

Lectures on quantum gases

Lecture 4

Cold Collisions

Atoms with internal structure

Jook Walraven

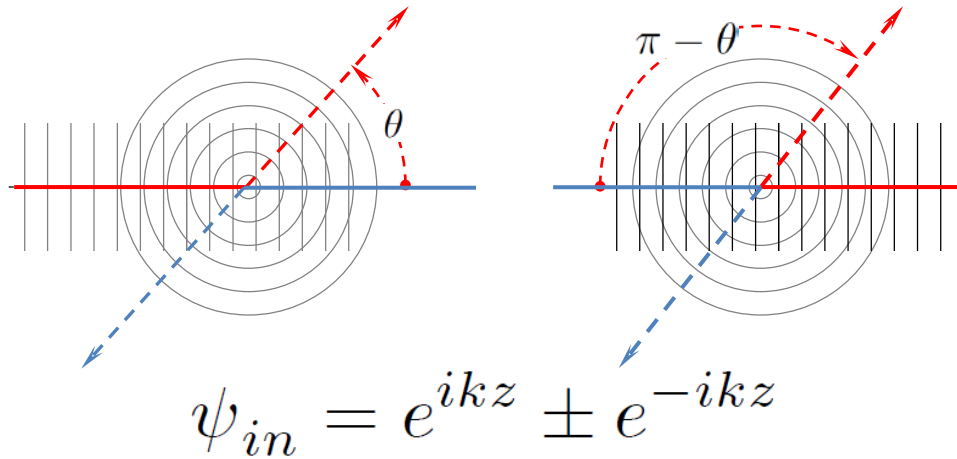
University of Amsterdam

Lecture notes:

<https://staff.fnwi.uva.nl/j.t.m.walraven/walraven/JookWalraven.htm>

Identical atoms

Identical atoms



Bosons: symmetric under exchange

Fermions: antisymmetric under exchange

$$\psi_{sc} \underset{r \rightarrow \infty}{\simeq} [f(\theta) \pm f(\pi - \theta)] e^{ikr} / r$$

$$\psi \underset{r \rightarrow \infty}{\simeq} (e^{ikz} \pm e^{-ikz}) + [f(\theta) \pm f(\pi - \theta)] e^{ikr} / r$$

Identical atoms

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

$$e^{-ikz} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(-\cos \theta) \quad \left. \vphantom{\sum_{l=0}^{\infty}} \right\} \begin{array}{l} P_l(-u) = (-1)^l P_l(u) \end{array}$$

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

$$\psi_{in} = e^{ikz} \pm e^{-ikz} = 2 \sum_{l=\substack{even \\ odd}}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos \theta)$$

Conclusion: Bosons *even* partial waves; fermions *odd* partial waves

scattered waves

similar for scattered waves:

$$\psi_{sc} \underset{r \rightarrow \infty}{\simeq} \frac{e^{ikr}}{kr} \sum_{l=0}^{\infty} (2l+1) e^{i\eta_l} \sin \eta_l [1 \pm (-1)^l] P_l(\cos \theta)$$

$$f_{\pm}(\theta) \equiv f(\theta) \pm f(\pi - \theta) = \frac{2}{k} \sum_{l=\text{even/odd}} (2l+1) e^{i\eta_l} P_l(\cos \theta) \sin \eta_l$$

unlike atoms: $f(\theta) \simeq f_0 \simeq -a$

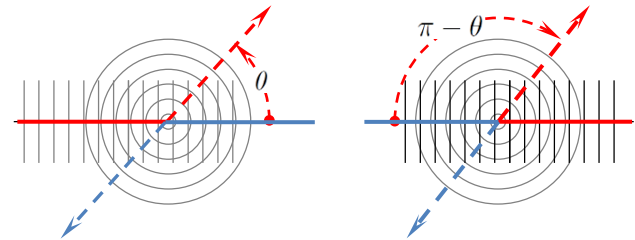
identical bosons: $f(\theta) + f(\pi - \theta) \simeq 2f_0 \simeq -2a$

identical fermions: $f(\theta) - f(\pi - \theta) \simeq 6f_1 \cos \theta \simeq -2a_1 (ka_1)^2 \cos \theta$

cross section

Differential cross section:

$$\frac{d\sigma_{\pm}(\theta, \phi)}{d\Omega} = |f(\theta) \pm f(\pi - \theta)|^2$$



$$\sigma_{\pm} = \int_0^{\pi/2} 2\pi \sin \theta |f(\theta) \pm f(\pi - \theta)|^2 d\theta$$

$$= 8\pi \sum_{l, l' = \text{even/odd}} (2l' + 1)(2l + 1) f_{l'}^* f_l \int_0^{\pi/2} P_{l'}(\cos \theta) P_l(\cos \theta) \sin \theta d\theta$$

$$= 8\pi \sum_{l = \text{even/odd}} (2l + 1)^2 |f_l|^2 \int_0^{\pi/2} [P_l(\cos \theta)]^2 \sin \theta d\theta$$

$$= 8\pi \sum_{l = \text{even/odd}} (2l + 1) |f_l|^2$$

$$\sigma_{\pm} = \frac{8\pi}{k^2} \sum_{l = \text{even/odd}} (2l + 1) \sin^2 \eta_l$$

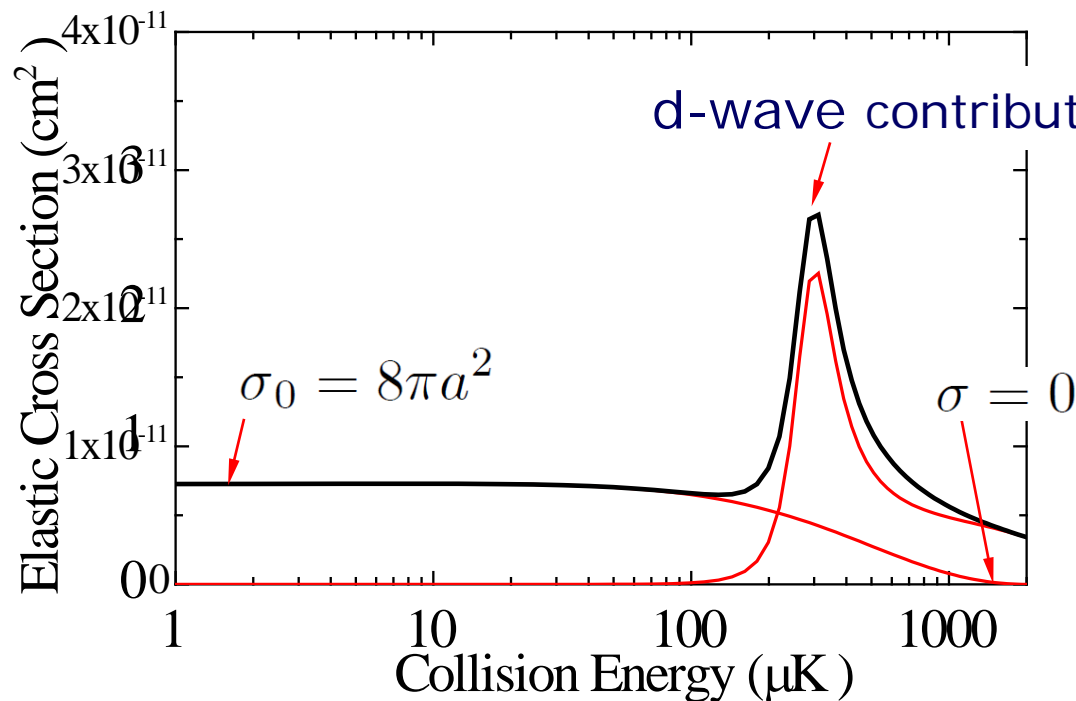
$$\sigma = \frac{8\pi}{k^2} \sin^2 \eta_0 \underset{k \rightarrow 0}{\approx} 8\pi a^2$$

$$\sigma = \frac{8\pi}{k^2} 3 \sin^2 \eta_1 \underset{k \rightarrow 0}{\approx} 8\pi a_1^2 (ka_1)^4$$

properties of elastic cross section

Bosons: s-wave scattering (low-energy limit)

$$\sigma_{\pm} = \frac{8\pi}{k^2} \sum_{l=\text{even/odd}} (2l+1) \sin^2 \eta_l \xrightarrow{\quad} \sigma_0 = \frac{8\pi}{k^2} \sin^2 \eta_0 \xrightarrow{\eta_0 = -ka} \sigma_0 = \frac{8\pi}{k^2} \sin^2 ka$$



$\eta_0 \rightarrow \pi$

$k \rightarrow 0$

$$\sigma = 0$$

$$\sigma_0 = 8\pi a^2$$

First Ramsauer minimum

NO p-wave !

atoms with internal structure

Schrödinger equation

$$\left[\frac{1}{2\mu} \left(p_r^2 + \frac{\mathbf{L}^2}{r^2} \right) + \mathcal{V}(r) \right] \psi(r, \theta, \phi) = E \psi(r, \theta, \phi)$$

thus far: fixed potential

What happens if we add internal structure?

First we recapitulate:

\mathbf{L}^2, L_z commute with r and p_r

separation of variables: $\psi = R_l(r) Y_l^m(\theta, \phi)$

$$\mathbf{L}^2 Y_l^m(\theta, \phi) = l(l+1)\hbar^2 Y_l^m(\theta, \phi)$$

$$L_z Y_l^m(\theta, \phi) = m\hbar Y_l^m(\theta, \phi).$$

$$\left[\frac{\hbar^2}{2\mu} \left(-\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} \right) + \underbrace{\frac{l(l+1)\hbar^2}{2\mu r^2}}_{\mathcal{V}_{\text{eff}}(r)} + \mathcal{V}(r) \right] R_l(r) = E R_l(r)$$

good for systems like helium

Interactions between alkali atoms

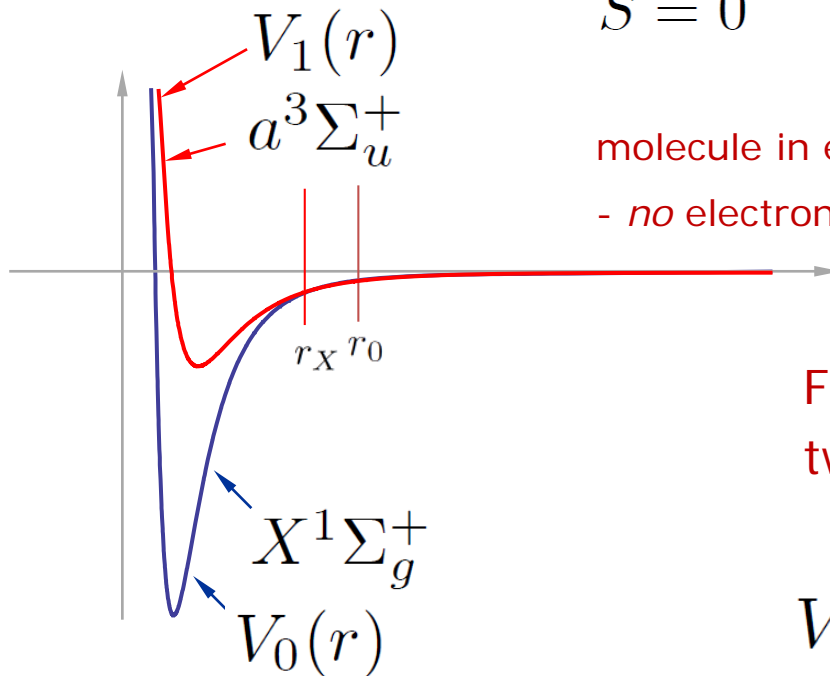
$$\mathbf{S} = \mathbf{s}_1 + \mathbf{s}_2$$



$$S = 0$$



$$S = 1$$



molecule in electronic ground state

- no electronic angular momentum: $\Lambda = 0$

For two ground-state alkali atoms
two (not more than two) potentials

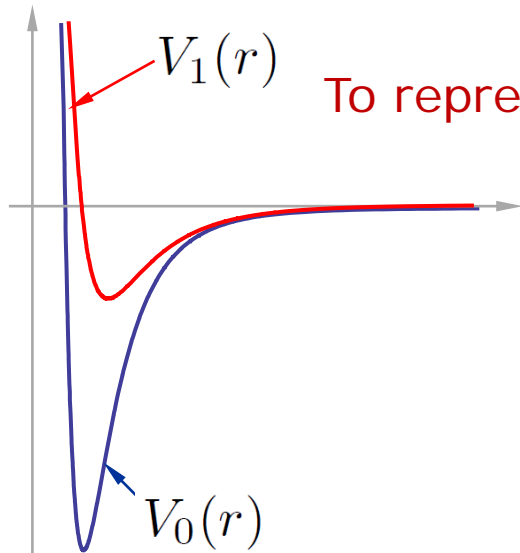
$$V_S(r) \rightarrow \begin{cases} S = 1 & V_1(r) & \text{triplet} \\ S = 0 & V_0(r) & \text{singlet} \end{cases}$$

Conclusion: exchange determines interatomic interaction

To solve Schrödinger equation

we turn to the basis: $|\psi\rangle = |R_l\rangle |lm_l; \psi_e\rangle |S, M_S\rangle$

Interactions between alkali atoms



To represent exchange we construct a *spin hamiltonian*:

$$\mathcal{V}(r) = V_D(r) + J(r)\mathbf{s}_1 \cdot \mathbf{s}_2$$

$$J(r) = V_1(r) - V_0(r)$$

$$V_D(r) = \frac{1}{4}[V_0(r) + 3V_1(r)]$$

$$\mathbf{s}_1 \cdot \mathbf{s}_2 = \frac{1}{2} (\mathbf{S}^2 - \mathbf{s}_1^2 - \mathbf{s}_2^2)$$

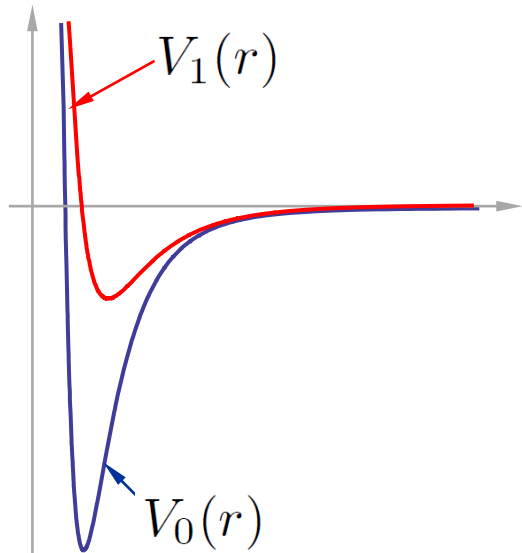
Properties of operator $\mathcal{V}(r)$:

$$\left. \begin{aligned} \mathcal{V}(r) |0, 0\rangle &= V_0(r) |0, 0\rangle \\ \mathcal{V}(r) |1, M_S\rangle &= V_1(r) |1, M_S\rangle \end{aligned} \right\} \rightarrow \mathcal{V}(r) |S, M_S\rangle = V_S(r) |S, M_S\rangle$$

Hamiltonian including exchange:

$$\mathcal{H} = \frac{1}{2\mu} \left(p_r^2 + \frac{\mathbf{L}^2}{r^2} \right) + \mathcal{V}(r)$$

Interactions between alkali atoms



Let us add magnetic field:

$$\mathcal{H}_Z = \gamma_e \mathbf{s}_1 \cdot \mathbf{B} + \gamma_e \mathbf{s}_2 \cdot \mathbf{B} = \gamma_e \mathbf{S} \cdot \mathbf{B} = \gamma_e B S_z$$

$$\gamma_e = g_s \mu_B / \hbar$$

$$\Delta E_Z = g_s \mu_B B M_S$$

$$M_S = m_{s_1} + m_{s_2} \text{ is good quantum number}$$

$$\mathbf{s}_1 \cdot \mathbf{s}_2 = \frac{1}{2} (\mathbf{S}^2 - \mathbf{s}_1^2 - \mathbf{s}_2^2)$$

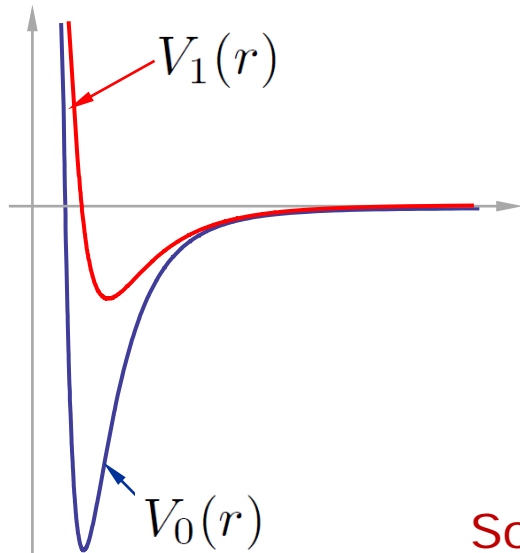
$$\mathbf{s}_1 \cdot \mathbf{s}_2 = s_{1z} s_{2z} + \frac{1}{2} (s_1^+ s_2^- + s_1^- s_2^+)$$

Hamiltonian including spin Zeeman term:

$$\mathcal{H} = \frac{1}{2\mu} \left(p_r^2 + \frac{\mathbf{L}^2}{r^2} \right) + \mathcal{V}(r) + \gamma_e B S_z$$

good basis states: $|\psi\rangle = |R_l^S\rangle |l, m_l\rangle |S, M_S\rangle$

Interactions between alkali atoms



Hamiltonian including spin Zeeman term:

$$\mathcal{H} = \frac{1}{2\mu} \left(p_r^2 + \frac{\mathbf{L}^2}{r^2} \right) + \mathcal{V}(r) + \gamma_e B S_z$$

$\mathcal{V}(r) = V_D(r) + J(r)\mathbf{s}_1 \cdot \mathbf{s}_2$

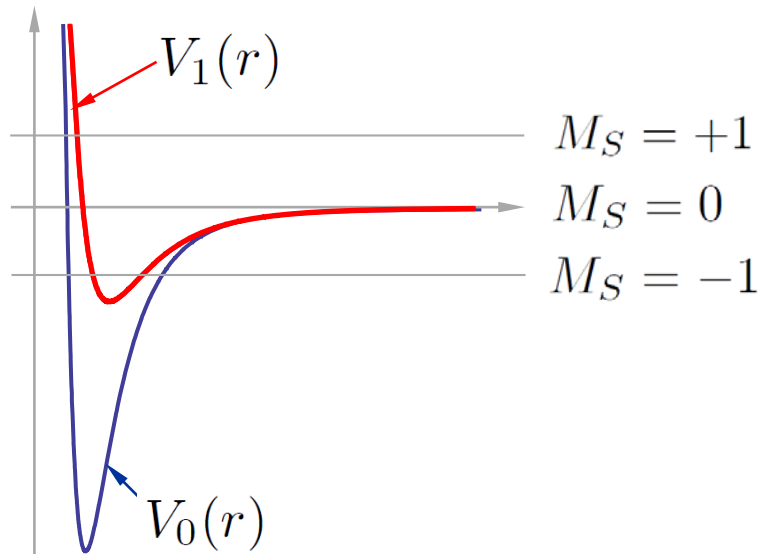
good basis states: $|\psi\rangle = |R_l^S\rangle |l, m_l\rangle |S, M_S\rangle$

Solve radial wave equation for given l , S and M_S :

$$R''_{S,l} + \frac{2}{r} R'_{S,l} + [\varepsilon - U_{S,l}(r)] R_{S,l} = 0$$

$$U_{S,l}(r) = U_S(r) + \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2} \gamma_e B M_S$$

Interactions between alkali atoms

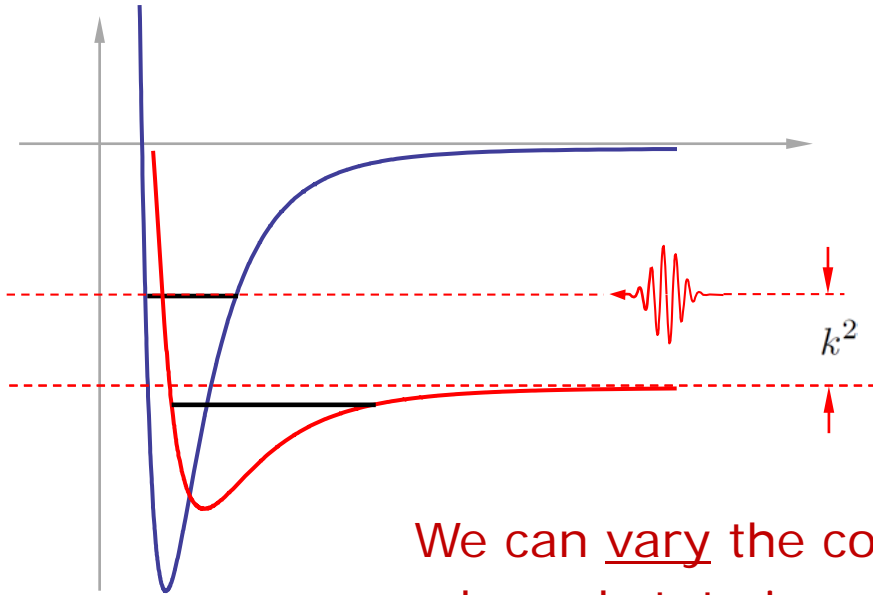


magnetic field lifts degeneracy of triplet potential

$$U_{S,l}(r) = U_S(r) + \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2} \gamma_e B M_S$$

This makes it possible to shift the triplet potential with respect to the singlet potential

Feshbach resonance

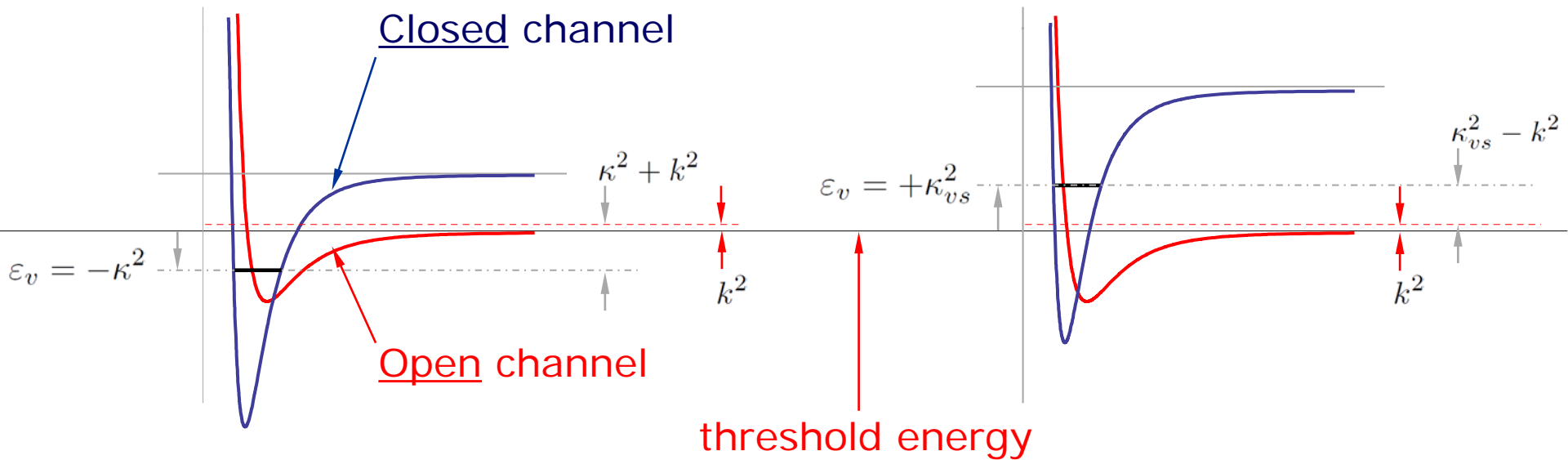


We can vary the collision energy to be resonant with a bound state in a closed channel

Any weak singlet-triplet coupling induces a scattering resonance in the open channel: Feshbach resonance

With cold alkali atoms we can tune to a Feshbach resonance at arbitrary, fixed (low) collisional energy by varying the magnetic field: Zeeman tuning

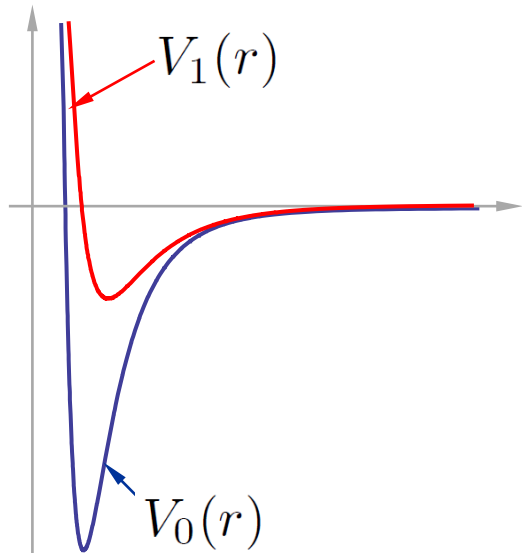
some nomenclature



Closed channel **below** threshold

Closed channel **above** threshold

Interactions between two alkali atoms



Solve radial wave equation for given l , S and M_S :

$$R''_{S,l} + \frac{2}{r} R'_{S,l} + [\varepsilon - U_{S,l}(r)] R_{S,l} = 0$$

$$U_{S,l}(r) = U_S(r) + \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2} \gamma_e B M_S$$

Solutions for given l , S and M_S :

Continuum states $\varepsilon > 0$: $\varepsilon_k = k^2 + \frac{2\mu}{\hbar^2} \gamma_e B M_S$

Bound states $\varepsilon < 0$: $\varepsilon_{v,l}^S = -\kappa_{v,S}^2 + l(l+1) \mathcal{R}_{v,l}^S + \frac{2\mu}{\hbar^2} \gamma_e B M_S$

\uparrow
 $\mathcal{R}_{v,l}^S = \langle R_{v,l}^S | r^{-2} | R_{v,l}^S \rangle$

Interactions between two alkali atoms

Hamiltonian including spin Zeeman term:

$$\mathcal{H} = \frac{1}{2\mu} \left(p_r^2 + \frac{\mathbf{L}^2}{r^2} \right) + \overset{\mathcal{V}(r) = V_D(r) + J(r)\mathbf{s}_1 \cdot \mathbf{s}_2}{\mathcal{V}(r)} + \gamma_e B S_z - (\gamma_1 i_{z1} + \gamma_2 i_{z2}) B$$

Add nuclear Zeeman terms (*unlike* atoms):

$$\mathcal{H}_Z = -\gamma_1 \mathbf{i}_1 \cdot \mathbf{B} - \gamma_2 \mathbf{i}_2 \cdot \mathbf{B}$$

$$\Delta E_Z = -(\gamma_1 m_1 + \gamma_2 m_2) B$$

Good basis states: $|\psi\rangle = |R_l^S\rangle |l, m_l\rangle |S, M_S\rangle |i_1, m_1\rangle |i_2, m_2\rangle$

Effective potential (including rotational and magnetic shifts):

$$U_{S,l}(r) = U_S(r) + \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2} [\gamma_e B M_S - (\gamma_1 m_1 + \gamma_2 m_2) B]$$

Interactions between two alkali atoms

Hamiltonian including spin Zeeman term:

$$\mathcal{H} = \frac{1}{2\mu} \left(p_r^2 + \frac{\mathbf{L}^2}{r^2} \right) + \overset{\mathcal{V}(r) = V_D(r) + J(r)\mathbf{s}_1 \cdot \mathbf{s}_2}{\mathcal{V}(r)} + \gamma_e B S_z - \gamma_n B I_z$$

Add nuclear Zeeman terms (*identical* atoms):

$$\mathbf{I} = \mathbf{i}_1 + \mathbf{i}_2 \quad M_I = m_1 + m_2$$

$$\mathcal{H}_Z = -\gamma_n \mathbf{i}_1 \cdot \mathbf{B} - \gamma_n \mathbf{i}_2 \cdot \mathbf{B} = -\gamma_n \mathbf{I} \cdot \mathbf{B}$$

Good basis states: $|\psi\rangle = |R_l^{S,I}\rangle |l, m_l\rangle |S, M_S\rangle |I, M_I\rangle$

Effective potential (including rotational and magnetic shifts):

$$U_{S,l}(r) = U_S(r) + \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2} [\gamma_e B M_S - \gamma_n B M_I]$$

Interactions between two alkali atoms

Add hyperfine interactions (*unlike* atoms):

$$\mathcal{H}_{\text{hf}} = \frac{a_1}{\hbar^2} \mathbf{i}_1 \cdot \mathbf{s}_1 + \frac{a_2}{\hbar^2} \mathbf{i}_2 \cdot \mathbf{s}_2$$

Is $M_F = M_S + M_I$ still a good quantum number?

$$\begin{array}{ccc} \downarrow & \downarrow & \\ M_I = m_1 + m_2 & & \\ \downarrow & & \\ M_S = m_{s_1} + m_{s_2} & & \end{array}$$

Answer: yes!

$$\mathbf{i} \cdot \mathbf{s} = i_z s_z + \frac{1}{2} (i_+ s_- + i_- s_+)$$

Is S still a good quantum number?

$$\begin{aligned} \mathcal{H}_{\text{hf}} &= \mathcal{H}_{\text{hf}}^+ + \mathcal{H}_{\text{hf}}^- \\ \mathcal{H}_{\text{hf}}^\pm &= \frac{a_1}{2\hbar^2} \mathbf{i}_1 \cdot (\mathbf{s}_1 \pm \mathbf{s}_2) \pm \frac{a_2}{2\hbar^2} \mathbf{i}_2 \cdot (\mathbf{s}_1 \pm \mathbf{s}_2) \end{aligned}$$

Interactions between two alkali atoms

Is S still a good quantum number?

$$\mathcal{H}_{\text{hf}} = \mathcal{H}_{\text{hf}}^+ + \mathcal{H}_{\text{hf}}^-$$

$$\mathcal{H}_{\text{hf}}^{\pm} = \frac{a_1}{2\hbar^2} \mathbf{i}_1 \cdot (\mathbf{s}_1 \pm \mathbf{s}_2) \pm \frac{a_2}{2\hbar^2} \mathbf{i}_2 \cdot (\mathbf{s}_1 \pm \mathbf{s}_2)$$

$$\mathcal{H}_{\text{hf}}^+ = \frac{a_1}{2\hbar^2} \mathbf{i}_1 \cdot \mathbf{S} + \frac{a_2}{2\hbar^2} \mathbf{i}_2 \cdot \mathbf{S}$$

identical atoms

\longrightarrow $\boxed{\mathcal{H}_{\text{hf}}^+ = \frac{a_1}{2\hbar^2} \mathbf{I} \cdot \mathbf{S}}$ $\mathcal{H}_{\text{hf}}^+$ can change M_S but not S and M_F

$$\mathbf{I} \cdot \mathbf{S} = I_z S_z + \frac{1}{2}(I_+ S_- + I_- S_+)$$

$$\mathbf{I} \cdot \mathbf{S} = \frac{1}{2}(\mathbf{F}^2 - \mathbf{I}^2 - \mathbf{S}^2) \quad \mathbf{F} = \mathbf{I} + \mathbf{S}$$

With $\mathcal{H}_{\text{hf}}^+$ in hamiltonian S remains a good quantum number!

Analysis shows that $\mathcal{H}_{\text{hf}}^-$ converts singlet in triplet and vice versa

Interactions between two alkali atoms

Hamiltonian including spin Zeeman term:

$$\mathcal{H} = \frac{1}{2\mu} \left(p_r^2 + \frac{\mathbf{L}^2}{r^2} \right) + \overset{\mathcal{V}(r) = V_D(r) + J(r)\mathbf{s}_1 \cdot \mathbf{s}_2}{\mathcal{V}(r)} + \gamma_e B S_z - \underbrace{(\gamma_1 i_{z1} + \gamma_2 i_{z2}) B}_{(-\gamma_n B I_z)} + \mathcal{H}_{\text{hf}}^+ + \mathcal{H}_{\text{hf}}^-$$

all terms conserve M_F

*only term
not singlet/triplet conserving*

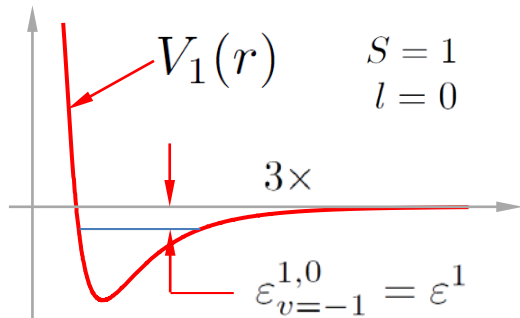
Good basis states: $|\psi\rangle = |R_l^S\rangle |l, m_l\rangle |S, M_S\rangle |i_1, m_1\rangle |i_2, m_2\rangle$

$$|\psi\rangle = |R_l^{S,I}\rangle |l, m_l\rangle |S, M_S\rangle |I, M_I\rangle$$

Effective potential:

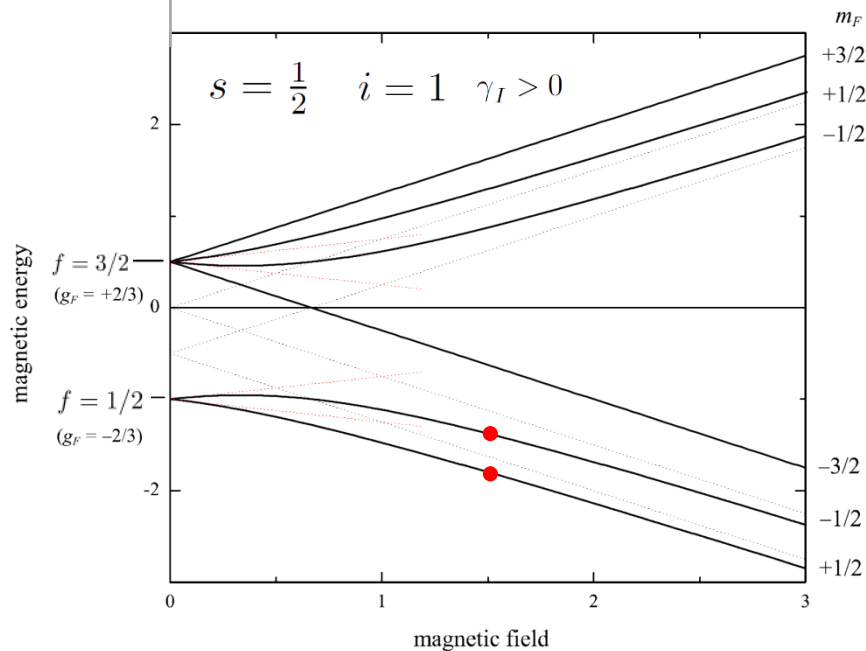
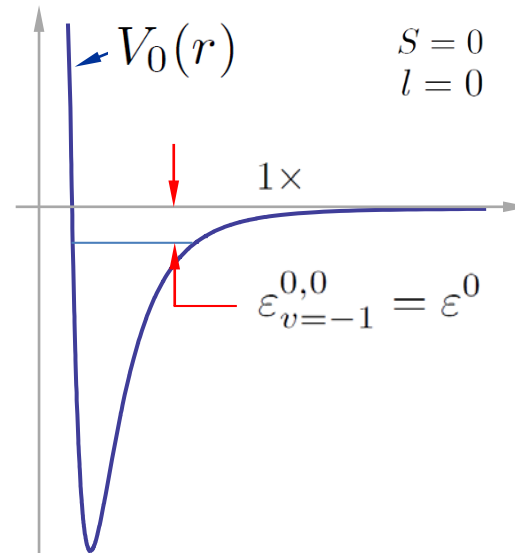
$$U_{S,l}(r) = U_S(r) + \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2} [\gamma_e B M_S - \underbrace{(\gamma_1 m_1 + \gamma_2 m_2) B}_{(-\gamma_n B M_I)}]$$

Example: two ${}^6\text{Li}$ atoms



$\gamma_I > 0$

$s = \frac{1}{2} \quad i = 1 \rightarrow f = \frac{1}{2}, \frac{3}{2}$



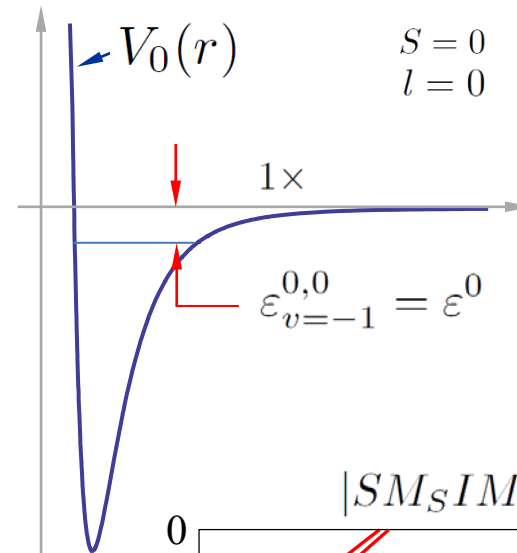
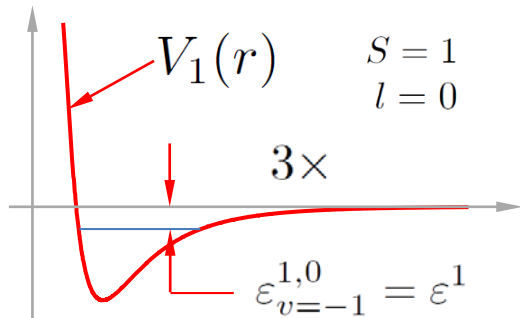
Find all s-wave molecules with $M_F=0$

$S=0 \left\{ \begin{array}{l} I=0,2 \\ I=1 \end{array} \right. X^1\Sigma_g^+ \quad \begin{array}{l} l=0,2,4,\dots \\ l=1,3,5,\dots \end{array}$

$S=1 \left\{ \begin{array}{l} I=0,2 \\ I=1 \end{array} \right. a^3\Sigma_u^+ \quad \begin{array}{l} l=1,3,5,\dots \\ l=0,2,4,\dots \end{array}$

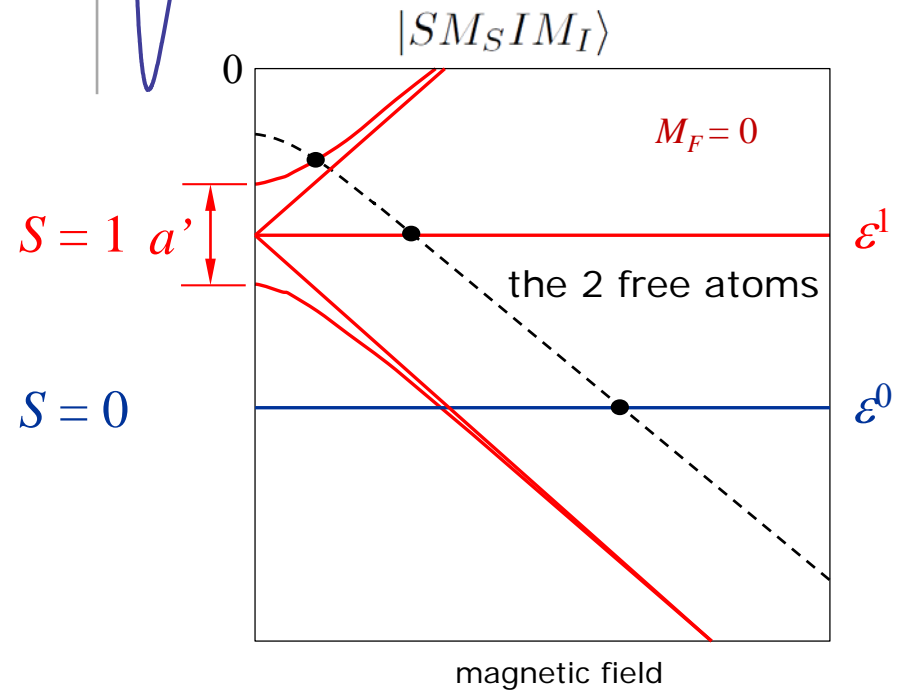
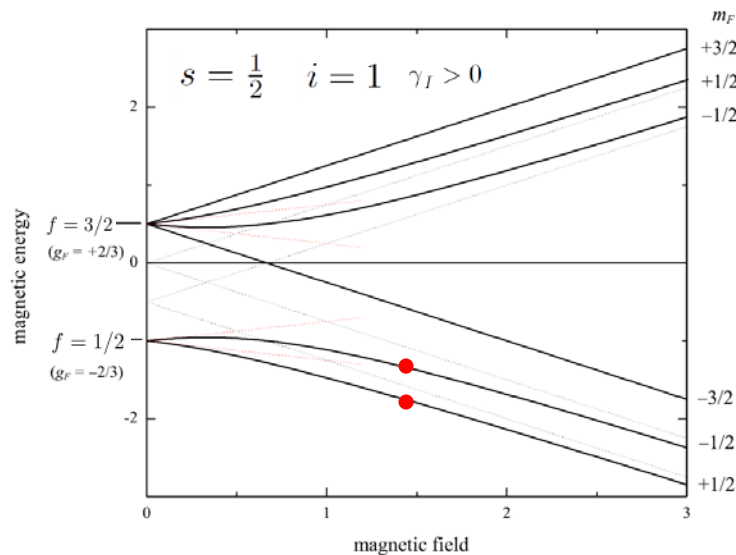
→ free atom pair with $M_F=0$

Example: two ${}^6\text{Li}$ atoms

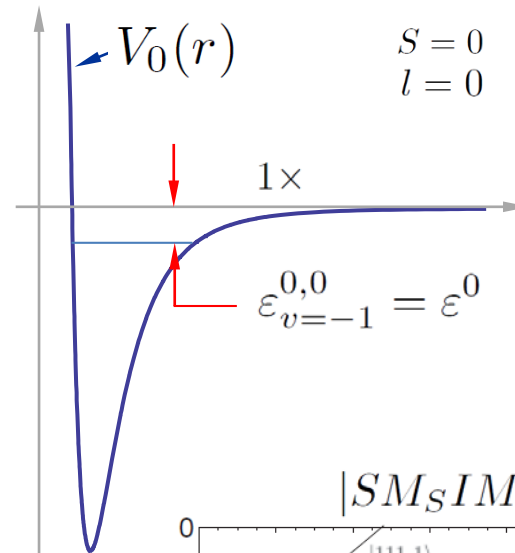
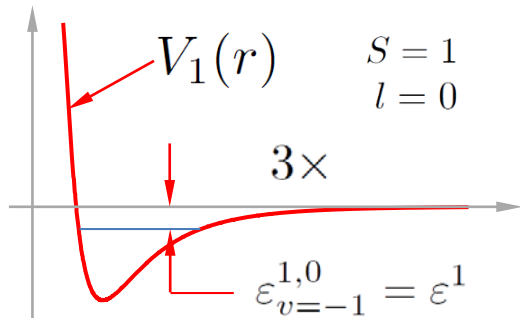


$M_F=0$

$$\begin{array}{l}
 S=0 \left\{ \begin{array}{l} I=0,2 \\ I=1 \end{array} \right. X^1\Sigma_g^+ \quad \begin{array}{l} l=0,2,4,\dots \\ l=1,3,5,\dots \end{array} \\
 S=1 \left\{ \begin{array}{l} I=0,2 \\ I=1 \end{array} \right. a^3\Sigma_u^+ \quad \begin{array}{l} l=1,3,5,\dots \\ l=0,2,4,\dots \end{array}
 \end{array}$$

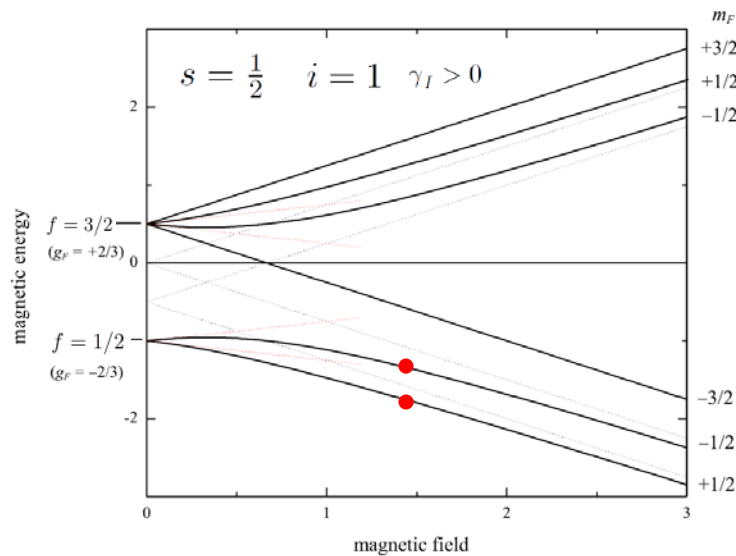


Example: two ${}^6\text{Li}$ atoms



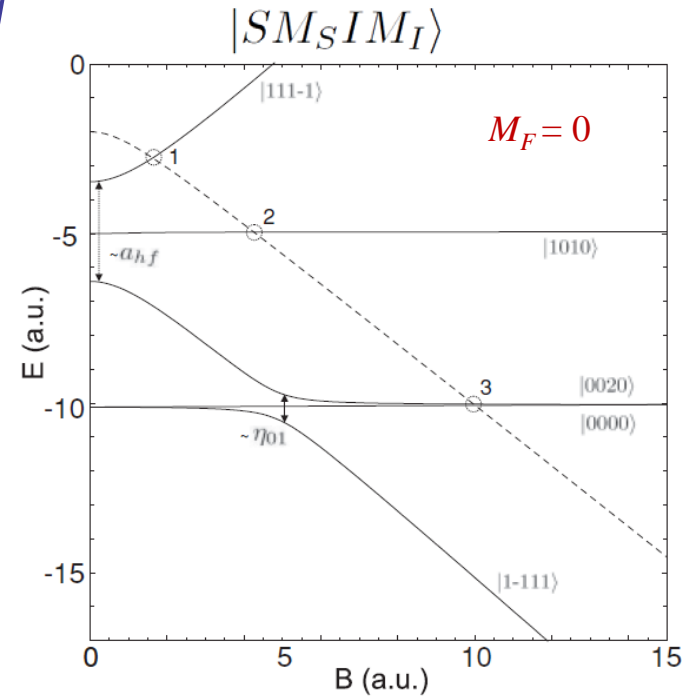
$M_F=0$

$$\begin{array}{l}
 S=0 \left\{ \begin{array}{l} I=0,2 \\ I=1 \end{array} \right. X^1\Sigma_g^+ \quad \begin{array}{l} l=0,2,4,\dots \\ l=1,3,5,\dots \end{array} \\
 S=1 \left\{ \begin{array}{l} I=0,2 \\ I=1 \end{array} \right. a^3\Sigma_u^+ \quad \begin{array}{l} l=1,3,5,\dots \\ l=0,2,4,\dots \end{array}
 \end{array}$$



$S=1$

$S=0$



Atoms with internal structure

1. We symmetrized the pair wavefunction
2. We found that identical atoms scatter according to even or odd partial waves
3. We derived the expression for the cross section
4. We introduce spin in the atoms
5. We found triplet and singlet potentials
6. We searched for terms coupling the singlet and triplet potentials
7. We found that Part of HF interaction is non-singlet-triplet conserving
8. We found that MF remains a good quantum number
9. We studied the magnetic structure of the pairs
10. We know where to search for Feshbach resonances