Lectures on quantum gases

Lecture 4

Collisions between atoms
(role of internal structure)

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

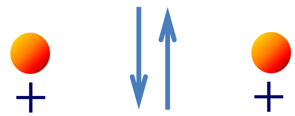
$$\mathbf{L}^2\,Y_l^m(\theta,\phi)=l(l+1)\hbar^2\,Y_l^m(\theta,\phi)$$
$$L_z\,Y_l^m(\theta,\phi)=m\hbar\,Y_l^m(\theta,\phi).$$

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

good for systems like helium

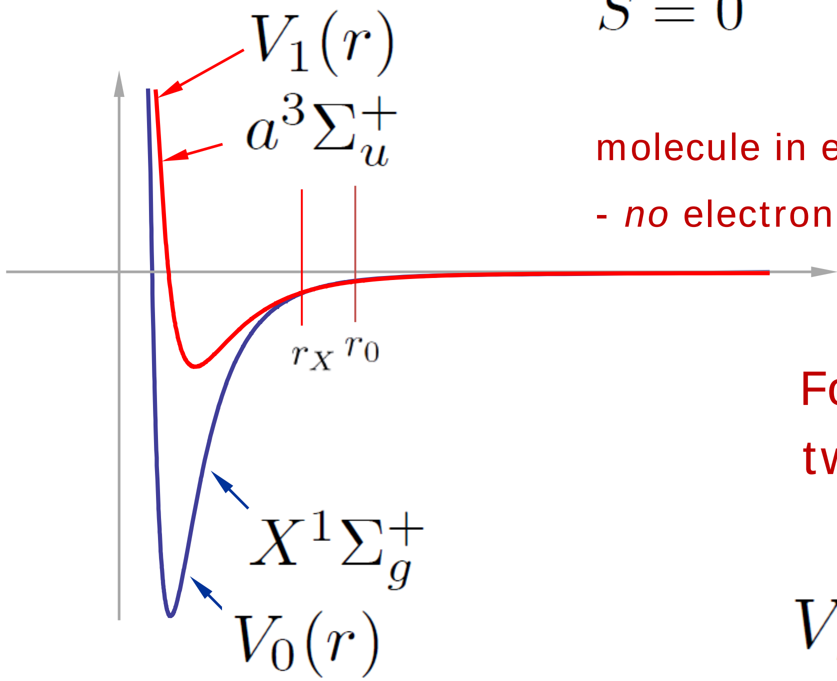
Interactions between alkali atoms

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



$S = 0$

$S = 1$



molecule in electronic ground state

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

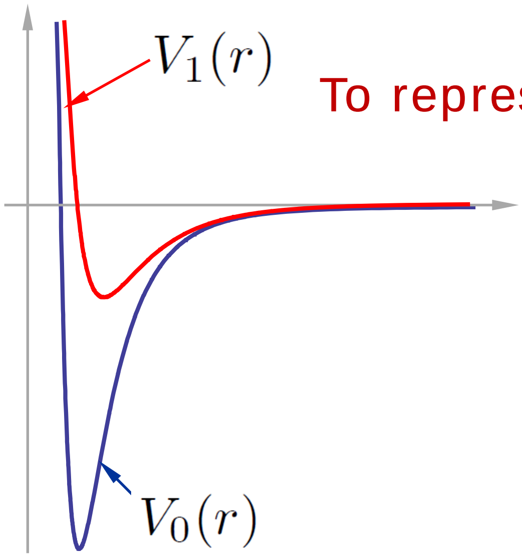
For two ground-state alkali atoms
two (not more than two) potentials

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

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*:

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

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

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

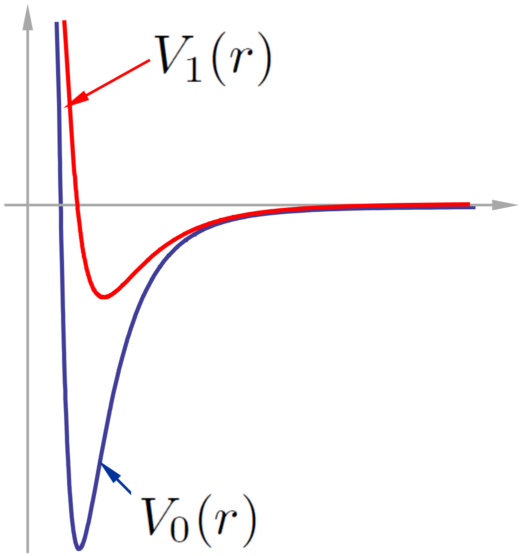
$$\boxed{\mathbf{s}_1 \cdot \mathbf{s}_2 = \tfrac{1}{2}\left(\mathbf{S}^2 - \mathbf{s}_1^2 - \mathbf{s}_2^2\right)}$$

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

Interactions between alkali atoms



Let us add magnetic field:

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

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

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

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

$$\boxed{\mathbf{s}_1 \cdot \mathbf{s}_2 = \tfrac{1}{2}\left(\mathbf{S}^2 - \mathbf{s}_1^2 - \mathbf{s}_2^2\right)}$$

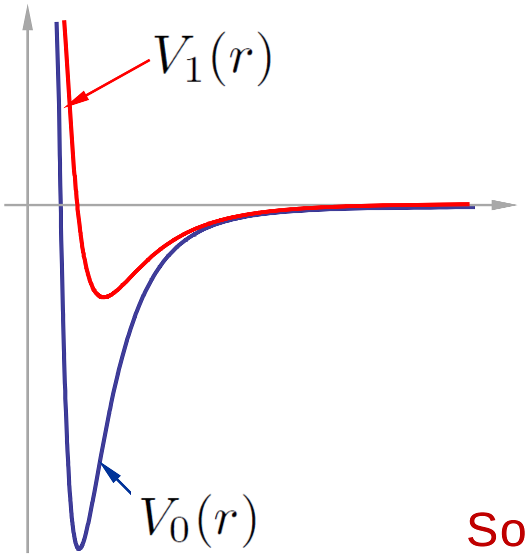
$$\boxed{\mathbf{s}_1 \cdot \mathbf{s}_2 = s_{1z} s_{2z} + \tfrac{1}{2}(s_1^+ s_2^- + s_1^- s_2^+)}$$

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:

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

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

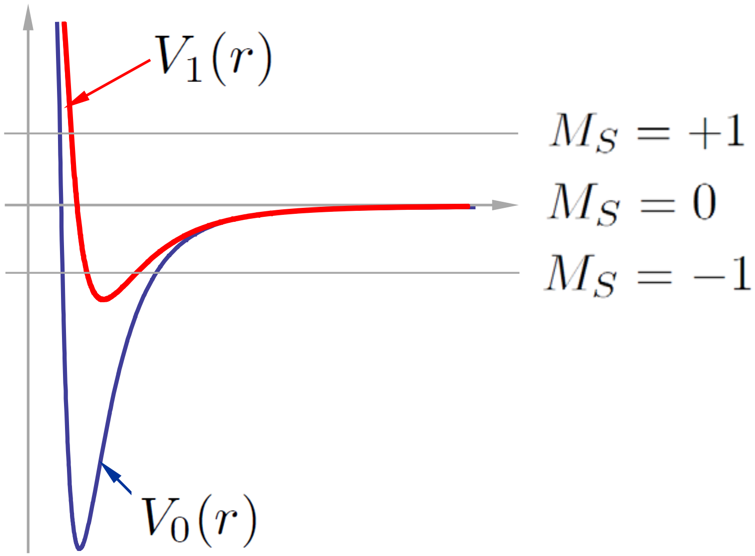
good basis states: $|\psi\rangle = |R^S_{v,l}\rangle|S, M_S\rangle|l, m_l\rangle$

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

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

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

Interactions between alkali atoms

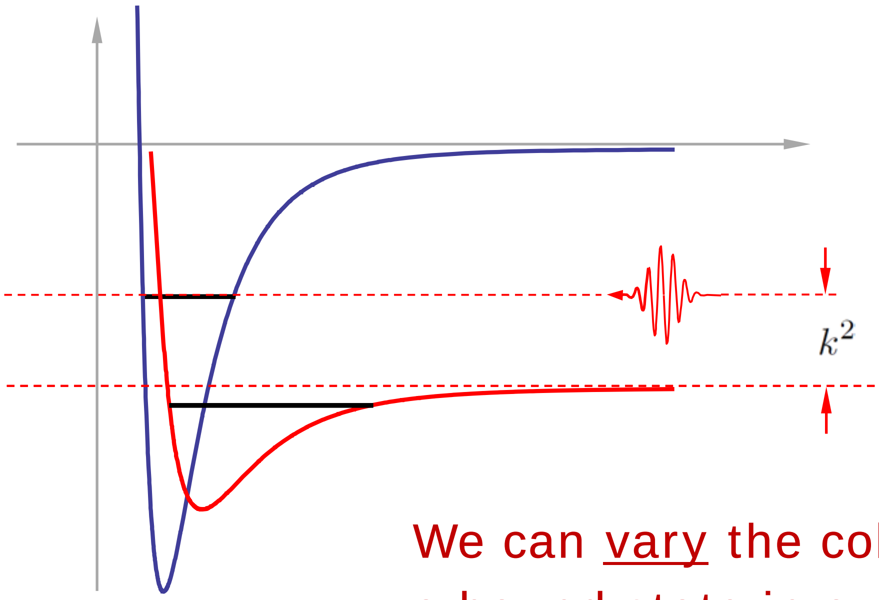


magnetic field lifts degeneracy of triplet potential

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

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

Feshbach resonance

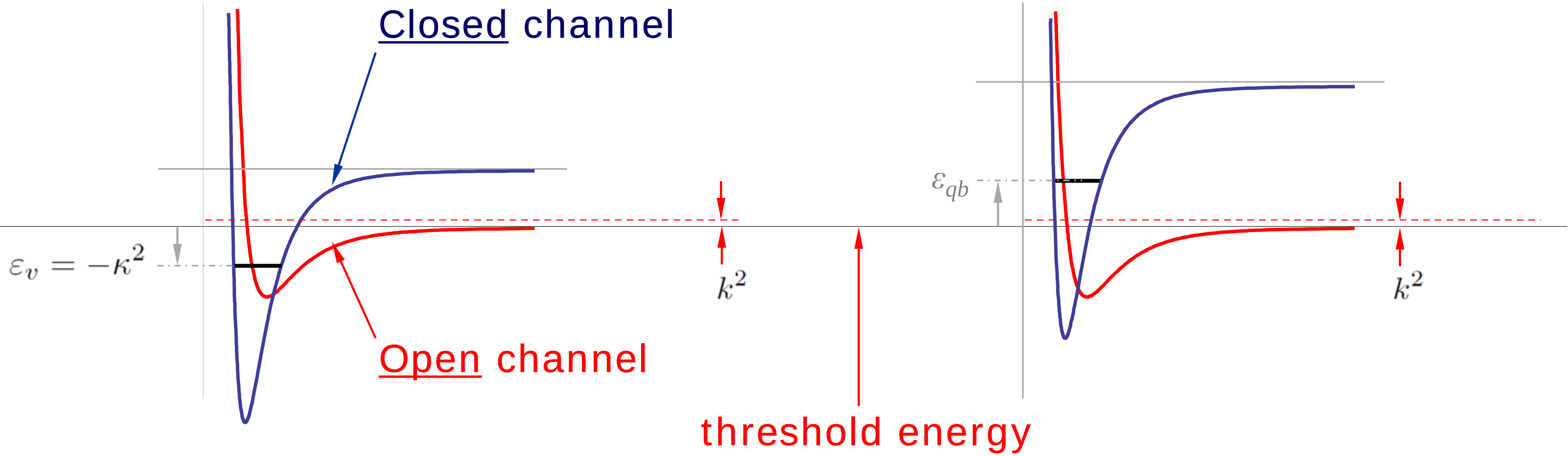


We can <u>vary</u> the collision energy to be resonant with a bound state in a closed channel

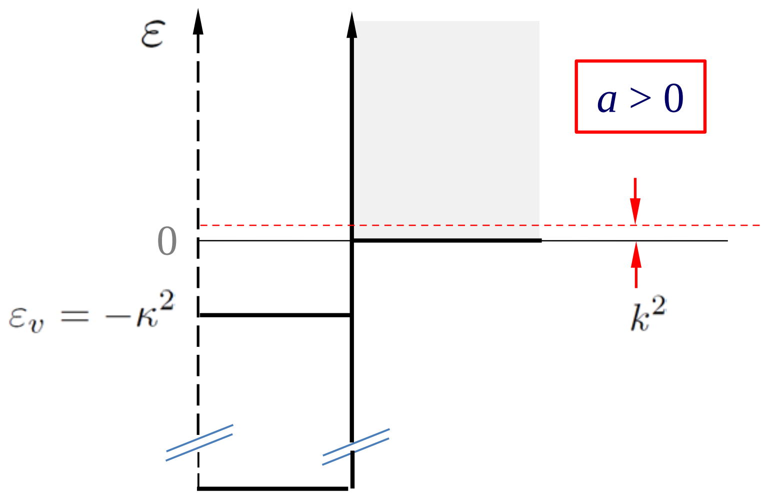
Any weak singlet-triplet coupling induces a scattering resonance in the open channel: Feshbach resonance

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

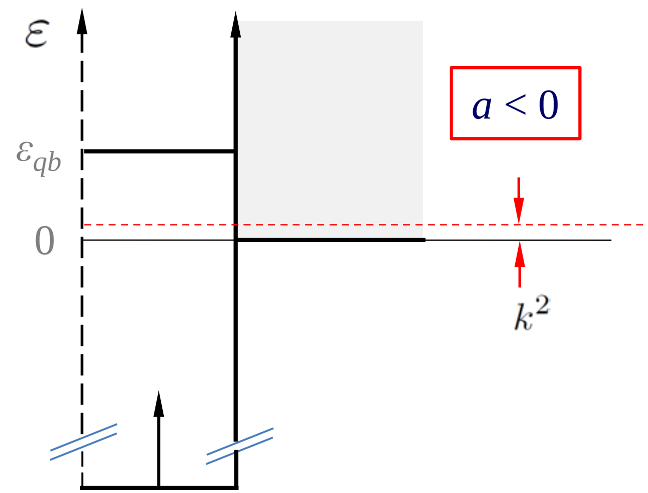
some nomenclature



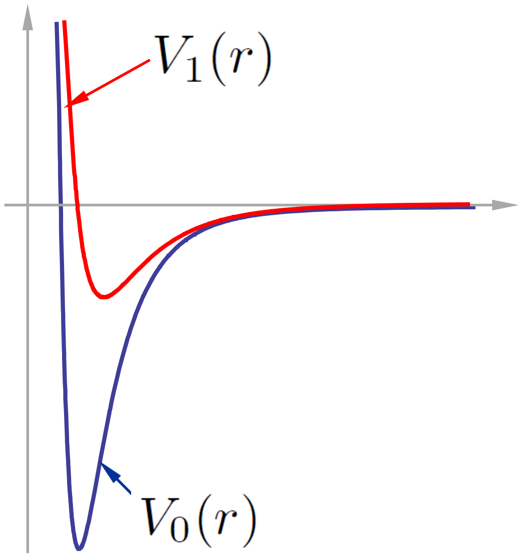
Closed channel: below threshold



Closed channel: above threshold



Interactions between two alkali atoms



$$\mathcal{H} = \underbrace{\frac{1}{2\mu}\left(p_r^2 + \frac{\mathbf{L}^2}{r^2}\right) + \mathcal{V}(r)}_{\mathcal{H}_0} + \gamma_e B\, S_z$$

$$|\psi\rangle = |R_{v,l}^S\rangle |S, M_S\rangle |l, m_l\rangle$$

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

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

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

Solutions for given l, S and M_S :

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

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

$$\langle R_{v,l}^S | \mathcal{H}_0 | R_{v,l}^S \rangle \qquad \mathcal{R}_{v,l}^S = \langle R_{v,l}^S | r^{-2} | R_{v,l}^S \rangle$$

Interactions between two alkali atoms

Hamiltonian including spin Zeeman term:

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

$$\mathcal{H} = \frac{1}{2\mu}\left(p_r^2 + \frac{\mathbf{L}^2}{r^2}\right) + \mathcal{V}(r) + \gamma_e B\, S_z - (\gamma_1 i_{z1} + \gamma_2 i_{z2})\, B$$

<u>Add nuclear Zeeman terms (*unlike* atoms):</u>

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

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

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):

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

Interactions between two alkali atoms

Hamiltonian including spin Zeeman term:

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

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

<u>Add nuclear Zeeman terms (*identical* atoms):</u>

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

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

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):

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

Interactions between two alkali atoms

Add hyperfine interactions (*unlike* atoms):

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

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

$$M_I = m_1 + m_2$$

$$M_S = m_{s_1} + m_{s_2}$$

Answer: yes!

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

Is S still a good quantum number?

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

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

Interactions between two alkali atoms

Is S still a good quantum number?

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

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

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

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

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

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

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

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

Interactions between two alkali atoms

Hamiltonian including spin Zeeman term:

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

$$\mathcal{H} = \frac{1}{2\mu}\left(p_r^2 + \frac{\mathbf{L}^2}{r^2}\right) + \mathcal{V}(r) + \gamma_e B\, S_z \underbrace{- (\gamma_1 i_{z1} + \gamma_2 i_{z2})\, B}_{(-\gamma_n B\, I_z)} + \mathcal{H}_{\rm hf}^{+} + \mathcal{H}_{\rm hf}^{-}$$

all terms conserve M_F

only term

not singlet/triplet conserving

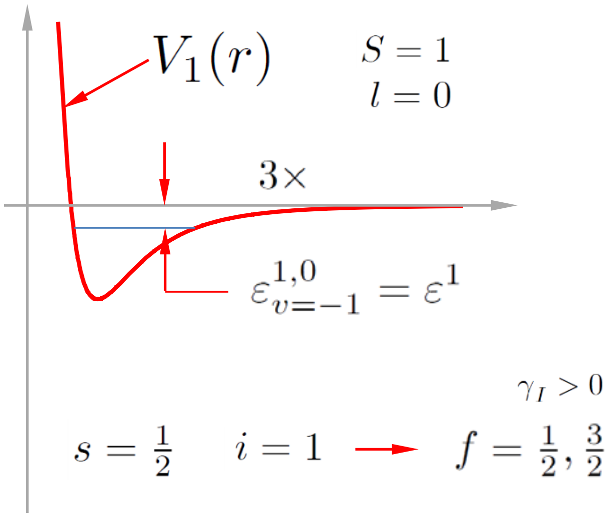
Good basis states: $|\psi\rangle = |R_l^S\rangle |l, m_l\rangle |S, M_S\rangle |i_1, m_1\rangle |i_2, m_2\rangle$

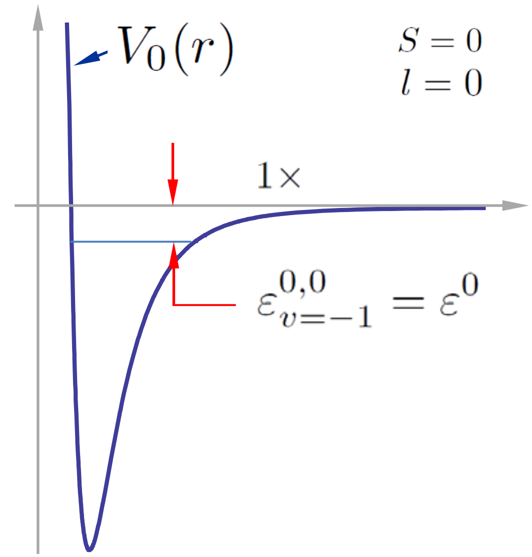
$$|\psi\rangle = |R_l^{S,I}\rangle |l, m_l\rangle |S, M_S\rangle |I, M_I\rangle$$

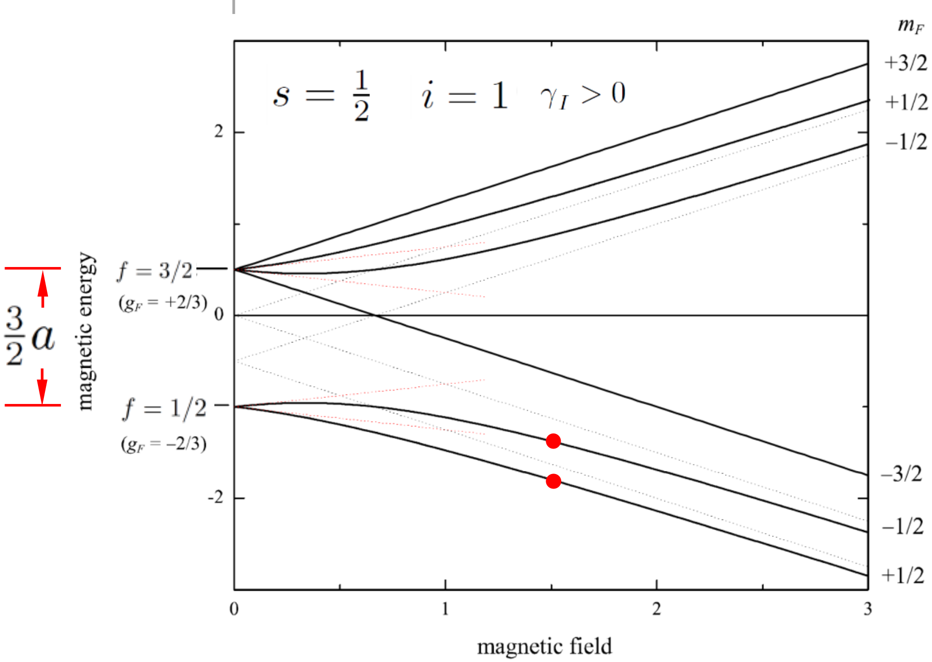
Effective potential:

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

Example: two ^{6}Li atoms







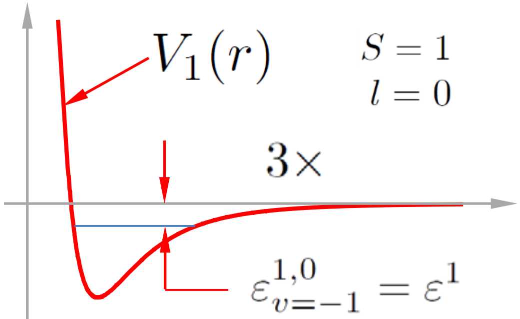
Find all s-wave molecules with $M_F=0$

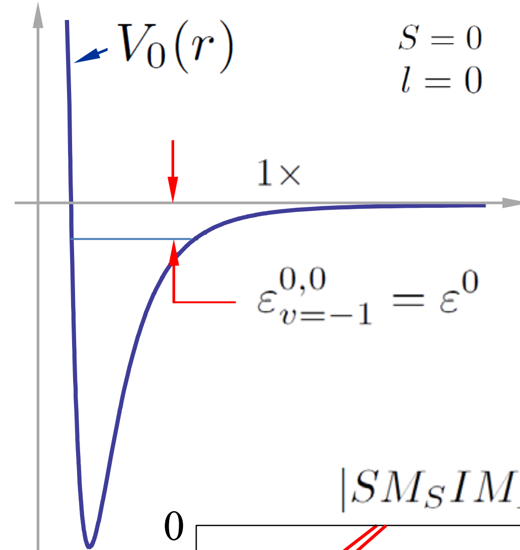
$$S=0\ \begin{cases} I=0,2 \\ I=1 \end{cases}\quad X^1\Sigma_g^+\quad \begin{matrix} l=0,2,4,\cdots \\ l=1,3,5,\cdots \end{matrix}$$

$$S=1\ \begin{cases} I=0,2 \\ I=1 \end{cases}\quad a^3\Sigma_u^+\quad \begin{matrix} l=1,3,5,\cdots \\ l=0,2,4,\cdots \end{matrix}$$

free atom pair with $M_F=0$

Example: two ^{6}Li atoms

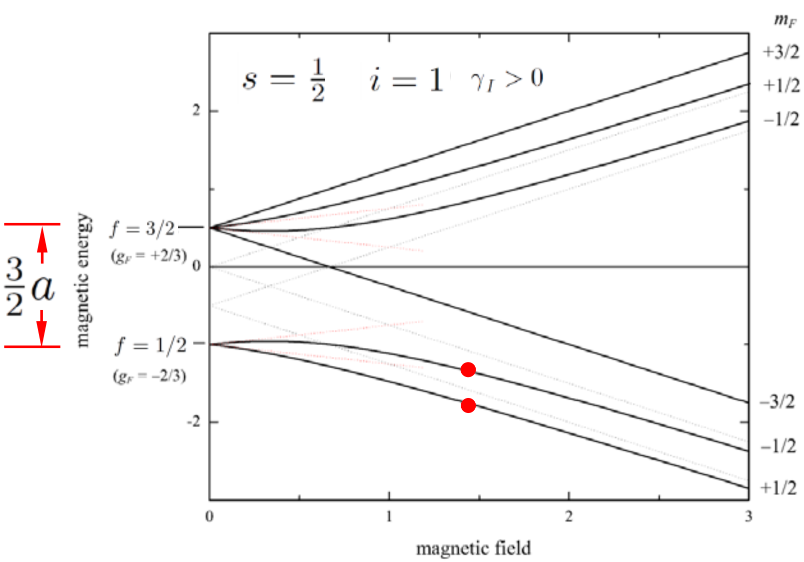


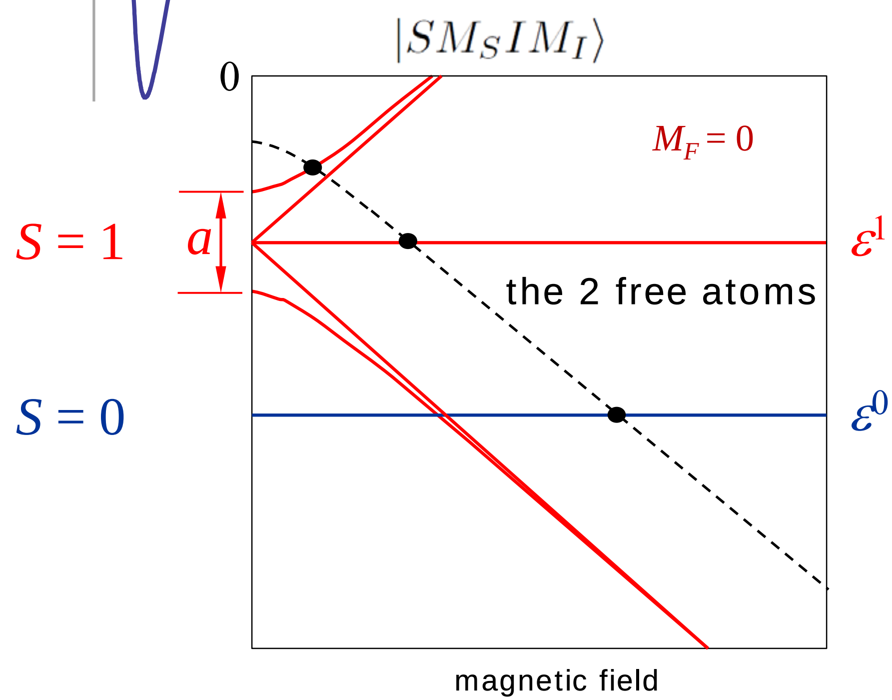


$M_F = 0$

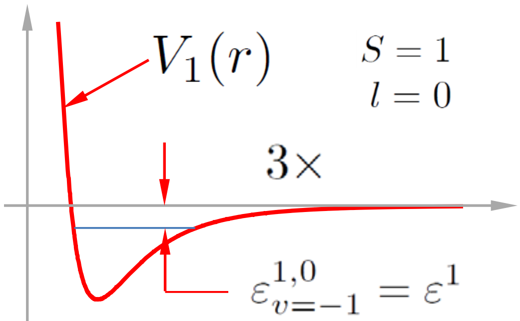
$$S=0 \quad \left\{ \begin{array}{l} I = 0,2 \\ I = 1 \end{array} \right. \quad X^1\Sigma_g^+ \quad \begin{array}{l} l = 0,2,4,\cdots \\ l = 1,3,5,\cdots \end{array}$$

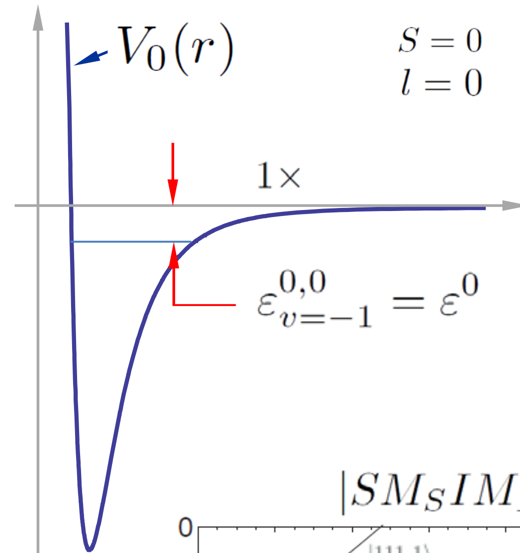
$$S=1 \quad \left\{ \begin{array}{l} I = 0,2 \\ I = 1 \end{array} \right. \quad a^3\Sigma_u^+ \quad \begin{array}{l} l = 1,3,5,\cdots \\ l = 0,2,4,\cdots \end{array}$$





Example: two ^{6}Li atoms

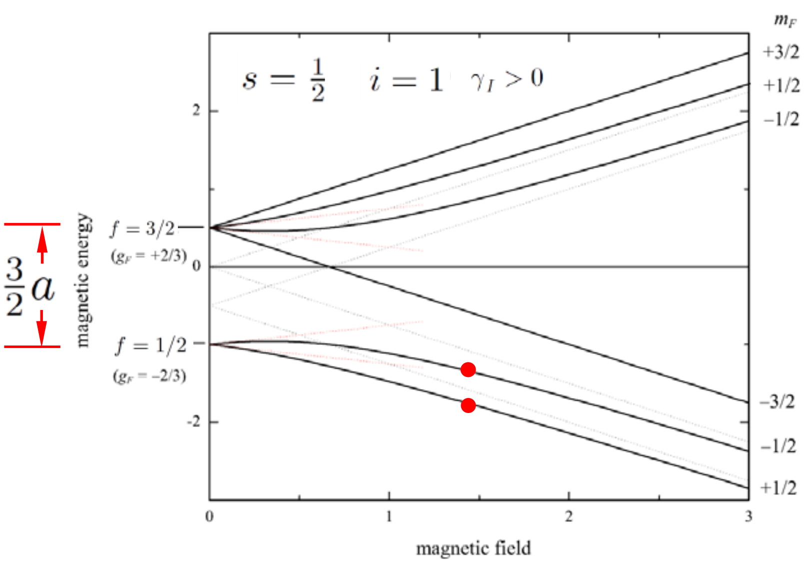




$M_F = 0$

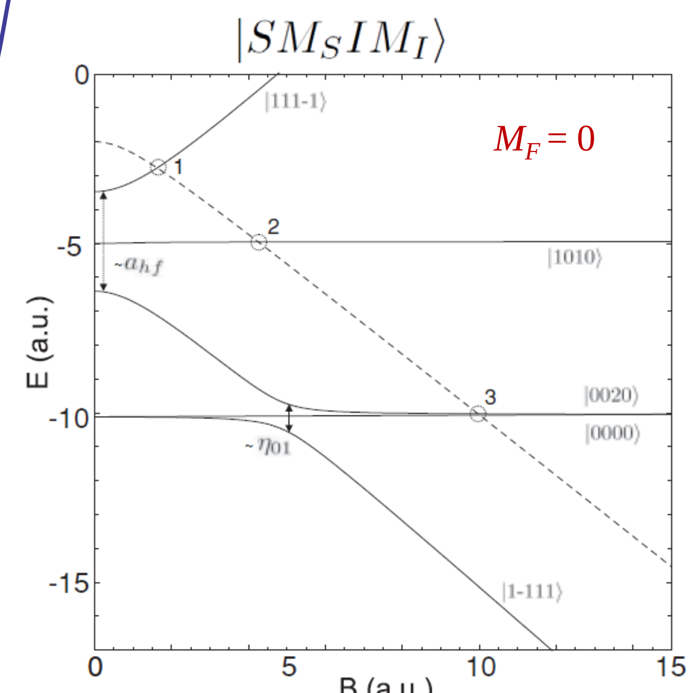
$$S=0 \quad \left\{ \begin{array}{l} I = 0,2 \\ I = 1 \end{array} \right. \quad X^1\Sigma_g^+ \quad \begin{array}{l} l = 0,2,4,\cdots \\ l = 1,3,5,\cdots \end{array}$$

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



$S = 1$

$S = 0$



Diagonalization of Hamiltonian

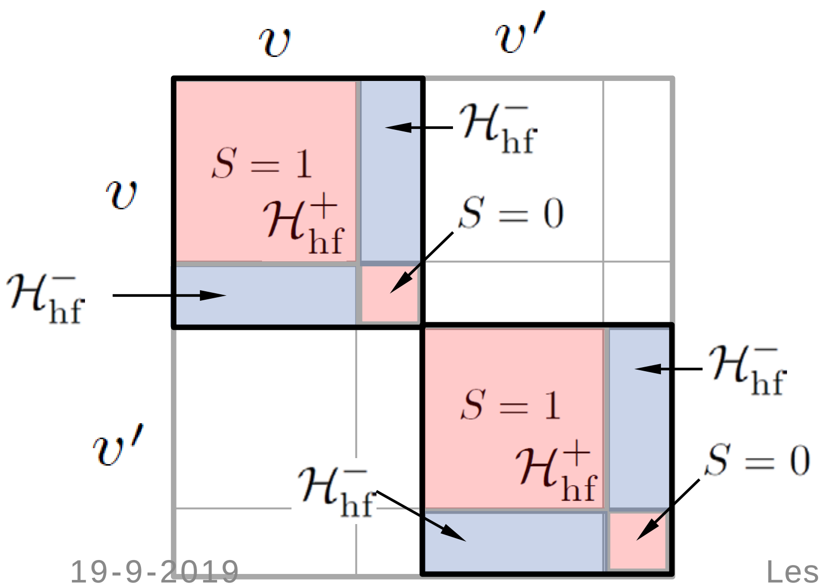
$$\mathcal{H} = \frac{1}{2\mu}\left(p_r^2 + \frac{\mathbf{L}^2}{r^2}\right) + \mathcal{V}(r) \; + \gamma_e B\, S_z \; - (\gamma_1 i_{z1} + \gamma_2 i_{z2})\, B \; + \mathcal{H}_{\mathrm{hf}}^{+} + \mathcal{H}_{\mathrm{hf}}^{-}$$

$$\boxed{\det |\langle\beta|\mathcal{H}|\alpha\rangle - \underline{I}E| = 0} \qquad |\alpha\rangle = |R_{l,v}^{S}\rangle \overbrace{|S, M_S\rangle|i_1, m_1\rangle|i_2, m_2\rangle}^{|\sigma\rangle}$$

$$\langle\beta|\mathcal{H}|\alpha\rangle = \left[\varepsilon_v^{S,l} + (\gamma_e M_S - \gamma_1 m_1 + \gamma_2 m_2)\, B\right] \langle\beta|\alpha\rangle + \langle\beta|\mathcal{H}_{\mathrm{hf}}^{+} + \mathcal{H}_{\mathrm{hf}}^{-}|\alpha\rangle$$

$$= \varepsilon_v^{S,l}(B)\delta_{v,v'}\delta_{\sigma,\sigma'} + \underbrace{\langle\sigma'|\mathcal{H}_{\mathrm{hf}}^{+}|\sigma\rangle}_{=0 \text{ for } S \neq S'}\delta_{v,v'} \; + \underbrace{\langle\sigma'|\mathcal{H}_{\mathrm{hf}}^{-}|\sigma\rangle}_{=0 \text{ for } S = S'}\underbrace{\langle R_{v'}^{S',l}|R_v^{S,l}\rangle}$$

Franck-Condon factor (only part that depends on radial wavefunction)



Atoms with internal structure

1. We introduce spin in the atoms
2. We found triplet and singlet potentials
3. We searched for terms coupling the singlet and triplet potentials
4. We found that part of HF interaction is singlet-triplet non-conserving
5. We found that M_F remains a good quantum number
6. We studied the magnetic structure of the pairs
7. We know where to search for Feshbach resonances