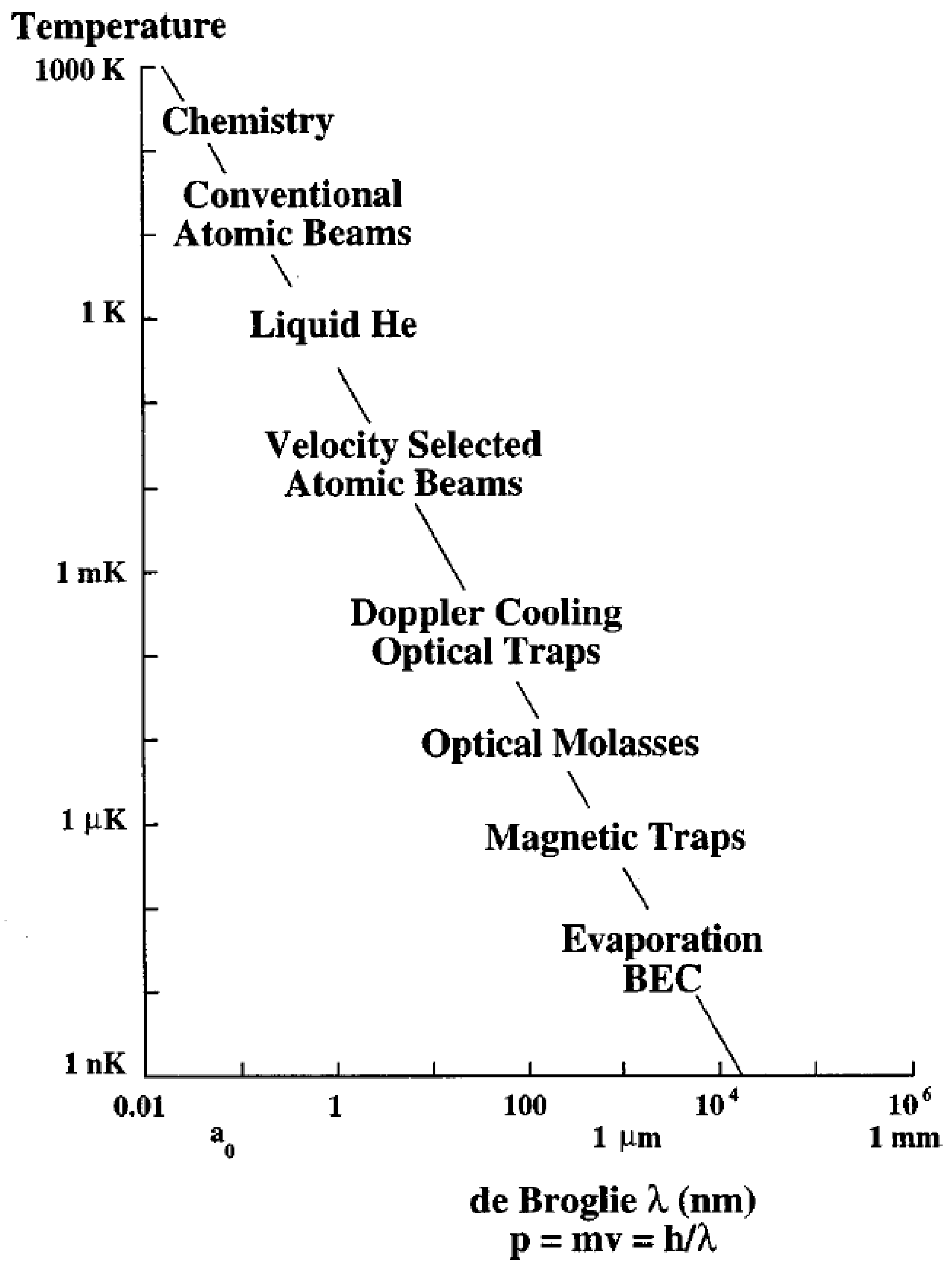
Cold Collisions

蔡錦俊 Chin-Chun Tsai
國立成功大學 物理系(光電系合聘)
Department of Physics, and Department of Photonics,
National Cheng-Kung University

Temperature:

Different scale of temperature and de Broglie wavelength (Na) for various physical phenomena

Photoassociation discussed below is less than 1 mK which corresponding to 21 MHz of energy spread of free state atom pair.



Motivations for using cold collisions:

Study the atoms free from spectral line broadening and shifts that arise from atomic motions and collisions

Advantages:

I. Cold collisions are highly quantum-mechanical in nature

II. Cold collisions are simple, involving only a few partial waves

III. Cold collisions are sensitive to long-range interatomic forces

IV. Long collision times can significantly affect the collision dynamics

V. Spontaneous emission during the collision may occur to change the collision channels involved.

Basic collision processes for cold atoms:

1,i. Excite by lasers at large R

2,ii. Spontaneous decay

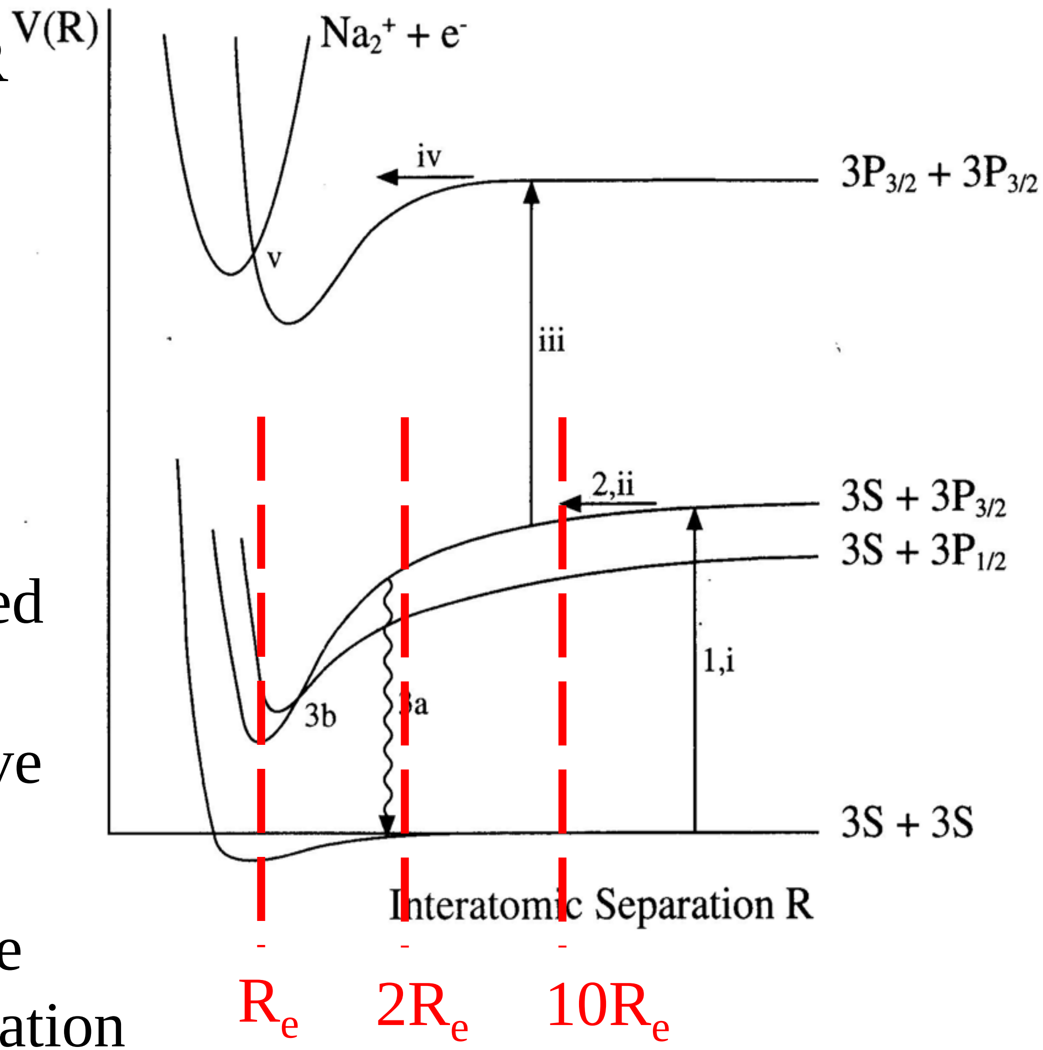
3a. Radiate to bound or free ground state

3b. Fine-structure changing collisions

iii. Excite to the doubly excited state

iv. Spontaneous decay or move toward to the small R

v. Auto-ionization, associative ionization, and pre-dissociation may occur.



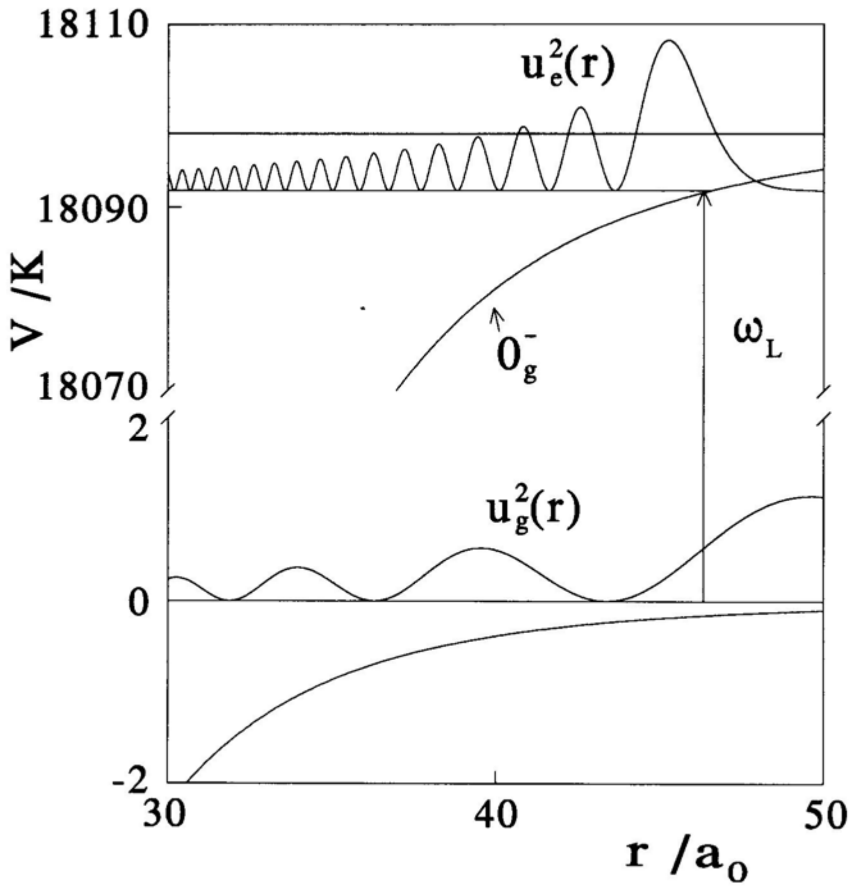
The long-range behaviors – wave functions:

The square of the wave functions is the probabilities of the atoms to be appeared

The amplitude of the wave functions is larger at the outer turning points

There are nodes and anti-nodes

Wavefunction tunneling occurs at the potential barrier



The long-range behaviors – potential curves:

$$V = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \frac{V_{ij}(a, b)}{R^{i+j+1}},$$

where

$$V_{ij}(a, b) = (-)^j \sum_{|m|=0}^{\min(i,j)} d_m(i, j) Q^i_m(a) Q^j_{-m}(b)$$

$$d_m(i, j) = (i + j)!((i - m)!(i + m)! \times (j - m)!(j + m)!)^{-1/2},$$

$$Q^i_m(a) = \sqrt{\frac{4\pi}{2i + 1}}\, r^i_a Y^m_i(\theta_a, \phi_a)$$

1. Asymptote ns + ns

$$C_{2n}(X\,^1\Sigma^+_g) \equiv C_{2n}(^3\Sigma^+_u), \quad n = 3, 4, 5 \cdots$$

$$C_6(\nu) = E^{\text{disp}}_{1111}(\nu, \nu),$$

$$C_8(\nu) = E^{\text{disp}}_{1122}(\nu, \nu) + E^{\text{disp}}_{2211}(\nu, \nu),$$

$$C_{10}(\nu) = E^{\text{disp}}_{1133}(\nu, \nu) + E^{\text{disp}}_{3311}(\nu, \nu) + E^{\text{disp}}_{2222}(\nu$$

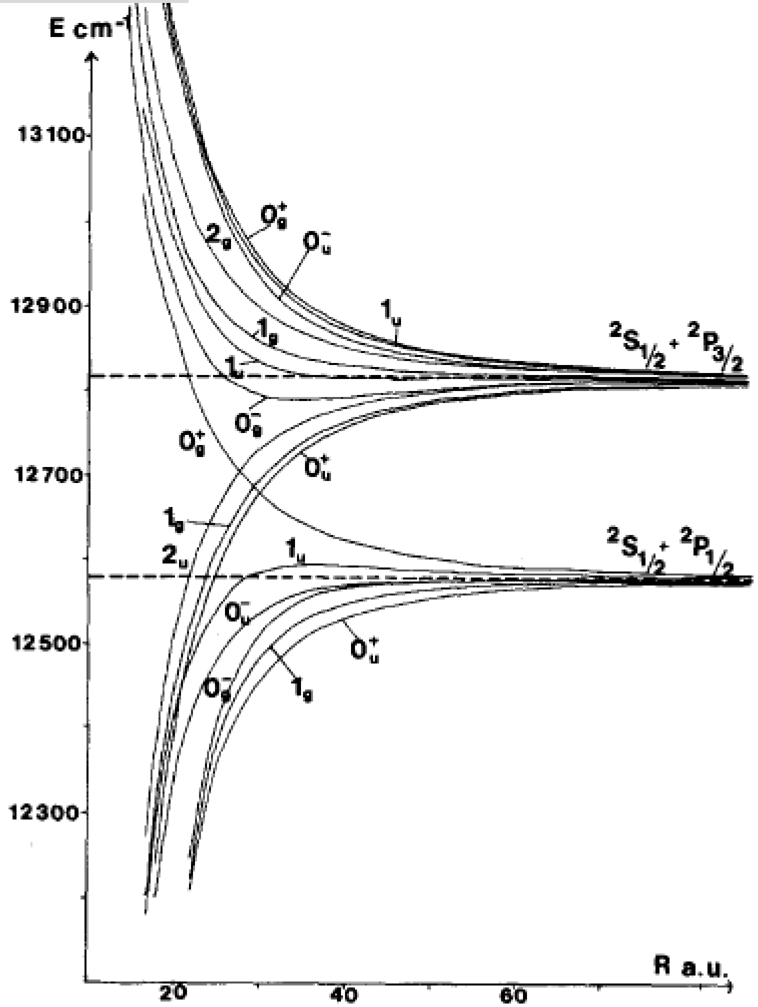


FIG. 4. Potential energy curves for the 16 molecular states of Rb_2 corresponding to the asymptote $5s + 5p$.

The long-range behaviors – potential curves:

2. Asymptote ns + np

$$C_3(^1\Lambda_g^{(+)}, {}^3\Lambda_u^{(+)}) = -C_3(^1\Lambda_u^{(+)}, {}^3\Lambda_g^{(+)})$$

for $\Lambda = 0, 1,$

$$C_3(^1\Sigma_g^+, {}^3\Sigma_u^+) = 2C_3(^1\Pi_u, {}^3\Pi_g).$$

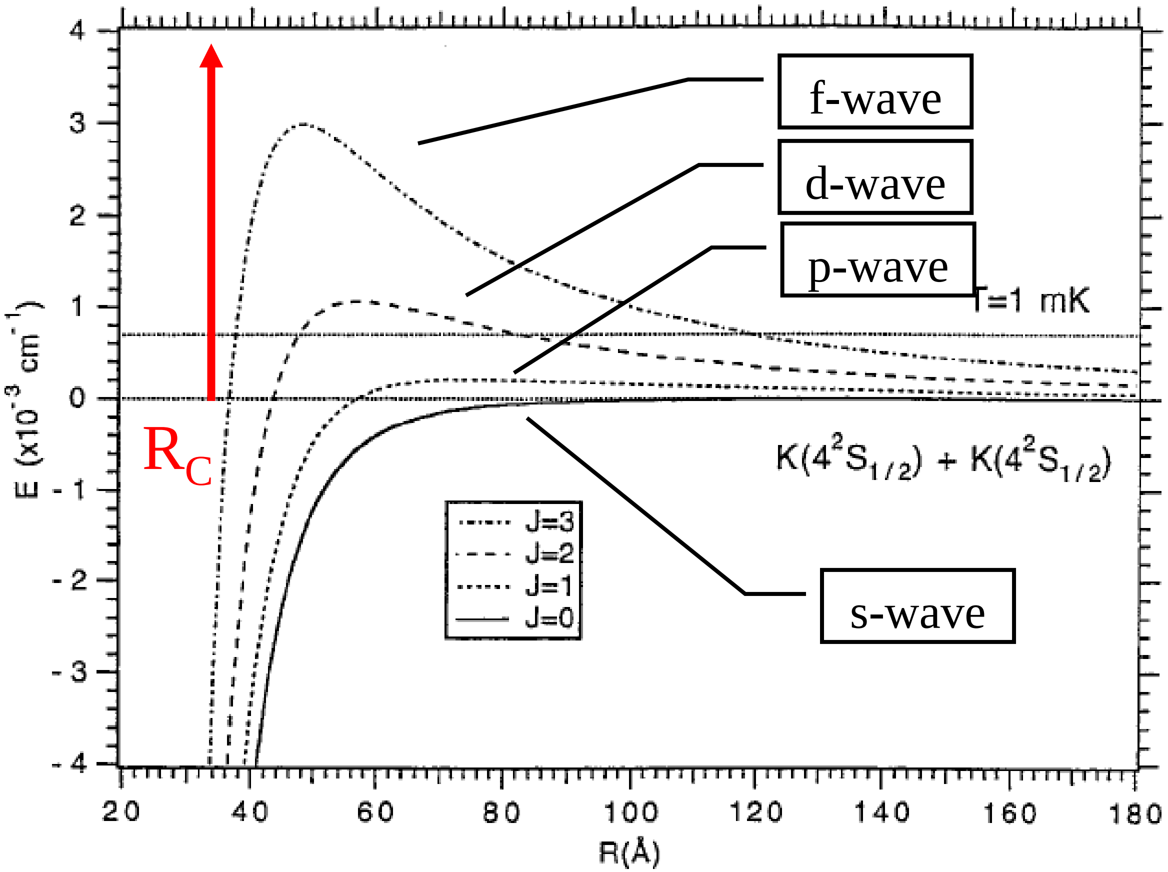
Furthermore,

$$C_n(^1\Lambda_k) \equiv C_n(^3\Lambda_l)$$

Asymptote	Molecular states	Molecule	Results	C_3	C_6	C_8 dispersion + induction	C_{10} dispersion + induction
			a	0	−1 383	−75 783	−4 816 675
			b	0	−1 390	−120 000	. . .
		Li_2	c	0	−1 381 ± 8	−82 615 ± 2288	. . .
			d	0	−1 389 ± 8	−80 890	. . .
			e	0	−1 390	. . .	. . .
			a	0	−1 698	−102 810	−6 939 128
		Na_2	f	0	−1 680	−164 000	. . .
			e	0	−1 580	. . .	. . .
			a	0	−4 721	−389 404	−40 694 332
$ns + ns$	$X\,^1\Sigma_g^+, {}^3\Sigma_u^+$	K_2	e	0	−3 820	. . .	. . .
			g	0	−3 890	−446 000	−54 900 000
$ns + np$	$^1\Sigma_u^+, {}^3\Sigma_g^+$	K_2	a	−18.68	−10 126	−2 454 301	
			h	−17.54	−9 651	−1 892 000	

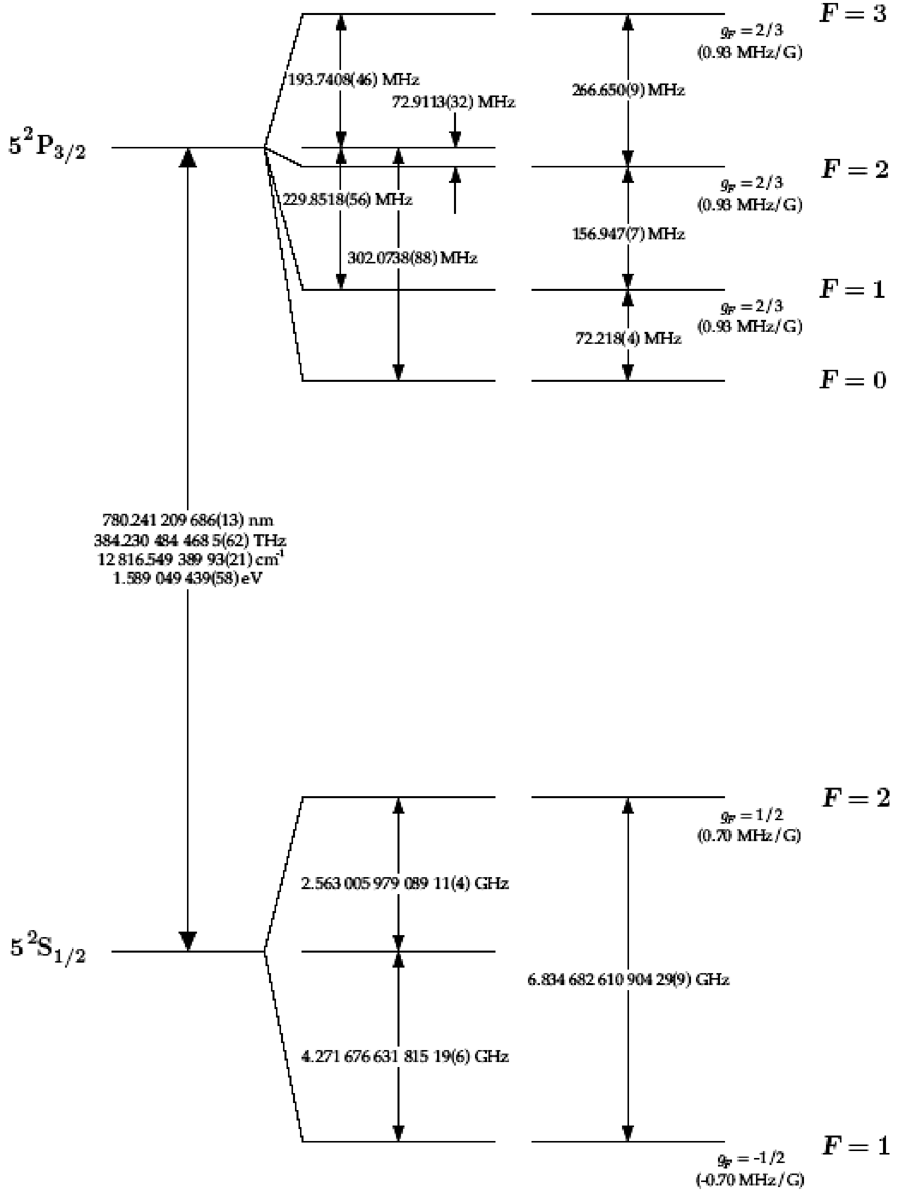
The long-range behaviors – partial wave involved:

$$U_J = V + \{\hbar^2[J(J+1) - \Omega^2]/2\mu R^2$$



Effective potential with rotational energy to form a centrifugal barrier.

Hyperfine levels of the ^{87}Rb D_2 line



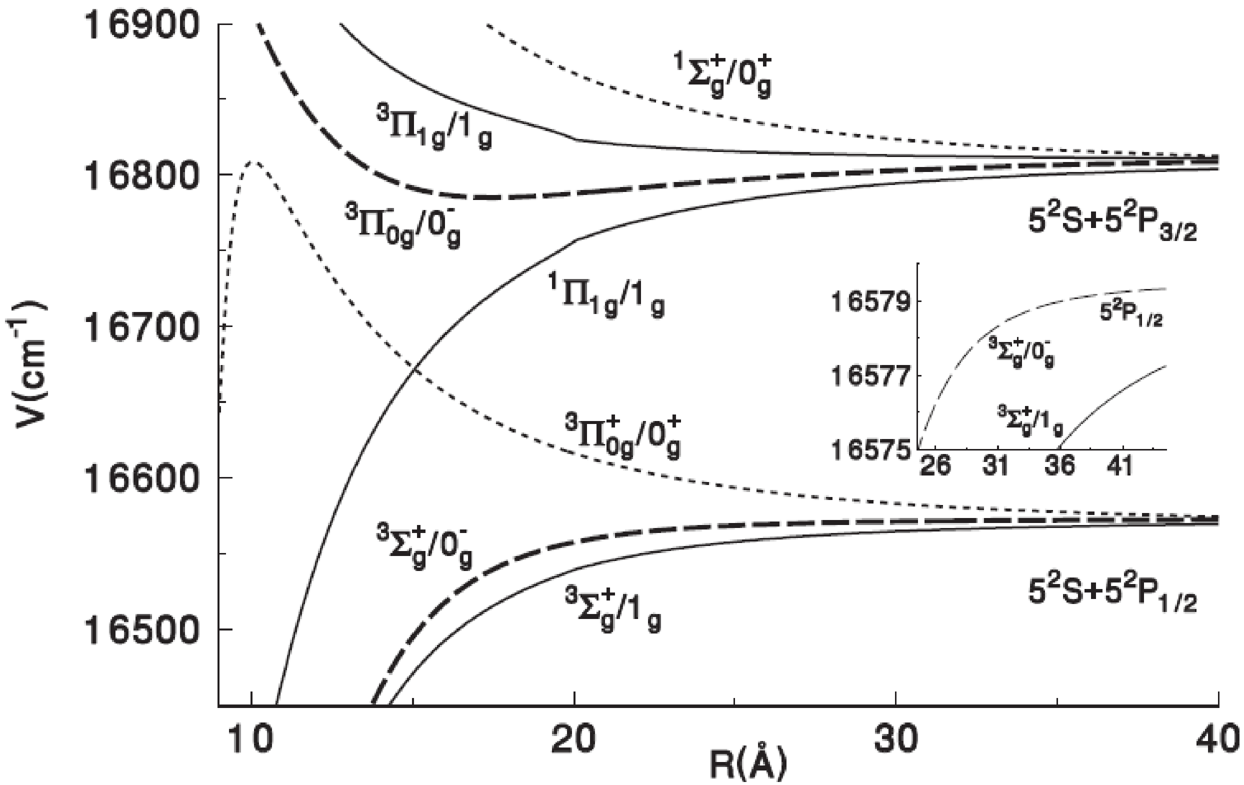
Adiabatic molecular fine structure potentials:

Ground states

^{87}Rb (5s $^2S_{1/2}$, F=1)
^{87}Rb (5s $^2S_{1/2}$, F=2)

Designation
(nl $^{2S+1}L_J$, F)

S=Σs_i, L=Σl_i
J=S+L
F=J+I



Excited states

^{87}Rb (5p $^2P_{1/2}$, F=1, or 2)

Adiabatic molecular hyperfine potentials:

Ground states

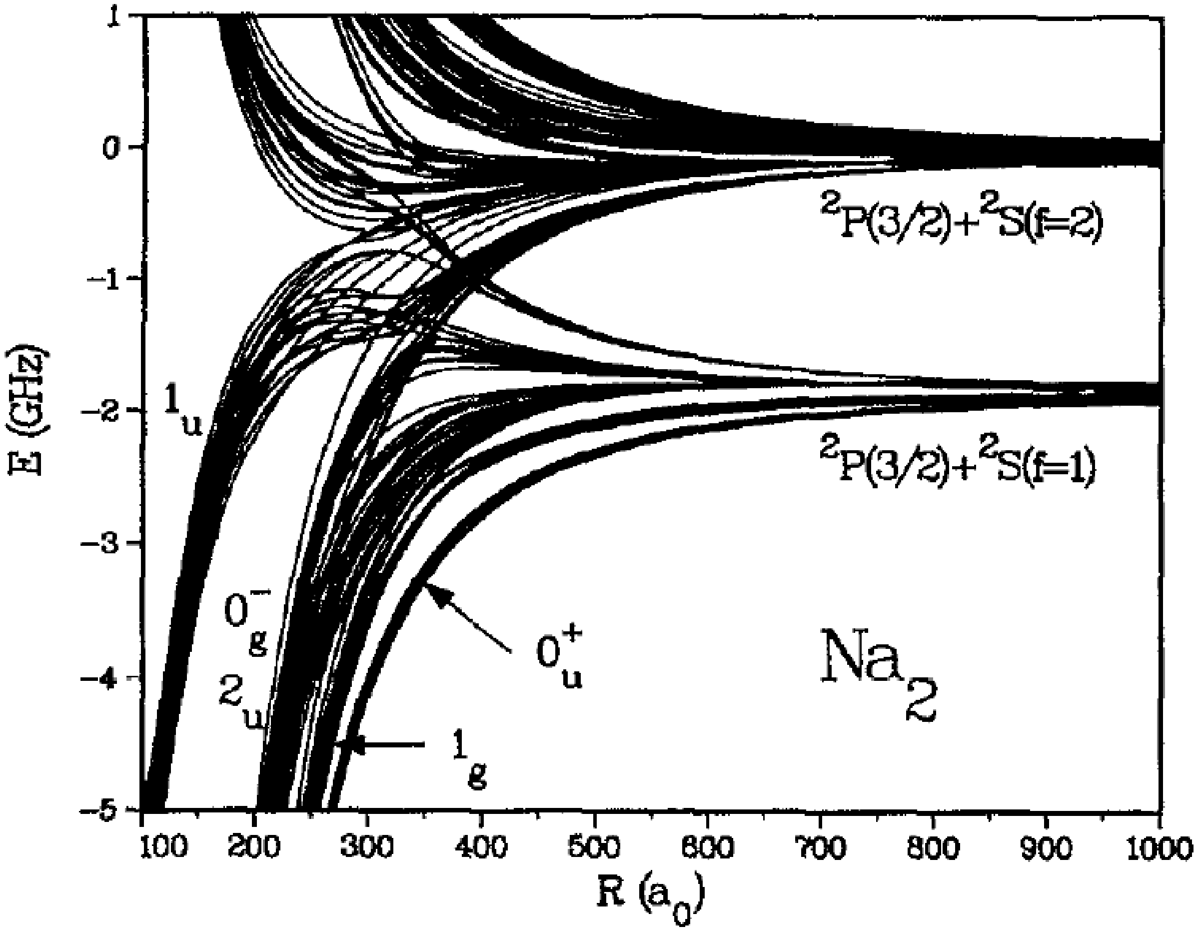
Na (3s $^2S_{1/2}$, F=1)
Na (3s $^2S_{1/2}$, F=2)

Designation
(nl $^{2S+1}L_J$, F)

$S=\Sigma s_i$, $L=\Sigma l_i$
J=S+L
F=J+I

Excited states

Na (3p $^2P_{1/2}$, F=1, or 2) …



Adiabatic molecular hyperfine potentials:

Ground states

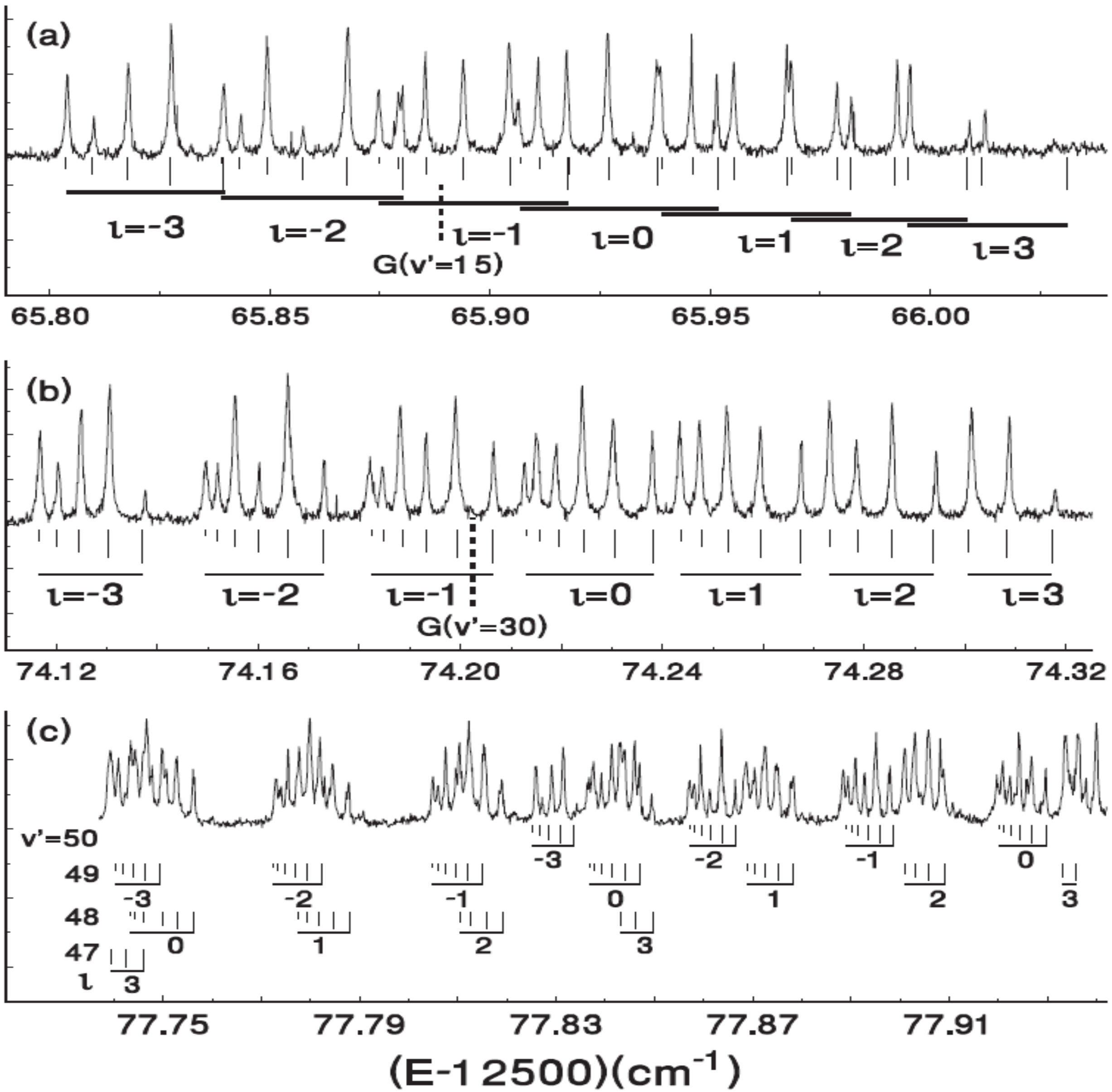
^{87}Rb (5s $^2S_{1/2}$, F=1)
^{87}Rb (5s $^2S_{1/2}$, F=2)

Designation
(nl $^{2S+1}L_J$, F)

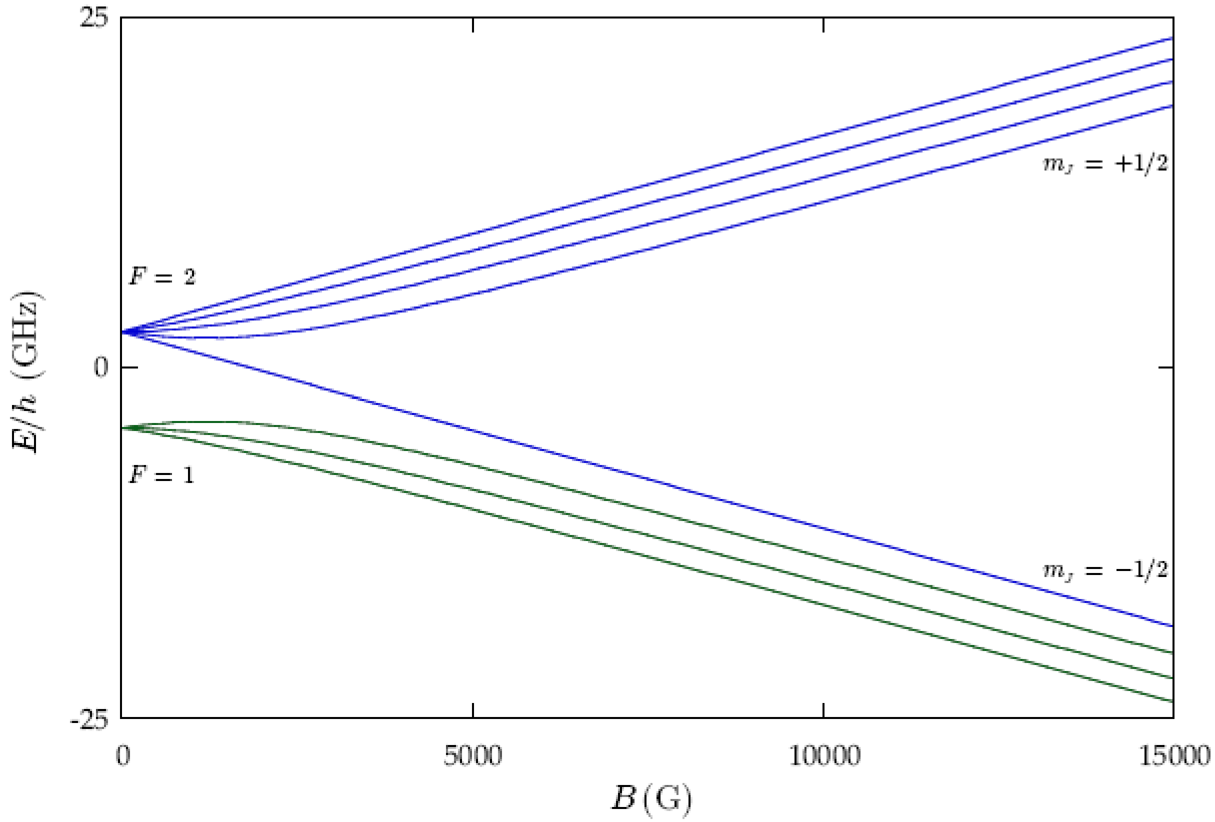
$S=\Sigma s_i$, $L=\Sigma l_i$
J=S+L
F=J+I

Excited states

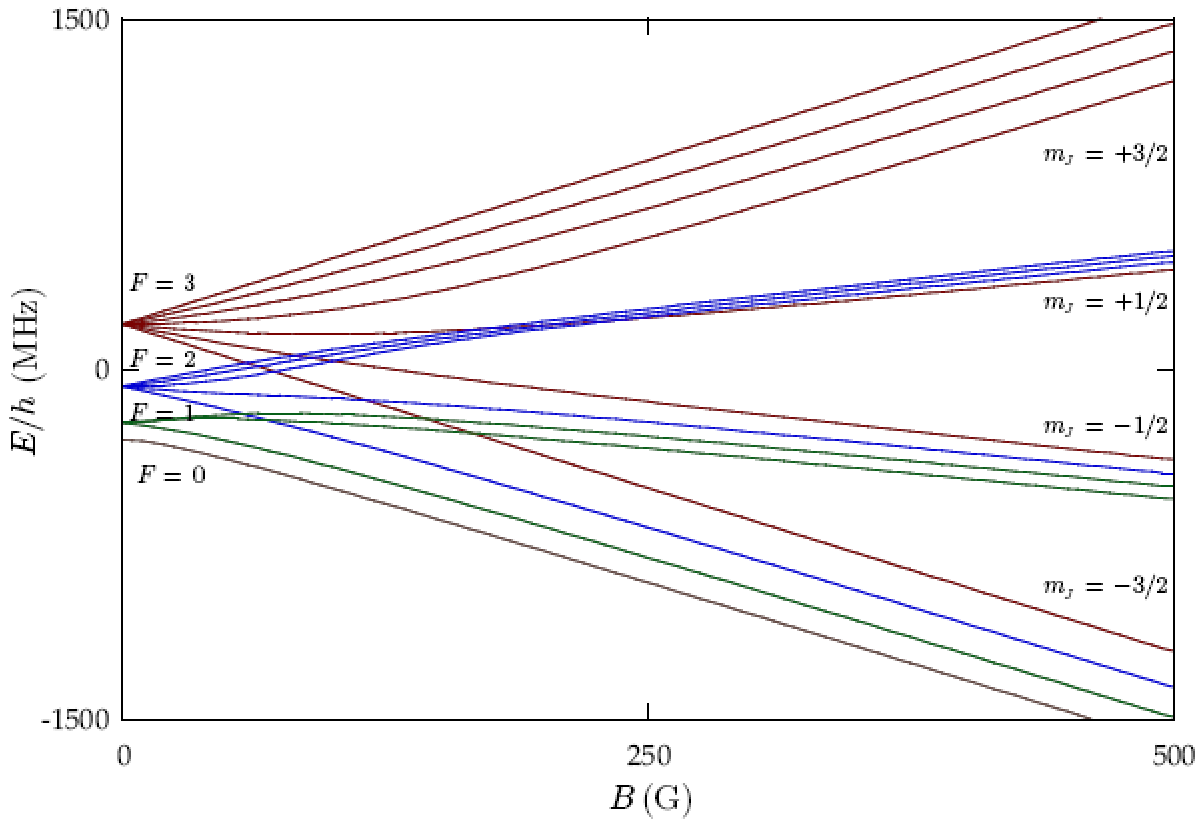
^{87}Rb (5p $^2P_{1/2}$,
F=1, or 2)



^{87}Rb 5s $^2S_{1/2}$ ground state levels with hyperfine structure in an external magnetic field.



^{87}Rb 5p $^2P_{3/2}$ excited state levels with hyperfine structure in an external magnetic field.



Symmetries in the collision

Two atoms collide with channels doubled

Ground state collisions

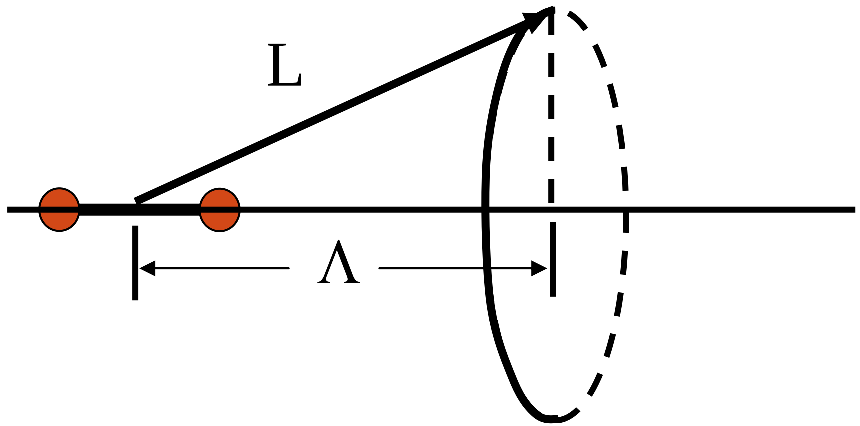
Atom1, Rb 5s $^2S_{1/2}$ Atom2, Rb 5s $^2S_{1/2}$

Electron spin	$s_1=1/2$	$s_2=1/2$	total $S=s_1+s_2$
Angular momentum	$l_1=0$	$l_2=0$	total $L=l_1+l_2$

S=0 or 1 and L=0

R (interatomic distance)

Symmetries in collision – Electronic states



Orbital angular momentum, L, is a constant of motion as long as the effect of electron spin is small or neglected.

A precession of L takes place about the field direction (internuclear axis) with constant component M_L= L, L-1, …., -L, and $\Lambda=|M_L|$

Λ is the electronic angular momentum along the internuclear axis.
Λ=0, 1, 2, …, L, called Σ, Π, Δ… Electronic states.

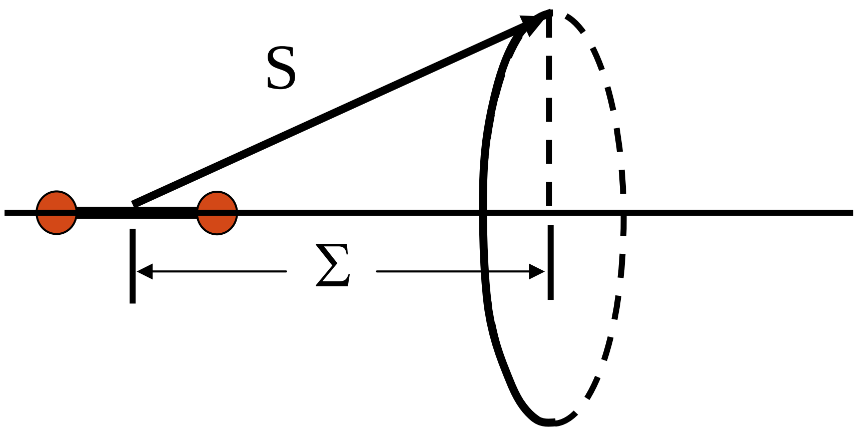
Symmetries in collision – Electronic spin

Electronic spin $S=\Sigma s_i$, where s_i is the individual electron spin.

Fine structure of electron bands shows a multiplet structure.

For $\Lambda \neq 0$, the internal magnetic field causes a precession of S about the field direction (internuclear axis).

Components of the precession:
$\Sigma = S, S-1, S-2, \ldots, -S$



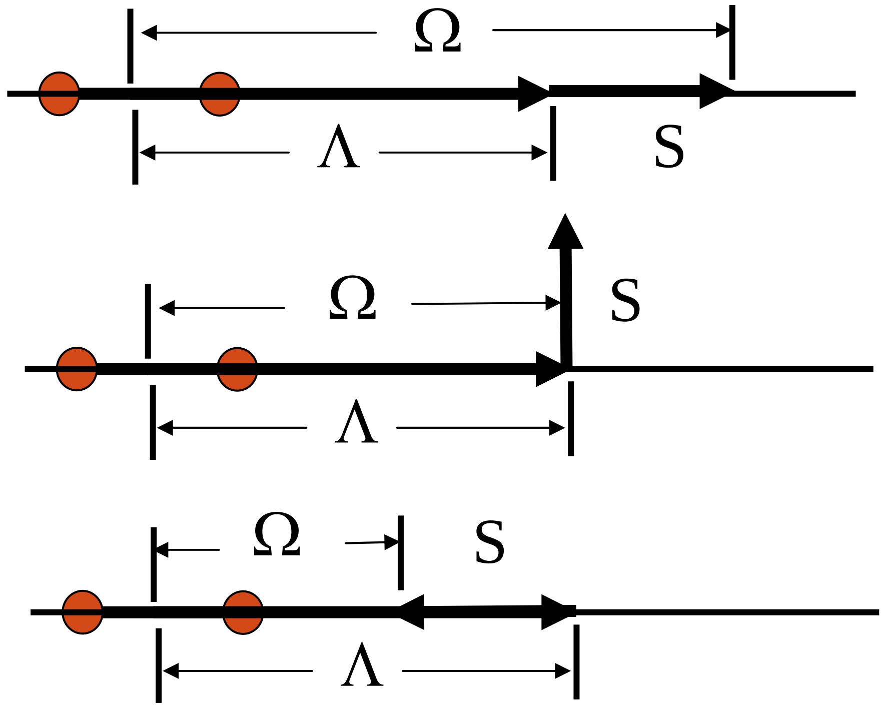
(note Σ can be positive and negative)

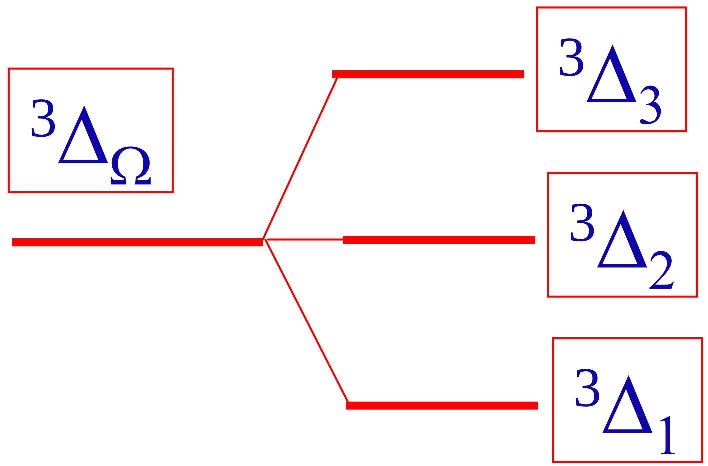
Symmetries in collision –Total angular momentum

The quantum number of the resultant electronic angular momentum about the internuclear axis is Ω:

For example (S=1) :

$$\Omega = |\Lambda + \Sigma|$$

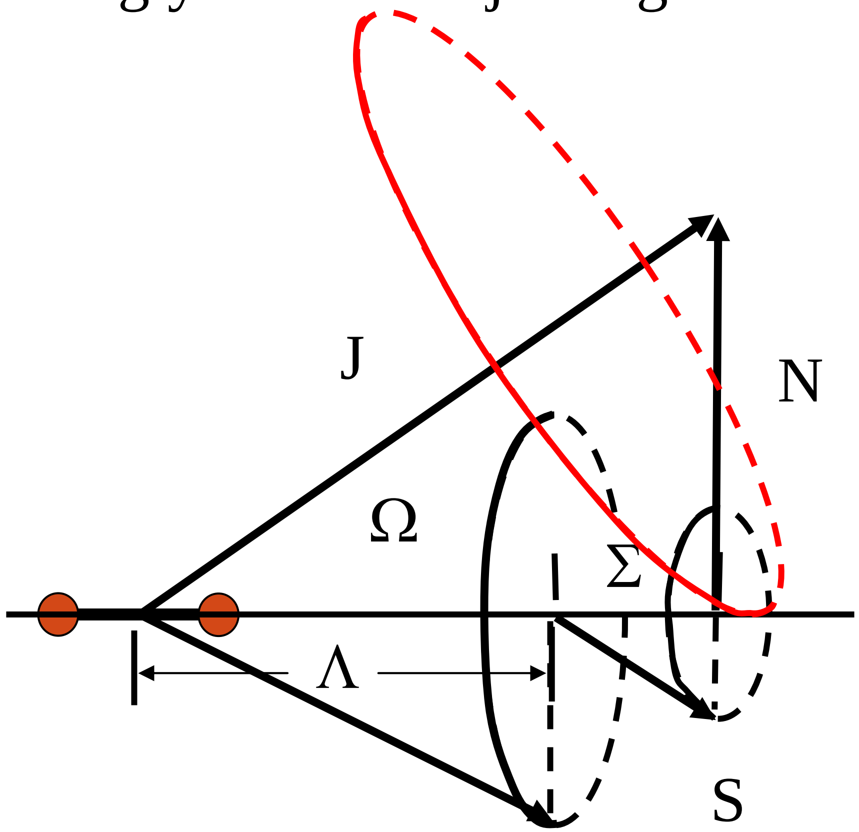




Symmetries in collision – Hund's coupling cases

Hund's case(*a*):

the interaction of the nuclear rotation with the electronic motion is very weak, whereas the electronic motion itself coupled very strongly to the line joining the nuclei.



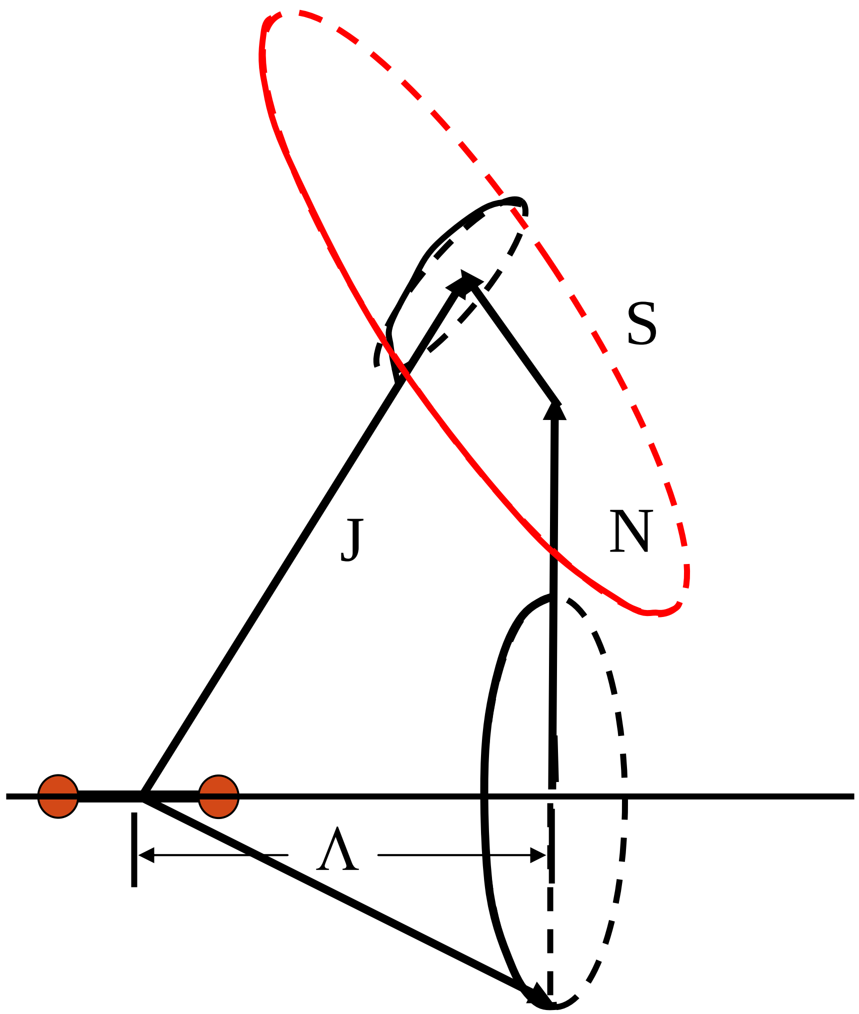
N: angular momentum of nuclear rotation

J: total angular momentum

$^{2S+1}\Lambda_{\Omega}$

Symmetries in collision – Hund's coupling cases

Hund's case(*b*):



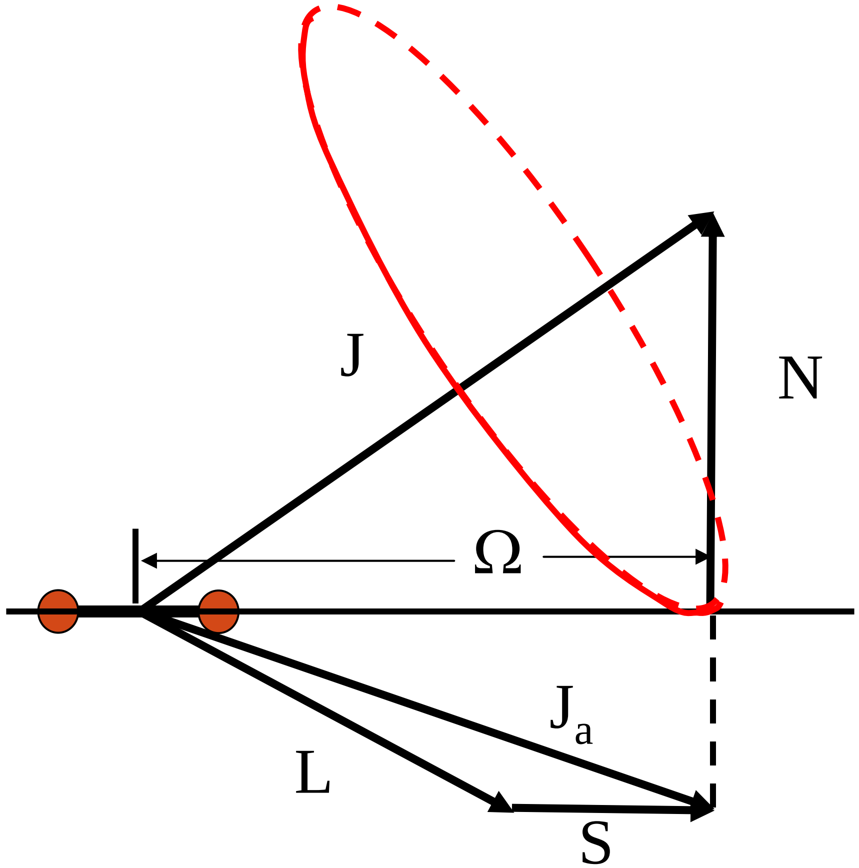
N: angular momentum of nuclear rotation

J: total angular momentum

$^{2S+1}\Lambda$

Hund's case(c):

the interaction between L and S may be stronger than the interaction with the nuclear axis, e.g. heavy molecules or molecules with large separation between atoms.



J_a: the resultant of L and S.

For large separation between atoms, J_a will be the resultant of J_{a1} and J_{a2}, where $J_{a1}=L_1+S_1$ is the resultant of atom1.

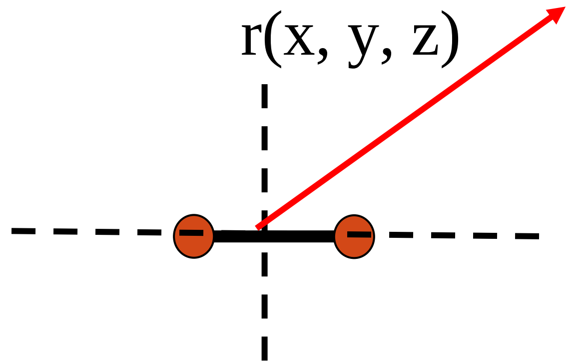
Ω

Symmetries Properties of electronic eigenfunctions

Plane symmetry

$$\hat{i}\,\Psi(x,y,z) = \Psi(x,y,-z)$$

Non-degenerate states, L=0 or Ω=0,
+: even symmetry as +
-: odd symmetry as -
Degenerate states, both + and –
belong to the same eigenvalue



Case(a) $$^{2S+1}\Lambda^{\pm}_{g/u,\Omega}$$

Center symmetry:

$$\hat{i}\,\Psi(x,y,z) = \Psi(-x,-y,-z)$$

+: even symmetry as gerade state, g
-: odd symmetry as ungerade state, u

Case(c) $$\Omega^{\pm}_{g/u}$$

Symmetries Properties of electronic eigenfunctions

Total wavefunction for electrons (fermions) should be anti-symmetry.

For unlike atoms, there is no center symmetry, *i.e.* without *g/u* and the non-degenerate states are Σ^+ and Σ^-.

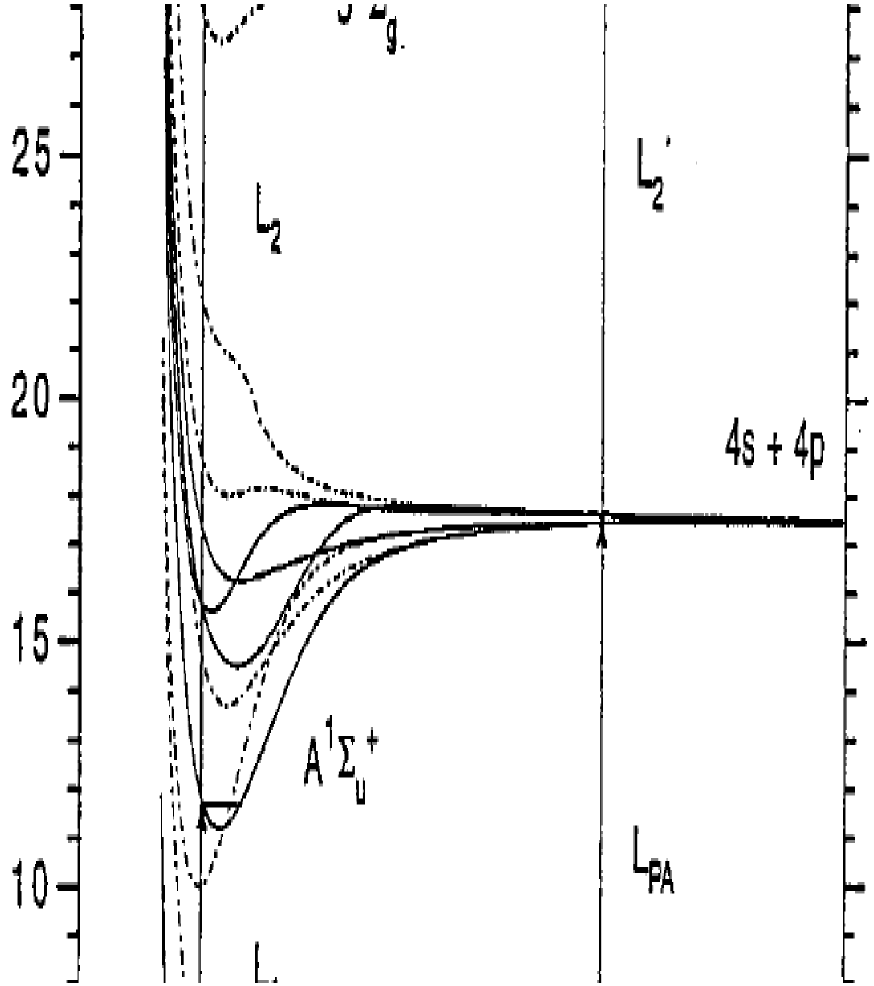
For like atoms, there is a center symmetry, *i.e. g/u states.*

For both atoms are in the same state, they have equal energy when the two atoms are interchanged.

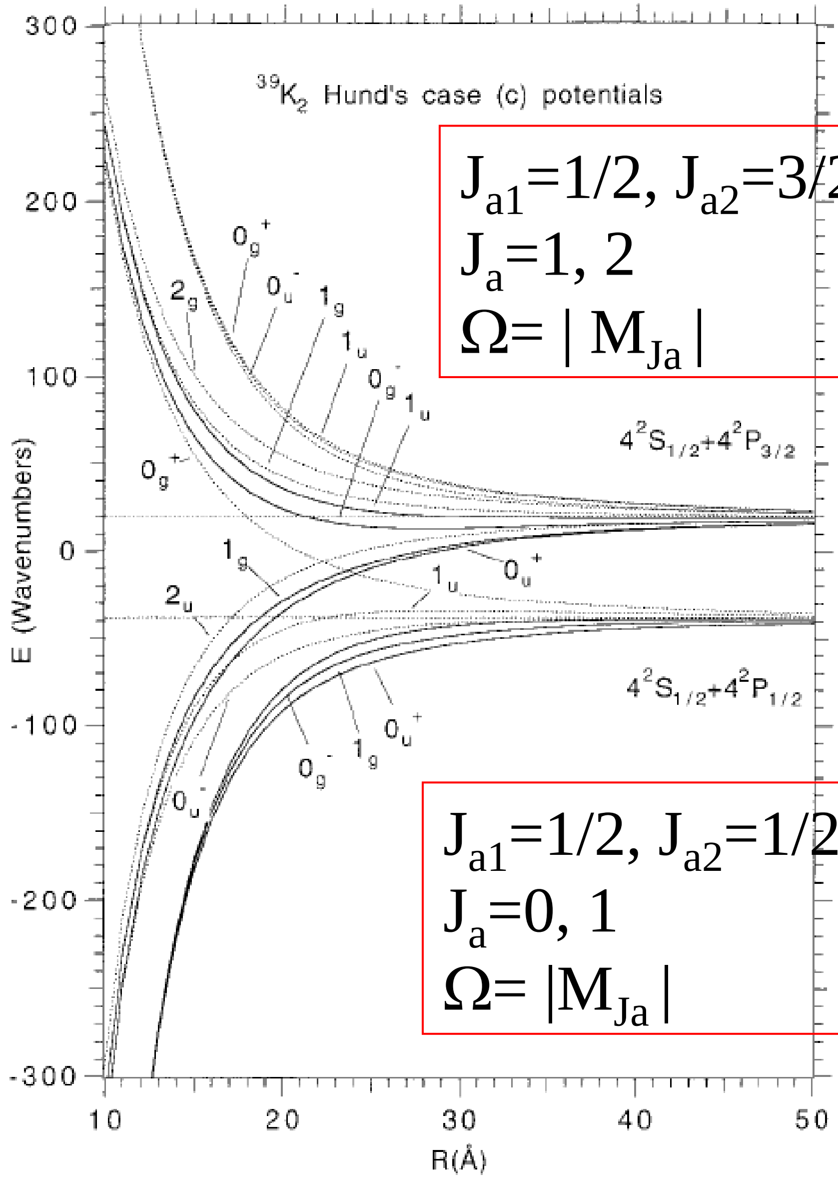
e.g. ns $^2S_{1/2}$+ns $^2S_{1/2}$ $\quad$ $^1\Sigma_g^+$, $^3\Sigma_u^-$

$J_1=1/2+J_1=1/2$ $\quad$ 1_u, 0_g^+, 0_u^-

ns+np in Hund's coupling case(a) and case(c)



Case(*a*)



J_{a1}=1/2, J_{a2}=3/2
J_a=1, 2
$\Omega = | M_{Ja} |$

J_{a1}=1/2, J_{a2}=1/2
J_a=0, 1
$\Omega = |M_{Ja}|$

Case(*c*)

How about doubly excited states, np+np.

$L_1=0, L_2=1$

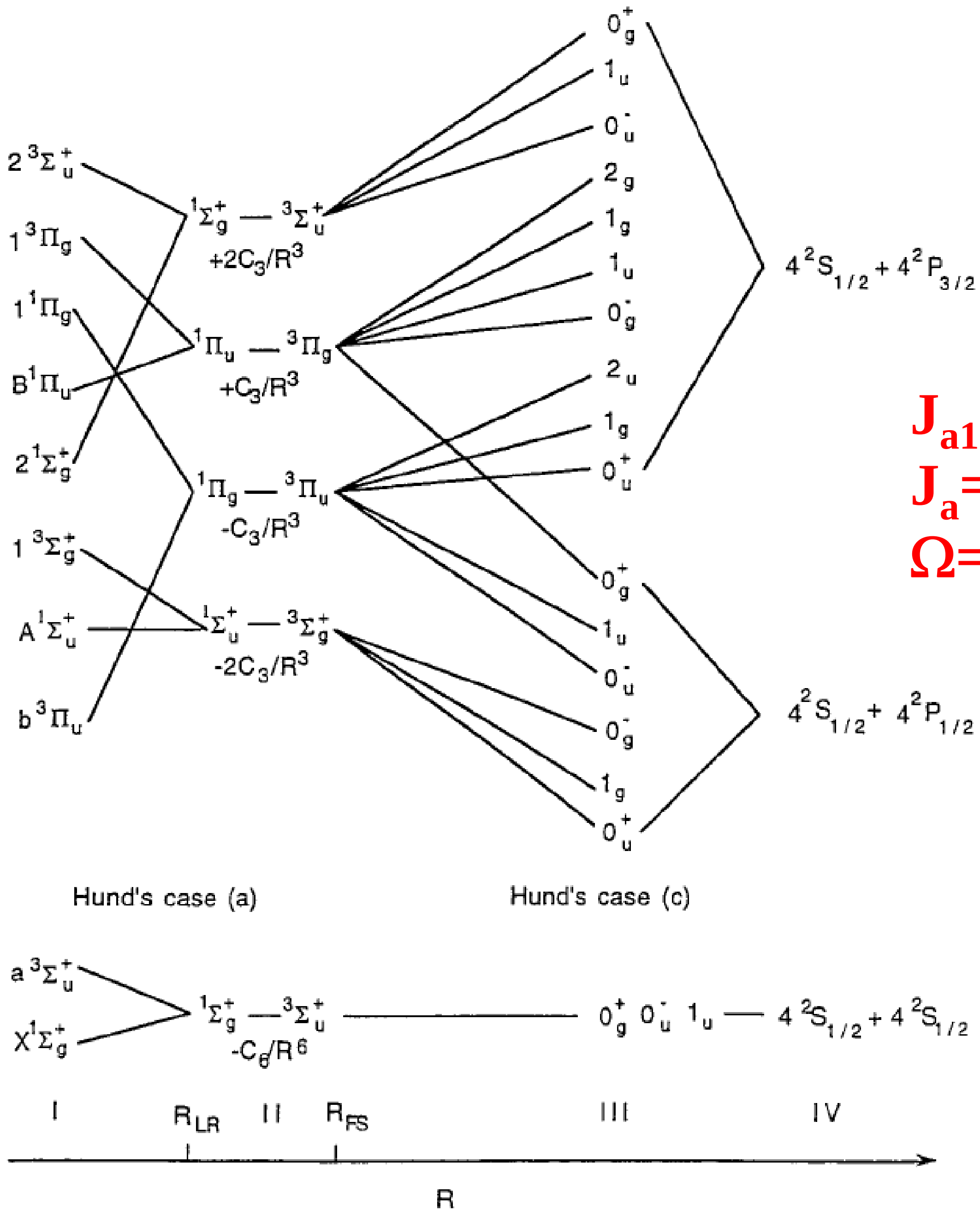
$L=0, 1$

$\Lambda=| M_L |$

$S_1=1/2, S_2=1/2$

$S=0, 1$

$2S+1=1, 3$



$J_{a1}=1/2, J_{a2}=3/2$

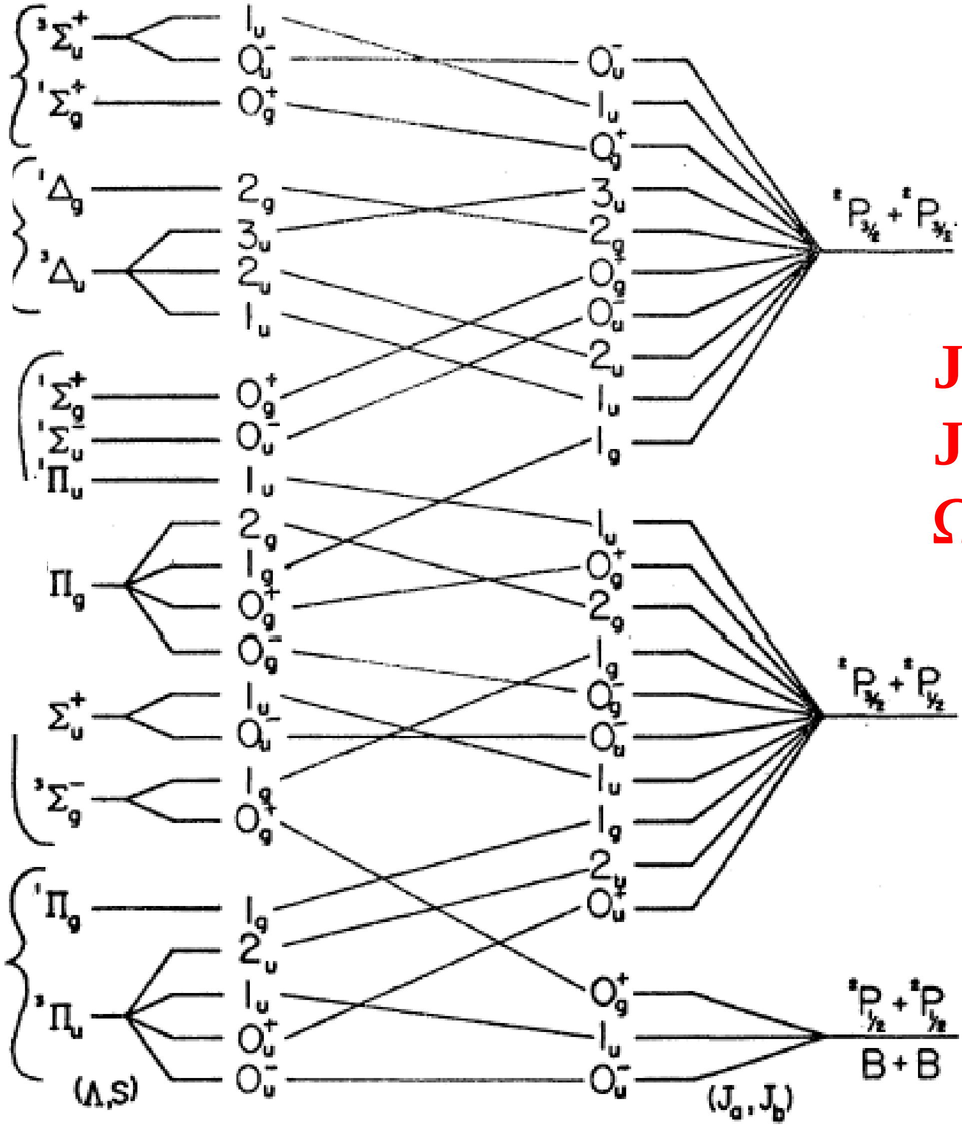
$J_a=1, 2$

$\Omega= | M_{Ja} |$

How about doubly excited states, np+np.

$L_1=0,\ L_2=1$
$L=0,\ 1$
$\Lambda=|\ M_L\ |$

$S_1=1/2,\ S_2=1/2$
$S=0,\ 1$
$2S+1=1,\ 3$

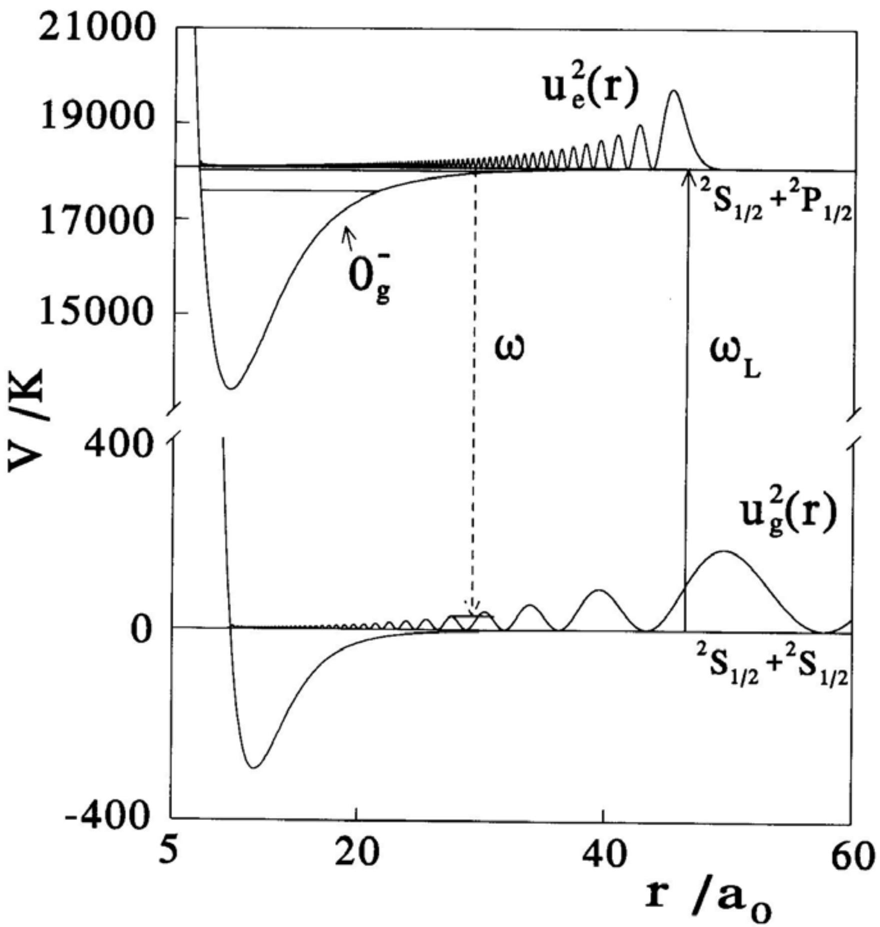


$J_{a1}=3/2,\ J_{a2}=3/2$
$J_a=0,\ 1,\ 2,\ 3$
$\Omega=|\ M_{Ja}\ |$

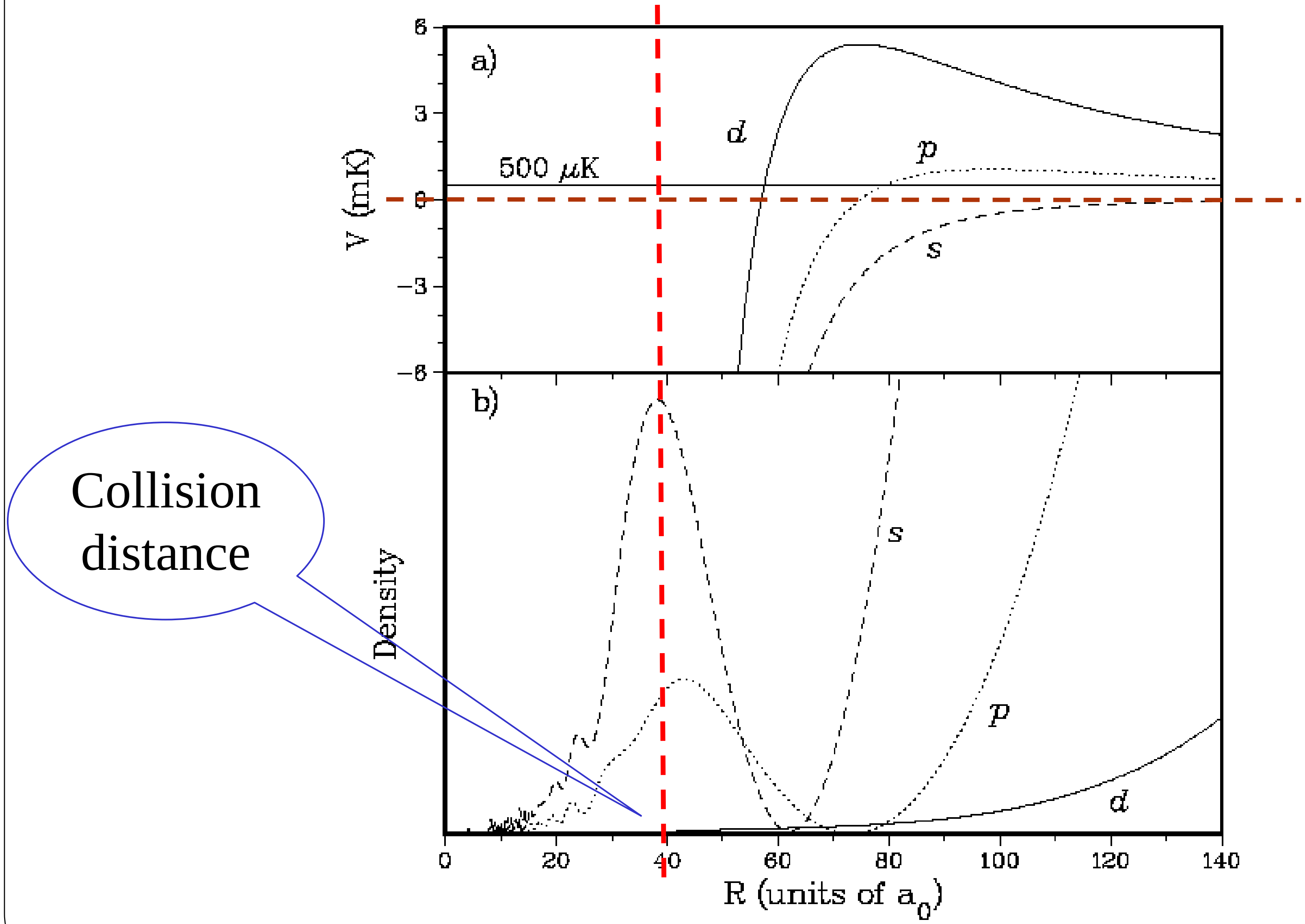
Cold atom photoassociation

Excitation of a colliding pair of Rb atoms by a photon (ω_L) leads to the formation of an excited Rb2 molecule in the 0_g^- excited state.

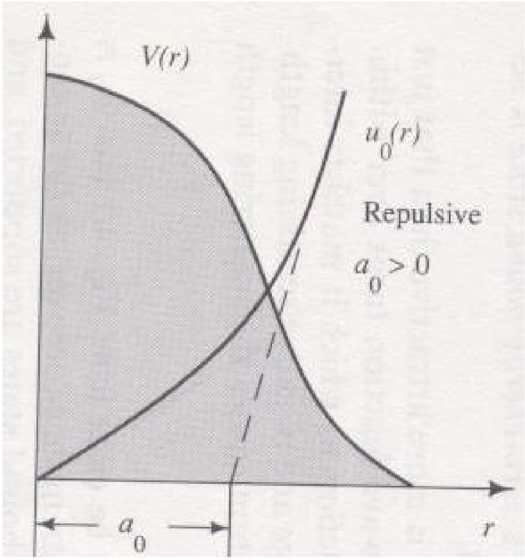
Spontaneous fluorescence radiates a photon (ω) from excited state 0_g^- to the free state of bound molecular ground state $X\ ^1\Sigma_g^+$.

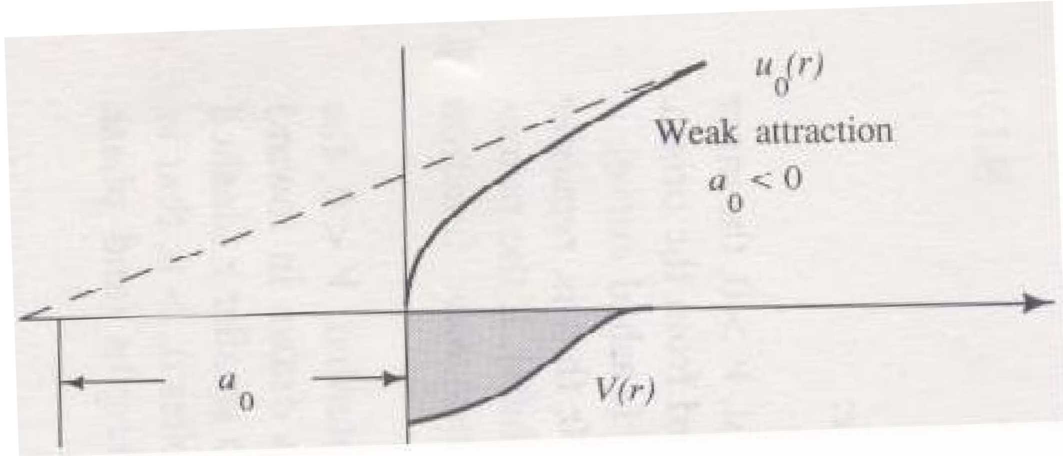


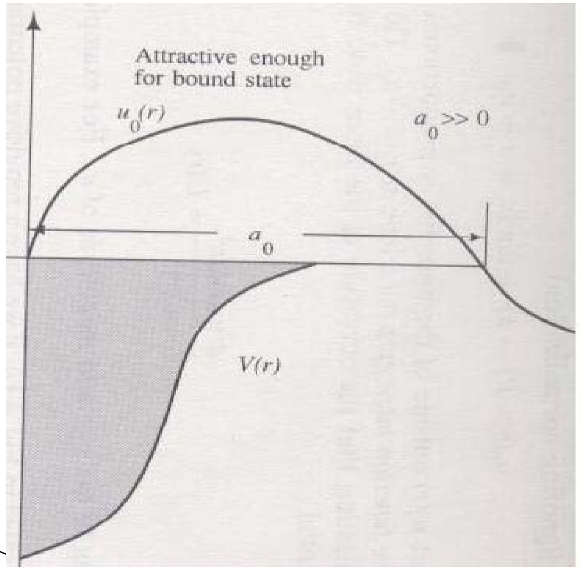
The s-wave scattering length *a*, why?

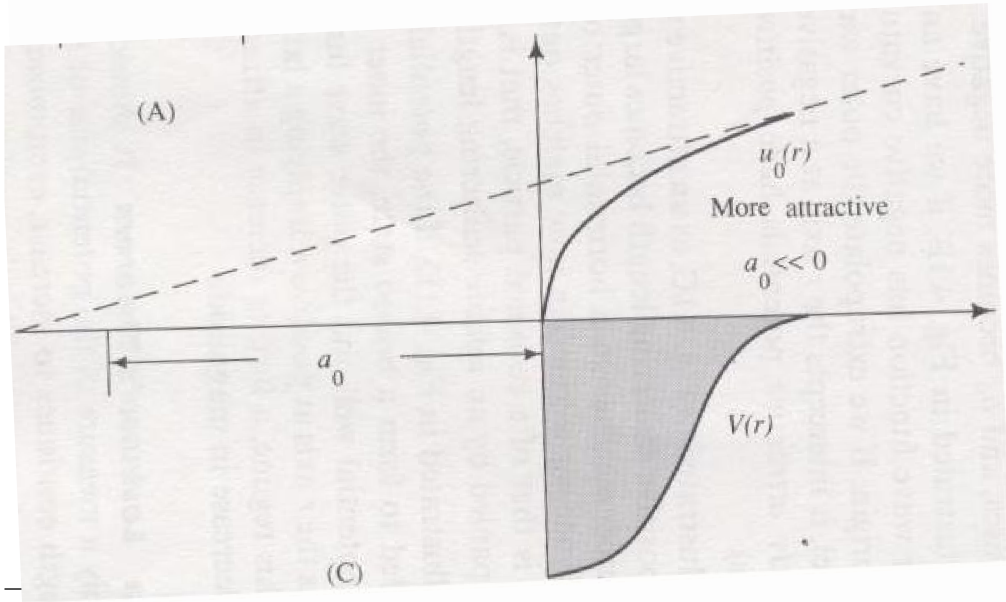


The s-wave scattering length *a*, how?









The s-wave scattering length *a*, how?

A. Determined by the interaction potential.

B. Determined by the free state wave function.

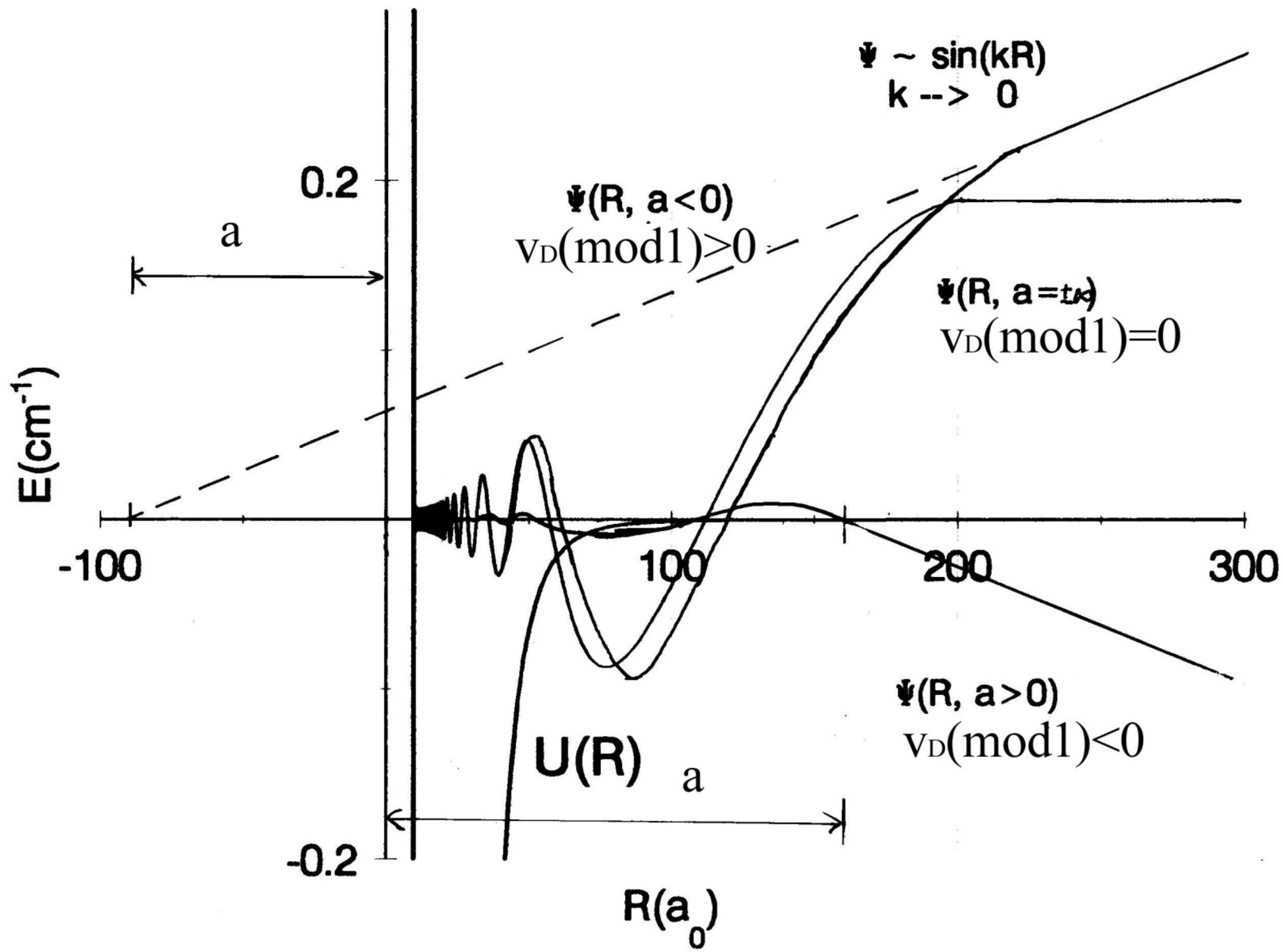
C. Determined by the last bound state and the long range potential.

D. Using different type of resonances to determine the collision processes in a certain channel or channels.

…..

The s-wave scattering length *a*, how?

Long Range Wavefunction and Scattering Length



The s-wave scattering length *a*, how?

$$\left[\frac{d^2}{dr^2}+k^2-\frac{\ell(\ell+1)}{r^2}+V(r)\right]rR_{k\ell}(r)=0$$

$\ell = 0,1,2.....correspondent\ s\ wave, p\ wave, d\ wave...$

(i) $r \gg R\ (potentail\ range)$, $V(r) \to 0$

(ii) extremely low kinetic energy i.e. $k \to 0$

(iii) for $\ell=0 \Rightarrow$ S-wave , why S-wave ?

$$\begin{cases} \dfrac{d^2}{dr^2}rR_{k,\ell=0}(r)=\dfrac{d^2}{dr^2}U(r)=0 \ \Rightarrow\ U(r)=C(r-a) \quad a: \text{ S-wave scattering length} \\ \qquad \text{simple geometrical meaning : intersecton of } U_{\ell=0}(r) \text{ v.s. r} \\ U(r)=A_\ell'\dfrac{1}{k}\sin(kr+\delta_{\ell=0})=A_\ell'\dfrac{1}{k}\sin\left[k(r+\dfrac{1}{k}\delta_{\ell=0})\right] \end{cases}$$

radial boundry condition $\dfrac{1}{r}\dfrac{\frac{d}{dr}U(r)}{dr}$, $k\cot\left[k(r+\dfrac{1}{k}\delta_{\ell=0})\right]=\dfrac{1}{r-a}$

$\lim\limits_{k\to 0} k\cot\delta_{\ell=0}=\dfrac{1}{-a}$ (evne not the true wavefunction : Sakurai)

$\sigma=\dfrac{4\pi}{k^2}\sum\limits_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell=4\pi a^2$ (s-wave total cross section)

$$\therefore \begin{cases} \sigma_{tot}=4\pi a^2 \\ a=-\lim\limits_{k\to 0}\dfrac{\tan\delta_{\ell=0}}{k} \end{cases}$$