Cold Collisions

Atoms with internal structure

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Lecture notes:
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Identical atoms
Identical atoms

Bosons: symmetric under exchange

Fermions: antisymmetric under exchange

$$\psi_{in} = e^{ikz} \pm e^{-ikz}$$

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

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

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

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

\[ P_l(-u) = (-1)^l P_l(u) \]

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

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

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

similar for scattered waves:

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

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

Unlike atoms: \( f(\theta) \simeq f_0 \simeq -a \)

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

Identical fermions: \( f(\theta) - f(\pi - \theta) \simeq 6f_1 \cos \theta \simeq -2a_1 (k^2 a_1)^2 \cos \theta \)
Differential cross section:

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

\[
\sigma_{\pm} = \int_{0}^{\pi/2} 2\pi \sin \theta |f(\theta) \pm f(\pi - \theta)|^2 d\theta
\]

\[
= 8\pi \sum_{l,l' = \text{even/odd}} (2l' + 1)(2l + 1) f_{l'}^* f_l \int_{0}^{\pi/2} P_{l'}(\cos \theta) P_l(\cos \theta) \sin \theta d\theta
\]

\[
= 8\pi \sum_{l = \text{even/odd}} (2l + 1)^2 |f_l|^2 \int_{0}^{\pi/2} [P_l(\cos \theta)]^2 \sin \theta d\theta
\]

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

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

\[
\sigma = \frac{8\pi}{k^2} \sin^2 \eta_0 \approx 8\pi a^2
\]

\[
\sigma = \frac{8\pi}{k^2} 3 \sin^2 \eta_1 \approx 8\pi a_1^2 (ka_1)^4
\]
properties of elastic cross section

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

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

\[ \sigma_0 = \frac{8\pi}{k^2} \sin^2 \eta_0 \]

\[ \eta_0 = -k\alpha \]

\[ \eta_0 \to \pi \]

\[ k \to 0 \]

\[ \sigma = 0 \]

\[ \sigma_0 = 8\pi a^2 \]

First Ramsauer minimum

NO p-wave!
atoms with internal structure
Schrödinger equation

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

thus far: fixed potential

What happens if we add internal structure?

First we recapitulate:

\( L^2, L_z \) commute with \( r \) and \( p_r \)

separation of variables:

\[
\psi = R_l(r) Y^m_l(\theta, \phi)
\]

\[
L^2 Y^m_l(\theta, \phi) = l(l + 1) \hbar^2 Y^m_l(\theta, \phi)
\]

\[
L_z Y^m_l(\theta, \phi) = m \hbar Y^m_l(\theta, \phi).
\]

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

\( V_{\text{eff}}(r) \)

good for systems like helium
Interactions between alkali atoms

\[ S = s_1 + s_2 \]

\[ V_1(r) \]

\[ \alpha^3 \Sigma^{+}_{u} \]

\[ r_X r_0 \]

\[ X^1 \Sigma^{+}_g \]

\[ V_0(r) \]

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*:

\[
\mathcal{V}(r) = V_D(r) + J(r)s_1 \cdot s_2
\]

\[
J(r) = V_1(r) - V_0(r)
\]

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

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

\[
\mathcal{V}(r)|0,0\rangle = V_0(r)|0,0\rangle
\]

\[
\mathcal{V}(r)|1,M_S\rangle = V_1(r)|1,M_S\rangle
\]

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:

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

\[ \gamma_e = g_s \mu_B / \hbar \]

\[ \Delta E_Z = g_s \mu_B B M_S \]

\[ M_S = m_{s_1} + m_{s_2} \] is good quantum number

\[ \mathbf{s}_1 \cdot \mathbf{s}_2 = \frac{1}{2} \left( \mathbf{S}^2 - s_1^2 - s_2^2 \right) \]

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

Hamiltonian including spin Zeeman term:

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

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:

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

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 \( M_S \):

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

\[ U_{S,l}(r) = U_S(r) + \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2 \gamma_e B} M_S \]
Interactions between alkali atoms

The magnetic field lifts the degeneracy of the triplet potential.

\[ V_{1}(r) \]

\[ V_{0}(r) \]

\[ M_{S} = +1 \]
\[ M_{S} = 0 \]
\[ M_{S} = -1 \]

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

\[ U_{S,l}(r) = U_{S}(r) + \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2}\gamma_eB M_S \]
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 Fesbach resonance at arbitrary, fixed (low) collisional energy by varying the magnetic field: Zeeman tuning.
some nomenclature

Closed channel below threshold

Closed channel above threshold

Open channel

threshold energy

\[ \varepsilon_v = -\kappa^2 \]

\[ \varepsilon_v = +\kappa_{vs}^2 \]

\[ \kappa^2 + k^2 \]

\[ \kappa_{vs}^2 - k^2 \]
Interactions between two alkali atoms

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

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

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

Solutions for given \( l, S \) and \( M_S \):

Continuum states \( \varepsilon > 0 \):

\[
\varepsilon_k = k^2 + \frac{2\mu}{\hbar^2} \gamma_e B M_S
\]

Bound states \( \varepsilon < 0 \):

\[
\varepsilon_{v,l}^S = -\kappa_{v,S}^2 + l(l+1) R_{v,l}^S + \frac{2\mu}{\hbar^2} \gamma_e B M_S
\]

\[
R_{v,l}^S = \langle R_{v,l}^S | r^{-2} | R_{v,l}^S \rangle
\]
Interactions between two alkali atoms

Hamiltonian including spin Zeeman term:

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

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: \( |\psi\rangle = |R_i^S\rangle |l, m_l\rangle |S, M_S\rangle |i_1, m_{i_1}\rangle |i_2, m_{i_2}\rangle \)

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:

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

Add nuclear Zeeman terms (identical atoms):

$$I = i_1 + i_2 \quad M_I = m_1 + m_2$$

$$\mathcal{H}_Z = -\gamma_n i_1 \cdot B - \gamma_n i_2 \cdot B = -\gamma_n I \cdot B$$

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

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):

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

Is \( M_F = M_S + M_I \) still a good quantum number?

\[ M_I = m_1 + m_2 \]
\[ M_S = m_{s_1} + m_{s_2} \]

Answer: yes!

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

Is \( S \) still a good quantum number?

\[ \mathcal{H}_{hf} = \mathcal{H}_{hf}^+ + \mathcal{H}_{hf}^- \]
\[ \mathcal{H}_{hf}^\pm = \frac{a_1}{2\hbar^2} \mathbf{i}_1 \cdot (\mathbf{s}_1 \pm \mathbf{s}_2) \pm \frac{a_2}{2\hbar^2} \mathbf{i}_2 \cdot (\mathbf{s}_1 \pm \mathbf{s}_2) \]
Interactions between two alkali atoms

Is $S$ still a good quantum number?

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

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

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

identical atoms

$\mathcal{H}_{hf}^+ = \frac{a_1}{2\hbar^2} \mathbf{I} \cdot \mathbf{S}$

$\mathcal{H}_{hf}^+$ can change $M_S$ but not $S$ and $M_F$

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

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

$F = I + S$

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

Analysis shows that $\mathcal{H}_{hf}^-$ converts singlet in triplet and vice versa
Interactions between two alkali atoms

Hamiltonian including spin Zeeman term:

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

all terms conserve \( M_F \)

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:

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

\[-\gamma_n B M_I \]
Example: two $^6\text{Li}$ atoms

$$V_1(r) \quad S = 1 \quad l = 0$$

$$\varepsilon^{1,0}_{v=-1} = \varepsilon^1$$

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

$$\gamma_I > 0$$

$$V_0(r) \quad S = 0 \quad l = 0$$

$$\varepsilon_{v=-1}^{0,0} = \varepsilon^0$$

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

$$S = 0 \begin{cases} I = 0, 2 & X^1\Sigma_g^+ \\ I = 1 & l = 0, 2, 4, \ldots \end{cases}$$

$$S = 1 \begin{cases} I = 0, 2 & a^3\Sigma_u^+ \\ I = 1 & l = 1, 3, 5, \ldots \end{cases}$$

free atom pair with $M_F = 0$

Les Houches 2018
Example: two $^6\text{Li}$ atoms

$M_F = 0$

$S = 0$

$M_F = 0$

$S = 0$

$S = 1$

$S = 1$

$S = 0$

$S = 0$

$S = 0$

$S = 1$

$S = 1$

$S = 1$
Example: two $^6\text{Li}$ atoms

$V_1(r)$ \hspace{1cm} $S = 1$ \hspace{1cm} $l = 0$

$V_0(r)$ \hspace{1cm} $S = 0$ \hspace{1cm} $l = 0$

$M_F = 0$

$S = 0$

$M_F = 0$

$S = 1$

$S = 0$
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