Ultracold quantum scattering - Part III: Hyperfine structure

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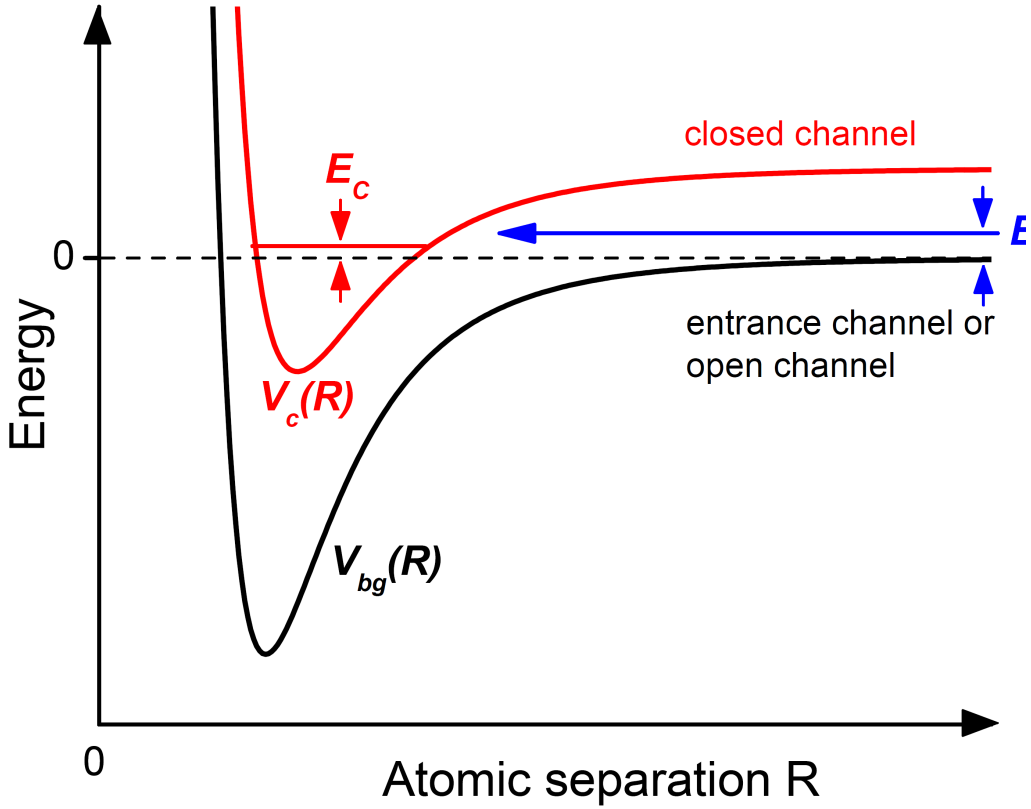
Magnetic Feshbach resonances in ultracold collisions

Origin of Fesbhach resonances

Cold Molecules: Theory, Experiment, Applications.
CRC Press, 2009



$|f_{1'}m_{1'}f_{2'}m_{2'}l'm_{l'}>$

$|f_1 m_1 f_2 m_2 l m_l>$

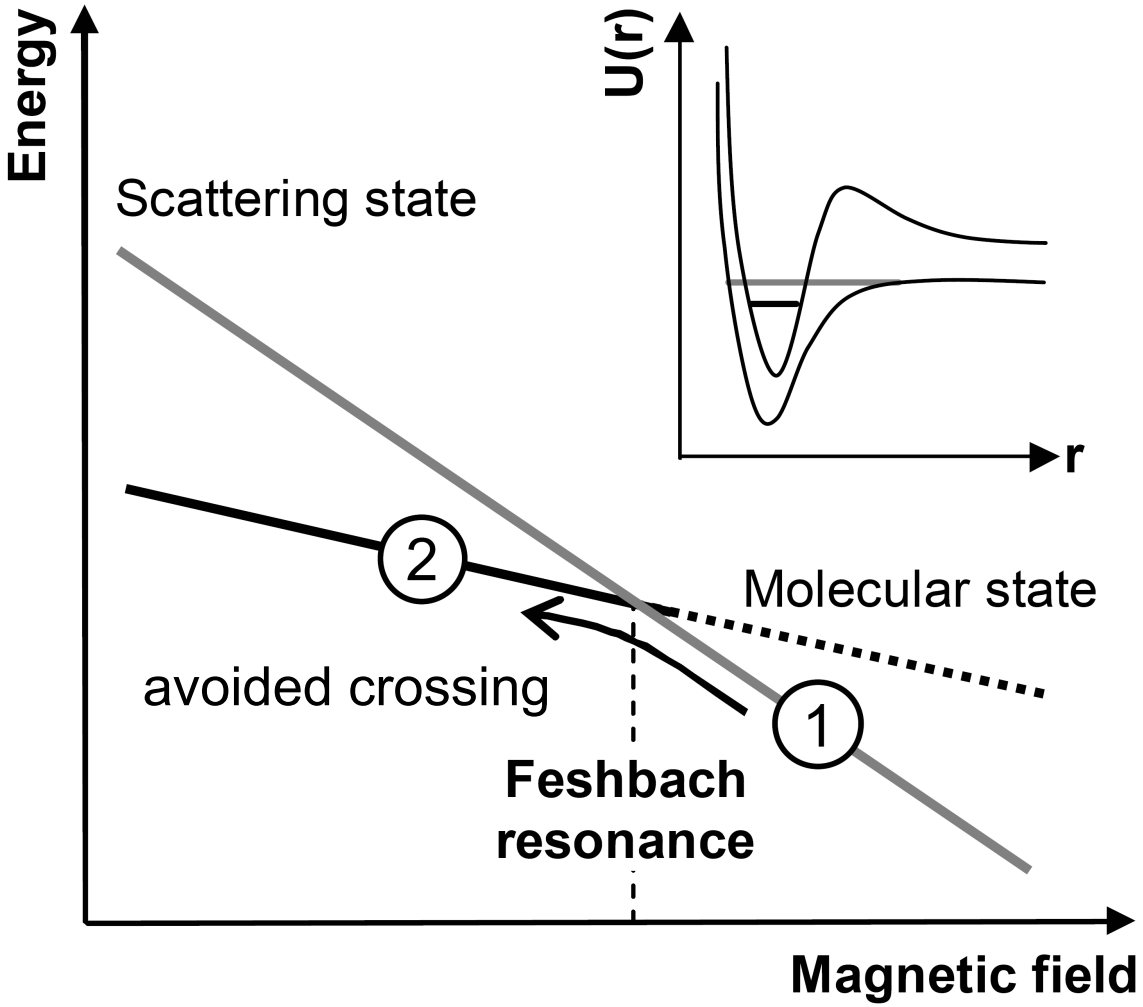
$|\alpha> \equiv |f_1 m_1 f_2 m_2 l m_l> \rightarrow |f_1 m_1> + |f_2 m_2>$

open: $E_\alpha = E_{f1m1} + E_{f2m2} < E_{total}$

closed: $E_\alpha = E_{f1m1} + E_{f2m2} > E_{total}$

Crossing between atomic and molecular states

Int. Rev. Phys. Chem. **25**(4), 496 (2006)

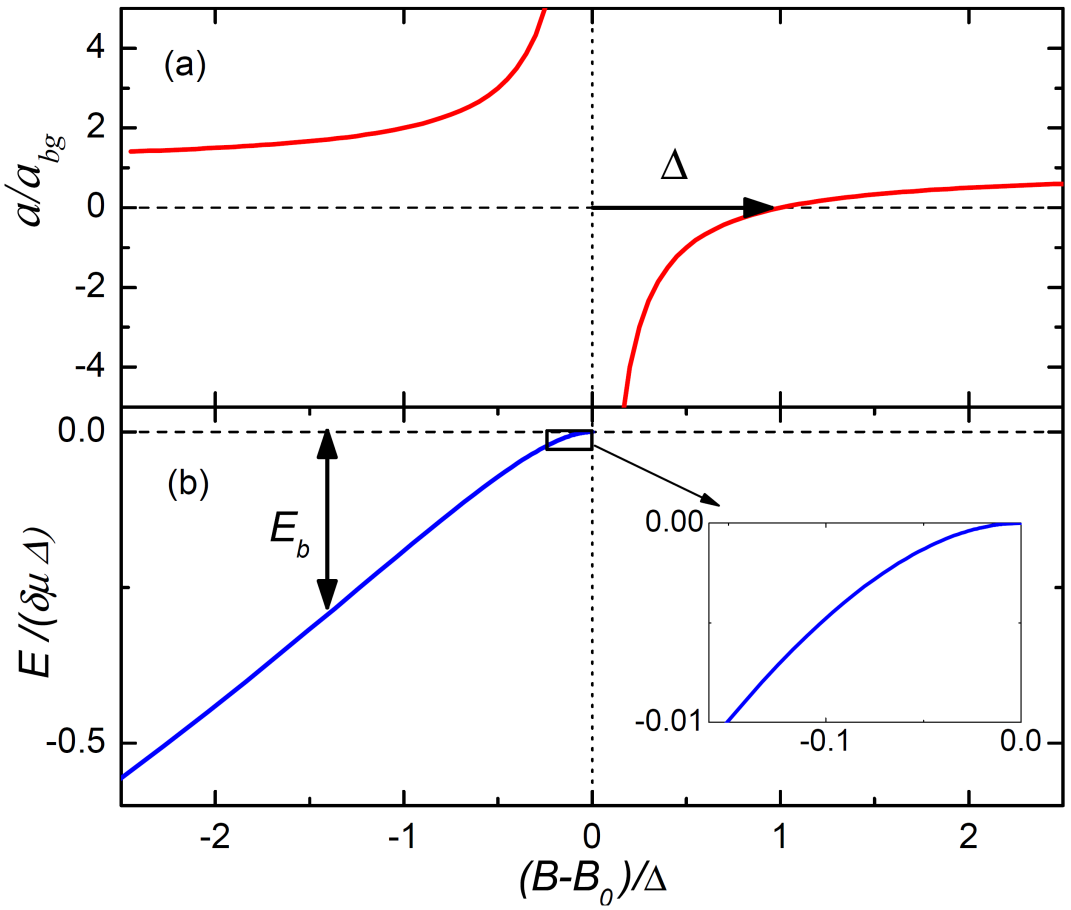


$E=\Sigma \mu_i B_i$

$\mu_{open} \neq \mu_{closed}$

Scattering length and binding energy

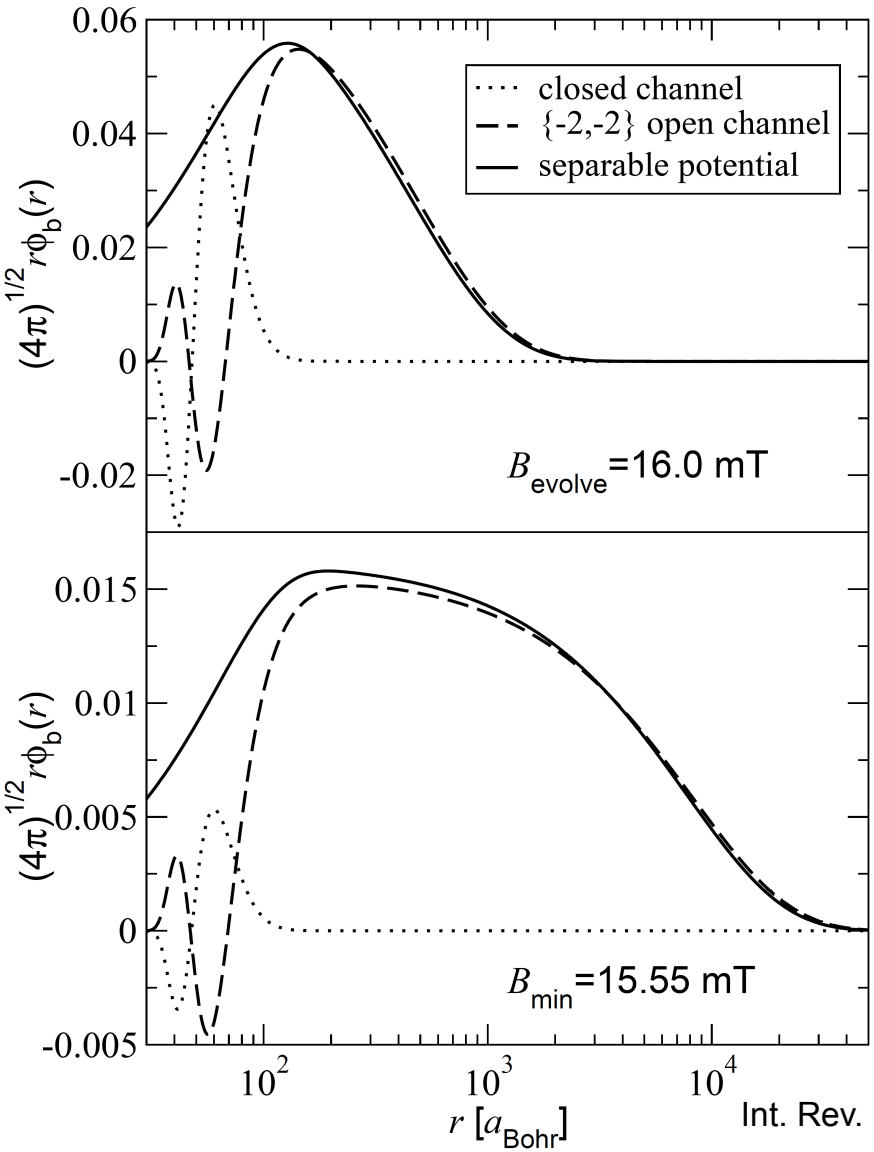
Cold Molecules: Theory, Experiment, Applications.
CRC Press, 2009



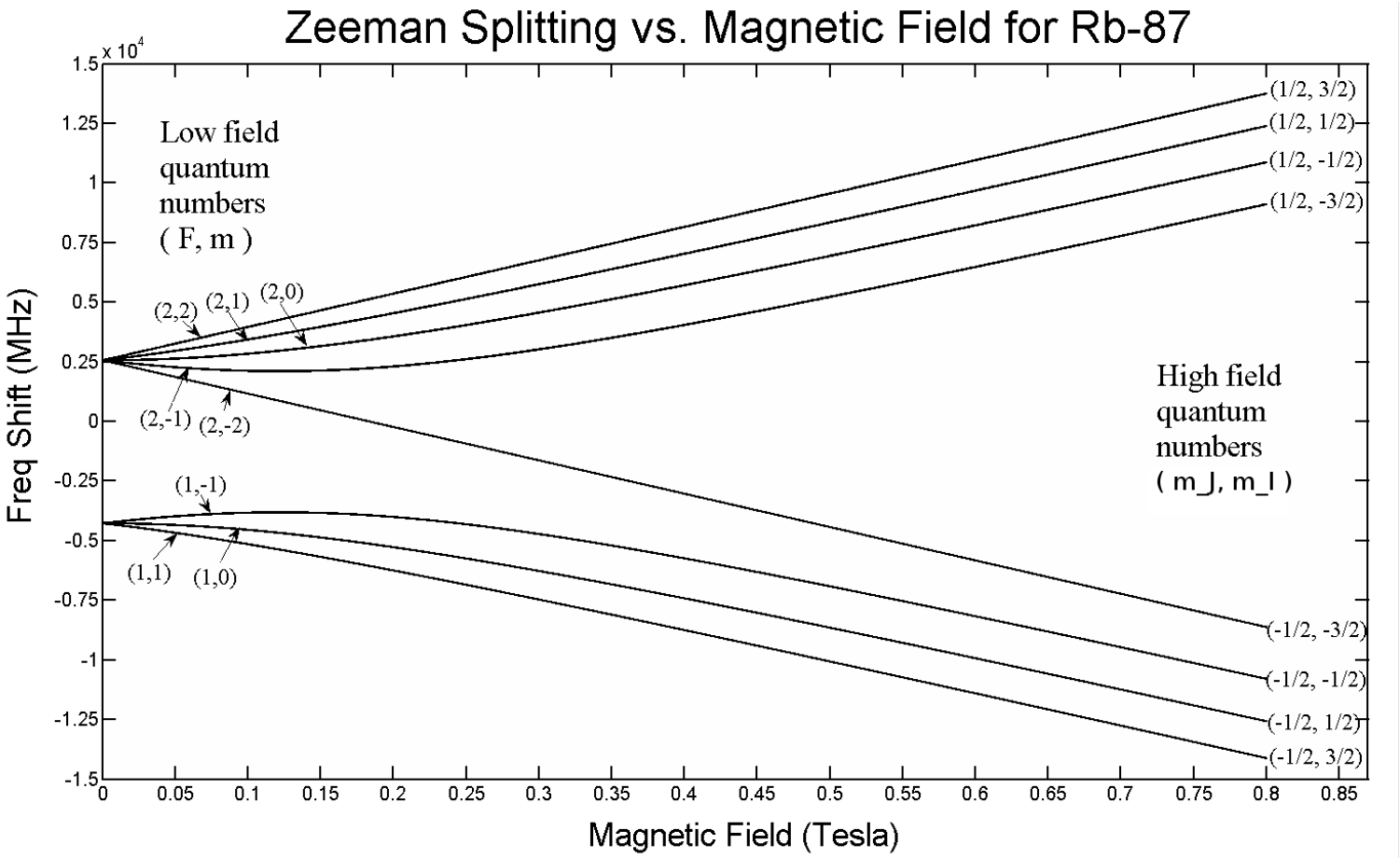
$$a(B) = a_{bg}\left(1 - \frac{\Delta B}{B - B_0}\right)$$

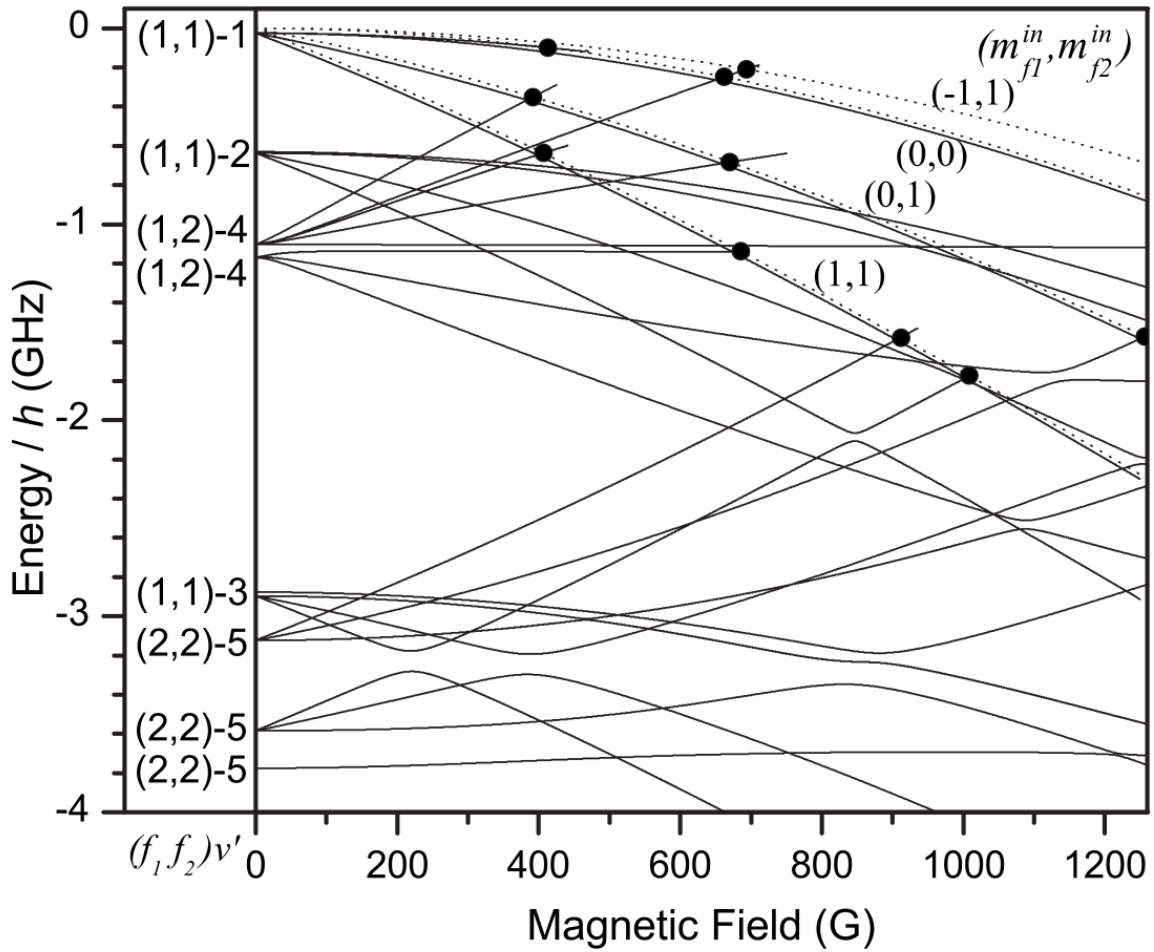
$$E_{top} = \frac{-h^2}{2\mu a^2}$$

Very weakly bound states



Int. Rev. Phys. Chem. **25**(4), 496 (2006)


Zeeman Splitting vs. Magnetic Field for Rb-87
x 10^4
Freq Shift (MHz)
Magnetic Field (Tesla)
Low field quantum numbers (F, m)
High field quantum numbers (m_J, m_I)
(2,2)
(2,1)
(2,0)
(2,-1)
(2,-2)
(1,-1)
(1,1)
(1,0)
(1/2, 3/2)
(1/2, 1/2)
(1/2, -1/2)
(1/2, -3/2)
(-1/2, -3/2)
(-1/2, -1/2)
(-1/2, 1/2)
(-1/2, 3/2)


0
-1
-2
-3
-4
Energy / h (GHz)
(1,1)-1
(1,1)-2
(1,2)-4
(1,2)-4
(1,1)-3
(2,2)-5
(2,2)-5
(2,2)-5
$(f_1 f_2)v'$
$(m_{f1}^{in}, m_{f2}^{in})$
(-1,1)
(0,0)
(0,1)
(1,1)
0
200
400
600
800
1000
1200
Magnetic Field (G)

Cold collisions in magnetic field

Cold collisions in magnetic field

$$\hat{H} = -\frac{\hbar^2}{2\mu}\frac{1}{R}\frac{d^2}{dR^2}R + \frac{\hat{\mathbf{l}}^2}{2\mu R^2} + \hat{V}(R) + \hat{H}_A + \hat{H}_B\,, \tag{1}$$

where $\hat{\mathbf{l}}$ is the rotational angular momentum operator. $\hat{V}(R)$ is the interaction potential, which depends on the total spin S and its projection M_S

$$\hat{V}(R) = \sum_{S,M_S} V_S(R)|S,M_S\rangle\langle S,M_S|\,. \tag{2}$$

The atomic Hamiltonian, $\hat{H}_j$ ($j = A^+, B$), including hyperfine and Zeeman interactions, is given by

$$\hat{H}_j = \zeta_j \hat{\mathbf{i}}_j \cdot \hat{\mathbf{s}}_j + g_e \mu_B \hat{\mathbf{s}}_j \cdot \mathbf{B} + g_j \mu_N \hat{\mathbf{i}}_j \cdot \mathbf{B}\,, \tag{3}$$

with $\hat{\mathbf{s}}_j$ and $\hat{\mathbf{i}}_j$ the electron and nuclear spin operators, ζ_j denoting the hyperfine coupling constant, $g_{e/j}$ the electron and nuclear g factors, $\mu_{B/N}$ the Bohr and nuclear magnetons, and $\mathbf{B}$ the magnetic field.

Coupled-channel multi-partial-wave scattering

$$\mathbf{\Psi}(R,\theta,\phi) = \sum_{\chi} \Phi_{\chi}(R)|l, m_l\rangle|s_1, m_{s_1}\rangle|i_1, m_{i_1}\rangle|s_2, m_{s_2}\rangle|i_2, m_{i_2}\rangle/R\,, \quad (4)$$

$$\chi = l, m_l, s_1, m_{s_1}, s_2, m_{s_2}, i_1, m_{i_1}, i_2, m_{i_2}$$

$$\hat{H}\mathbf{\Psi}(R,\theta,\phi) = E\mathbf{\Psi}(R,\theta,\phi) \quad (5)$$

Coupled-channel multi-partial-wave scattering

in a matrix form

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dR^2} + \mathbf{W}(R)\right)\mathbf{\Phi}(R) = E\mathbf{\Phi}(R)\,, \tag{6}$$

where

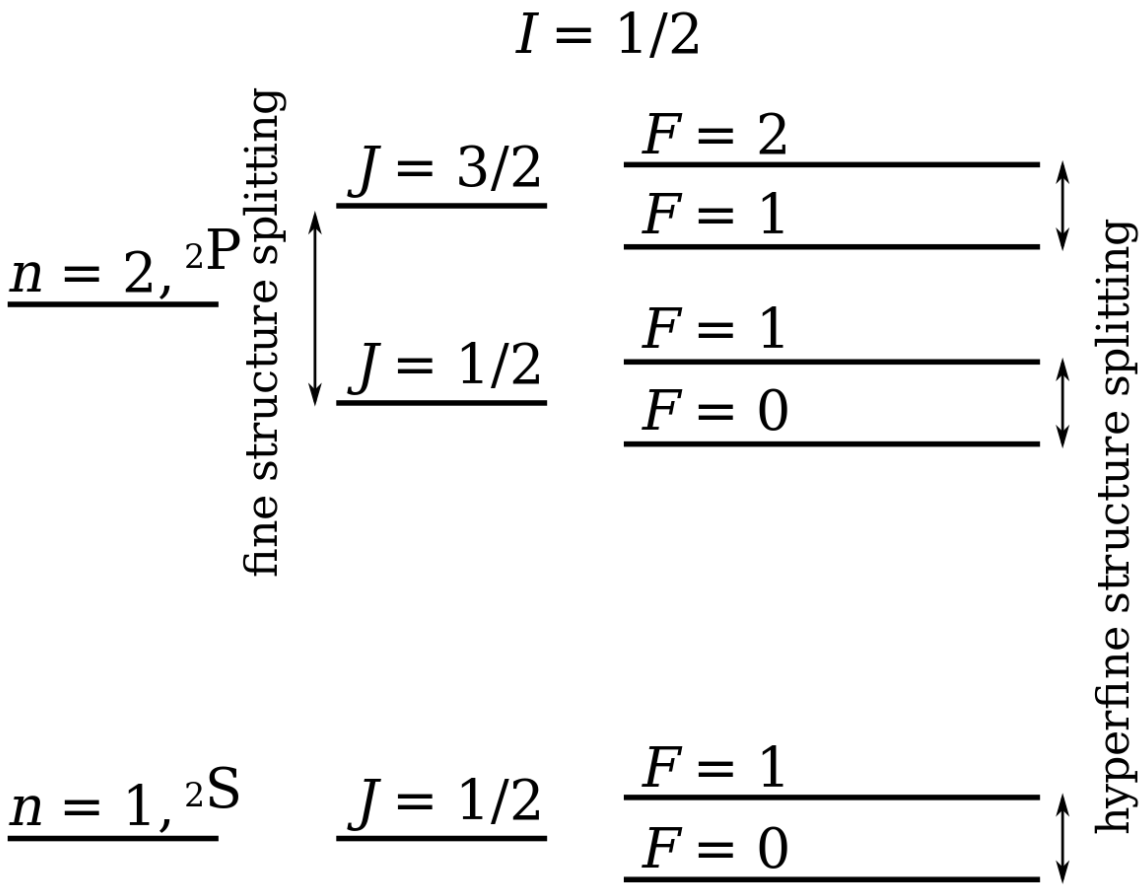
$$W_{\chi\chi'}(R) = \delta_{\chi\chi'}\frac{\hbar^2 l(l+1)}{2\mu R^2} + \langle\chi|\hat{V}(R) + \hat{H}_A + \hat{H}_B|\chi'\rangle \tag{7}$$

where

$$|\chi\rangle = |l, m_l\rangle|s_1, m_{s_1}\rangle|i_1, m_{i_1}\rangle|s_2, m_{s_2}\rangle|i_2, m_{i_2}\rangle \tag{8}$$

Atomic hyperfine structure

Atomic fine and hyperfine structure



atomic term $^{2S+1}\mathbf{L_J}$: S couples with L to J. J couples with I to F.

Atomic hyperfine structure

In general situations, an electronic spin $\underline{S}$ and a nuclear spin $\underline{I}$ are coupled by an interaction

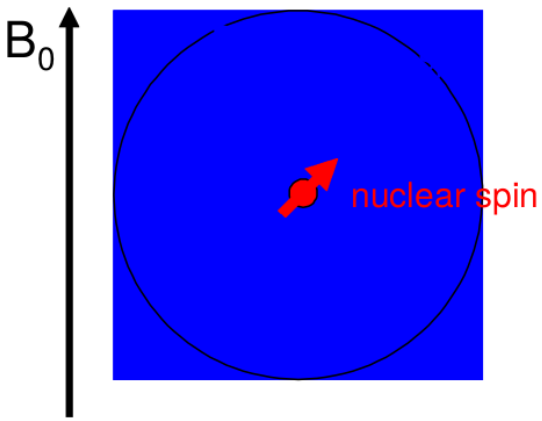
$$\hat{H}_{\mathrm{hfi}} = \underline{\hat{I}} \cdot \underline{\underline{A}} \cdot \underline{\hat{S}}$$

The second rank tensor A is called the hyperfine tensor and it can be described by its three principal axes values A_{XX}, A_{YY}, A_{ZZ} along the principal axis system $\hat{X},\hat{Y},\hat{Z}$.

In many situations, the hyperfine interaction is a scalar, independent of the spin direction. This case is e.g. the Fermi contact interaction between s-like electrons at the nuclear site.

In this situation, the hfi leads to a scalar interaction term: $\hat{H}_{\mathrm{hfi}} = a \cdot \underline{\hat{I}} \cdot \underline{\hat{S}} = h \cdot A \cdot \underline{\hat{I}} \cdot \underline{\hat{S}}$

The hfi coupling constant a = h·A is often given in frequency units: e.g. A = 65 MHz.



The Hamiltonian of an electronic spin $\hat{\underline{S}}$ and a nuclear spin $\hat{\underline{I}}$ in a magnetic field $\underline{B}_0$ along the z-direction:

$$\hat{H} = g_e \mu_B B_0 \hat{S}_z - g_n \mu_K B_0 \hat{I}_z + h \cdot A \, \underline{\hat{I}} \cdot \underline{\hat{S}}$$

Atomic hyperfine structure

This Hamiltonian is solved by diagonalisation, leading to the energy eigenvalues and the eigenstates. As the base states for the quantum mechanical treatment, we take product states between the electron spin states $|S,m_S\rangle$ and the nuclear spin states $|I, m_I\rangle$

$$|\psi\rangle = |S, m_S\rangle \cdot |I, m_I\rangle \qquad m_S = -S, -S+1,\ldots,S-1,S \qquad m_I = -I, -I+1,\ldots,I-1,I$$

There are $(2S+1)\cdot(2I+1)$ base states.

In order to avoid a too clumsy notation, one usually omits the S, I in the base states and writes: $|\psi\rangle = |m_S m_I\rangle = |m_S\rangle \cdot |m_I\rangle$

For the case S =1/2 I =1/2, we have 4 base states:

$$|1\rangle = \left|+\tfrac{1}{2}\ +\tfrac{1}{2}\right\rangle \qquad |2\rangle = \left|+\tfrac{1}{2}\ -\tfrac{1}{2}\right\rangle \qquad |3\rangle = \left|-\tfrac{1}{2}\ +\tfrac{1}{2}\right\rangle \qquad |4\rangle = \left|-\tfrac{1}{2}\ -\tfrac{1}{2}\right\rangle$$

The operators S_z and I_z are diagonal in the base states.

$$\hat{S}_z|1\rangle = \hat{S}_z\left|+\tfrac{1}{2}\ +\tfrac{1}{2}\right\rangle = \frac{1}{2}\cdot\left|+\tfrac{1}{2}\ +\tfrac{1}{2}\right\rangle = \frac{1}{2}\cdot|1\rangle \qquad \hat{S}_z|2\rangle = +\frac{1}{2}\cdot|2\rangle \qquad \hat{S}_z|3\rangle = -\frac{1}{2}\cdot|3\rangle \qquad \hat{S}_z|4\rangle = -\frac{1}{2}\cdot|4\rangle$$

$$\hat{I}_z|1\rangle = +\frac{1}{2}\cdot|1\rangle \qquad \hat{I}_z|2\rangle = -\frac{1}{2}\cdot|2\rangle \qquad \hat{I}_z|3\rangle = +\frac{1}{2}\cdot|3\rangle \qquad \hat{I}_z|4\rangle = -\frac{1}{2}\cdot|4\rangle$$

Atomic hyperfine structure

$$\hat{H}_{\mathrm{hfi}} = h A \underline{\hat{I}} \cdot \underline{\hat{S}} = h A (\hat{I}_x \hat{S}_x + \hat{I}_y \hat{S}_y + \hat{I}_z \hat{S}_z)$$

$$\hat{H}_{\mathrm{hfi}} = h A \left(\hat{I}_z \hat{S}_z + \frac{1}{2} (\hat{I}_+ \hat{S}_- + \hat{I}_- \hat{S}_+) \right)$$

$$\hat{S}_+ |3\rangle = |1\rangle \quad \hat{S}_+ |4\rangle = |2\rangle \quad \hat{S}_- |1\rangle = |3\rangle \quad \hat{S}_- |2\rangle = |4\rangle$$

$$\hat{I}_+ |2\rangle = |1\rangle \quad \hat{I}_+ |4\rangle = |3\rangle \quad \hat{I}_- |1\rangle = |2\rangle \quad \hat{I}_- |3\rangle = |4\rangle$$

S operates on the electronic spin only leaving the nuclear spin state unaffected. Similarly I only operates on the nuclear spin.

$$\hat{I}_+ \hat{S}_- |2\rangle = \hat{I}_+ |4\rangle = |3\rangle \qquad \hat{I}_- \hat{S}_+ |3\rangle = \hat{I}_- |1\rangle = |2\rangle$$

$$\hat{H}_{\mathrm{hfi}} = h A \left(\hat{I}_z \hat{S}_z + \frac{1}{2} (\hat{I}_+ \hat{S}_- + \hat{I}_- \hat{S}_+) \right)$$

Is diagonal with matrix elements $\pm hA/4$

Couples the states $|2\rangle$ and $|3\rangle$ with matrix elements $hA/2$

Note: For quantum mechanical calculations with spins, it is generally vary practical to express the operators S_x, S_y, I_x, I_y in terms of the shift operators S_+, S_-, I_+, I_-. The matrix elements of these operators are easy to evaluate: S_+ shifts a state $|m_S\rangle$ to $|m_S+1\rangle$, unless $|m_S\rangle$ is the highest state. S_- shifts $|m_S\rangle$ to $|m_S-1\rangle$, unless $|m_S\rangle$ is the lowest state.

Atomic hyperfine structure

Matrix elements of the Hamilton operator

$$H = g_e \mu_B B_0 \hat{S}_z - g_n \mu_K B_0 \hat{I}_z + h A \underline{\hat{I}} \cdot \underline{\hat{S}}$$

	$\lvert 1\rangle = \lvert +\frac{1}{2}\ +\frac{1}{2}\rangle$	$\lvert 2\rangle = \lvert +\frac{1}{2}\ -\frac{1}{2}\rangle$	$\lvert 3\rangle = \lvert -\frac{1}{2}\ +\frac{1}{2}\rangle$	$\lvert 4\rangle = \lvert -\frac{1}{2}\ -\frac{1}{2}\rangle$
$\langle 1\rvert = \langle +\frac{1}{2}\ +\frac{1}{2}\rvert$	$\frac{1}{2} g_e \mu_B B_0 - \frac{1}{2} g_n \mu_K B_0 + \frac{hA}{4}$	0	0	0
$\langle 2\rvert = \langle +\frac{1}{2}\ -\frac{1}{2}\rvert$	0	$+\frac{1}{2} g_e \mu_B B_0 + \frac{1}{2} g_n \mu_K B_0 - \frac{hA}{4}$	$\frac{hA}{2}$	0
$\langle 3\rvert = \langle -\frac{1}{2}\ +\frac{1}{2}\rvert$	0	$\frac{hA}{2}$	$-\frac{1}{2} g_e \mu_B B_0 - \frac{1}{2} g_n \mu_K B_0 - \frac{hA}{4}$	0
$\langle 4\rvert = \langle -\frac{1}{2}\ -\frac{1}{2}\rvert$	0	0	0	$-\frac{1}{2} g_e \mu_B B_0 + \frac{1}{2} g_n \mu_K B_0 + \frac{hA}{4}$

Atomic hyperfine structure

The following operators are frequently found in calculations of spin systems:

$$\hat{J}^2, \hat{J}_z, \hat{J}_x, \hat{J}_y, \hat{J}_+, \hat{J}_-$$

The operator symbol J stands for any angular momentum operator like $\underline{L}$, $\underline{S}$, $\underline{I}$, $\underline{J} = \underline{L}+\underline{S}$, $\underline{F} = \underline{J}+\underline{I}$ etc.

The quantum states are written as:

$|Jm_J\rangle$ J is the spin number, m_J the projection of the spin onto the quantisation axis, usually taken as the z-axis.

Fundamental relations for the operators and the states are:

$$\hat{J}^2|Jm_J\rangle = J(J+1)|Jm_J\rangle$$ Diagonal with eigenvalue J(J+1)

$$\hat{J}_z|Jm_J\rangle = m_J|Jm_J\rangle$$ Diagonal with eigenvalue m_J

$$\hat{J}_+|Jm_J\rangle = \sqrt{J(J+1) - m_J(m_J+1)}\,|Jm_J+1\rangle$$ "Shifts" one state up.

$$\hat{J}_-|Jm_J\rangle = \sqrt{J(J+1) - m_J(m_J-1)}\,|Jm_J-1\rangle$$ "Shifts" one state down.

$$\hat{J}_+ = \hat{J}_x + i\hat{J}_y \qquad \hat{J}_- = \hat{J}_x - i\hat{J}_y$$

$$\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-) \qquad \hat{J}_y = \frac{-i}{2}(\hat{J}_+ - \hat{J}_-)$$

Atomic hyperfine structure

Whereas the diagonal operators can easily be calculated, matrix element tables for the operators J_+ and J_- are very convenient for practical quantum mechanical calculations.

J_+, J_-	|-1/2>	|+1/2>
<-1/2|	0	1
<+1/2|	1	0

J_+, J_-	|-1>	| 0>	|+1>
<-1|	0	$\sqrt{2}$	0
< 0|	$\sqrt{2}$	0	$\sqrt{2}$
<+1|	0	$\sqrt{2}$	0

J_+, J_-	|-3/2>	|-1/2>	|+1/2>	|+3/2>
<-3/2|	0	$\sqrt{3}$	0	0
<-1/2|	$\sqrt{3}$	0	$\sqrt{4}$	0
<+1/2|	0	$\sqrt{4}$	0	$\sqrt{3}$
<+3/2|	0	0	$\sqrt{3}$	0

J_+, J_-	|-5/2>	|-3/2>	|-1/2>	|+1/2>	|+3/2>	|+5/2>
<-5/2|	0	$\sqrt{5}$	0	0	0	0
<-3/2|	$\sqrt{5}$	0	$\sqrt{8}$	0	0	0
<-1/2|	0	$\sqrt{8}$	0	$\sqrt{9}$	0	0
<+1/2|	0	0	$\sqrt{9}$	0	$\sqrt{8}$	0
<+3/2|	0	0	0	$\sqrt{8}$	0	$\sqrt{5}$
<+5/2|	0	0	0	0	$\sqrt{5}$	0

J_+, J_-	|-2>	|-1>	| 0>	|+1>	|+2>
<-2|	0	$\sqrt{4}$	0	0	0
<-1|	$\sqrt{4}$	0	$\sqrt{6}$	0	0
< 0|	0	$\sqrt{6}$	0	$\sqrt{6}$	0
<+1|	0	0	$\sqrt{6}$	0	$\sqrt{4}$
<+2|	0	0	0	$\sqrt{4}$	0

Computer laboratory

Computer laboratory - Hyperfine spectra

Task I (1 pt.): Calculate and plot atomic hyperfine spectra (in MHz) of ^{6}Li and ^{85}Rb atoms as a function of the magnetic field strength (between 0 and 2000 Gauss).

Task* II (0.2 pt.): Calculate and plot molecular hyperfine spectrum (in MHz) of a mixture of ^{6}Li and ^{87}Rb atoms as a function of the magnetic field strength (between 0 and 2000 Gauss). Plot spectra for different projections of the total angular momentum M.

Computer laboratory - Hyperfine spectra

Hyperfine coupling constants are: $A_{^6\mathrm{Li}}$=152.1 MHz, $A_{^{85}\mathrm{Rb}}$=1011.9 MHz

$S_{^6\mathrm{Li}}=S_{^{85}\mathrm{Rb}}=\frac{1}{2}$

$I_{^6\mathrm{Li}}=1$, $I_{^{85}\mathrm{Rb}}=\frac{5}{2}$

Electron and nuclear g factors are: g_e=2.002319, $g_N(^6\mathrm{Li})$=-0.000447, $g_N(^{85}\mathrm{Rb})$=-0.000294

Bohr magneton: $\mu_B = \frac{e\hbar}{2m_e}$. Nuclear magneton: $\mu_N = \frac{e\hbar}{2m_p}$.

$m_p = 1836.15 m_e$

Use atomic units: $\hbar=m_e=e=1$ in calculations.