



UNIVERSITY of
TASMANIA

KYA323

Atomic physics

Andy McCulloch





Hyperfine structure

McIntyre Ch. 11 // Foot Ch. 6



UNIVERSITY of
TASMANIA

Learning outcomes

Week 2, lecture 1

McIntyre §11.1 – 11.4: Hyperfine structure

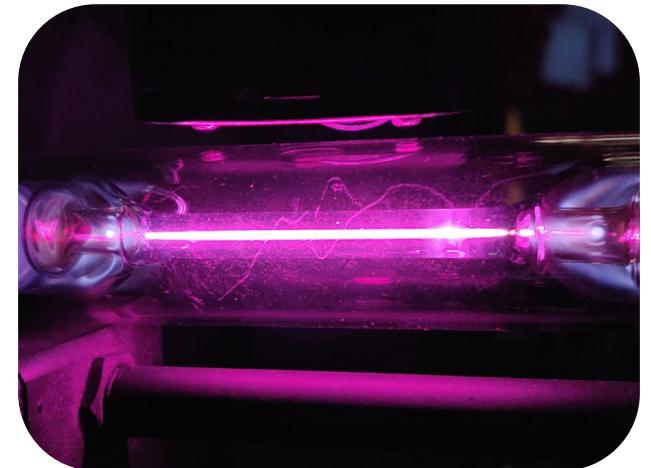
- The Hyperfine interaction
 - What is it?
 - What is the Hamiltonian, and how do I solve it?
- Angular momentum
 - A review
 - Ladder operators
 - Matrix representation
- Hyperfine structure
 - Degenerate perturbation theory

The hydrogen spectrum returns

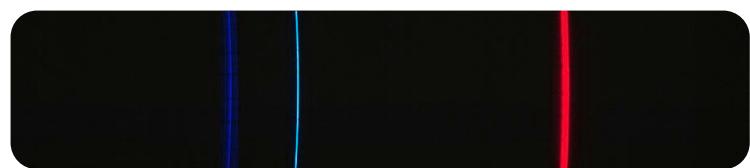
Careful experimentation reveals an energy structure of hydrogen beyond $1/n^2$

Additional energy levels arise from perturbations to the zeroth-order Coulomb Hamiltonian

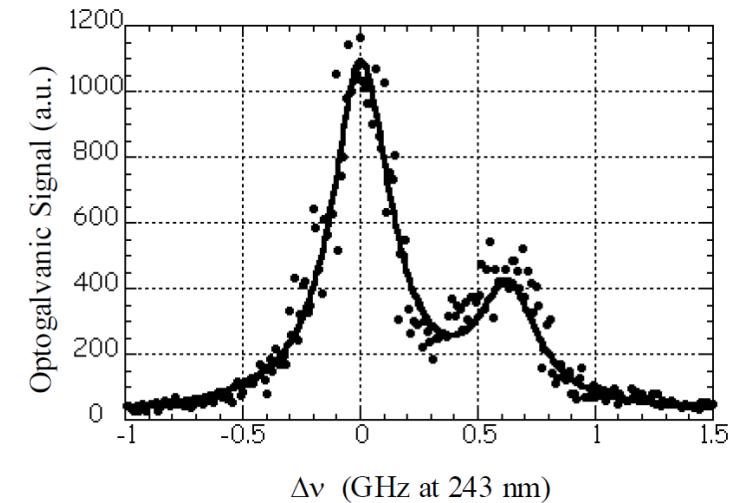
We are going to study an important perturbation, they *hyperfine* interaction, which will lead us into the world of angular momentum coupling



A hydrogen discharge lamp



The hydrogen emission spectrum



Ground state splitting of hydrogen

The hyperfine interaction

The nuclear charge is not a true point charge, but rather has a charge distribution

The finite distribution gives rise to higher electromagnetic multipole moments:

$$V(\mathbf{R}) = \sum_{i=1}^N \frac{q_i}{4\pi\epsilon_0 |\mathbf{r}_i - \mathbf{R}|} = \frac{1}{4\pi\epsilon_0} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} (-1)^m I_{\ell}^{-m}(\mathbf{R}) \sum_{i=1}^N q_i R_{\ell}^m(r_i)$$

where the *regular solid harmonics* are

$$R_{\ell}^m(r_i) \equiv \sqrt{\frac{4\pi}{2\ell+1}} r^{\ell} Y_{\ell}^m(r_i)$$

And the *irregular solid harmonics* are

$$I_{\ell}^m(\mathbf{R}) \equiv \sqrt{\frac{4\pi}{2\ell+1}} \frac{Y_{\ell}^m(\hat{\mathbf{R}})}{R^{\ell+1}}$$



*Multipole moments
(an artist's impression)*

The *hyperfine interaction* arises from the interaction of the magnetic moment of the nucleus and the internal magnetic field caused by the electronic motion (\mathbf{L}) and the electron's spin (\mathbf{S})

Magnetic moments

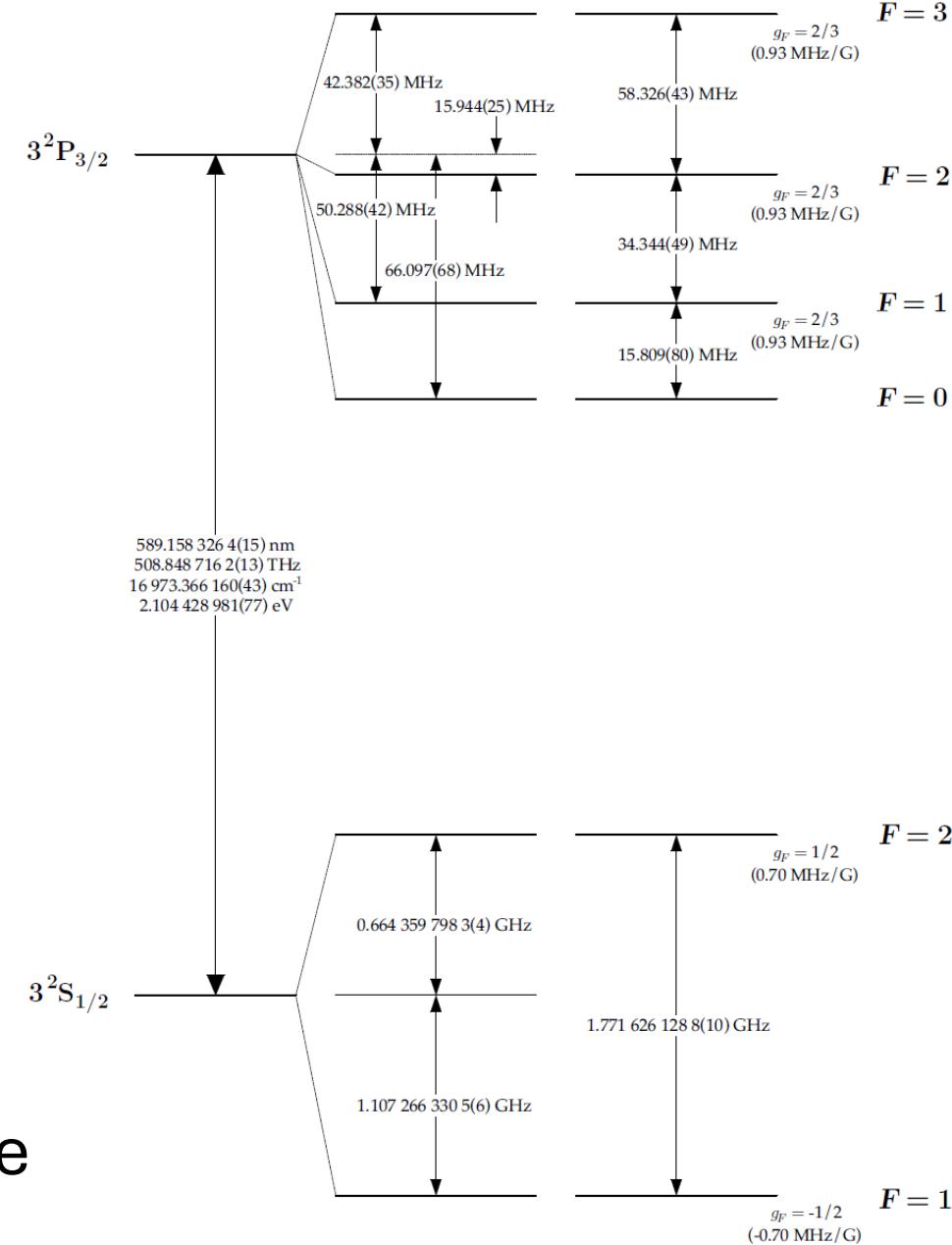
The (spin) magnetic moment of the electron is

$$\mu_e = -g_e \frac{e}{2m_e} \mathbf{S} = -g_e \mu_B \frac{\mathbf{S}}{\hbar}$$

The proton is also a spin-1/2 particle, and the nuclear spin is denoted by \mathbf{I} , with magnetic moment

$$\mu_p = g_p \frac{e}{2m_p} \mathbf{I} = g_p \mu_N \frac{\mathbf{I}}{\hbar}$$

In reality: $g_e \approx 2$, $g_p \approx 5.6$, and $m_p \approx 1836 \times m_e$ which gives $\mu_p \ll \mu_e$, and thus the hyperfine effect is small: GHz in PHz!



Sodium D₂ transition hyperfine structure

Hyperfine interaction Hamiltonian

The Hamiltonian is

$$H'_{hf} = \boxed{\boldsymbol{\mu}_p \cdot \frac{\mu_0}{4\pi} \frac{e\mathbf{L}}{mr^3}} + \boxed{\frac{\mu_0}{4\pi} \frac{1}{r^3} \left[\boldsymbol{\mu}_e \cdot \boldsymbol{\mu}_p - 3 \frac{(\boldsymbol{\mu}_e \cdot \mathbf{r})(\boldsymbol{\mu}_p \cdot \mathbf{r})}{r^2} \right]} - \boxed{\frac{\mu_0}{4\pi} \frac{8\pi}{3} \boldsymbol{\mu}_e \cdot \boldsymbol{\mu}_p \delta(\mathbf{r})}$$

Interaction between proton and orbital magnetic moment of electron

Interaction between proton and spin magnetic moment of electron
for $r \neq 0$

Fermi contact interaction:
the interaction between proton and spin magnetic moment of electron
for $r = 0$

Inserting the spin operators, for hydrogen we have:

$$H'_{hf} = \frac{\mu_0}{4\pi} \frac{g_e \mu_B g_p \mu_N}{\hbar^2} \left[\frac{2}{g_e} \frac{1}{r^3} \mathbf{I} \cdot \mathbf{L} - \frac{1}{r^3} \mathbf{S} \cdot \mathbf{I} + \frac{3}{r^5} (\mathbf{S} \cdot \mathbf{r})(\mathbf{I} \cdot \mathbf{r}) + \frac{8\pi}{3} \mathbf{S} \cdot \mathbf{I} \delta(\mathbf{r}) \right]$$

Hyperfine perturbation

Perturbation theory demands that we compute the matrix elements of the perturbation Hamiltonian, H'_{hf} . For simplicity, we consider the 1s state:

$$H'_{hf} = \frac{\mu_0}{4\pi} \frac{g_e \mu_B g_p \mu_N}{\hbar^2} \frac{8\pi}{3} \mathbf{S} \cdot \mathbf{I} \delta(\mathbf{r})$$

Depends on both space
(position) and spin

which has matrix elements of the form

$$\langle space | \langle spin | H'_{hf} | spin \rangle | space \rangle$$

which factors into

$$\frac{\mu_0}{4\pi} \frac{g_e \mu_B g_p \mu_N}{\hbar^2} \frac{8\pi}{3} \langle space | \delta(\mathbf{r}) | space \rangle \langle spin | \mathbf{S} \cdot \mathbf{I} | spin \rangle$$



Computing the matrix elements

Calculating the spatial component is easy:

$$\langle \text{space} | \delta(\mathbf{r}) | \text{space} \rangle = \int_{\text{space}} \psi_{1s}^*(r, \theta, \varphi) \delta(\mathbf{r}) \psi_{1s}(r, \theta, \varphi) d^3r$$
$$= |\psi_{1s}(0)|^2 = 1/\pi a_0^3$$

But how to compute the spin matrix elements? We didn't include the spin of the electron or proton when solving for the energy eigenstates...

Our mission: develop tools to calculate these matrix elements

MISSION: POSSIBLE

Angular momentum 101

In quantum, you studied:

- Spin angular momentum **S**
- Orbital angular momentum **L**

which have different physical origins but share similarities.

We denote the generalised angular momentum **J**, which obeys the same eigenvalue equations as both spin and orbital angular momentum, namely:

$$\begin{aligned} \mathbf{J}^2 |j m_j\rangle &= j(j+1)\hbar^2 |j m_j\rangle \\ J_z |j m_j\rangle &= m_j \hbar |j m_j\rangle \end{aligned}$$

$|j m_j\rangle$ are simultaneous eigenstates of \mathbf{J}^2 and J_z with eigenvalues j (integer or half-integer) and $m_j = -j, -j+1, \dots, j-1, j$ respectively

The components of angular momentum do not commute:

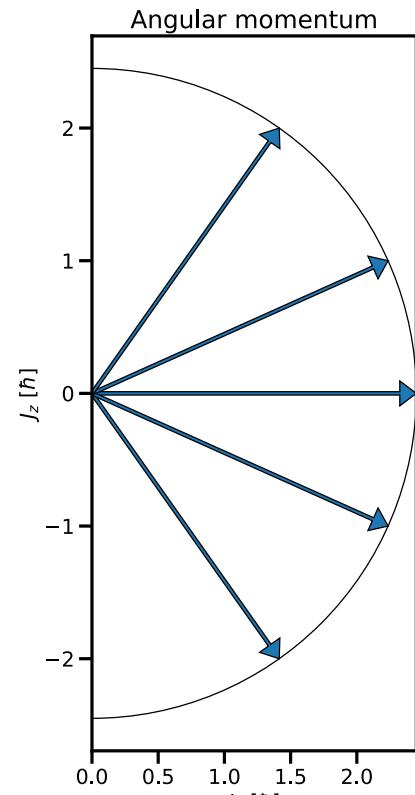
$$[J_x, J_y] = i\hbar J_z, [J_y, J_z] = i\hbar J_x, [J_z, J_x] = i\hbar J_y$$

but do commute with \mathbf{J}^2 :

$$[\mathbf{J}^2, J_x] = [\mathbf{J}^2, J_y] = [\mathbf{J}^2, J_z] = 0$$



The Stern-Gerlach experiment



*The projection of **J** onto the z-axis*

Matrix representation

We can represent angular momentum operators as matrices in the angular momentum basis. Conventionally:

- Write separate matrices for each value of j
- Use eigenstates of the angular momentum component operator J_z as the basis

For example:

$$j = \frac{1}{2} \Rightarrow J^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad J_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

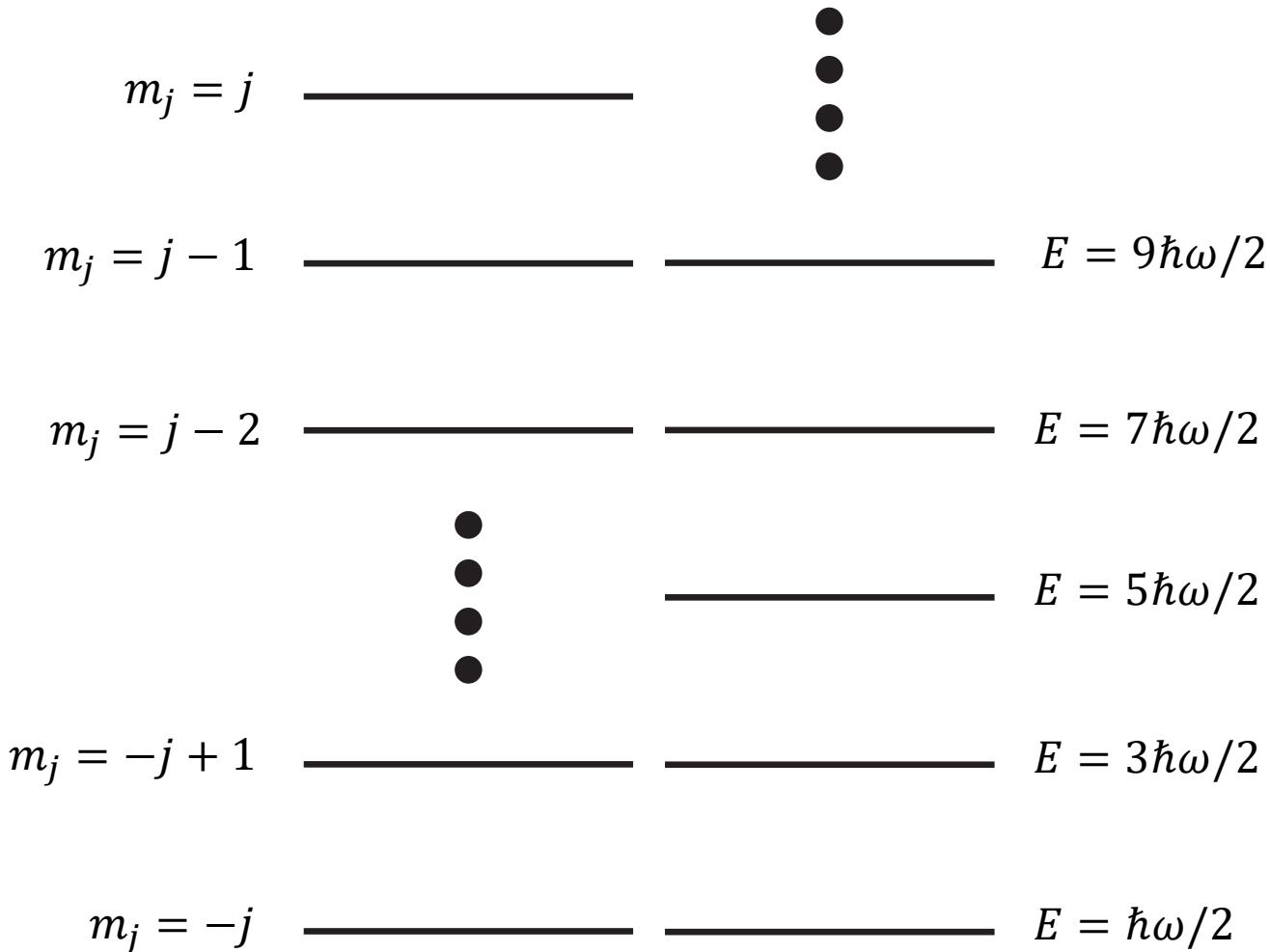
$$j = 1 \Rightarrow J^2 = 2\hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad J_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Ladder operators

The manifold of angular momentum component states looks similar to the harmonic oscillator...

Look for operators which connect states within a given j manifold
(c.f. a and a^\dagger):

$$J_+ = J_x + iJ_y$$
$$J_- = J_x - iJ_y$$



Polar Bear



Poll Everywhere



A QR code to Poll Everywhere
<https://pollev.com/andym360>

Do the operators J_+ and J_- represent physical observables?

Yes



No



Raising and lowering

J_{\pm} are not Hermitian \Rightarrow not observables

Properties/relations:

$$J_+ = J_-^\dagger$$

$$[J_+, J_-] = 2\hbar J_z$$

$$[J^2, J_{\pm}] = 0$$

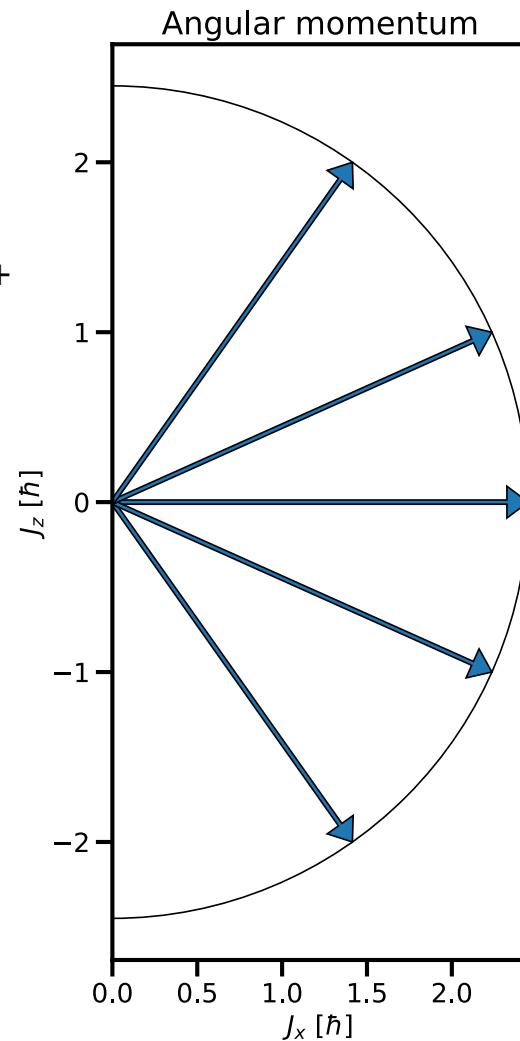
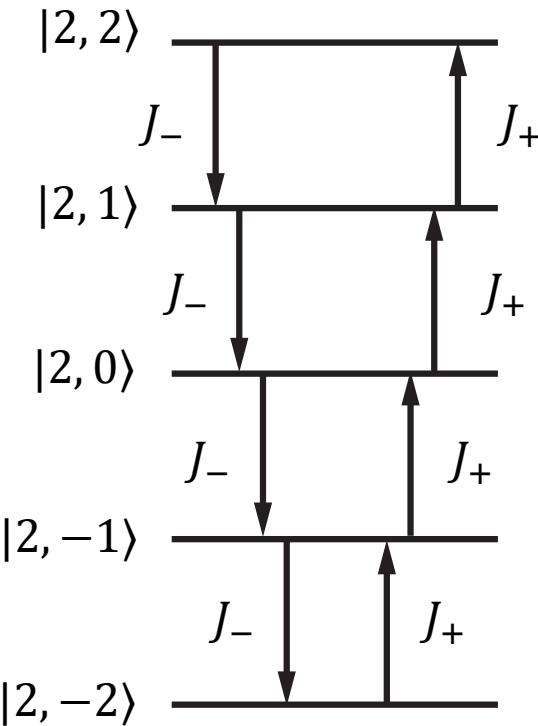
$$[J_z, J_+] = +\hbar J_+, \quad [J_z, J_-] = -\hbar J_-$$

These commutation relations imply that J_+ and J_- raise and lower the angular momentum component by \hbar and hence change m_j

$$J_{\pm}|j, m_j\rangle = \hbar[j(j+1) - m_j(m_j \pm 1)]^{1/2}|j, m_j \pm 1\rangle$$

with

$$J_+|j, j\rangle = J_-|j, -j\rangle = 0$$



Raising and lowering m_j for $j = 2$

Diagonalisation of the hyperfine perturbation

We want to find the hyperfine matrix elements: the full state vector must include the spatial wave function, and spin vectors for the electron and proton

$$|\psi_{1s}\rangle \equiv \psi_{1s}(r, \theta, \varphi) |+\rangle_e |-\rangle_p$$

where

$$S_z |\pm\rangle_e = \pm \frac{\hbar}{2} |\pm\rangle_e, \quad \mathbf{S}^2 |\pm\rangle_e = \frac{3\hbar^2}{4} |\pm\rangle_e$$

$$I_z |\pm\rangle_p = \pm \frac{\hbar}{2} |\pm\rangle_p, \quad \mathbf{I}^2 |\pm\rangle_p = \frac{3\hbar^2}{4} |\pm\rangle_p$$

We can write $|+\rangle_e |-\rangle_p$ a number of ways:

$$\begin{aligned} |+\rangle_e |-\rangle_p &= \left| s = \frac{1}{2}, m_s = \frac{1}{2} \right\rangle \left| I = \frac{1}{2}, m_I = -\frac{1}{2} \right\rangle \\ &= \left| s = \frac{1}{2}, m_s = \frac{1}{2}, I = \frac{1}{2}, m_I = -\frac{1}{2} \right\rangle = \left| s = \frac{1}{2}, I = \frac{1}{2}, m_s = \frac{1}{2}, m_I = -\frac{1}{2} \right\rangle \\ &= \left| m_s = \frac{1}{2}, m_I = -\frac{1}{2} \right\rangle = |+ -\rangle \end{aligned}$$



Cooking with gas

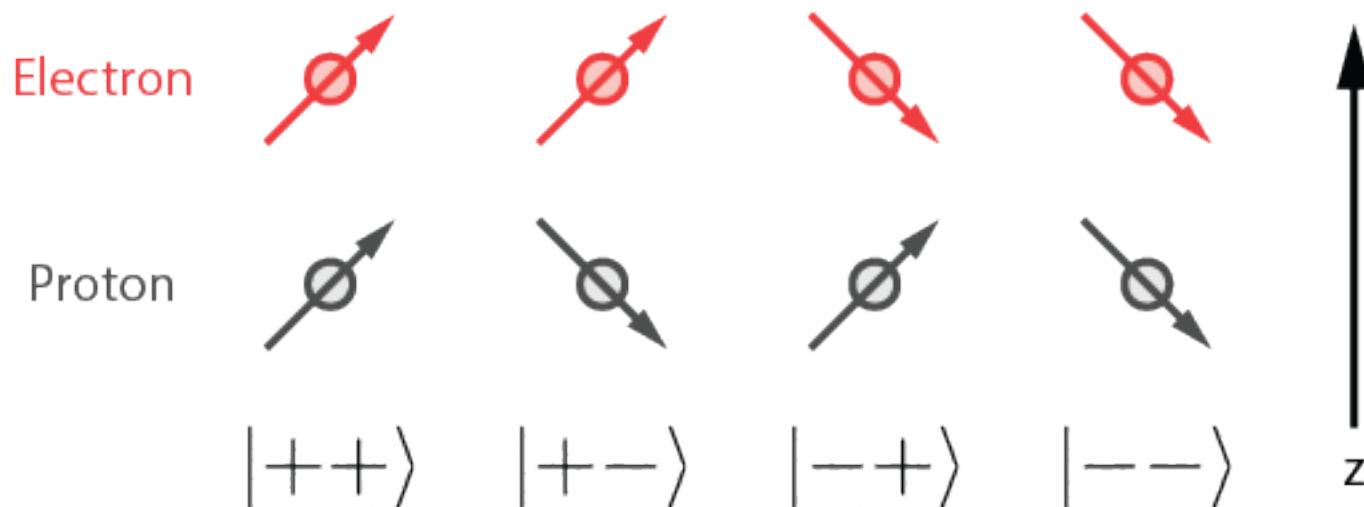
s and I do not change $\Rightarrow |\text{Electron spin, proton spin}\rangle$

The uncoupled basis

The electron-proton spin states exist in a new vector space, spanned by the basis states

$$|++\rangle, |+-\rangle, |-+\rangle, |--\rangle$$

The basis is formed from the eigenstates of S_z and I_z , is called the *uncoupled basis*



Electron and proton spin states

Consider the ground state of Hydrogen: $|\psi_{1s}\rangle$. Is this state degenerate?

Yes, clearly

67%

No, obviously

33%

Matrix representation of S_z and I_z

Zeroth-order hydrogen ground state is fourfold degenerate \Rightarrow must use **degenerate** perturbation theory.

The spin operators act only on their own part of the state:

$$S_z|+-\rangle = S_z|+\rangle_e|-\rangle_p = +\frac{\hbar}{2}|+\rangle_e|-\rangle_p = \frac{\hbar}{2}|+-\rangle$$

or more generally

$$\begin{aligned} S_z|m_s m_I\rangle &= m_s \hbar |m_s m_I\rangle \\ S_I|m_s m_I\rangle &= m_I \hbar |m_s m_I\rangle \end{aligned}$$

S_z and I_z commute

The matrix representations are then:

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad I_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad \begin{matrix} ++ \\ +- \\ -+ \\ -- \end{matrix}$$



Degenerate perturbation theory

What is the problem?

$$E_n^{(1)} = H'_{nn} = \langle n^{(0)} | H' | n^{(0)} \rangle$$

$$|n^{(1)}\rangle = \sum_{m \neq n} \frac{\langle m^{(0)} | H' | n^{(0)} \rangle}{(E_n^{(0)} - E_m^{(0)})} |m^{(0)}\rangle = \sum_{m \neq n} \frac{H'_{mn}}{(E_n^{(0)} - E_m^{(0)})} |m^{(0)}\rangle$$

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle m^{(0)} | H' | n^{(0)} \rangle|^2}{(E_n^{(0)} - E_m^{(0)})}$$

Imagine that states $n = 2$ and $n = 3$ are degenerate, so want to solve

$$(H_0 - E_n^{(0)}) |n_1\rangle = (E_n^{(1)} - H') |n^0\rangle$$

If we are looking for $E_2^{(1)}$

$$H_0 - E_2^{(0)} = \begin{pmatrix} E_1^{(0)} - E_2^{(0)} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E_4^{(0)} - E_2^{(0)} \end{pmatrix}$$
$$E_2^{(1)} - H' = \begin{pmatrix} E_2^{(1)} - H'_{11} & -H'_{12} & -H'_{13} & -H'_{14} \\ -H'_{21} & E_2^{(1)} - H'_{22} & -H'_{23} & -H'_{24} \\ -H'_{31} & -H'_{32} & E_2^{(1)} - H'_{33} & -H'_{34} \\ -H'_{41} & -H'_{43} & -H'_{43} & E_2^{(1)} - H'_{44} \end{pmatrix}$$

$$\begin{pmatrix} E_2^{(1)} - H'_{22} & -H'_{23} \\ -H'_{32} & E_2^{(1)} - H'_{33} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0$$

How do we perform degenerate perturbation theory?

Ladder operators and the hyperfine Hamiltonian

Recall the hyperfine Hamiltonian is proportional to the operator

$$\mathbf{S} \cdot \mathbf{I} = S_x I_x + S_y I_y + S_z I_z$$

which can be rewritten

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

Most operations will be zero

$$S_+ |++\rangle = 0, \quad I_- |+-\rangle = 0$$

Non-zero off-diagonal values constructed from states which can be raised or lowered, e.g.

$$S_+ |-+\rangle = \hbar[s(s+1) - m_s(m_s+1)]^{1/2} |++\rangle$$

$$= \hbar \left[\frac{3}{4} + \frac{1}{4} \right]^{1/2} |++\rangle = \hbar |++\rangle$$

$$I_+ |-+\rangle = \hbar \left[\frac{3}{4} - \frac{1}{4} \right] |--\rangle = \frac{\hbar}{2} |--\rangle$$



The ladder operator



Matrix representation of $\mathbf{S} \cdot \mathbf{I}$

We need to compute the values of $\mathbf{S} \cdot \mathbf{I} |m_s m_I\rangle$, e.g.

$$\begin{aligned}\mathbf{S} \cdot \mathbf{I} |-+\rangle &= \left[\frac{1}{2}(S_+ I_- + S_- I_+) + S_z I_z \right] |-+\rangle \\ &= 0 + \frac{1}{2}\hbar\hbar|+-\rangle + \frac{1}{2}\hbar\left(-\frac{1}{2}\right)\hbar|-+\rangle \\ &= \frac{1}{4}\hbar^2[2|+-\rangle - |-+\rangle]\end{aligned}$$

Which can be projected onto our basis, giving:

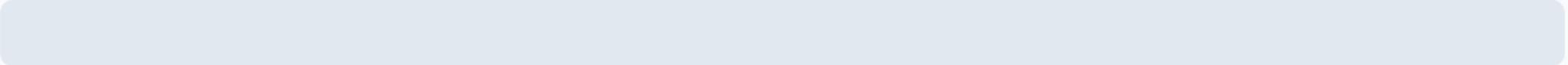
$$\mathbf{S} \cdot \mathbf{I} = \frac{\hbar^2}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{array}{c} ++ \\ +- \\ -+ \\ -- \end{array}$$



Matrix projection

Are the states $|m_s, m_j\rangle$ (i.e. $|++\rangle$, $|+-\rangle$, $| -+\rangle$, and $|--\rangle$) eigenstates of $\mathbf{S} \cdot \mathbf{I}$?

Yes

A horizontal progress bar consisting of a grey rectangular bar with rounded ends, representing 0% completion.

0%

No

A horizontal progress bar consisting of a solid blue rectangular bar with rounded ends, representing 100% completion.

100%



Eigenstates of the hyperfine Hamiltonian

The operator $\mathbf{S} \cdot \mathbf{I}$ is not diagonal \Rightarrow uncoupled basis not eigenstates!

The hyperfine Hamiltonian is:

$$H'_{hf} = \frac{A}{\hbar^2} \mathbf{S} \cdot \mathbf{I} \quad \text{where} \quad A = \frac{2\mu_0}{3} g_e \mu_B g_p \mu_N |\psi_{1s}(0)|^2$$

which then becomes

$$H'_{hf} = \frac{A}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \begin{matrix} ++ \\ +- \\ -+ \\ -- \end{matrix}$$

Degenerate perturbation theory: we must diagonalise H' in the degenerate subspace.

By inspection:

$$E_1 = A/4, \quad |E_1\rangle = |++\rangle$$

$$E_2 = A/4, \quad |E_2\rangle = |--\rangle$$

Show that

$$E_3 = A/4, \quad |E_3\rangle = 1/\sqrt{2}[|+-\rangle + |-+\rangle]$$

$$E_4 = -3A/4, \quad |E_4\rangle = 1/\sqrt{2}[|+-\rangle - |-+\rangle]$$

Hyperfine structure of the ground state

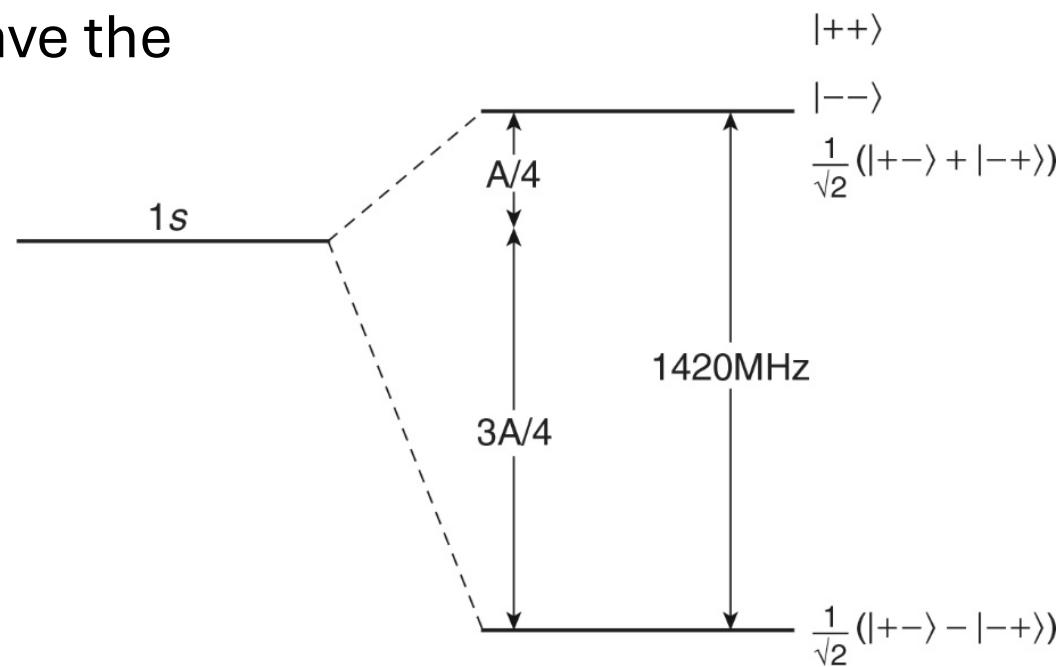
- Perturbation partially lifts degeneracy
- States $|++\rangle$, $|--\rangle$, and $1/\sqrt{2}[|+-\rangle + |-+\rangle]$ have the same energy $A/4$ whereas the state $1/\sqrt{2}[|+-\rangle - |-+\rangle]$ has the energy $-3A/4$

What is the energy spacing?

$$\begin{aligned}\Delta E_{hf} = A &= \frac{2\mu_0}{3} g_e \mu_B g_p \mu_N |\psi_{1s}(0)|^2 \\ &= \frac{2\mu_0}{3} \frac{g_e \mu_B g_p \mu_N}{\pi a_0^3} = \alpha^4 m_e c^2 \frac{2}{3} g_e g_p \left(\frac{m_e}{m_p} \right) \\ &= 5.88 \times 10^{-6} \text{ eV} = h \times 1420.4057517667(9) \text{ MHz}\end{aligned}$$

Recall that the energy scale in hydrogen is

$$\begin{aligned}1 \text{ Ry} &= hcR_\infty = 13.6 \text{ eV} \\ \Rightarrow A &< 10^{-6} \text{ Ry}\end{aligned}$$



Hyperfine splitting of the ground state of hydrogen

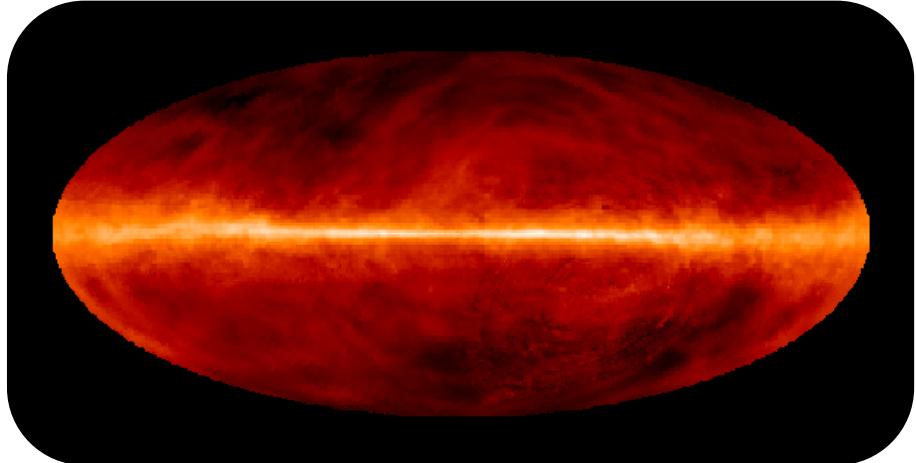
(Hyper)fine details



The 21cm line fundamental for astronomy and cosmology



A hydrogen maser is an excellent frequency reference

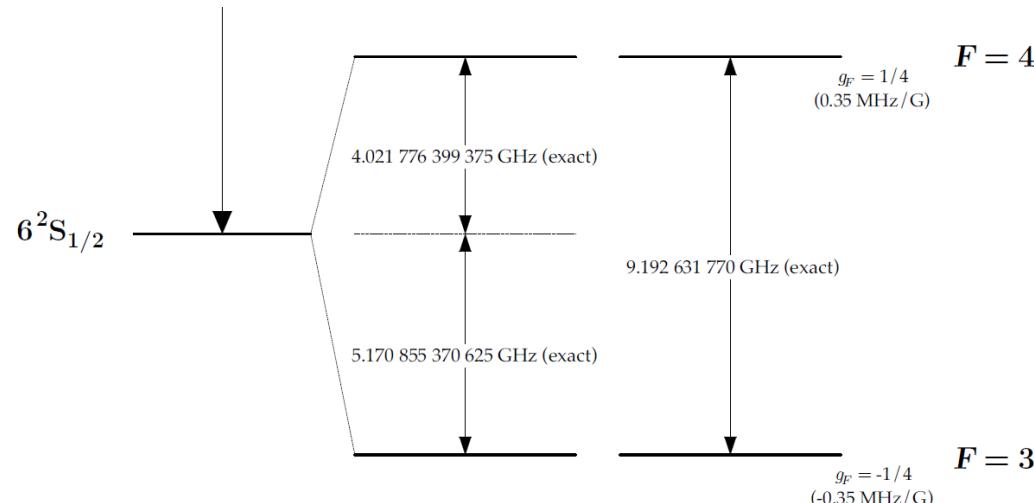


The galaxy at 21 cm

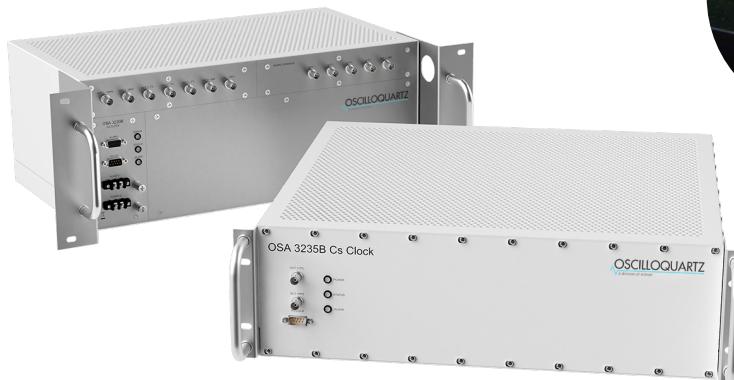


Real-time bonus: treats!?

How (be very specific) is the second defined?



Hyperfine splitting for the ground state of caesium



The ground-state splitting of caesium defines the second and is the core of an atomic clock



An (atomic) fountain clock



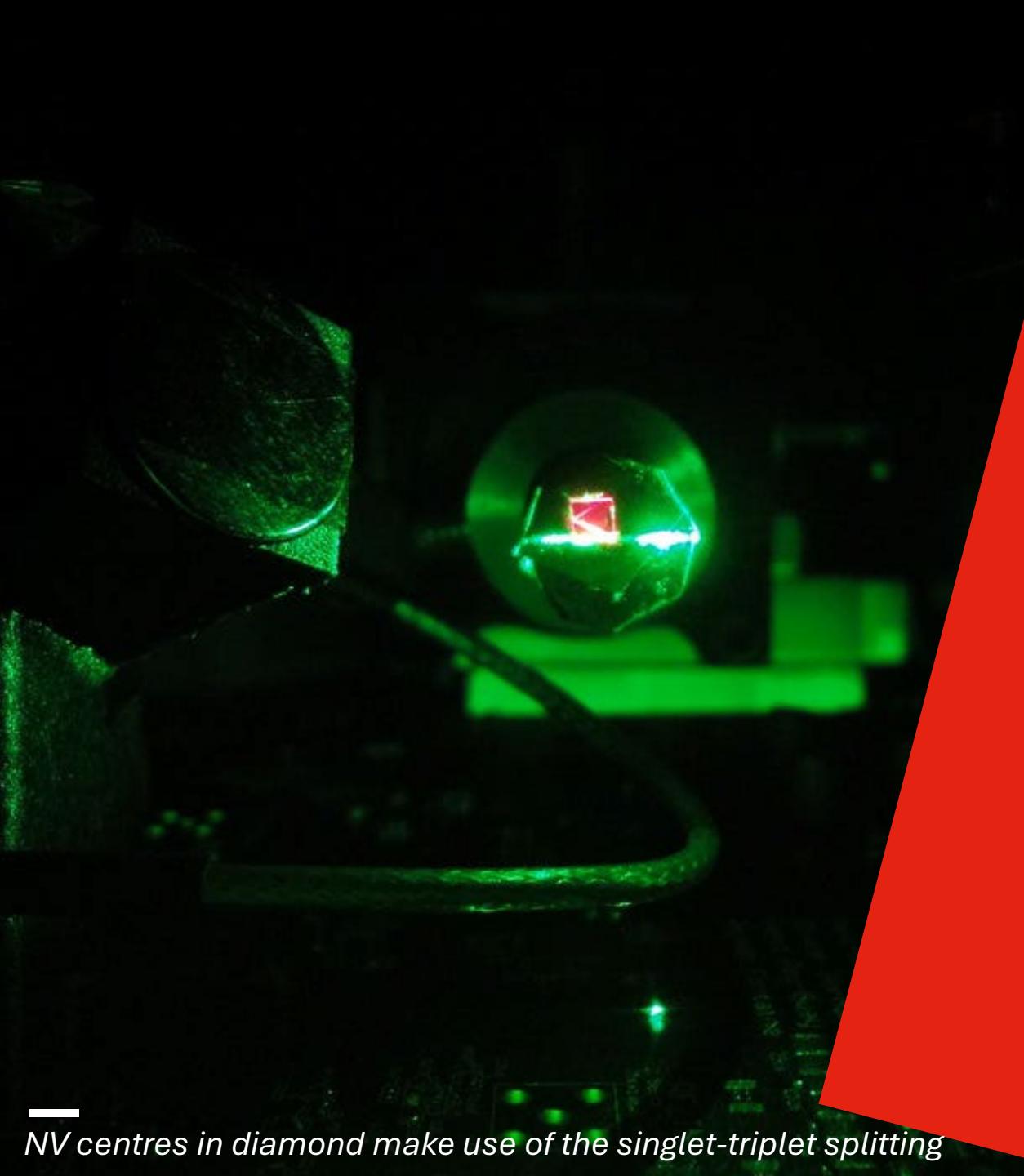
UNIVERSITY of
TASMANIA

Summary

Problems

M7.7, M11.6, M11.9

- The Hyperfine interaction
 - The finite extent of the nuclear charge leads to higher-order interactions
- Angular momentum
 - Generalised angular momenta obey the same relations as familiar angular momenta
 - The coupled basis describes the state space for the hyperfine interaction
- Hyperfine structure
 - Interaction between electron and nucleus leads to a splitting of the ground-state energy



Addition of angular momenta

McIntyre Ch. 11 // Foot Ch. 6



UNIVERSITY of
TASMANIA

Learning outcomes

Week 2, lecture 2

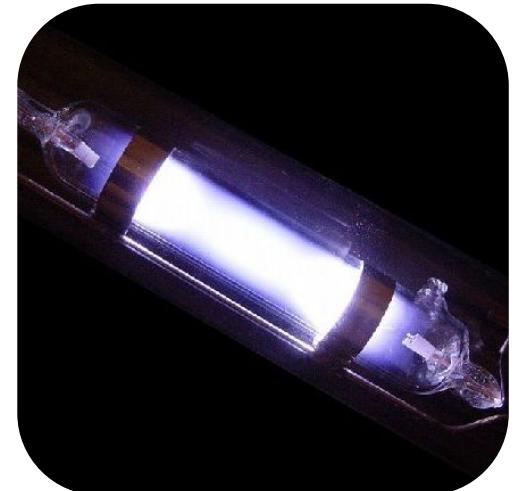
McIntyre §11.5: Addition of angular momenta

- Total angular momentum
 - What is it, and why do we need it?
 - What are the coupled and uncoupled bases?
 - What is the connection the total angular momentum to the hyperfine interaction?

Nuclear spin is extremely quantum, right?

Nuclear Spin Attenuates the Anesthetic Potency of Xenon Isotopes in Mice: Implications for the Mechanisms of Anesthesia and Consciousness

Conclusions: Xenon isotopes with nuclear spin are less potent than those without, and polarizability cannot account for the difference. The lower anesthetic potency of Xe may be the result of it participating in conscious processing and therefore partially antagonizing its own anesthetic potency. Nuclear spin is a quantum property, and our results are consistent with theories that implicate quantum mechanisms in consciousness.



A reason to be sceptical? See A Mathematical Model for the Determination of Total Area Under Glucose Tolerance and Other Metabolic Curves

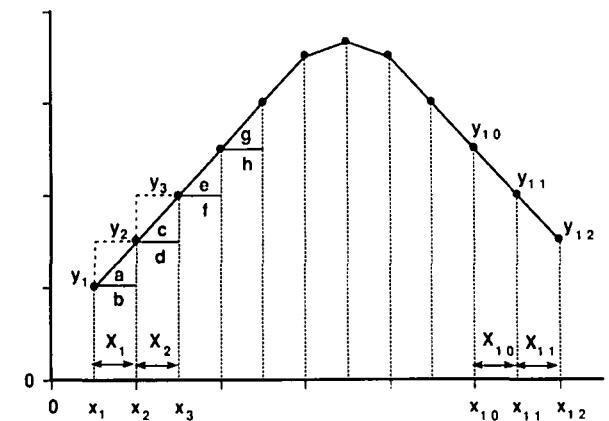
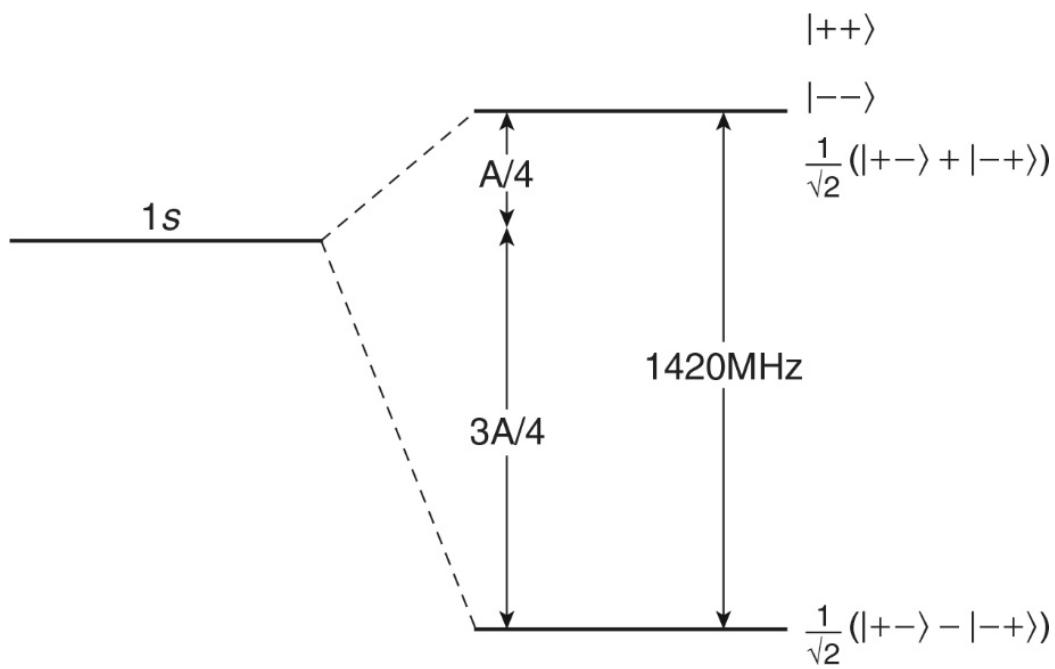


Figure 1—Total area under the curve is the sum of individual areas of triangles a, c, e, and g and rectangles b, d, f, and h.

A kettle of fish

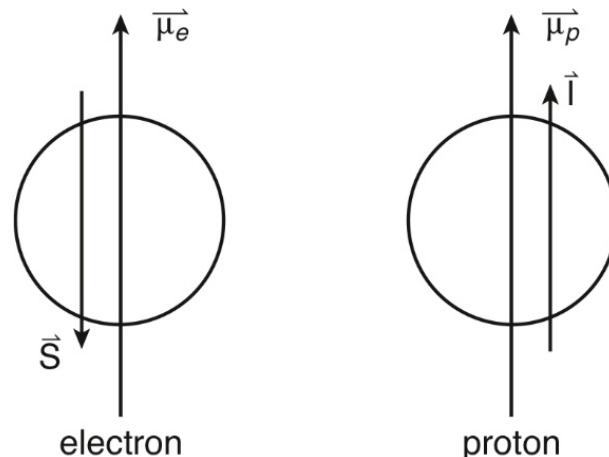
We saw that the energy of $|+ +\rangle$ and $|--\rangle$ was raised. Why does this correspond to a *lower* energy?



Hyperfine splitting of the ground state of hydrogen

$$H'_{hf} = \frac{A}{\hbar^2} \mathbf{S} \cdot \mathbf{I}$$

Classical dipole interaction:
energy minimised when magnetic
dipoles are anti-aligned



The states $|+ +\rangle$ and $|--\rangle$ correspond to magnetic moments which are anti-aligned

Alignment problems

It (hopefully!) makes sense that states $|+ +\rangle$ and $|- -\rangle$ are degenerate, but what about the other eigenstates?

Discussion:

What distinguishes the states

$$|E_3\rangle = \frac{1}{\sqrt{2}}[|+ -\rangle + |- +\rangle] \text{ and } |E_4\rangle = \frac{1}{\sqrt{2}}[|+ -\rangle - |- +\rangle]$$

Why are these states separated in energy?

The question: what is special about these hyperfine basis states (as compared to the uncoupled basis), and how can we generalise the theory, i.e. pick the correct basis states to start with?



Think-pair-share

The good, the bad, and the ugly

Classical

Interacting magnetic dipoles exert torques on each other

⇒ angular momentum of each particle not conserved, the magnitude remains constant, but the direction changes

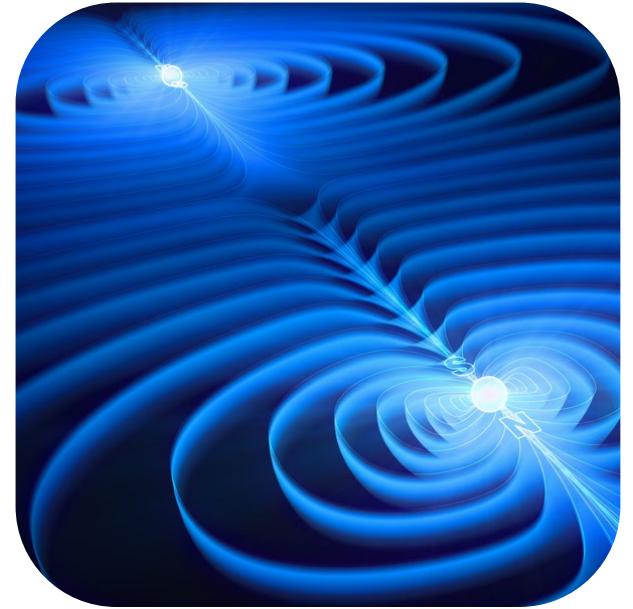
Quantum

The spin observables \mathbf{S}^2 and \mathbf{I}^2 commute with the Hyperfine Hamiltonian, but S_z and I_z do not

Consequence: quantum numbers s and I are “good” quantum numbers, m_s and m_I are “bad”

- The hyperfine eigenstates are superpositions of the $|m_s\ m_I\rangle$ basis (the *uncoupled* basis)

To find good quantum numbers, and hence a convenient basis, we need a conserved quantity



Interacting magnetic dipoles



A bad quantum number



Total angular momentum

Angular momentum of particles not conserved, but total angular momentum is conserved

Eigenstates of the total angular momentum of the system \Leftrightarrow basis in which hyperfine Hamiltonian is diagonal

We continue with the Hydrogen ground state (no orbital angular momentum) and define the total angular momentum \mathbf{F} as

$$\mathbf{F} = \mathbf{S} + \mathbf{I}$$

The operator \mathbf{F} quacks like a spin as it obeys the commutation relations of an angular momentum:

Show that $[F_x, F_y] = i\hbar F_z$



♪ ♪ ♪ It's the final
quantum number ♪ ♪ ♪

The coupled basis

As \mathbf{F} acts as an angular momentum, there must be a set of basis states $|F M_F\rangle$ which are eigenstates of \mathbf{F}^2 and F_z . This basis is called the *coupled basis*.

How to find the quantum numbers F and M_F ?

- Find the eigenstates and eigenvalues of the operators \mathbf{F}^2 and F_z

How to find the eigenstates and eigenvalues \mathbf{F}^2 and F_z

- Diagonalise the matrices for \mathbf{F}^2 and F_z

We know the matrices for \mathbf{S} , \mathbf{I} , S_z , and S_I in the uncoupled basis, so we will use these



Matrix mayhem

Our basis:

$$|++\rangle, |+-\rangle, |-+\rangle, |--\rangle$$

Operators:

$$\begin{aligned} \mathbf{J}^2 |j m_j\rangle &= j(j+1)\hbar^2 |j m_j\rangle \\ J_z |j m_j\rangle &= m_j \hbar |j m_j\rangle \end{aligned}$$

Matrices:

$$\mathbf{S}^2 = \frac{3\hbar^2}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \begin{array}{l} ++ \\ +- \\ -+ \\ -- \end{array}$$

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad I_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad \begin{array}{l} ++ \\ +- \\ -+ \\ -- \end{array}$$

$$\mathbf{S} \cdot \mathbf{I} = \frac{\hbar^2}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \begin{array}{l} ++ \\ +- \\ -+ \\ -- \end{array}$$

Matrix elements:

$$O_{ij} = \langle i | O | j \rangle$$

Matrix representation:

$$O = \begin{pmatrix} \langle 1 | O | 1 \rangle & \langle 1 | O | 2 \rangle & \langle 1 | O | 3 \rangle & \langle 1 | O | 4 \rangle \\ \langle 2 | O | 1 \rangle & \langle 2 | O | 2 \rangle & \langle 2 | O | 3 \rangle & \langle 2 | O | 4 \rangle \\ \langle 3 | O | 1 \rangle & \langle 3 | O | 2 \rangle & \langle 3 | O | 3 \rangle & \langle 3 | O | 4 \rangle \\ \langle 4 | O | 1 \rangle & \langle 4 | O | 2 \rangle & \langle 4 | O | 3 \rangle & \langle 4 | O | 4 \rangle \end{pmatrix} \quad \begin{array}{l} |1\rangle \\ |2\rangle \\ |3\rangle \\ |4\rangle \end{array}$$

Calculated last class

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

$$J_{\pm} |j, m_j\rangle = \hbar [j(j+1) - m_j(m_j \pm 1)]^{1/2} |j, m_j \pm 1\rangle$$

Total angular momentum component

Use previously obtained matrices $F_z = S_z + I_z$:

$$F_z = \hbar \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad \begin{matrix} ++ \\ +- \\ -+ \\ -- \end{matrix}$$

F_z is diagonal $\Rightarrow |m_s m_I\rangle$ are eigenstates. We have:

$$\begin{aligned} F_z |m_s m_I\rangle &= (S_z + I_z) |m_s m_I\rangle \\ &= (m_s + m_I) \hbar |m_s m_I\rangle \end{aligned}$$

and by definition

$$F_z |F M_F\rangle = M_F \hbar |F M_F\rangle$$

so we have

$$M_F = m_s + m_I$$

The allowed values of $m_s = \pm 1/2$ and $m_I = \pm 1/2$ mean the values of M_F are 1, 0, 0, and -1.

$|+-\rangle$ and $|--\rangle$ are degenerate, having $M_F = 0$. This means there is an ambiguity around the state which corresponds to $M_F = 0$.



Total angular momentum

Need to find the matrix \mathbf{F}^2 :

We have used the fact $[\mathbf{S}, \mathbf{I}] = 0$

$$\begin{aligned}\mathbf{F}^2 &= (\mathbf{S} + \mathbf{I})^2 = \mathbf{S}^2 + \mathbf{I}^2 + \mathbf{S} \cdot \mathbf{I} + \mathbf{I} \cdot \mathbf{S} \\ &= \mathbf{S}^2 + \mathbf{I}^2 + 2\mathbf{S} \cdot \mathbf{I}\end{aligned}$$

Recall

$$\mathbf{J}^2 |j m_j\rangle = j(j+1) |j m_j\rangle$$

$|m_s m_I\rangle$ are eigenstates of \mathbf{S}^2 and $\mathbf{I}^2 \Rightarrow$ the matrices will be $3/4 \hbar^2 \hat{1}$

We have previously computed $\mathbf{S} \cdot \mathbf{I}$, and so

$$\mathbf{F}^2 = \hbar^2 \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} \quad \begin{matrix} ++ \\ +- \\ -+ \\ -- \end{matrix}$$



The final eigenvalues

$$\mathbf{F}^2 = \hbar^2 \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} \quad \begin{array}{l} ++ \\ +- \\ -+ \\ -- \end{array}$$

\mathbf{F}^2 is block diagonal \Rightarrow eigenvalues are $2\hbar^2$ for the states $|++\rangle$ and $|--\rangle$

The eigenvalue equation for \mathbf{F}^2 is given by

$$\mathbf{F}^2 |F M_F\rangle = F(F+1)\hbar^2 |F M_F\rangle$$

so we find $F = 1$ for $|++\rangle$ and $|--\rangle$.

How to find the other states?

- Diagonalise the submatrix within the space of $|+-\rangle$ and $|-+\rangle$

The eigenvalues of the submatrix are $2\hbar^2$ and 0 \Rightarrow $F = 1$ and 0

Diagonalisation is the same as rotating in Hilbert space, so normally one will “undiagonalise” other matrices.

In the case of F_z , as the states $|+-\rangle$ and $|-+\rangle$ are degenerate with $M_F = 0$, the F_z matrix is proportional to the identity matrix with the degenerate subspace. As rotations have no effect on the identity, this degeneracy – the ambiguity of the state associated with $M_F = 0$ – means that the diagonalisation of \mathbf{F}^2 does not undiagonalise F_z



Bases covered

We can now construct the eigenstates $|F M_F\rangle$ of the coupled basis in terms of the uncoupled basis:

Coupled basis	Uncoupled basis
$ 11\rangle$	$ + +\rangle$
$ 10\rangle$	$1/\sqrt{2}[+ -\rangle + - +\rangle]$
$ 1, -1\rangle$	$ --\rangle$
$ 00\rangle$	$1/\sqrt{2}[+ -\rangle - - +\rangle]$

\uparrow *Triplet state*
 \downarrow *Singlet state*

These states are referred to as the *triplet* state ($F = 1$) and the singlet ($F = 0$) state, and are exactly the eigenstates that we found when we did degenerate perturbation theory on the hyperfine Hamiltonian.

Take a breather

Started with 2 spin-1/2 particles

- Found total angular momentum could be 0 or 1 ($F = s + I = 1$ and $F = s - I = 0$)
- For each value of F the magnetic quantum numbers run from $-M_F$ to M_F in unit steps
- Learned how to express the coupled basis in terms of the uncoupled basis

We now have two complete orthonormal bases to use. The best one to use will depend on the problem, e.g. for the hyperfine Hamiltonian, the coupled basis is the “good” basis as the basis eigenstates are the energy eigenstates



Zoidberg...

Hyperfine interaction MKII

Knowing the coupled basis, the hyperfine problem should be easy to solve. Recall

$$H'_{hf} = \frac{A}{\hbar^2} \mathbf{S} \cdot \mathbf{I}$$

Show that for the ground state of Hydrogen,

$$E_{hf}^{(1)} = \begin{cases} +A/4; & F = 1 \\ -3A/4; & F = 0 \end{cases}$$

Finding \mathbf{F}^2 , we showed

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

so we need to find the matrices \mathbf{F}^2 , \mathbf{S}^2 , and \mathbf{I}^2

The matrix returns

All states have the quantum numbers $s = 1/2$ and $I = 1/2$, so the coupled states are eigenstates of \mathbf{S}^2 and \mathbf{I}^2 with eigenvalues $3\hbar^2/4$, so in the coupled basis

$$\mathbf{S}^2 = \mathbf{I}^2 = \frac{3\hbar^2}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{matrix} 11 \\ 10 \\ 1, -1 \\ 00 \end{matrix}$$

\mathbf{F}^2 can be found from the eigenvalue equation
 $\mathbf{F}^2 |\mathbf{F} M_F\rangle = F(F+1)\hbar^2 |\mathbf{F} M_F\rangle$

$$\mathbf{F}^2 = \frac{\hbar^2}{4} \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{matrix} 11 \\ 10 \\ 1, -1 \\ 00 \end{matrix}$$

and so we find

$$H'_{hf} = \frac{A}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix} \begin{matrix} 11 \\ 10 \\ 1, -1 \\ 00 \end{matrix}$$

which is (very unsurprisingly) diagonal.

To find $E_{hf}^{(1)}$, we must still use degenerate perturbation theory, which means:

- diagonalising the Hamiltonian in the degenerate space

Done! By inspection:

$$E_{hf}^{(1)} = \begin{cases} +A/4; & F = 1 \\ -3A/4; & F = 0 \end{cases}$$

No need for the degenerate

It is worth noting that we can apply non-degenerate perturbation theory when the matrix H'_{hf} is diagonal.

How do we calculate $E_{hf}^{(1)}$ with non-degenerate perturbation theory?

- Need to calculate the expectation values of the perturbation $\langle F M_F | H'_{hf} | F M_F \rangle$

As the states $|F M_F\rangle$ are the eigenstates of \mathbf{F}^2 , \mathbf{S}^2 , and \mathbf{I}^2 :

$$\begin{aligned} E_{hf}^{(1)} &= \langle F M_F | H'_{hf} | F M_F \rangle = \frac{A}{2\hbar^2} \langle F M_F | \mathbf{F}^2 - \mathbf{S}^2 - \mathbf{I}^2 | F M_F \rangle \\ &= \frac{A}{2\hbar^2} [F(F+1) - s(s+1) - I(I+1)]\hbar^2 \\ &= \frac{A}{2} \left[F(F+1) - \frac{3}{2} \right] \\ &= \begin{cases} +A/4; & F = 1 \\ -3A/4; & F = 0 \end{cases} \end{aligned}$$

which is (unsurprisingly!) the same as the previous times we have computed this.

Let us return to the beginning

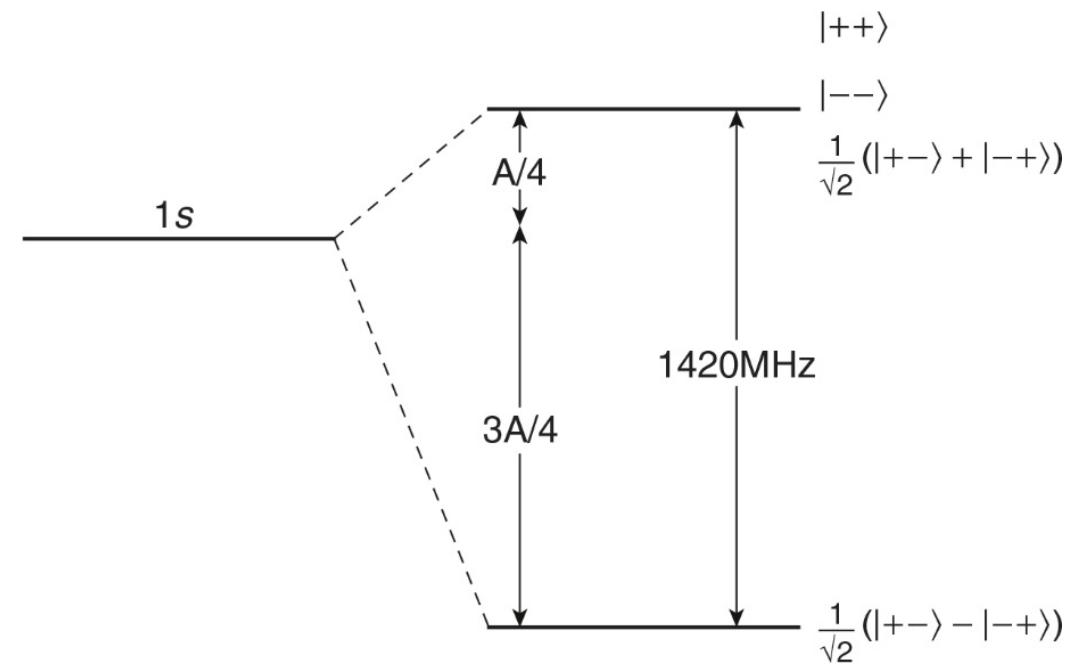
Discussion:

What distinguishes the states

$$|E_3\rangle = 1/\sqrt{2}[|+-\rangle + |-+\rangle] \text{ and } |E_4\rangle = 1/\sqrt{2}[|+-\rangle - |-+\rangle]$$

Why are these states separated in energy?

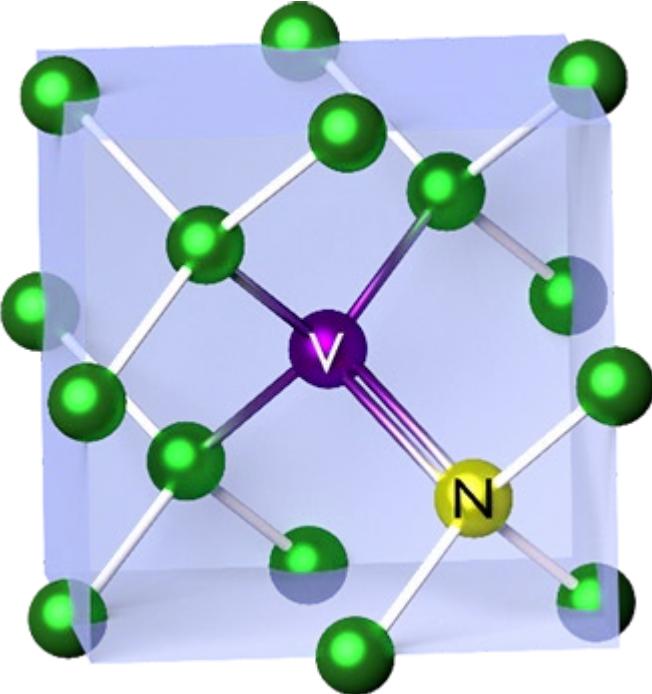
Coupled basis	Uncoupled basis
$ 11\rangle$	$ ++\rangle$
$ 10\rangle$	$1/\sqrt{2}[+-\rangle + -+\rangle]$
$ 1,-1\rangle$	$ --\rangle$
$ 00\rangle$	$1/\sqrt{2}[+-\rangle - -+\rangle]$



Hyperfine splitting of the ground state of hydrogen

Quantum information and NV centres

A relatively simple *pseudo-atom* is the Nitrogen-Vacancy (NV) centre in diamond



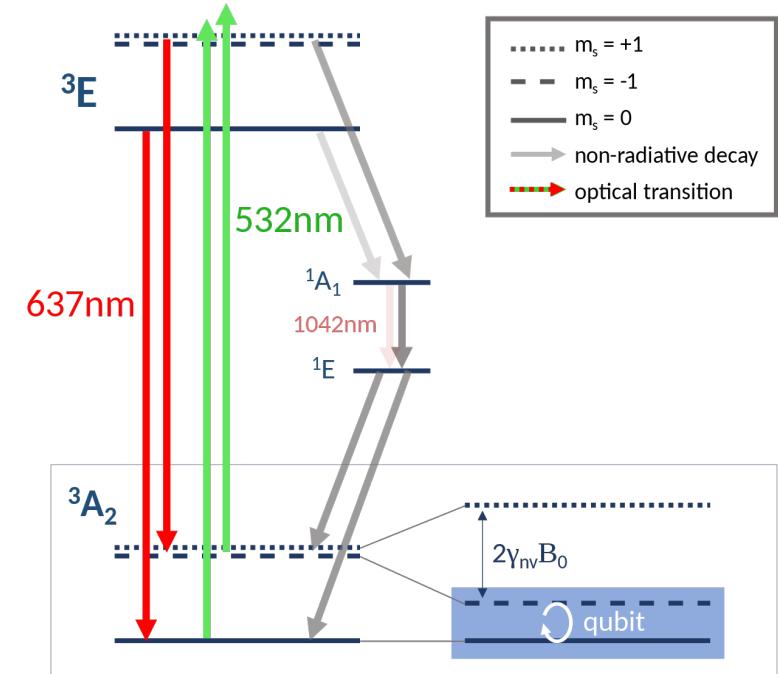
The structure of an NV centre

Excitation is spin conserving, but decay prefers the $m_s = 0$ state

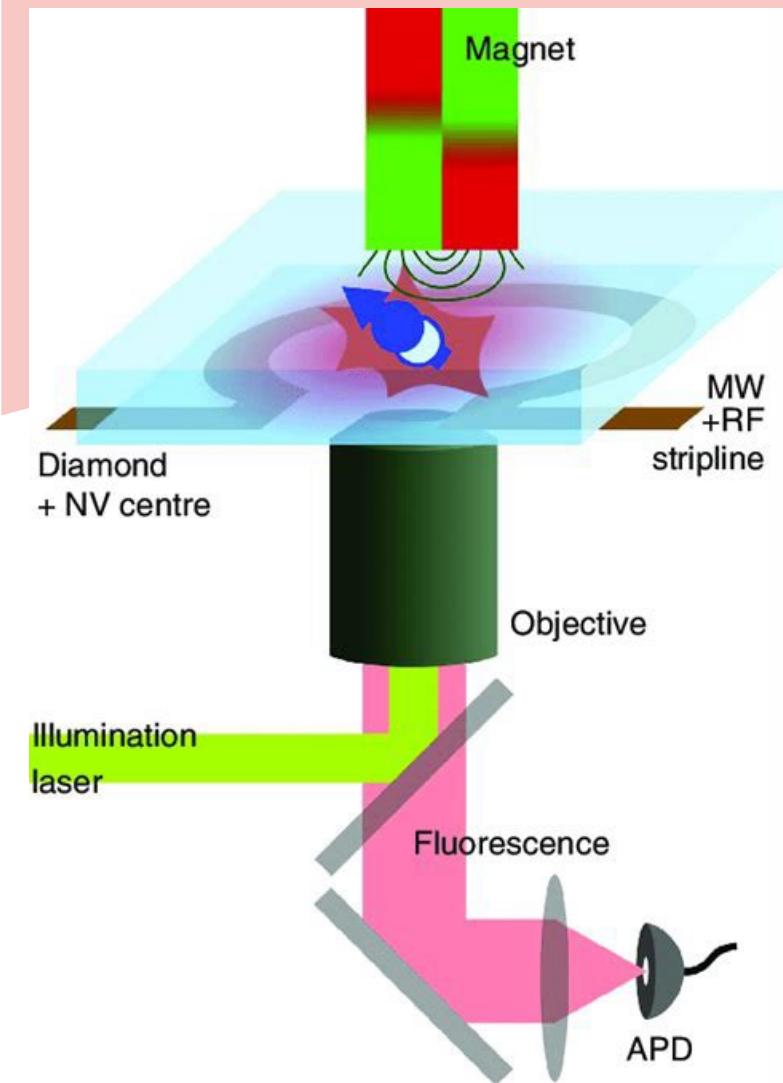
Electrons can be initialised in the ground state

If the electron is excited to $m_s = \pm 1$, fluorescence decreases

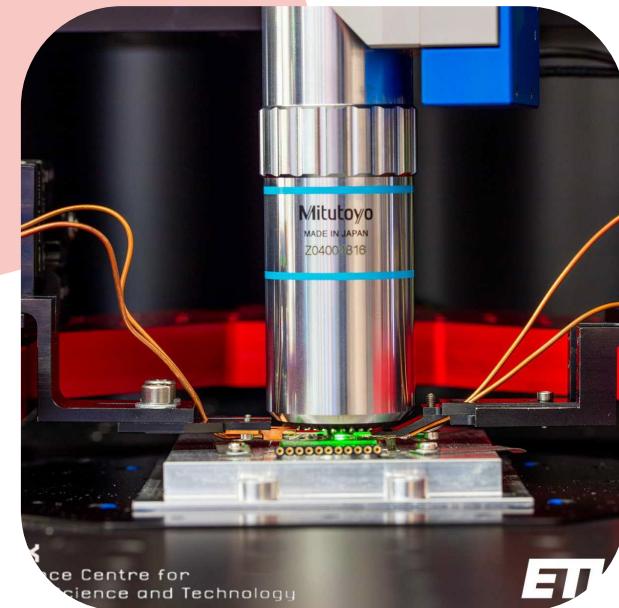
Room temperature single-atom system, with applications in sensing and quantum computing



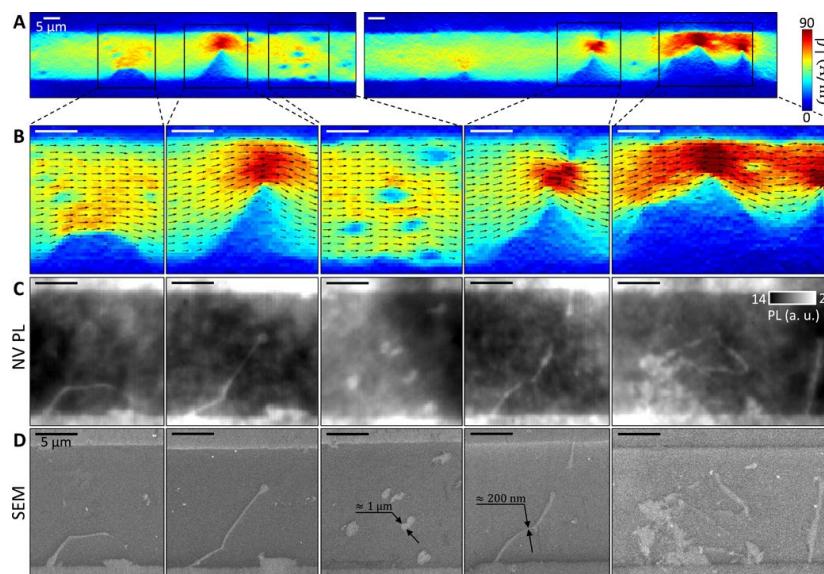
Energy level structure of an NV-centre in diamond



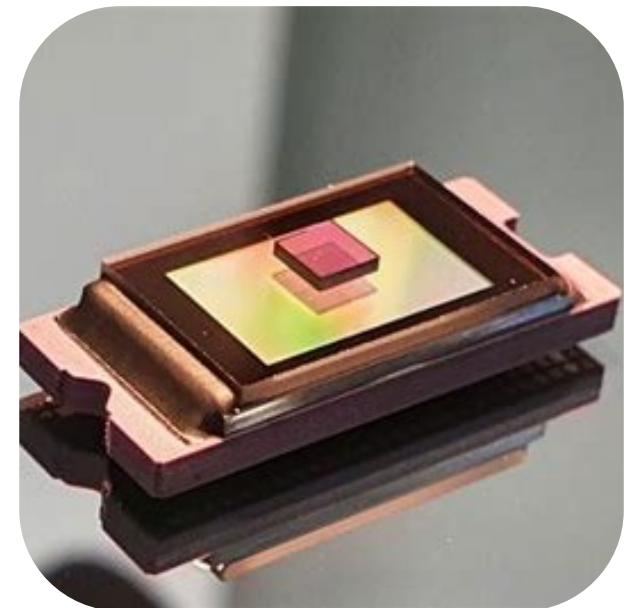
A schematic for quantum control of a NV centre



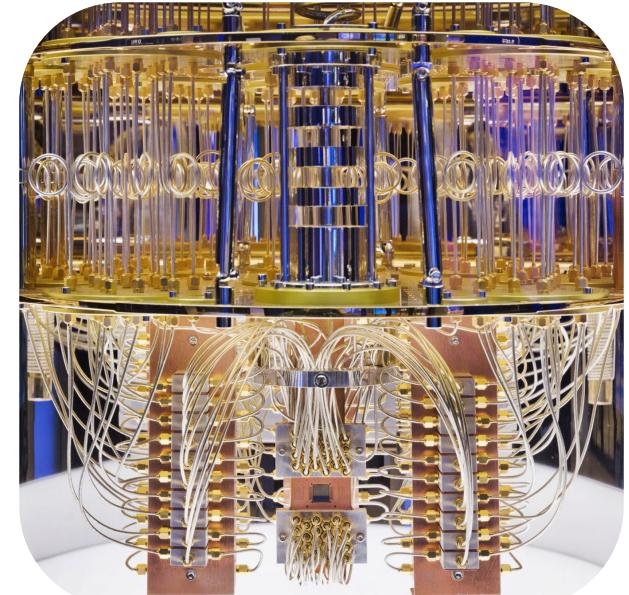
A setup for quantum control of an NV centre



Current density sensing in graphene



NV centres as a basis for quantum computing



c.f. superconductors



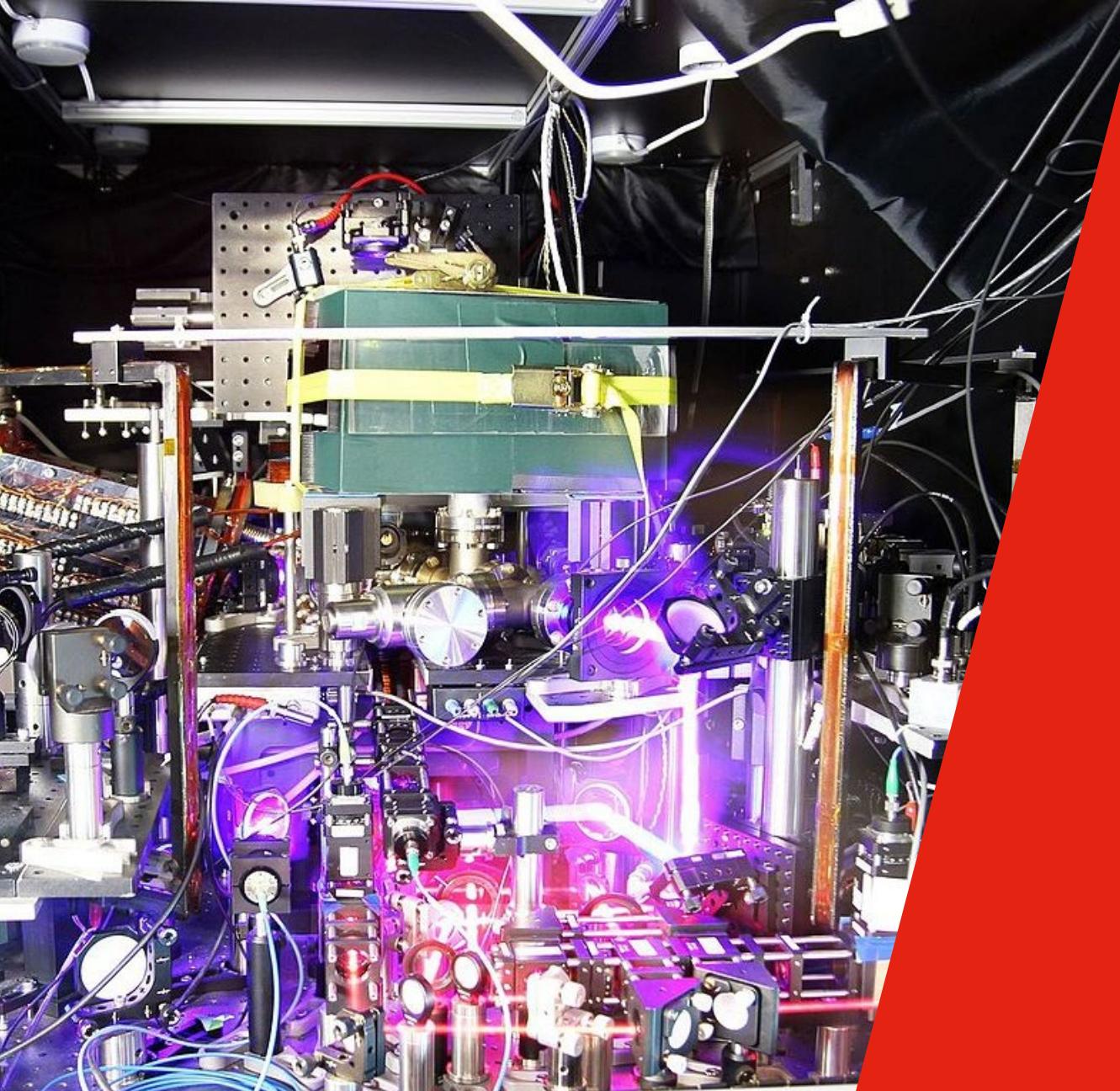
UNIVERSITY of
TASMANIA

Summary

- Total angular momentum
 - We can describe a system of two angular momenta using either the uncoupled or coupled basis
 - Solving problems in the coupled basis is much simpler, and is often illuminating
 - Diagonalisation is an important tool for performing angular momentum – and more general quantum mechanical – calculations

Problems

M11.8, M11.10, M11.18



Addition of generalised angular momenta

Chapter 11



UNIVERSITY of
TASMANIA

Learning outcomes

Week 2, lecture 3

McIntyre §11.6: Addition of generalised angular momenta

- Connecting bases
 - How do we move between the coupled basis and uncoupled basis
- Clebsch-Gordan coefficients
 - What they are, why you'll want to use them, and how to use them

Where are we, and where are we going?

We have seen how to add the angular momenta of two spin-1/2 particles, but we want to add *any* two angular momenta

Discussion:

Why do we care about the addition of angular momenta?

Directly finding the eigenstates of \mathbf{F} will always work, but will get ugly quickly!

We seek a recipe to allow us to convert between the *coupled* and *uncoupled* bases, and the starting point is the ladder operators.



The plan:

Recall that the generalised ladder operators obey

$$J_{\pm}|j, m_j\rangle = \hbar[j(j+1) - m_j(m_j \pm 1)]^{1/2}|j, m_j \pm 1\rangle$$

Recall also that for a spin-1/2 system, we have

Coupled basis	Uncoupled basis
$ 11\rangle$	$ + +\rangle$
$ 10\rangle$	$1/\sqrt{2}[+ -\rangle + - +\rangle]$
$ 1, -1\rangle$	$ --\rangle$
$ 00\rangle$	$1/\sqrt{2}[+ -\rangle - - +\rangle]$

The state $|11\rangle = |+ +\rangle$ is an eigenstate in both the coupled and uncoupled basis

⇒ we can apply the ladder operators to these states, and learn how they are related



Plug and play

Let's go:

$$F_- |11\rangle = F_- |++\rangle$$

$$F_- |11\rangle = (S_- + I_-) |++\rangle$$

$$F_- |11\rangle = S_- |++\rangle + I_- |++\rangle$$

$$\sqrt{2}\hbar |10\rangle = \hbar(|+-\rangle + |-+\rangle)$$

or

$$|10\rangle = 1/\sqrt{2}[|+-\rangle + |-+\rangle]$$

as we found previously (unsurprisingly!)

We can repeat this process to show that

$$|1,-1\rangle = |--\rangle$$

But we have only changed M_F , not F

In order to find the state $|00\rangle$, we can use orthogonality to find a state that is orthogonal to $|10\rangle$ and comprises the same uncoupled states, i.e.

$$|00\rangle = a|+-\rangle + b|-+\rangle$$

for some a and b . Then we have

$$0 = \langle 10|00\rangle$$

$$= \frac{1}{\sqrt{2}} (\langle +-| + \langle -+|)(a|+-\rangle + b|-+\rangle)$$

$$= \frac{1}{\sqrt{2}} (a + b)$$

$$\Rightarrow |00\rangle = 1/\sqrt{2}[|+-\rangle - |-+\rangle]$$



Matrix mayhem – final edition

Our basis:

$$|11\rangle, |10\rangle, |1, -1\rangle, |00\rangle$$

Operators:

$$\mathbf{F}^2|F M_F\rangle = F(F+1)\hbar^2|F M_F\rangle$$

$$F_z|F M_F\rangle = M_F\hbar|F M_F\rangle$$

Matrices:

$$\mathbf{F}^2 = \frac{\hbar^2}{4} \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \begin{matrix} |11\rangle \\ |10\rangle \\ |1, -1\rangle \\ |00\rangle \end{matrix}$$

$$F_z = \hbar \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \begin{matrix} |11\rangle \\ |10\rangle \\ |1, -1\rangle \\ |00\rangle \end{matrix}$$

$$F_{\pm}|F M_F\rangle = \hbar[F(F+1) - M_F(M_F \pm 1)]^{1/2}|F M_F \pm 1\rangle$$

What is the matrix for F_- ?

$$\langle 1 1|F_-|1 1\rangle = \langle 1 1|\hbar[2 - 0]^{1/2}|1 0\rangle = 0$$

$$\langle 1 0|F_-|1 1\rangle = \sqrt{2}$$

$$F_- = \hbar \begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \begin{matrix} |11\rangle \\ |10\rangle \\ |1, -1\rangle \\ |00\rangle \end{matrix}$$

State generation

This procedure of using ladder operators and orthogonality generates all states in **any** coupled basis

Consider two angular momenta J_1 and J_2 coupled to form total angular momentum J

$$J = J_1 + J_2$$

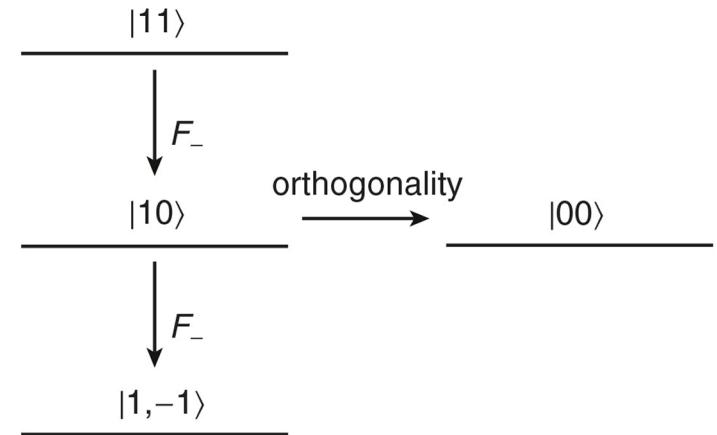
The J_i are characterised by quantum numbers j_i, m_i and J is characterised by J, M . Specifying all eigenvalues, we have

Uncoupled basis

$$|j_1 j_2 m_1 m_2\rangle$$

Coupled basis

$$|j_1 j_2 J M\rangle$$



Generation of the coupled states for two spin-1/2 particles

Eigenstates of which operators?

The uncoupled basis vectors are eigenstates of J_1^2, J_2^2, J_{1z} , and J_{2z}

The coupled basis vectors are eigenstates of J_1^2, J_2^2, J^2 and J_z

Generalisation

For a given problem, the values j_1 and j_2 are fixed, so by convention they are not used to label states in the coupled basis

Coupled basis	Uncoupled basis
$ 11\rangle$	$\left \begin{array}{cccc} 1 & 1 & 1 & 1 \\ 2 & 2 & 2 & 2 \end{array} \right\rangle$
$ 10\rangle$	$\frac{1}{\sqrt{2}} \left(\left \begin{array}{cccc} 1 & 1 & 1 & -1 \\ 2 & 2 & 2 & 2 \end{array} \right\rangle + \left \begin{array}{cccc} 1 & 1 & -1 & 1 \\ 2 & 2 & 2 & 2 \end{array} \right\rangle \right)$
$ 1, -1\rangle$	$\left \begin{array}{cccc} 1 & 1 & -1 & -1 \\ 2 & 2 & 2 & 2 \end{array} \right\rangle$
$ 00\rangle$	$\frac{1}{\sqrt{2}} \left(\left \begin{array}{cccc} 1 & 1 & 1 & -1 \\ 2 & 2 & 2 & 2 \end{array} \right\rangle - \left \begin{array}{cccc} 1 & 1 & -1 & 1 \\ 2 & 2 & 2 & 2 \end{array} \right\rangle \right)$

convention \Leftrightarrow convenience: we can immediately distinguish between the coupled and uncoupled basis



In the general case, the state generation procedure will produce values of

$$J = j_1 + j_2, j_1 + j_2 - 1, j_1 + j_2 - 2, \dots |j_1 - j_2|$$

that is, integer steps between the extreme values of $j_1 + j_2$ and $j_1 - j_2$ (noting that $J \geq 0!$)

For each allowed value of J , the allowed values of M are

$$M = -J, -J + 1, \dots, J - 1, J$$

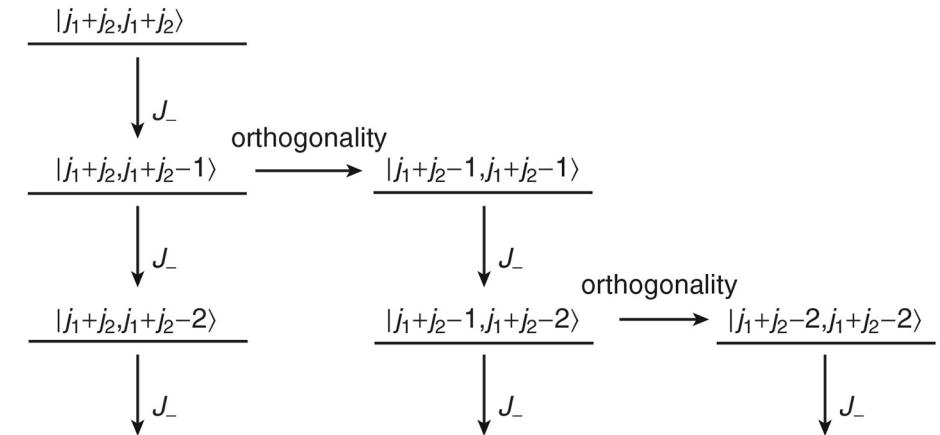
that is, integer steps between $-J$ and J

Generating generalised states

The general state generation procedure is as shown over:

In addition to generating the states, it provides the coefficients needed to express the uncoupled basis states in terms of the coupled basis states (or vice versa). These coefficients are called the *Clebsch-Gordan* coefficients

This recipe is great, but can be tedious for large angular momentum values



Generation of the coupled states for generalised angular momenta j_1 and j_2

$$|22\rangle = |1111\rangle$$

$$|21\rangle = \frac{1}{\sqrt{2}}|1110\rangle + \frac{1}{\sqrt{2}}|1101\rangle$$

$$|20\rangle = \frac{1}{\sqrt{6}}|111-1\rangle + \sqrt{\frac{2}{3}}|1100\rangle + \frac{1}{\sqrt{6}}|11-11\rangle$$

$$|2-1\rangle = \frac{1}{\sqrt{2}}|110-1\rangle + \frac{1}{\sqrt{2}}|11-10\rangle$$

$$|2-2\rangle = |11-1-1\rangle$$

$$|11\rangle = \frac{1}{\sqrt{2}}|1110\rangle - \frac{1}{\sqrt{2}}|1101\rangle$$

$$|10\rangle = \frac{1}{\sqrt{2}}|111-1\rangle - \frac{1}{\sqrt{2}}|11-11\rangle$$

$$|1-1\rangle = \frac{1}{\sqrt{2}}|110-1\rangle - \frac{1}{\sqrt{2}}|11-10\rangle$$

$$|00\rangle = \frac{1}{\sqrt{3}}|111-1\rangle - \frac{1}{\sqrt{3}}|1100\rangle + \frac{1}{\sqrt{3}}|11-11\rangle$$

The coupled states $|JM\rangle$ for $j_1 = 1$ and $j_2 = 1$

Relating the bases

Remember that we seek a general formula for relating the coupled and uncoupled states. This can be found using the completeness relation, which for the uncoupled basis looks like

$$\sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} |j_1 j_2 m_1 m_2\rangle \langle j_1 j_2 m_1 m_2| = \mathbf{1}$$

Acting this projection operator on a coupled state gives

$$|JM\rangle = \left[\sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} |j_1 j_2 m_1 m_2\rangle \langle j_1 j_2 m_1 m_2| \right] |JM\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} (\langle j_1 j_2 m_1 m_2 | JM \rangle) |j_1 j_2 m_1 m_2\rangle$$

or

$$|JM\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} C_{m_1 m_2 M}^{j_1 j_2 J} |j_1 j_2 m_1 m_2\rangle$$

where the products connecting the bases, $\langle j_1 j_2 m_1 m_2 | JM \rangle$, are the *Clebsch-Gordan* coefficients

Clebsch-Gordan coefficients (and the cursed table)

34. Clebsch-Gordan coefficients 010001-1

34. CLEBSCH-GORDAN COEFFICIENTS, SPHERICAL HARMONICS, AND d FUNCTIONS

Note: A square-root sign is to be understood over every coefficient, e.g., for $-8/15$ read $-\sqrt{8/15}$.

$l_1 \times l_2 \times l_3$	m_1	m_2	m_3	Notation:	J	J	\dots
M_1	M_2	M_3			M	M	\dots
$1/2 \times 1/2$	± 1	± 1	± 1	m_1, m_2	J	J	\dots
$1 \times 1/2$	$\pm 1/2$	$\pm 1/2$	$\pm 1/2$	m_1, m_2	M	M	\dots
2×1	± 1	± 1	± 1	m_1, m_2	m_1, m_2	m_3	\dots
1×1	± 1	± 1	± 1	m_1, m_2	m_1, m_2	m_3	\dots
$Y_\ell^{-m} = (-1)^m Y_\ell^m$	$d_{m,\ell}^j = \sqrt{\frac{4\pi}{2\ell+1}} Y_\ell^m e^{-im\theta}$	$(j_1 j_2 m_1 m_2 j_1 j_2 JM)$	$= (-1)^J j_1 j_2 (j_2 j_1 m_2 m_1 j_2 j_1 JM)$				
$d_{m',m}^j = (-1)^{m-m'} d_{m,m'}^j = d_{-m,-m'}^j$							
$2 \times 3/2$	$\pm 3/2$	$\pm 1/2$	$\pm 3/2$	m_1, m_2	J	J	\dots
2×2	± 2	± 2	± 2	m_1, m_2	J	J	\dots
$d_{3/2,3/2}^{3/2} = \frac{1+\cos\theta}{2} \cos \frac{\theta}{2}$							
$d_{3/2,1/2}^{3/2} = -\sqrt{3/10} \cos \frac{\theta}{2} \sin \frac{\theta}{2}$	$d_{2,2}^{3/2} = \left(\frac{1+\cos\theta}{2}\right)^2$						
$d_{3/2,-1/2}^{3/2} = \sqrt{3/10} \cos \frac{\theta}{2} \sin \frac{\theta}{2}$	$d_{2,1}^{3/2} = -\frac{1+\cos\theta}{2} \sin \theta$	$d_{1,1}^{3/2} = \frac{1+\cos\theta}{2} (2\cos\theta - 1)$	$d_{1,-1}^{3/2} = -\frac{1+\cos\theta}{2} (2\cos\theta + 1)$	$d_{2,0}^{3/2} = \frac{\sqrt{6}}{4} \sin^2 \theta$			
$d_{3/2,-3/2}^{3/2} = -\frac{1-\cos\theta}{2} \sin \frac{\theta}{2}$	$d_{2,-2}^{3/2} = -\frac{1-\cos\theta}{2} \sin \theta$	$d_{1,0}^{3/2} = -\sqrt{\frac{3}{2}} \sin \theta \cos \theta$	$d_{1,-2}^{3/2} = -\frac{1-\cos\theta}{2} (2\cos\theta + 1)$	$d_{2,0}^{3/2} = \left(\frac{3}{2}\right) \cos^2 \theta - \frac{1}{2}$			
$d_{1/2,1/2}^{3/2} = \frac{3\cos\theta - 1}{2} \cos \frac{\theta}{2}$	$d_{2,-1}^{3/2} = -\frac{1-\cos\theta}{2} \sin \theta$	$d_{1,0}^{3/2} = -\sqrt{\frac{3}{2}} \sin \theta \cos \theta$	$d_{1,-2}^{3/2} = -\frac{1-\cos\theta}{2} (2\cos\theta + 1)$	$d_{2,0}^{3/2} = \left(\frac{3}{2}\right) \cos^2 \theta - \frac{1}{2}$			
$d_{1/2,-1/2}^{3/2} = \frac{3\cos\theta + 1}{2} \sin \frac{\theta}{2}$	$d_{2,-2}^{3/2} = \left(\frac{1-\cos\theta}{2}\right)^2$	$d_{1,-1}^{3/2} = \frac{1-\cos\theta}{2} (2\cos\theta + 1)$	$d_{1,2}^{3/2} = \frac{1-\cos\theta}{2} (2\cos\theta - 1)$	$d_{2,0}^{3/2} = \left(\frac{3}{2}\right) \cos^2 \theta - \frac{1}{2}$			

Figure 34.1: The sign convention is that of Wigner (*Group Theory*, Academic Press, New York, 1959), also used by Condon and Shortley (*The Theory of Atomic Spectra*, Cambridge Univ. Press, New York, 1933), Rose (*Elementary Theory of Angular Momentum*, Wiley, New York, 1957), and Cohen (*Tables of the Clebsch-Gordan Coefficients*, North American Rockwell Science Center, Thousand Oaks, Calif., 1974). The coefficients here have been calculated using computer programs written independently by Cohen and at LBNL.

Notation:

m_1	m_2	Notation:	J	J	\dots
m_1	m_2		M	M	\dots
\cdot	\cdot		M_1	M_2	\dots
\cdot	\cdot		m_1	m_2	\dots
\cdot	\cdot			m_3	\dots
\cdot	\cdot				M_3

Coefficients

$1/2 \times 1/2$

	1		
$+1/2$	$+1/2$	1	0
$+1/2$	$-1/2$	$1/2$	$1/2$
$-1/2$	$+1/2$	$1/2$	$-1/2$
$-1/2$	$-1/2$	1	

Coupled basis

$|11\rangle$

Uncoupled basis

$\left| \begin{array}{cccc} 1 & 1 & 1 & 1 \\ 2 & 2 & 2 & 2 \end{array} \right\rangle$

$|10\rangle$

$\frac{1}{\sqrt{2}} \left(\left| \begin{array}{cccc} 1 & 1 & 1 & -1 \\ 2 & 2 & 2 & 2 \end{array} \right\rangle + \left| \begin{array}{cccc} 1 & 1 & -1 & 1 \\ 2 & 2 & 2 & 2 \end{array} \right\rangle \right)$

$|00\rangle$

$\frac{1}{\sqrt{2}} \left(\left| \begin{array}{cccc} 1 & 1 & 1 & -1 \\ 2 & 2 & 2 & 2 \end{array} \right\rangle - \left| \begin{array}{cccc} 1 & 1 & -1 & 1 \\ 2 & 2 & 2 & 2 \end{array} \right\rangle \right)$

$|1, -1\rangle$

$\left| \begin{array}{cccc} 1 & 1 & -1 & -1 \\ 2 & 2 & 2 & 2 \end{array} \right\rangle$



Consider a system of two angular momenta with $j_1 = 1$ and $j_2 = 1/2$.

- What are the possible states of this system in the uncoupled basis
- What are the allowed values of the coupled angular momentum quantum numbers J and M ?
- Write down all the possible states of this system in the coupled basis $|JM\rangle$
- Use the Clebsch-Gordan coefficients to express the coupled basis states $|JM\rangle$ in terms of the uncoupled basis states $|j_1 j_2 m_1 m_2\rangle$

$1 \times 1/2$	$\begin{matrix} 3/2 \\ +3/2 \end{matrix}$	$\begin{matrix} 3/2 & 1/2 \\ +1/2 & +1/2 \end{matrix}$	$\begin{matrix} +1 & +1/2 \\ 0 & +1/2 \end{matrix}$	$\begin{matrix} +1 & -1/2 \\ 0 & +1/2 \end{matrix}$	$\begin{matrix} 1/3 & 2/3 \\ 2/3 & -1/3 \end{matrix}$	$\begin{matrix} 3/2 & 1/2 \\ -1/2 & -1/2 \end{matrix}$	$\begin{matrix} 0 & -1/2 \\ -1 & +1/2 \end{matrix}$	$\begin{matrix} 2/3 & 1/3 \\ 1/3 & -2/3 \end{matrix}$	$\begin{matrix} 3/2 \\ -3/2 \end{matrix}$
2×1	$\begin{matrix} 3 \\ +3 \end{matrix}$	$\begin{matrix} 3 \\ 3 \end{matrix}$	$\begin{matrix} 2 \\ 2 \end{matrix}$	$\begin{matrix} -1 & -1/2 \\ -1 & -1/2 \end{matrix}$		1			

Extract from the table of Clebsch-Gordan coefficients



Consider a system of two particles. Particle #1 has spin 1 and particle 2 has spin 1/2 . The system is in a state with total spin $\frac{1}{2}$ and z-component $-\hbar/2$. If you measure the z-component of the spin of particle #1, what are the possible results, and what are the probabilities of the measurements? What about for particle #2?

$1 \times 1/2$	$\begin{matrix} 3/2 \\ +3/2 \end{matrix}$	$\begin{matrix} 3/2 & 1/2 \\ +1/2 & +1/2 \end{matrix}$	$\begin{matrix} 3/2 & 1/2 \\ -1/2 & -1/2 \end{matrix}$	$\begin{matrix} 3/2 & 1/2 \\ 1/3 & 2/3 \end{matrix}$	$\begin{matrix} 0 & -1/2 \\ 2/3 & -1/3 \end{matrix}$	$\begin{matrix} 0 & -1/2 \\ -1 & +1/2 \end{matrix}$	$\begin{matrix} 2/3 & 1/3 \\ 1/3 & -2/3 \end{matrix}$	$\begin{matrix} 3/2 \\ -3/2 \end{matrix}$
2×1	$\begin{matrix} 3 \\ +3 \end{matrix}$	$\begin{matrix} 3 \\ 3 \end{matrix}$	$\begin{matrix} 2 \\ 2 \end{matrix}$	$\begin{matrix} -1 \\ -1 \end{matrix}$	$\begin{matrix} -1/2 \\ -1/2 \end{matrix}$	$\begin{matrix} 1 \\ 1 \end{matrix}$		

Extract from the table of Clebsch-Gordan coefficients



Cursed table treats

Consider coupled spins with $J_1 = 3/2$ and $J_2 = 1$. What is the state $\left| \frac{5}{2}, -\frac{1}{2} \right\rangle$ in the coupled basis expressed in the uncoupled basis?

- a) What are the possible states of this system in the uncoupled basis
- b) What are the allowed values of the coupled angular momentum quantum numbers J and M ?
- c) Write down all the possible states of this system in the coupled basis $|JM\rangle$
- d) Use the Clebsch-Gordan coefficients to express the coupled basis states $|JM\rangle$ in terms of the uncoupled basis states $|j_1 j_2 m_1 m_2\rangle$

$3/2 \times 1$	$\begin{matrix} 5/2 \\ +5/2 \\ \hline +3/2 & +1 \end{matrix}$	$\begin{matrix} 5/2 & 3/2 \\ +3/2 & +3/2 \\ \hline +3/2 & 0 & 2/5 & 3/5 & 5/2 & 3/2 & 1/2 \\ +1/2 & +1 & 3/5 & -2/5 & +1/2 & +1/2 & +1/2 \end{matrix}$	$\begin{matrix} +3/2 & -1 & 1/10 & 2/5 & 1/2 \\ +1/2 & 0 & 3/5 & 1/15 & -1/3 & 5/2 & 3/2 & 1/2 \\ -1/2 & +1 & 3/10 & -8/15 & 1/6 & -1/2 & -1/2 & -1/2 \end{matrix}$	$\begin{matrix} +1/2 & -1 & 3/10 & 8/15 & 1/6 \\ -1/2 & 0 & 3/5 & -1/15 & -1/3 & 5/2 & 3/2 \\ -3/2 & +1 & 1/10 & -2/5 & 1/2 & -3/2 & -3/2 \end{matrix}$	$\begin{matrix} -1/2 & -1 & 3/5 & 2/5 & 5/2 \\ -3/2 & 0 & 2/5 & -3/5 & -5/2 \\ -3/2 & -1 & 1 & & \end{matrix}$
----------------	---	--	---	---	--

Zeroing in

Shown are two versions of tabulated Clebsch-Gordan coefficients

The complete table is illustrative because, as we shall see, to compute transition probabilities between states, the angular overlap integrals of wave functions can be expressed in terms of Clebsch-Gordan coefficients. We can therefore see that some transitions are *allowed* (non-zero transition probability) whilst others are forbidden.

$1 \times 1/2$	$\begin{matrix} 3/2 \\ +3/2 \\ +1 \\ +1/2 \\ 1 \end{matrix}$	$\begin{matrix} 3/2 & 1/2 \\ +1/2 & +1/2 \end{matrix}$	$\begin{matrix} 3/2 & 1/2 \\ -1/2 & -1/2 \end{matrix}$	$\begin{matrix} 3/2 & 1/2 \\ 1/3 & 2/3 \\ 2/3 & -1/3 \end{matrix}$	$\begin{matrix} 0 & -1/2 \\ -1 & +1/2 \end{matrix}$	$\begin{matrix} 2/3 & 1/3 \\ 1/3 & -2/3 \end{matrix}$	$\begin{matrix} 3/2 \\ -3/2 \end{matrix}$
2×1	$\begin{matrix} 3 \\ +3 \end{matrix}$	$\begin{matrix} 3 \\ 3 \end{matrix}$	$\begin{matrix} 2 \end{matrix}$				$\begin{matrix} -1 & -1/2 \\ 1 \end{matrix}$

Table of non-zero Clebsch-Gordan coefficients

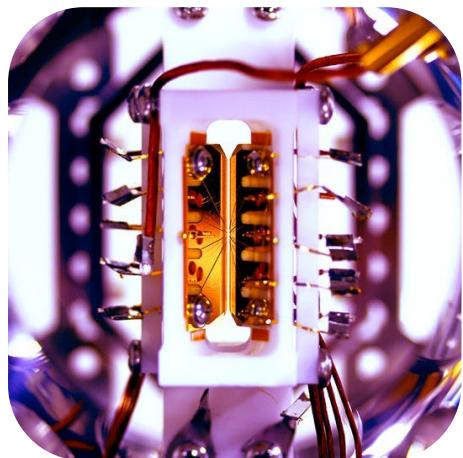
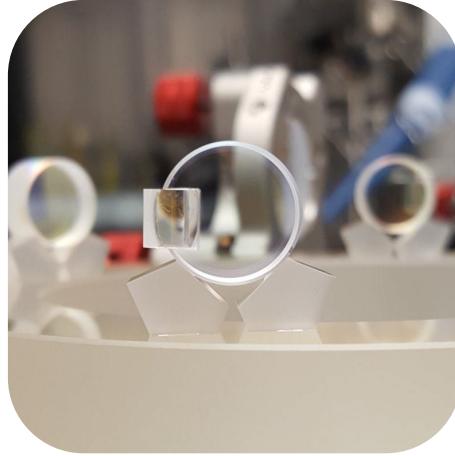
$j_1 = 1$	J	$\frac{3}{2}$	$\frac{3}{2}$	$\frac{3}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
$j_2 = \frac{1}{2}$	M	$\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$
m_1	m_2						
1	$\frac{1}{2}$	1	0	0	0	0	0
1	$-\frac{1}{2}$	0	$\frac{1}{\sqrt{3}}$	0	0	$\sqrt{\frac{2}{3}}$	0
0	$\frac{1}{2}$	0	$\sqrt{\frac{2}{3}}$	0	0	$-\frac{1}{\sqrt{3}}$	0
0	$-\frac{1}{2}$	0	0	$\sqrt{\frac{2}{3}}$	0	0	$\frac{1}{\sqrt{3}}$
-1	$\frac{1}{2}$	0	0	$\frac{1}{\sqrt{3}}$	0	0	$-\sqrt{\frac{2}{3}}$
-1	$-\frac{1}{2}$	0	0	0	1	0	0

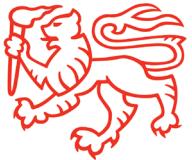
“Complete” table of Clebsch-Gordan coefficients

Isn't this all a bit abstract?

Why Clebsch-Gordan coefficients matter

- Spectroscopy and atomic structure: determining fine and hyperfine structures in atomic spectra, essential for identifying elements and their isotopes.
- Quantum computing and information: efficiently managing quantum states and operations in quantum algorithms
- Magnetic resonance techniques: crucial for applications in nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI)
- Chemical bonding and molecular physics: essential in predicting chemical reactivity and properties of new materials





UNIVERSITY of
TASMANIA

Summary

Problems

M11.12, M11.13, M11.16

- Angular momentum coupling
 - Ladder operators can generate states with the same value of M_J
 - Orthogonality can be used to generate states with different J
 - States in the coupled basis are labelled using only $|J\ M_J\rangle$ whilst states in the uncoupled basis are labelled $|J_1\ J_2\ m_{J_1}\ m_{J_2}\rangle$
 - Clebsch-Gorden coefficients connect the coupled basis and uncoupled basis
 - Important to know how to read and use the table of Clebsch-Gorden coefficients