



UNIVERSITY OF  
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NST Part II Physics  
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# ADVANCED QUANTUM PHYSICS

## Handout 5

- 
- ▶ Symmetry transformations
  - ▶ The Wigner-Eckart theorem (selection rules)
  - ▶ Combining magnetic moments

# Symmetries

- There is a close connection in quantum mechanics between invariance under *symmetry operations* and *conservation laws* :

time translation :  $t \rightarrow t + \tau$  energy conservation

spatial translation :  $\mathbf{r} \rightarrow \mathbf{r} + \mathbf{a}$  linear momentum conservation

spatial rotation :  $r_i \rightarrow \sum_j R_{ij} r_j$  angular momentum conservation

spatial inversion :  $\mathbf{r} \rightarrow -\mathbf{r}$  conservation of parity

- These, and other, symmetry principles (in particular, gauge invariance) underpin the form of all the fundamental interactions

# Symmetry Transformations

- A *symmetry transformation* involves viewing a given system from a different perspective, e.g. from a different position or angle

Such a transformation can be considered, equivalently, to be either

- *active* (move the system, keeping the axes fixed), or
- *passive* (move the axes, keeping the system fixed)

- In quantum mechanics, a symmetry transformation is implemented by introducing an operator  $U$  which transforms physical states as

$$|\psi\rangle \rightarrow |\psi'\rangle = \hat{U}|\psi\rangle$$

If a system is *invariant* under the symmetry transformation, then all probabilities and normalisations are left unchanged

We then have, for any pair of states  $|\psi\rangle$  and  $|\phi\rangle$ ,

$$|\langle\phi'|\psi'\rangle|^2 = |\langle\hat{U}\phi|\hat{U}\psi\rangle|^2 = |\langle\phi|\psi\rangle|^2$$

(5.3.1)

## Symmetry transformations (2)

- A theorem due to Wigner states that there are just two ways in which the condition (5.3.1) can be satisfied for all states  $|\psi\rangle$  and  $|\phi\rangle$  :
  - 1) The simplest possibility is that all overlaps  $\langle\phi|\psi\rangle$  remain unchanged after the transformation :

$$\langle \hat{U}\phi | \hat{U}\psi \rangle = \langle \phi | \psi \rangle$$

We then have

$$\langle \phi | \hat{U}^\dagger \hat{U} | \psi \rangle = \langle \phi | \psi \rangle$$

For this to hold for all states  $|\psi\rangle$  and  $|\phi\rangle$ , the operator  $U$  must be *unitary* :

$$\boxed{\hat{U}^\dagger \hat{U} = I ; \quad \hat{U}^{-1} = \hat{U}^\dagger}$$

- 2) The second possibility is that the overlaps  $\langle\phi|\psi\rangle$  become conjugated :

$$\langle \hat{U}\phi | \hat{U}\psi \rangle = \langle \phi | \psi \rangle^* = \langle \psi | \phi \rangle$$

In this case, the operator  $U$  is (by definition) *antiunitary*

## Symmetry transformations (3)

- The symmetry transformations we shall consider all involve *unitary* (not antiunitary) symmetry operators
- The prime example of a symmetry transformation requiring an *antiunitary* operator is *time-reversal symmetry*  $t \rightarrow -t$  :

The weak interactions (responsible for nuclear  $\beta$ -decay for example) were unexpectedly found *not* to be invariant under time-reversal symmetry

→ the rate for a weak interaction process  $i \rightarrow f$  is not necessarily the same as the rate for the time-reversed process  $i \leftarrow f$

## Symmetry transformations (4)

- *Continuous symmetries*, such as spatial translations and rotations, can be taken to be arbitrarily close to the identity transformation

For such infinitesimal transformations, the operator  $U$  must be of the form

$$\hat{U}(\epsilon) = \hat{I} + i\epsilon\hat{T} + \mathcal{O}(\epsilon^2) \quad (5.6.1)$$

and  $U(\epsilon)$  must be *unitary* (not antiunitary) because  $I$  itself is unitary

- Unitarity of the operator  $U(\epsilon)$  then gives

$$\begin{aligned}\hat{I} &= \hat{U}(\epsilon)^\dagger \hat{U}(\epsilon) = [\hat{I} + i\epsilon\hat{T} + \mathcal{O}(\epsilon^2)]^\dagger [\hat{I} + i\epsilon\hat{T} + \mathcal{O}(\epsilon^2)] \\ &= \hat{I} + i\epsilon(\hat{T} - \hat{T}^\dagger) + \mathcal{O}(\epsilon^2)\end{aligned}$$

Hence the operator  $T$  must be Hermitian :

$$\boxed{\hat{T}^\dagger = \hat{T}}$$

(the factor of  $i$  was introduced in equation (5.6.1) to make  $T$  Hermitian)

- The operator  $T$  is known as the generator of the symmetry transformation

## Symmetry transformations (5)

- A finite transformation  $U(\theta)$  can be built up from an infinitely large number of infinitesimal transformations  $U(\epsilon)$

To see this, divide the finite transformation  $\theta$  into a large number,  $N$ , of infinitesimal transformations :

$$\epsilon = \frac{\theta}{N}$$

Then  $U(\theta)$  is

$$\begin{aligned}\hat{U}(\theta) &= (I + i\epsilon\hat{T})^N = \left(I + i\frac{\theta}{N}\hat{T}\right)^N \\ &= I + i\theta\hat{T} + \frac{N-1}{2N}[i\theta\hat{T}]^2 + \dots\end{aligned}$$

- Taking the limit  $N \rightarrow \infty$ , we obtain

$$\boxed{\hat{U}(\theta) = \exp(i\theta\hat{T})}$$

## Symmetry transformations (6)

- Matrix elements of an observable  $A$  transform as

$$\langle \phi | \hat{A} | \psi \rangle \rightarrow \langle \hat{U} \phi | \hat{A} | \hat{U} \psi \rangle = \langle \phi | \hat{U}^\dagger \hat{A} \hat{U} | \psi \rangle$$

Hence the effect of a symmetry transformation on a matrix element can be obtained by transforming the observable as

$$\hat{A} \rightarrow \hat{U}^\dagger \hat{A} \hat{U}$$

while leaving the states of the system unchanged

- Suppose the matrix elements of an observable  $A$  are left unchanged by a symmetry transformation; then, for any pair of states  $|\psi\rangle$  and  $|\phi\rangle$ , we have

$$\langle \phi | \hat{A} | \psi \rangle = \langle \phi | \hat{U}^\dagger \hat{A} \hat{U} | \psi \rangle$$

In this case,  $A$  must commute with all symmetry operators  $U$ :

$$\hat{A} = \hat{U}^\dagger \hat{A} \hat{U} \quad \Rightarrow \quad [\hat{A}, \hat{U}] = 0 \quad (5.8.1)$$

## Symmetry transformations (7)

- For a continuous symmetry, equation (5.8.1) can be applied to infinitesimal symmetry transformations of the form  $\hat{U} = I + i\epsilon\hat{T}$

This shows that  $A$  must also commute with the generator  $T$ :

$$[\hat{A}, \hat{T}] = 0$$

- In particular, if the Hamiltonian  $H$  of a system is invariant under a symmetry operation, then we have

$$\langle \phi | \hat{H} | \psi \rangle = \langle \hat{U}\phi | \hat{H} | \hat{U}\psi \rangle \quad \Rightarrow \quad [\hat{H}, \hat{T}] = 0$$

Ehrenfest's theorem then immediately gives

$$\frac{d}{dt} \langle \psi | \hat{T} | \psi \rangle = \frac{i}{\hbar} \langle \psi | [\hat{H}, \hat{T}] | \psi \rangle = 0$$

The generator  $T$  is therefore *conserved*; its expectation values remain constant:

*symmetries  $\Leftrightarrow$  conservation laws*

## Symmetry transformations (8)

- For an energy eigenstate,  $\hat{H}|\psi\rangle = E|\psi\rangle$ , we have

$$\hat{H}|\psi'\rangle = \hat{H}\hat{U}|\psi\rangle = \hat{U}\hat{H}|\psi\rangle = E\hat{U}|\psi\rangle = E|\psi'\rangle$$

Provided the state  $|\psi'\rangle$  is a distinct state to  $|\psi\rangle$ , the energy level  $E$  must then be degenerate :

*symmetries  $\Leftrightarrow$  degeneracies*

- Symmetries often determine whether processes are allowed or forbidden :

*symmetries  $\Leftrightarrow$  selection rules*

We shall focus on *rotational symmetry*, and the *Wigner-Eckart Theorem*

*“ arguably the most important theorem in all of quantum mechanics ”*

( D. Griffiths & D. Schroeter, “Quantum Mechanics”, 3<sup>rd</sup> edn., CUP, 2018; p255 )

## Time Translation

- The time-translation operator  $U(\tau)$  shifts the origin of the time coordinate by an amount  $\tau$  :

$$\hat{U}(\tau)|\psi(t)\rangle = |\psi(t + \tau)\rangle$$

If all probabilities are preserved by the time translation,

$$|\langle\phi(t + \tau)|\psi(t + \tau)\rangle|^2 = |\langle\phi(t)|\psi(t)\rangle|^2$$

then  $U(\tau)$  is unitary :

$$\hat{U}^\dagger(\tau)\hat{U}(\tau) = I$$

- For an *infinitesimal* time translation,  $U(\tau)$  must be of the form

$$\hat{U}(\tau) = \hat{I} - \frac{i}{\hbar}\hat{H}\tau + \mathcal{O}(\tau^2)$$

where the factor of  $1/\hbar$  has been introduced so that the generator  $H$  has dimensions of energy

## Time translation (2)

- A *finite* time translation is generated by the exponential operator

$$\hat{U}(\tau) = \exp(-i\hat{H}\tau/\hbar); \quad |\psi(t+\tau)\rangle = \exp(-i\hat{H}\tau/\hbar)|\psi(t)\rangle$$

Choosing  $t = 0$ , and relabelling  $\tau \rightarrow t$ , all states must have a time-dependence given by

$$|\psi(t)\rangle = \exp(-i\hat{H}t/\hbar)|\psi(0)\rangle \tag{5.12.1}$$

- Hence all states must satisfy the differential equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$

- The Hamiltonian  $H$  is seen to be the generator of time translations  
( this can be regarded as the *definition* of  $H$  )

*The time-dependent Schrödinger equation is a consequence of invariance under time translations*

## Spatial Translations

- Consider applying a spatial translation  $\mathbf{a} = (a_x, a_y, a_z)$  to a system such that, for the  $n$ 'th particle,

$$\langle \psi' | \hat{\mathbf{r}}_n | \psi' \rangle = \langle \psi | \hat{\mathbf{r}}_n | \psi \rangle + \mathbf{a} \quad (5.13.1)$$

- Introduce the operator  $U(\mathbf{a})$  defined such that

$$|\psi\rangle \rightarrow |\psi'\rangle = \hat{U}(\mathbf{a})|\psi\rangle$$

If all measurement outcomes are unaffected by the spatial translation, so that  $|\langle \phi' | \psi' \rangle|^2 = |\langle \phi | \psi \rangle|^2$ , then the operator  $U(\mathbf{a})$  is unitary :

$$\hat{U}^\dagger(\mathbf{a})\hat{U}(\mathbf{a}) = \hat{I}$$

- From equation (5.13.1), the operator  $U(\mathbf{a})$  must also satisfy

$$\langle \psi | \hat{U}^\dagger(\mathbf{a}) \hat{\mathbf{r}}_n \hat{U}(\mathbf{a}) | \psi \rangle = \langle \psi | \hat{\mathbf{r}}_n | \psi \rangle + \mathbf{a}$$

For this to hold for all states  $|\psi\rangle$ , we must have the operator relation

$$\hat{U}^\dagger(\mathbf{a}) \hat{\mathbf{r}}_n \hat{U}(\mathbf{a}) = \hat{\mathbf{r}}_n + \mathbf{a} \quad (5.13.2)$$

## Spatial translations (2)

- For an *infinitesimal* translation, we can set

$$\hat{U}(\mathbf{a}) = \hat{I} - \frac{i}{\hbar} \hat{\mathbf{P}} \cdot \mathbf{a} + \mathcal{O}(a^2) \quad \left( \hat{T}_i \rightarrow -\frac{1}{\hbar} \hat{P}_i \right)$$

where  $\hat{\mathbf{P}}$  is a vector of Hermitian generators :

$$\hat{\mathbf{P}} = (\hat{P}_1, \hat{P}_2, \hat{P}_3) = (\hat{P}_x, \hat{P}_y, \hat{P}_z)$$

- In this case, equation (5.13.2) is

$$\left( \hat{I} + \frac{i}{\hbar} \hat{\mathbf{P}} \cdot \mathbf{a} + \mathcal{O}(a^2) \right) \hat{\mathbf{r}}_n \left( \hat{I} - \frac{i}{\hbar} \hat{\mathbf{P}} \cdot \mathbf{a} + \mathcal{O}(a^2) \right) = \hat{\mathbf{r}}_n + \mathbf{a}$$

Multiplying out, and keeping terms up to order  $O(a)$ , gives

$$\hat{\mathbf{r}}_n + \frac{i}{\hbar} (\hat{\mathbf{P}} \cdot \mathbf{a}) \hat{\mathbf{r}}_n - \hat{\mathbf{r}}_n \frac{i}{\hbar} (\hat{\mathbf{P}} \cdot \mathbf{a}) = \hat{\mathbf{r}}_n + \mathbf{a}$$

Hence, for the  $n$ 'th particle, we obtain the commutation relation

$$\frac{i}{\hbar} [\hat{\mathbf{P}} \cdot \mathbf{a}, \hat{\mathbf{r}}_n] = \mathbf{a} ; \quad \frac{i}{\hbar} \sum_{k=1}^3 [\hat{P}_k, \hat{r}_{nj}] a_k = a_j \quad (5.14.1)$$

## Spatial translations (3)

- Equation (5.14.1) must hold for any choice of  $\mathbf{a}$ , so we must have

$$[\hat{r}_{nj}, \hat{P}_k] = i\hbar \delta_{jk} \quad (\text{for particle } n)$$

Thus the generators ( $P_x, P_y, P_z$ ) commute in the same way with the position operators of each particle  $n$ , the non-zero commutators being

$$[\hat{x}_n, \hat{P}_x] = i\hbar, \quad [\hat{y}_n, \hat{P}_y] = i\hbar, \quad [\hat{z}_n, \hat{P}_z] = i\hbar$$

- In summary, invariance of a system under spatial translations implies the existence of a vector operator  $\mathbf{P} = (P_x, P_y, P_z)$  satisfying the commutation relations above
- The generators ( $P_x, P_y, P_z$ ) are associated with the system as a whole  
→ we identify  $\mathbf{P}$  as the total momentum operator for the system

## Spatial translations (4)

- The Hamiltonian for an *isolated* system must be invariant under spatial translations (the energy eigenvalues can not depend on where the system happens to be located)

$$\langle \phi | \hat{H} | \psi \rangle = \langle \hat{U}(\mathbf{a})\phi | \hat{H} | \hat{U}(\mathbf{a})\psi \rangle = \langle \phi | \hat{U}^\dagger(\mathbf{a}) \hat{H} \hat{U}(\mathbf{a}) | \psi \rangle$$

Hence we must have, for *all* operators  $U(\mathbf{a})$ ,

$$\hat{U}^\dagger(\mathbf{a}) \hat{H} \hat{U}(\mathbf{a}) = \hat{H} ; \quad [\hat{H}, \hat{U}(\mathbf{a})] = 0$$

- In particular, considering an infinitesimal spatial translation, we must have

$$[\hat{H}, \hat{P}_j] = 0$$

Ehrenfest's theorem then gives

$$\boxed{\frac{d}{dt} \langle \psi | \hat{\mathbf{P}} | \psi \rangle = 0}$$

*Conservation of total momentum for an isolated system is a consequence of invariance under spatial translations*

## Spatial translations (5)

- The order in which spatial translations are applied is irrelevant, so the associated unitary operators must commute :

$$\hat{U}(\mathbf{b})\hat{U}(\mathbf{a}) = \hat{U}(\mathbf{a})\hat{U}(\mathbf{b})$$

- In particular, for two infinitesimal translations, this is

$$\left( I - \frac{i}{\hbar} \hat{\mathbf{P}} \cdot \mathbf{b} + .. \right) \left( I - \frac{i}{\hbar} \hat{\mathbf{P}} \cdot \mathbf{a} + .. \right) = \left( I - \frac{i}{\hbar} \hat{\mathbf{P}} \cdot \mathbf{a} + .. \right) \left( I - \frac{i}{\hbar} \hat{\mathbf{P}} \cdot \mathbf{b} + .. \right)$$

Multiplying out then gives, for all  $\mathbf{a}, \mathbf{b}$ ,

$$\begin{aligned} (\hat{\mathbf{P}} \cdot \mathbf{b})(\hat{\mathbf{P}} \cdot \mathbf{a}) &= (\hat{\mathbf{P}} \cdot \mathbf{a})(\hat{\mathbf{P}} \cdot \mathbf{b}) \\ \Rightarrow \quad \sum_{j,k} \hat{P}_k \hat{P}_j b_k a_j &= \sum_{j,k} \hat{P}_j \hat{P}_k a_j b_k \end{aligned}$$

- Equating the coefficients of  $a_j b_k$  on both sides then shows that the components  $P_x, P_y, P_z$  of total momentum must mutually commute :

$$[\hat{P}_j, \hat{P}_k] = 0 \quad (j, k = 1, 2, 3)$$

## Spatial translations (6)

- Consider, for example, a one-dimensional system described by states  $\psi(x)$  which depend on the spatial coordinate  $x$  :

Applying a spatial translation transforms the wavefunction  $\psi(x)$  as

$$\psi(x) \rightarrow \psi'(x) = \psi(x - a) \equiv \hat{U}(a)\psi(x)$$

- For the case of an *infinitesimal* translation, the transformed wavefunction is

$$\psi(x - a) = \psi(x) - a \frac{\partial \psi(x)}{\partial x} + \dots = \left( \hat{I} - a \frac{\partial}{\partial x} + \dots \right) \psi(x)$$

Hence

$$\hat{U}(a) = \hat{I} - a \frac{\partial}{\partial x} + \dots \equiv \hat{I} - \frac{i}{\hbar} a \hat{P}_x + \dots$$

$$\Rightarrow \boxed{\hat{P}_x = -i\hbar \frac{\partial}{\partial x}}$$

- Thus the form  $\hat{P} = -i\hbar\nabla$ , originally introduced in an ad-hoc manner, can now be seen to be a direct consequence of translation invariance

## Spatial Rotations

- A spatial rotation is a real, linear transformation of the form

$$r_i \rightarrow r'_i = \sum_j R_{ij} r_j$$

that leaves all three-vector scalar products  $\mathbf{x} \cdot \mathbf{y}$  unchanged :

$$\sum_i x'_i y'_i = \sum_i \left( \sum_j R_{ij} x_j \right) \left( \sum_k R_{ik} y_k \right) = \sum_i x_i y_i$$

- This can be written as

$$\sum_i \sum_{j,k} R_{ij} R_{ik} x_j y_k = \sum_i \sum_{j,k} \delta_{ij} \delta_{ik} x_j y_k$$

For this to hold for all possible values of  $x_j$  and  $y_k$ , we must have

$$\sum_i R_{ij} R_{ik} = \delta_{jk}$$

- In matrix notation, this is

$$R^T R = I$$

$$[R^T]_{ji} = R_{ij}$$

## Spatial Rotations (2)

- The determinant of the matrix  $R$  must be

$$\det R = \pm 1 \quad \begin{cases} \det(R^T) = \det(R) \\ \det(AB) = \det(A)\det(B) \end{cases}$$

- “Rotations” with  $\det R = -1$  are in fact spatial *inversions* (see later) :

$$R = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad (x, y, z) \rightarrow (-x, -y, -z)$$

- Infinitesimal rotations (with  $\det R = +1$ ) must be of the form

$$R_{ij} = \delta_{ij} + \omega_{ij} + \mathcal{O}(\omega^2) ; \quad R = I + \omega + \mathcal{O}(\omega^2)$$

The condition  $R^T R = I$  then gives

$$I = [I + \omega + \mathcal{O}(\omega^2)]^T [I + \omega + \mathcal{O}(\omega^2)] = I + \omega^T + \omega + \mathcal{O}(\omega^2)$$

$$\Rightarrow \boxed{\omega^T = -\omega}$$

## Spatial Rotations (3)

- The (real) matrix  $\omega$  of infinitesimal parameters is therefore of the form

$$\omega = \begin{pmatrix} \omega_{11} & \omega_{12} & \omega_{13} \\ \omega_{21} & \omega_{22} & \omega_{23} \\ \omega_{31} & \omega_{32} & \omega_{33} \end{pmatrix} = \begin{pmatrix} 0 & \omega_3 & -\omega_2 \\ -\omega_3 & 0 & \omega_1 \\ \omega_2 & -\omega_1 & 0 \end{pmatrix}$$

This makes sense; to describe a rotation, we need *three* independent parameters :

$$\boldsymbol{\omega} = (\omega_1, \omega_2, \omega_3)$$

- the *direction* of the vector  $\boldsymbol{\omega}$  defines the *axis of rotation*
  - the *magnitude*  $|\boldsymbol{\omega}|$  defines the *angle of rotation* about the axis  $\boldsymbol{\omega}$
- To see this, consider a rotation through an angle  $\phi$  about the  $z$  axis; in this case, the matrix  $R$  is

$$R = \begin{pmatrix} \cos \phi & \sin \phi & 0 \\ -\sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

## Spatial Rotations (4)

- The infinitesimal version of this rotation is

$$\sin \phi \approx \phi ; \quad \cos \phi \approx 1 - \frac{1}{2}\phi^2$$

$$R = \begin{pmatrix} 1 & \phi & 0 \\ -\phi & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \mathcal{O}(\phi^2) ; \quad \omega = \begin{pmatrix} 0 & \phi & 0 \\ -\phi & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

The vector  $\omega$  in this case is therefore

$$\omega = (\omega_1, \omega_2, \omega_3) = (0, 0, \phi)$$

i.e., as advertised, a vector of length  $\phi$  along the axis of rotation ( $z$ )

- There is nothing special about the choice of  $z$  axis as rotation axis
  - ⇒ this interpretation of the vector  $\omega$  must hold for a general rotation about *any* axis

# Rotational Symmetry

*Now bring in Quantum Mechanics ...*

- Under a spatial rotation  $R$ , the states of a quantum system transform as

$$|\psi\rangle \rightarrow \hat{U}(R)|\psi\rangle$$

If the system is rotationally invariant, then the operator  $\hat{U}(R)$  is unitary :

$$\hat{U}(R)^\dagger \hat{U}(R) = \hat{I}$$

- Successive rotations combine to make another rotation :

$$\hat{U}(R_n) \cdots \hat{U}(R_2) \hat{U}(R_1) = \hat{U}(R_n \cdots R_2 R_1)$$

- Infinitesimal rotations can be written as

$$\hat{U}(\omega) = \hat{I} + \frac{i}{\hbar} (\boldsymbol{\omega} \cdot \hat{\mathbf{J}}) + \mathcal{O}(\omega^2)$$

where the generator  $\hat{\mathbf{J}}$  is a vector of Hermitian operators :

$$\hat{\mathbf{J}} = (\hat{J}_1, \hat{J}_2, \hat{J}_3) = (\hat{J}_x, \hat{J}_y, \hat{J}_z)$$

## Rotational symmetry (2)

- Consider three successive infinitesimal rotations of the form

$$R_1 = I + \omega' + \dots ; \quad R_2 = I + \omega + \dots ; \quad R_3 = (R_1)^{-1} = I - \omega' + \dots$$

$$\omega = \begin{pmatrix} 0 & \omega_3 & -\omega_2 \\ -\omega_3 & 0 & \omega_1 \\ \omega_2 & -\omega_1 & 0 \end{pmatrix} ; \quad \omega' = \begin{pmatrix} 0 & \omega'_3 & -\omega'_2 \\ -\omega'_3 & 0 & \omega'_1 \\ \omega'_2 & -\omega'_1 & 0 \end{pmatrix}$$

- This results in an overall rotation given by

$$\begin{aligned} R_3 R_2 R_1 &= (I - \omega' + \dots)(I + \omega + \dots)(I + \omega' + \dots) \\ &= I + \omega + \omega\omega' - \omega'\omega + \mathcal{O}(\omega^2, \omega'^2) \end{aligned}$$

where terms of order  $\omega\omega'$ ,  $\omega'\omega$  have been kept and are needed below

- The right-hand side above involves the matrix

$$\Omega \equiv \omega\omega' - \omega'\omega = \begin{pmatrix} 0 & \Omega_3 & -\Omega_2 \\ -\Omega_3 & 0 & \Omega_1 \\ \Omega_2 & -\Omega_1 & 0 \end{pmatrix} \quad \left\{ \begin{array}{l} \Omega_1 = \omega_3\omega'_2 - \omega_2\omega'_3 \\ \Omega_2 = \omega_1\omega'_3 - \omega_3\omega'_1 \\ \Omega_3 = \omega_2\omega'_1 - \omega_1\omega'_2 \end{array} \right.$$

## Rotational symmetry (3)

- The equation  $\hat{U}(R_3)\hat{U}(R_2)\hat{U}(R_1) = \hat{U}(R_3R_2R_1)$  then gives

$$\left[ \hat{I} - \frac{i}{\hbar}(\boldsymbol{\omega}' \cdot \hat{\mathbf{J}}) + \dots \right] \left[ \hat{I} + \frac{i}{\hbar}(\boldsymbol{\omega} \cdot \hat{\mathbf{J}}) + \dots \right] \left[ \hat{I} + \frac{i}{\hbar}(\boldsymbol{\omega}' \cdot \hat{\mathbf{J}}) + \dots \right]$$

$$= \hat{I} + \frac{i}{\hbar}(\boldsymbol{\omega} \cdot \hat{\mathbf{J}}) + \frac{i}{\hbar}(\boldsymbol{\Omega} \cdot \hat{\mathbf{J}}) + \dots$$

where

$$\boldsymbol{\omega} = (\omega_1, \omega_2, \omega_3) ; \quad \boldsymbol{\omega}' = (\omega'_1, \omega'_2, \omega'_3) ; \quad \boldsymbol{\Omega} = (\Omega_1, \Omega_2, \Omega_3)$$

Multiplying out the left-hand side above, we then find

$$(\boldsymbol{\omega}' \cdot \hat{\mathbf{J}})(\boldsymbol{\omega} \cdot \hat{\mathbf{J}}) - (\boldsymbol{\omega} \cdot \hat{\mathbf{J}})(\boldsymbol{\omega}' \cdot \hat{\mathbf{J}}) = i\hbar(\boldsymbol{\Omega} \cdot \hat{\mathbf{J}})$$

- Equating the coefficients of  $\omega_1\omega'_2$ ,  $\omega_2\omega'_3$ ,  $\omega_3\omega'_1$  on both sides then gives

$$\left. \begin{aligned} \hat{J}_1\hat{J}_2 - \hat{J}_2\hat{J}_1 &= i\hbar\hat{J}_3 \\ \hat{J}_2\hat{J}_3 - \hat{J}_3\hat{J}_2 &= i\hbar\hat{J}_1 \\ \hat{J}_3\hat{J}_1 - \hat{J}_1\hat{J}_3 &= i\hbar\hat{J}_2 \end{aligned} \right\}$$

$$[\hat{J}_i, \hat{J}_j] = i\hbar \sum_k \epsilon_{ijk} \hat{J}_k$$

We interpret  $\mathbf{J}$  as the total angular momentum operator for the system

## Rotational symmetry (4)

- Consider, for example, the rotation of a system through an angle  $\phi_0$  about the  $z$ -axis :

$$\psi(\phi) \rightarrow \psi'(\phi) = \hat{U}(\phi_0)\psi(\phi) = \psi(\phi + \phi_0)$$

For the case of an infinitesimal rotation, this gives

$$\psi(\phi + \phi_0) = \psi(\phi) + \phi_0 \frac{\partial \psi(\phi)}{\partial \phi} + \dots = \left( \hat{I} + \phi_0 \frac{\partial}{\partial \phi} + \dots \right) \psi(\phi)$$

- The vector  $\omega$  corresponding to this rotation is

$$\omega = (\omega_1, \omega_2, \omega_3) = (0, 0, \phi_0)$$

Hence the symmetry operator is

$$\hat{U}(\phi_0) = \hat{I} + \phi_0 \frac{\partial}{\partial \phi} + \dots \equiv \hat{I} + \frac{i}{\hbar} \phi_0 \hat{J}_z + \dots$$

$$\Rightarrow \boxed{\hat{J}_z = -i\hbar \frac{\partial}{\partial \phi}} \quad \text{(as on slide 1.30)}$$

# Scalar Operators

- A *scalar operator*  $K$  is an operator whose matrix elements remain invariant under rotations; i.e., for all states  $|\psi\rangle$  of the system, we have

$$\langle\psi'|\hat{K}|\psi'\rangle = \langle\psi|\hat{K}|\psi\rangle$$

Equivalently :

$$\langle\psi|\hat{U}(R)^\dagger\hat{K}\hat{U}(R)|\psi\rangle = \langle\psi|\hat{K}|\psi\rangle$$

$$\hat{U}(R)^\dagger\hat{K}\hat{U}(R) = \hat{K}$$

- Since  $U(R)$  is unitary, the scalar operator  $K$  must commute with all rotation operators :

$$[\hat{U}(R), \hat{K}] = 0$$

- In particular, this applies to infinitesimal rotations of the form

$$\hat{U}(\omega) = I + \frac{i}{\hbar}(\boldsymbol{\omega} \cdot \hat{\mathbf{J}}) + \mathcal{O}(\omega^2)$$

Since  $K$  commutes with  $U(\omega)$  for all  $\omega$ , it must also commute with  $\mathbf{J}$ :

$$[\hat{\mathbf{J}}, \hat{K}] = 0$$

(5.27.1)

## Scalar operators : angular momentum conservation

- This immediately also gives

$$(\hat{J}_\pm \equiv \hat{J}_1 \pm i\hat{J}_2)$$

$$[\hat{J}_z, \hat{K}] = 0 ; \quad [\hat{J}_\pm, \hat{K}] = 0 ; \quad [\hat{\mathbf{J}}^2, \hat{K}] = 0$$

- For an *isolated system*, the Hamiltonian  $H$  must be invariant under spatial rotations, i.e. the operator  $H$  must be a scalar operator :

$$\hat{U}(R)^\dagger \hat{H} \hat{U}(R) = \hat{H}$$

Equation (5.27.1) then gives

$$[\hat{H}, \hat{\mathbf{J}}] = 0$$

- Hence, from Ehrenfest's theorem :

$$\frac{d}{dt} \langle \psi(t) | \hat{\mathbf{J}} | \psi(t) \rangle = 0$$

Thus :

*Conservation of total angular momentum for an isolated system  
is a consequence of invariance under spatial rotations*

## Scalar operators : commutation relations

- Many commutation relations obtained earlier by hard graft can now be seen to be an immediate consequence of rotational invariance

For example, we can immediately write down (as in slides 1.29 and 1.31)

$$\hat{\mathbf{L}} : \quad [\hat{\mathbf{L}}, \hat{\mathbf{r}}^2] = [\hat{\mathbf{L}}, \hat{\mathbf{p}}^2] = [\hat{\mathbf{L}}, \hat{\mathbf{L}}^2] = [\hat{\mathbf{L}}, V(r)] = 0$$

$$\hat{\mathbf{L}}^2 : \quad [\hat{\mathbf{L}}^2, \hat{\mathbf{r}}^2] = [\hat{\mathbf{L}}^2, \hat{\mathbf{p}}^2] = [\hat{\mathbf{L}}^2, V(r)] = 0$$

These follow because the operators  $\mathbf{r}^2$ ,  $\mathbf{p}^2$ ,  $\mathbf{L}^2$ ,  $V(r)$  are clearly all scalar operators whose matrix elements are invariant under spatial rotations

- Similarly, for a particle with spin, with total angular momentum  $\mathbf{J} = \mathbf{L} + \mathbf{S}$ , we immediately have (as in slides 4.9 and 4.33)

$$\hat{\mathbf{J}} : \quad [\hat{\mathbf{J}}, \hat{\mathbf{L}}^2] = [\hat{\mathbf{J}}, \hat{\mathbf{S}}^2] = [\hat{\mathbf{J}}, \hat{\mathbf{J}}^2] = [\hat{\mathbf{J}}, \hat{\mathbf{L}} \cdot \hat{\mathbf{S}}] = 0$$

$$\hat{\mathbf{J}}^2 : \quad [\hat{\mathbf{J}}^2, \hat{\mathbf{L}}^2] = [\hat{\mathbf{J}}^2, \hat{\mathbf{S}}^2] = [\hat{\mathbf{J}}^2, \hat{\mathbf{L}} \cdot \hat{\mathbf{S}}] = 0$$

These relations follow because the operators  $\mathbf{L}^2$ ,  $\mathbf{S}^2$ ,  $\mathbf{J}^2$  and  $\mathbf{L} \cdot \mathbf{S}$  are all scalar operators

## Scalar operators : commutation relations (2)

- The product  $\mathbf{L} \cdot \mathbf{S}$  is not a scalar operator w.r.t.  $\mathbf{L}$  or  $\mathbf{S}$  separately, but only w.r.t. the *total* angular momentum  $\mathbf{J} = \mathbf{L} + \mathbf{S}$  ;

It is therefore not surprising (slide 4.34) that

$$[\hat{\mathbf{L}}, \hat{\mathbf{L}} \cdot \hat{\mathbf{S}}] \neq 0 ; \quad [\hat{\mathbf{S}}, \hat{\mathbf{L}} \cdot \hat{\mathbf{S}}] \neq 0$$

- For the relativistic corrections to the hydrogen atom,

$$\hat{H}_R \propto (\hat{\mathbf{p}}^2)^2 ; \quad \hat{H}_{SO} = \xi(r) \hat{\mathbf{L}} \cdot \hat{\mathbf{S}} ; \quad \hat{H}_D \propto \nabla^2 \phi(r)$$

rotational symmetry explains why  $H_R$ ,  $H_D$  and  $H_{SO}$  commute with all the operators in the coupled set,

$$[\hat{\mathbf{J}}^2, \hat{H}_{R,SO,D}] = [\hat{\mathbf{J}}, \hat{H}_{R,SO,D}] = [\hat{\mathbf{L}}^2, \hat{H}_{R,SO,D}] = [\hat{\mathbf{S}}^2, \hat{H}_{R,SO,D}] = 0$$

and why  $H_R$  and  $H_D$ , but not  $H_{SO}$ , commute with all the operators in the uncoupled set :

$$\begin{aligned} [\hat{L}_z, \hat{H}_{R,D}] &= 0 ; & [\hat{S}_z, \hat{H}_{R,D}] &= 0 \\ [\hat{L}_z, \hat{H}_{SO}] &\neq 0 ; & [\hat{S}_z, \hat{H}_{SO}] &\neq 0 \end{aligned}$$

## Scalar operators : matrix elements

- Consider an operator  $K$  which is a scalar operator with respect to an angular momentum operator  $\mathbf{J}$  :

$$[\hat{J}_z, \hat{K}] = 0 ; \quad [\hat{\mathbf{J}}^2, \hat{K}] = 0$$

- From the first of these relations, we obtain

$$0 = \langle j'm'_j | [\hat{J}_z, \hat{K}] | jm_j \rangle = (m'_j - m_j) \hbar \langle j'm'_j | \hat{K} | jm_j \rangle$$

Hence the matrix elements of  $K$  must be diagonal in  $m_j$  :

$$\langle j'm'_j | \hat{K} | jm_j \rangle = \langle j'm_j | \hat{K} | jm_j \rangle \delta_{m'_j m_j}$$

- Similarly, from the second commutation relation above, we obtain

$$0 = \langle j'm'_j | [\hat{\mathbf{J}}^2, \hat{K}] | jm_j \rangle = (j'(j'+1) - j(j+1)) \hbar^2 \langle j'm'_j | \hat{K} | jm_j \rangle$$

Hence the matrix elements of  $K$  must also be diagonal in  $j$  :

$$\boxed{\langle j'm'_j | \hat{K} | jm_j \rangle = \langle jm_j | \hat{K} | jm_j \rangle \delta_{j'j} \delta_{m'_j m_j}}$$

(5.31.1)

## Scalar operators : matrix elements (2)

- But equation (5.31.1) is not the end of the story – the expectation value  $\langle jm_j | \hat{K} | jm_j \rangle$  is in fact *independent of the quantum number  $m_j$*  :

$$\langle j'm'_j | \hat{K} | jm_j \rangle = C_j \delta_{j'j} \delta_{m'_j m_j}$$

where  $C_j$  is a constant depending only on  $j$

- This result, the *Wigner-Eckart theorem*, embodies the full impact of rotational symmetry on the structure of scalar operator matrix elements ...

## Scalar operators : the Wigner-Eckart theorem

- For operators  $K$  and  $\mathbf{J} = (J_x, J_y, J_z)$  satisfying the commutation relations

$$[\hat{J}_i, \hat{J}_j] = i\hbar \sum_k \epsilon_{ijk} \hat{J}_k ; \quad [\hat{\mathbf{J}}, \hat{K}] = 0$$

the **Wigner-Eckart Theorem** (for scalar operators) states that

$$\langle \alpha'' j'' m'' | \hat{K} | \alpha' j' m' \rangle = \langle \alpha'' j'' \| \hat{K} \| \alpha' j' \rangle \delta_{j'' j'} \delta_{m'' m'} \quad (5.33.1)$$

The quantities  $\alpha''$  and  $\alpha'$  have been introduced to represent any additional quantum numbers which might be needed, while the quantity

$$\langle \alpha'' j'' \| \hat{K} \| \alpha' j' \rangle$$

is an  $m$ -independent constant known as a “*reduced matrix element*”

The reduced matrix element is *not* a matrix element as such, but is rather the common, constant component of a related set of matrix elements

- The proof of equation (5.33.1) is given in the Appendix of the “Symmetries” handout, and is **non-examinable**

## Scalar operators : the Wigner-Eckart theorem (2)

- A particular case of equation (5.33.1) is

$$\langle \alpha jm | \hat{K} | \alpha jm \rangle = \langle \alpha j \| \hat{K} \| \alpha j \rangle$$

i.e. *the expectation values of a scalar operator are independent of  $m$*

(and are given by the appropriate reduced matrix element of  $K$ )

- The  $m$ -independence of matrix elements of scalar operators is intuitively reasonable, nay obvious :
  - the quantum number  $m$  arises from the definition of angular momentum eigenstates with respect to a particular, arbitrary choice of spatial direction (conventionally taken to be the  $z$  axis)
  - the matrix elements of a rotationally invariant operator cannot possibly depend on an arbitrary choice of spatial direction

## Scalar operators : the Wigner-Eckart theorem (3)

- The Hamiltonian  $H$  for an isolated system must be a scalar operator, and so must commute with the total angular momentum  $\mathbf{J}$  :

$$[\hat{H}, \hat{\mathbf{J}}] = 0$$

The operators  $H$  and  $\mathbf{J}$  therefore possess a set of simultaneous eigenstates; hence the energy eigenstates can be taken to be of the form

$$\hat{H}|\alpha jm\rangle = E_{\alpha jm}|\alpha jm\rangle$$

- From the Wigner-Eckart theorem, the expectation values of  $H$  are given by

$$E_{\alpha jm} = \langle \alpha jm | \hat{H} | \alpha jm \rangle = \langle \alpha j | \hat{H} | \alpha j \rangle$$

Hence the energy eigenvalues for an isolated system must be independent of the quantum number  $m$  :

$$E_{\alpha jm} \rightarrow E_{\alpha j} ; \quad \hat{H}|\alpha jm\rangle = E_{\alpha j}|\alpha jm\rangle$$

(5.35.1)

## Scalar operators : the Wigner-Eckart theorem (4)

- Thus, for an isolated system, energy levels with  $j > 0$  must inevitably be *degenerate*, with degeneracy  $g \geq 2j + 1$   
(there may be additional degeneracy if  $H$  possesses further symmetries)

This illustrates a general principle, that

*degeneracies are hardly ever accidental, but are indicative of an underlying symmetry principle*

(in this case, *rotational symmetry*)

- Equation (5.35.1) is in fact straightforward to obtain directly, using

$$\hat{J}_+ |\alpha jm\rangle = C |\alpha j, m+1\rangle; \quad C = \hbar \sqrt{j(j+1) - m(m+1)}$$

Then, since  $[\hat{H}, \hat{J}_+] = 0$  :

$$\begin{aligned} \hat{H}C|\alpha j, m+1\rangle &= \hat{H}\hat{J}_+|\alpha jm\rangle = \hat{J}_+\hat{H}|\alpha jm\rangle = E_{\alpha jm}\hat{J}_+|\alpha jm\rangle \\ &= E_{\alpha jm}C|\alpha j, m+1\rangle \end{aligned}$$

Hence

$$E_{\alpha j, m+1} = E_{\alpha jm}$$

## Scalar operators : the Wigner-Eckart theorem (5)

- Finally, we obtain an alternative formulation of the Wigner-Eckart theorem to that given in equation (5.33.1) ...

For the “trivial” angular momentum combination  $0 \otimes j = j$ , the Clebsch-Gordan coefficients are given by (see slide 1.77)

$$\langle 00; j'm' | j''m'' \rangle = \delta_{j''j'} \delta_{m''m'}$$

Equation (5.33.1) can therefore also be expressed as

$$\langle \alpha''j''m'' | \hat{K} | \alpha'j'm' \rangle = \langle \alpha''j'' \| \hat{K} \| \alpha'j' \rangle \langle 00; j'm' | j''m'' \rangle$$

- In this form, the Wigner-Eckart theorem generalises naturally from scalar operators to *vector operators* (and beyond) ...

# Vector Operators

- Define a *vector operator*

$$\hat{\mathbf{V}} = (\hat{V}_x, \hat{V}_y, \hat{V}_z) \equiv (\hat{V}_1, \hat{V}_2, \hat{V}_3)$$

as one whose expectation values transform under spatial rotations in the same way as ordinary three-vectors :

$$\langle \hat{V}_i \rangle' = \sum_j R_{ij} \langle \hat{V}_j \rangle \quad (i = 1, 2, 3)$$

- Setting  $\langle \hat{V}_i \rangle' = \langle \psi' | \hat{V}_i | \psi' \rangle$  and  $\langle \hat{V} \rangle = \langle \psi | \hat{V}_j | \psi \rangle$ , this is, for *any state*  $|\psi\rangle$ ,

$$\langle \psi | \hat{U}(R)^\dagger \hat{V}_i \hat{U}(R) | \psi \rangle = \sum_j R_{ij} \langle \psi | \hat{V}_j | \psi \rangle$$

Hence, equivalently, a vector operator can be defined as one which transforms under rotations as

$$\hat{U}(R)^\dagger \hat{V}_i \hat{U}(R) = \sum_j R_{ij} \hat{V}_j \quad \text{(5.38.1)}$$

## Vector operators (2)

- For an infinitesimal rotation of the form  $R = I + \boldsymbol{\omega} + \dots$ , equation (5.38.1) is

$$\left[ I - \frac{i}{\hbar} (\boldsymbol{\omega} \cdot \hat{\mathbf{J}} + \dots) \right] \hat{V}_i \left[ I + \frac{i}{\hbar} (\boldsymbol{\omega} \cdot \hat{\mathbf{J}} + \dots) \right] = \sum_j (\delta_{ij} + \omega_{ij} + \dots) \hat{V}_j$$

Equating terms of order  $\boldsymbol{\omega}$  on each side then gives (for  $i = 1, 2, 3$ )

$$\frac{i}{\hbar} \hat{V}_i (\boldsymbol{\omega} \cdot \hat{\mathbf{J}}) - \frac{i}{\hbar} (\boldsymbol{\omega} \cdot \hat{\mathbf{J}}) \hat{V}_i = \sum_j \omega_{ij} \hat{V}_j \quad (5.39.1)$$

where, for  $i = 1$ , for example, the right-hand side involves (see slide 5.21)

$$\omega_{11} = 0 , \quad \omega_{12} = \omega_3 , \quad \omega_{13} = -\omega_2$$

- Equating the coefficients of  $\omega_1, \omega_2, \omega_3$  on both sides of equation (5.39.1) for each value of  $i = 1, 2, 3$  in turn then gives the commutation relations

$$[\hat{J}_i, \hat{V}_j] = i\hbar \sum_k \epsilon_{ijk} \hat{V}_k \quad (5.39.2)$$

(which can also serve as yet another *definition* of a vector operator)

## Vector operators (3)

- The operators  $\mathbf{r}$ ,  $\mathbf{p}$ ,  $\mathbf{L}$  are all vector operators, so we immediately obtain

$$[\hat{J}_i, \hat{r}_j] = i\hbar \sum_k \epsilon_{ijk} \hat{r}_k ; \quad [\hat{J}_i, \hat{p}_j] = i\hbar \sum_k \epsilon_{ijk} \hat{p}_k$$
$$[\hat{J}_i, \hat{L}_j] = i\hbar \sum_k \epsilon_{ijk} \hat{L}_k$$

- Since the total angular momentum  $\mathbf{J}$  is itself a vector operator, we also obtain (slide 5.25) :

$$[\hat{J}_i, \hat{J}_j] = i\hbar \sum_k \epsilon_{ijk} \hat{J}_k$$

- For a single particle system, the total angular momentum is  $\mathbf{J} = \mathbf{L} = \mathbf{r} \wedge \mathbf{p}$ , so from equation (5.39.2) we immediately obtain

$$[\hat{L}_i, \hat{r}_j] = i\hbar \sum_k \epsilon_{ijk} \hat{r}_k ; \quad [\hat{L}_i, \hat{p}_j] = i\hbar \sum_k \epsilon_{ijk} \hat{p}_k$$
$$[\hat{L}_i, \hat{L}_j] = i\hbar \sum_k \epsilon_{ijk} \hat{L}_k$$

These commutation relations, obtained earlier by direct computation, are now seen to be a direct consequence of rotational invariance

## Vector operators : spherical components

- For vector operators, just as for scalars, rotational symmetry places tight constraints on the structure of matrix elements

These constraints are most naturally expressed in terms of the spherical components ( $V_{+1}$ ,  $V_{-1}$ ,  $V_0$ ) of  $\mathbf{V}$ , rather than the Cartesian components

- The spherical components of a vector operator  $\mathbf{V}$  are defined as

$$\hat{V}_{+1} \equiv -\frac{1}{\sqrt{2}}(\hat{V}_1 + i\hat{V}_2) , \quad \hat{V}_{-1} \equiv \frac{1}{\sqrt{2}}(\hat{V}_1 - i\hat{V}_2) , \quad \hat{V}_0 \equiv \hat{V}_3$$

( N.B.  $V_{+1}$  is not the same operator as  $V_1 \equiv V_x$  or as  $V_+ \equiv V_1 + iV_2$  )

- The full impact of rotational symmetry is again embodied in the (vector form of the) *Wigner-Eckart theorem* ....

## Vector operators : the Wigner-Eckart theorem

- For operators  $\mathbf{V}$  and  $\mathbf{J}$  satisfying the commutation relations

$$[\hat{J}_i, \hat{J}_j] = i\hbar \sum_k \epsilon_{ijk} \hat{J}_k ; \quad [\hat{J}_i, \hat{V}_j] = i\hbar \sum_k \epsilon_{ijk} \hat{V}_k \quad (5.42.1)$$

the **Wigner-Eckart theorem** (for vector operators) states that matrix elements of the spherical components  $V_m = (V_{+1}, V_{-1}, V_0)$  of  $\mathbf{V}$  are given by

$$\langle \alpha'' j'' m'' | \hat{V}_m | \alpha' j' m' \rangle = \langle \alpha'' j'' \| \hat{\mathbf{V}} \| \alpha' j' \rangle \langle 1m; j' m' | j'' m'' \rangle$$

( $m = -1, 0, +1$ )

reduced matrix element ;  
independent of  $m, m', m''$

“physics”

depends on the observable  $\mathbf{V}$

Clebsch-Gordan coefficient ;

carries the dependence on  $m, m', m''$

“geometry”

independent of the observable  $\mathbf{V}$

- The proof is given in the “Symmetries” handout, and is **non-examinable**

## Vector operators : the Wigner-Eckart theorem (2)

- The commutation relations in equation (5.42.1), and hence the Wigner-Eckart theorem itself, follow directly from rotational symmetry
- The “reduced matrix element”  $\langle \alpha'' j'' \| \hat{V} \| \alpha' j' \rangle$  is not a matrix element  
It is the common, constant component of a related set of matrix elements, and is a single (complex) number, not a vector
- The dependence of matrix elements on the arbitrary choice of quantisation axis (the  $z$  axis) is carried entirely by the Clebsch-Gordan coefficients

$$\langle 1m; j'm' | j''m'' \rangle$$

These are independent of the operator  $V$

The properties of these Clebsch-Gordan coefficients lead immediately to *selection rules* for vector operator matrix elements ....

## Vector operators : selection rules

- The Clebsch-Gordan coefficient

$$\langle 1m; j'm' | j''m'' \rangle$$

vanishes unless

$$m'' = m' + m \quad (m = -1, 0, +1)$$

and unless

$$j'' = 1 \otimes j' = \begin{cases} j', & j' \pm 1 \\ 1 & \end{cases} \quad \begin{matrix} (j' > 0) \\ (j' = 0) \end{matrix}$$

i.e. unless

$$j'' = j', \quad j' \pm 1 ; \quad j'' + j' \geq 1 ; \quad m'' = m' + m$$



( i.e. cannot have  $j' = j'' = 0$  , because  $\langle 1m; 00 | 00 \rangle = 0$  )

- It follows immediately from the Wigner-Eckart theorem that these same constraints (known as selection rules) must apply to vector operator matrix elements also ...

## Vector operators : selection rules (2)

- Thus: the vector operator matrix element  $\langle \alpha'' j'' m'' | \hat{V}_m | \alpha' j' m' \rangle$  can be non-zero only if

$$j'' = j', \quad j' \pm 1 ; \quad j'' + j' \geq 1 ; \quad m'' = m' + m$$

or, equivalently, only if  $(m = -1, 0, +1)$

$$\Delta j = 0, \pm 1 ; \quad 0 \leftrightarrow 0 ; \quad \Delta m = 0, \pm 1$$

- In particular, the matrix elements of any vector operator  $\hat{V}$  taken between states with zero angular momentum must vanish :

$$\langle \alpha'' 00 | \hat{V} | \alpha' 00 \rangle = 0$$

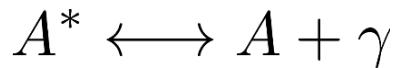
This follows because the relevant Clebsch-Gordan coefficients vanish :

$$\langle 1m; 00 | 00 \rangle = 0 \quad (m = \pm 1, 0)$$

which in turn follows because  $1 \otimes 0 \neq 0$

## Vector operators : selection rules (3)

- These selection rules can be applied immediately to electric dipole (E1) transitions in atoms :  
These are the dominant type of atomic transition, and involve the emission or absorption of a single photon



They are governed by a vector operator, the *electric dipole operator*,  $d$   
(see later)

- Besides rotational symmetry, selection rules for electric dipole transitions arise also from the requirement of parity invariance ...

## Spatial Inversion (Parity)

- The spatial inversion (parity) operation is defined as

$$\hat{P} : \quad \mathbf{r} \rightarrow -\mathbf{r} ; \quad (x, y, z) \rightarrow (-x, -y, -z)$$

e.g. for a system of  $N$  particles, the parity operation results in

$$\hat{P}|\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)\rangle = |\psi(-\mathbf{r}_1, -\mathbf{r}_2, \dots, -\mathbf{r}_N)\rangle$$

- The eigenvalues and eigenstates of the parity operator are defined by

$$\hat{P}|\psi\rangle = P|\psi\rangle$$

Applying the parity operator twice,  $(x, y, z) \rightarrow (-x, -y, -z) \rightarrow (x, y, z)$  brings us back to where we started :

$$\hat{P}^2|\psi\rangle = P^2|\psi\rangle = |\psi\rangle$$

Hence the eigenvalues of parity are restricted to

$$P = \pm 1$$

## Parity (2)

- For example, hydrogen atom wavefunctions  $|nlm_\ell\rangle$  are eigenstates of parity with eigenvalue (slide 1.35)

$$P = (-1)^\ell$$

- Consider a single-particle system with parity eigenstates  $|\psi_1\rangle$ ,  $|\psi_2\rangle$ , with corresponding parity eigenvalues  $P_1$ ,  $P_2$  :

$$\psi_1(-\mathbf{r}) = P_1 \psi(\mathbf{r}); \quad \psi_2(-\mathbf{r}) = P_2 \psi(\mathbf{r})$$

The matrix element of the position operator  $\mathbf{r}$  between these states is

$$\langle \psi_1(\mathbf{r}) | \hat{\mathbf{r}} | \psi_2(\mathbf{r}) \rangle = \int \psi_1^*(\mathbf{r}) \mathbf{r} \psi_2(\mathbf{r}) d^3\mathbf{r}$$

- Changing the integration variable from  $\mathbf{r}$  to  $-\mathbf{r}$  then gives

$$\langle \psi_1(\mathbf{r}) | \hat{\mathbf{r}} | \psi_2(\mathbf{r}) \rangle = - \int \psi_1^*(-\mathbf{r}) \mathbf{r} \psi_2(-\mathbf{r}) d^3\mathbf{r} = -P_1 P_2 \int \psi_1^*(\mathbf{r}) \mathbf{r} \psi_2(\mathbf{r}) d^3\mathbf{r}$$

Thus

$$\langle \psi_1(\mathbf{r}) | \hat{\mathbf{r}} | \psi_2(\mathbf{r}) \rangle = -P_1 P_2 \langle \psi_1(\mathbf{r}) | \hat{\mathbf{r}} | \psi_2(\mathbf{r}) \rangle$$

## Parity (3)

- Hence matrix elements of  $\hat{\mathbf{r}}$  vanish between states with the same parity :

$$\langle \psi_1(\mathbf{r}) | \hat{\mathbf{r}} | \psi_2(\mathbf{r}) \rangle = 0 \quad \text{if} \quad P_1 = P_2$$

Equivalently, this can be stated in the form of a *selection rule* :

The matrix element  $\langle \psi_1(\mathbf{r}) | \hat{\mathbf{r}} | \psi_2(\mathbf{r}) \rangle$  can be non-zero only if the eigenstates involved have *opposite parity* :

$$P_1 = -P_2 \quad \text{or} \quad P_1 \neq P_2$$

- e.g. for the hydrogen atom, we have

$$\langle n_1 \ell_1 m_1 | \hat{\mathbf{r}} | n_2 \ell_2 m_2 \rangle = 0 \quad \text{if} \quad (-1)^{\ell_1} = (-1)^{\ell_2}$$

Equivalently, we have the selection rule

$$(-1)^{\ell_1} \neq (-1)^{\ell_2} ; \quad \ell_1 + \ell_2 = 1, 3, 5, \dots$$

## Parity (4)

- Electromagnetic (EM) interactions are invariant under parity :

$$[\hat{H}_{\text{EM}}, \hat{P}] = 0$$

Therefore parity is conserved : the parity eigenvalue of the state of an isolated system cannot change in an electromagnetic interaction

(and similarly for the strong nuclear interaction, QCD)

[ As well as the “orbital” parity  $(-1)^\ell$ , all particles possess an *intrinsic* (internal) parity,  $P = \pm 1$ , which contributes to the overall parity of a state ]

- However the weak interactions do not conserve parity :

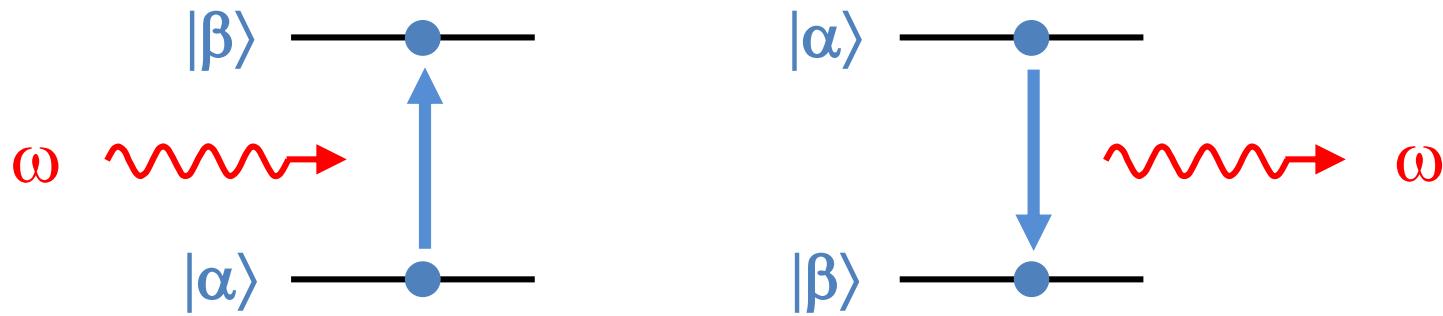
$$[\hat{H}_{\text{weak}}, \hat{P}] \neq 0$$

*Parity violation* was (unexpectedly) observed in 1956, in studies of the  $\beta$ -decay of polarised cobalt-60 nuclei ;

→ electrons were observed to be emitted preferentially towards the direction of the  ${}^{60}\text{Co}$  spin vector

# Atomic Transitions (Selection Rules)

- Consider the absorption or emission of a photon by an atom :



Electric dipole (E1) transitions between atomic states are governed by the matrix elements of a vector operator,  $d$  (see later)

- The Wigner-Eckart theorem (rotational symmetry) and parity invariance severely restrict the properties of these matrix elements

In particular, these symmetries determine which matrix elements are non-zero, and hence which atomic transitions are allowed,



*selection rules*

(for atomic transitions)

## Atomic transitions : selection rules (2)

- As will be shown later, the rate for photon emission or absorption,

$$|\alpha\rangle \longleftrightarrow |\beta\rangle + \gamma$$

via E1 transitions is of the form

$$\Gamma \propto \omega^3 |\langle \beta | \hat{\mathbf{d}} | \alpha \rangle|^2 \quad (\hbar\omega = |E_\alpha - E_\beta|)$$

where

$$\begin{aligned} |\langle \beta | \hat{\mathbf{d}} | \alpha \rangle|^2 &= |\langle \beta | \hat{d}_x | \alpha \rangle|^2 + |\langle \beta | \hat{d}_y | \alpha \rangle|^2 + |\langle \beta | \hat{d}_z | \alpha \rangle|^2 \\ &= |\langle \beta | \hat{d}_{+1} | \alpha \rangle|^2 + |\langle \beta | \hat{d}_{-1} | \alpha \rangle|^2 + |\langle \beta | \hat{d}_0 | \alpha \rangle|^2 \end{aligned}$$

For the hydrogen atom, the electric dipole operator is simply

$$\hat{\mathbf{d}} = -e\hat{\mathbf{r}}$$

where the vector  $\mathbf{r}$  is the position of the electron relative to the proton

- An E1 transition can therefore take place only if the dipole matrix element is non-zero for at least one spherical component of  $\mathbf{d}$  :

$$\langle \beta | \hat{d}_m | \alpha \rangle \neq 0 \quad (m = \pm 1, 0)$$

## Atomic transitions : zeroth-order hydrogen

- Consider the zeroth-order hydrogen atom, neglecting spin, with eigenstates  $|n\ell m_\ell\rangle$  :

$$|n_1\ell_1m_1\rangle \longleftrightarrow |n_2\ell_2m_2\rangle + \gamma$$

E1 transitions require, for at least one value of  $m = +1, -1, 0$ , that

$$\langle n_1\ell_1m_1 | \hat{d}_m | n_2\ell_2m_2 \rangle \neq 0$$

From the Wigner-Eckart theorem, this can happen only if the initial and final states satisfy the selection rules (see slide 5.45)

$$\Delta\ell = 0, \pm 1 ; \quad \ell_1 + \ell_2 \geq 1 ; \quad \Delta m_\ell = 0, \pm 1$$

- The possibility  $\Delta\ell = 0$  is excluded by the parity selection rule :

$$(-1)^{\ell_1} \neq (-1)^{\ell_2}$$

Thus a combination of rotational symmetry (the Wigner-Eckart theorem) and parity invariance gives the E1 selection rules

$$\boxed{\Delta\ell = \pm 1 ; \quad \Delta m_\ell = 0, \pm 1}$$

## Atomic transitions : zeroth-order hydrogen (2)

- At zeroth-order, the  $\Delta\ell$  rule restricts the allowed E1 transitions to

$$s \longleftrightarrow p ; \quad p \longleftrightarrow d ; \quad d \longleftrightarrow f ; \quad \dots$$

We can not have :

$$s \not\longleftrightarrow d ; \quad s \not\longleftrightarrow f ; \quad p \not\longleftrightarrow f ; \quad \dots$$

- There are no restrictions on the initial or final values of the principal quantum number  $n$  ;

e.g. for  $p \leftrightarrow d$  transitions, any of the following are allowed :

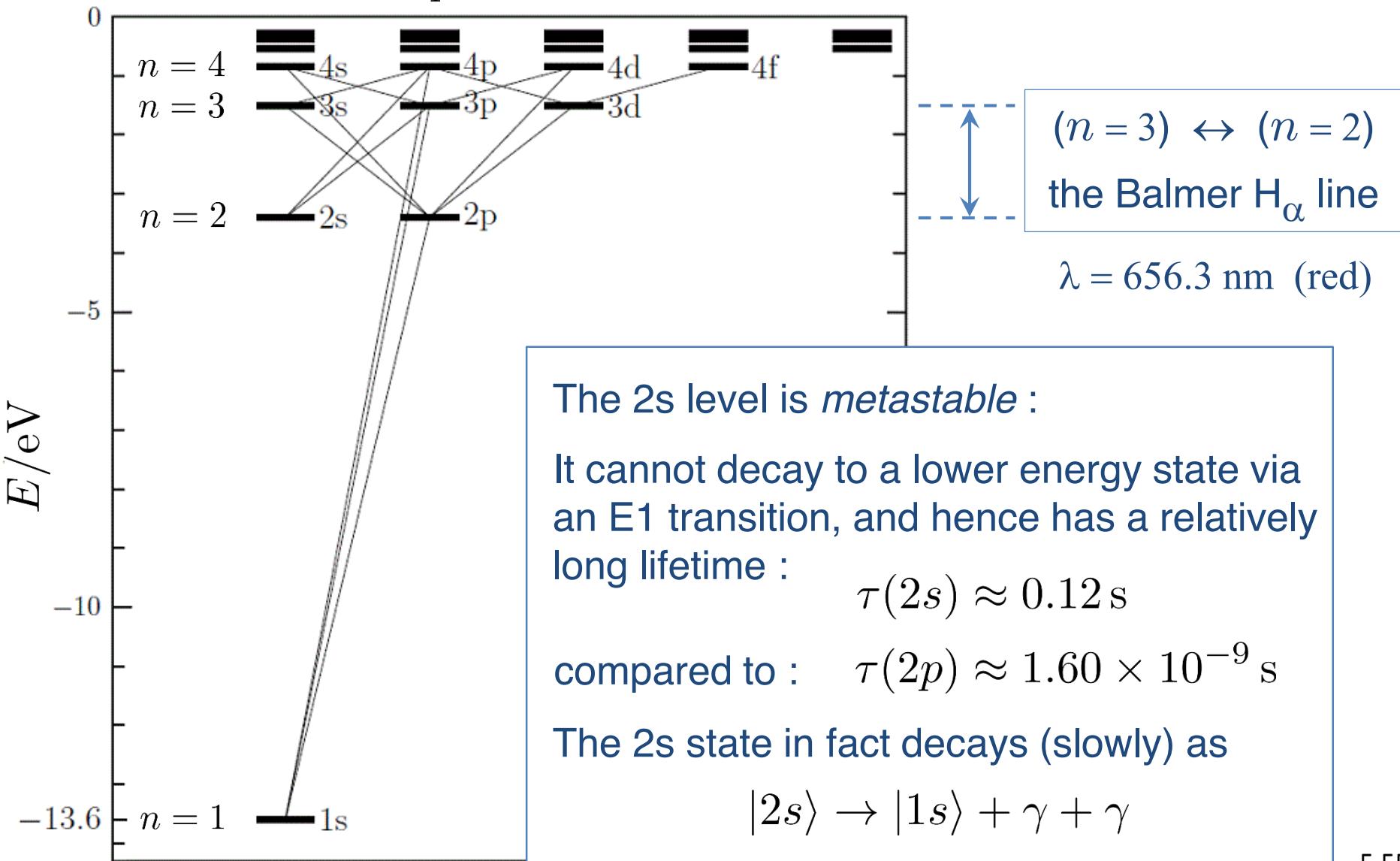
$$\{2p, 3p, 4p, \dots\} \longleftrightarrow \{3d, 4d, 5d, \dots\}$$

- The possible transitions are best illustrated by displaying the energy levels in the form of a *Grotian diagram* ...

## Atomic transitions : zeroth-order hydrogen (3)

$\ell = 0$        $\ell = 1$        $\ell = 2$        $\ell = 3$   
 $ns$              $np$              $nd$              $nf$

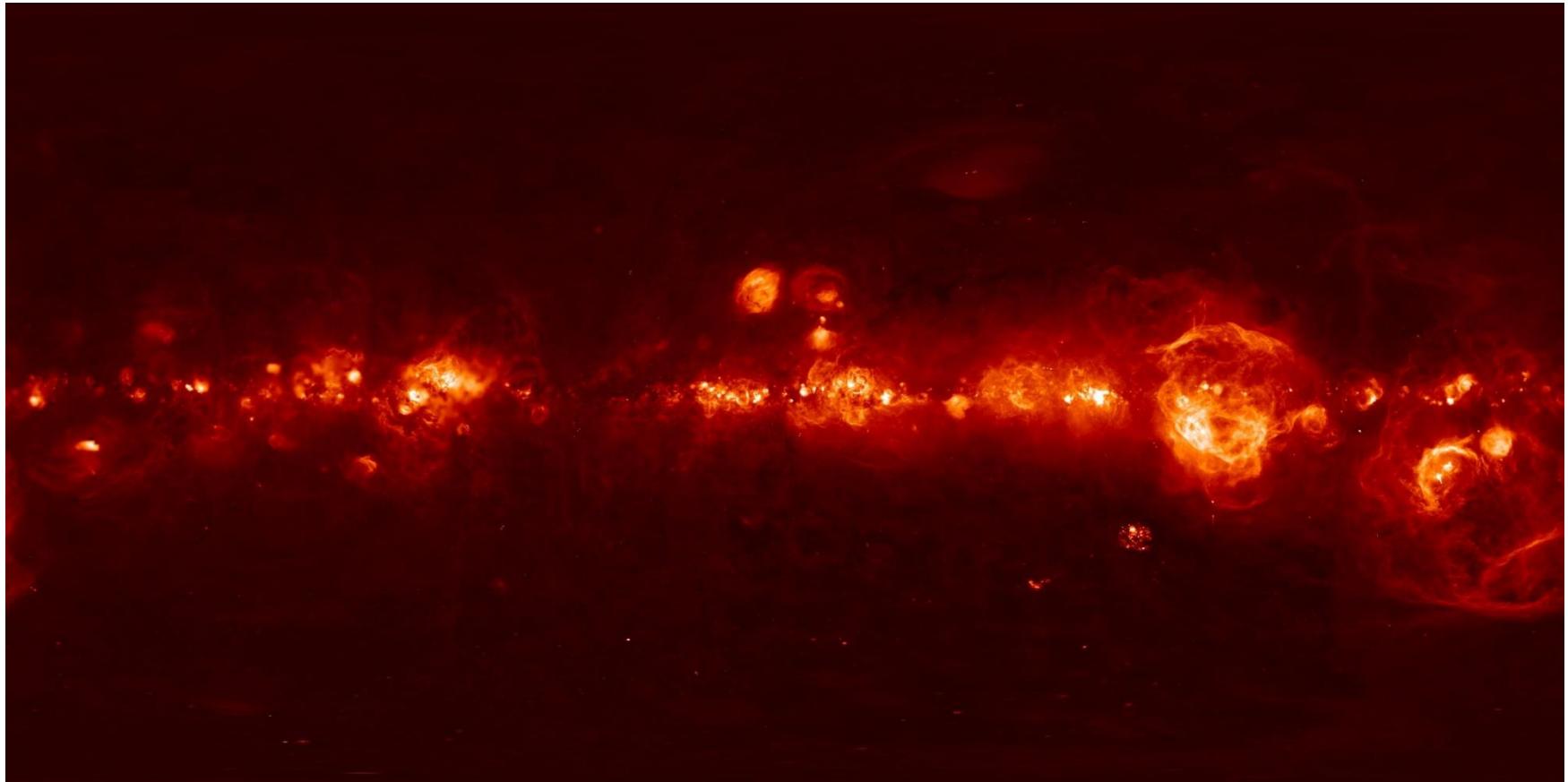
“Grotrian diagram”



## Atomic transitions : the H-alpha line

- A full map of the sky, as viewed in Balmer  $H_{\alpha}$  line emission :

[D. Finkbeiner, Ap. J. Suppl. 146 \(2003\) 407](#)



- $H_{\alpha}$  emission is a tracer of *ionised* hydrogen  
(star-forming regions, supernova remnants, ...)

## Atomic transitions : the H-alpha line (2)

- When an electron and proton in a region of ionised hydrogen recombine to form a neutral H atom, the atom will usually be formed in a highly excited (large  $n$ ) state ;
  - the excited H atom then cascades down to lower energy (lower  $n$ ) states by emitting one or more photons, until it reaches the ground state ( $n = 1$ ) (including, often, the emission of  $3 \rightarrow 2$  Balmer  $H_\alpha$  line photons)
- H and He are the dominant visible constituents of our home galaxy :

Milky Way

	mass
total mass	$10^{11} M_\odot$
stars	$5 \times 10^{10} M_\odot$
dark matter	$5 \times 10^{10} M_\odot$
ISG (mainly H, He)	$7 \times 10^9 M_\odot$

Interstellar gas (ISG)

	mass
ionised H (H II)	$1.1 \times 10^9 M_\odot$
neutral H (H I)	$2.9 \times 10^9 M_\odot$
molecular H ( $H_2$ )	$0.8 \times 10^9 M_\odot$
helium (He)	$1.8 \times 10^9 M_\odot$

## Atomic transitions : selection rules (z)

- In passing, we note a special case of the selection rules on slide 5.53 that apply to matrix elements of the  $z$  component of the position operator :

The operator  $z$  is the  $m = 0$  spherical component of the vector position operator  $\mathbf{r}$ ,

$$\hat{z} \equiv \hat{r}_0$$

Therefore, for a given matrix element of the operator  $z$  to be non-zero,

$$\langle n_1 \ell_1 m_1 | \hat{z} | n_2 \ell_2 m_2 \rangle \neq 0$$

the initial and final states must satisfy the selection rules

$$\boxed{\Delta \ell = \pm 1 , \quad \Delta m_\ell = 0} \quad (\hat{z})$$

- This result will be needed later for analysis of the *linear Stark effect*

## Atomic transitions : hydrogen with fine structure

- Now “switch on” electron spin and consider the hydrogen atom with fine structure effects included :
  - the total angular momentum operator is now  $\mathbf{J} = \mathbf{L} + \mathbf{S}$ , not  $\mathbf{J} = \mathbf{L}$

Hence, with fine structure, the selection rules for E1 transitions apply to the quantum numbers  $j$  and  $m_j$ , not to  $\ell$  and  $m_\ell$  :

$$\boxed{\Delta j = 0, \pm 1 ; \quad j_1 + j_2 \geq 1 ; \quad \Delta m_j = 0, \pm 1}$$

- In addition, the selection rules obtained above for zeroth-order hydrogen (with spin neglected) continue to apply, i.e. we still also have

$$\Delta \ell = \pm 1 ; \quad \Delta m_\ell = 0, \pm 1$$

This is because the operator responsible for the transitions (the dipole operator  $\mathbf{d}$ ) does not depend on the electron spin operator  $\mathbf{S}$

## Atomic transitions : hydrogen with fine structure (2)

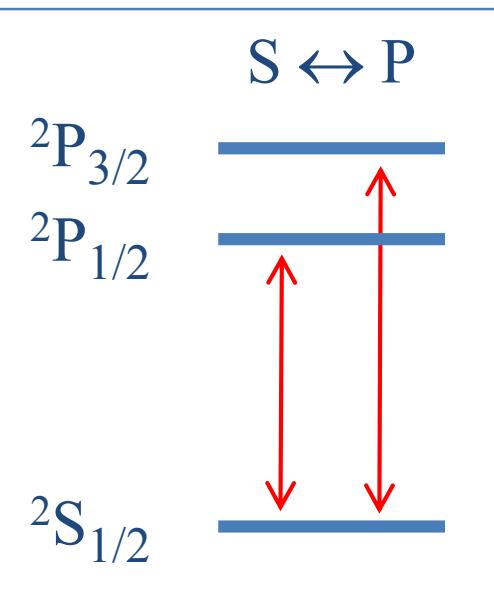
-- Thus the allowed E1 transitions are (for any  $n_1$  and  $n_2$ ) :

$$S \leftrightarrow P : \quad ^2S_{1/2} \leftrightarrow ^2P_{1/2}; \quad ^2S_{1/2} \leftrightarrow ^2P_{3/2}$$

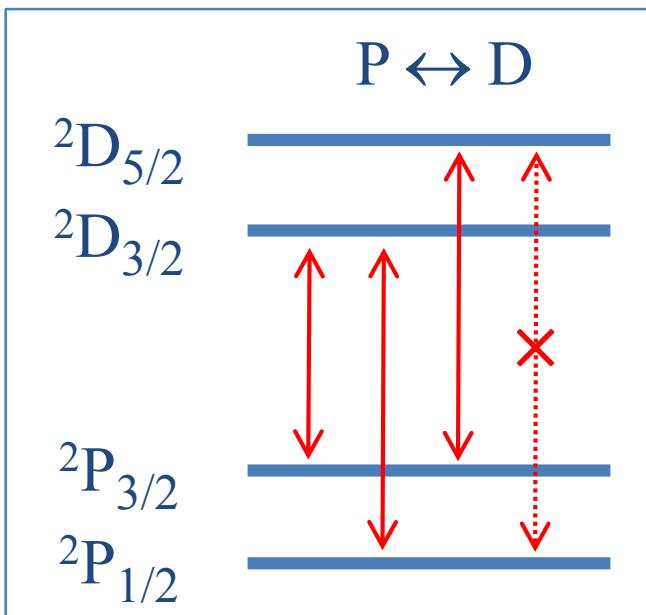
$$P \leftrightarrow D : \quad ^2P_{1/2} \leftrightarrow ^2D_{3/2}; \quad ^2P_{3/2} \leftrightarrow ^2D_{3/2}; \quad ^2P_{3/2} \leftrightarrow ^2D_{5/2}$$

$$D \leftrightarrow F : \quad ^2D_{3/2} \leftrightarrow ^2F_{5/2}; \quad ^2D_{5/2} \leftrightarrow ^2F_{5/2}; \quad ^2D_{5/2} \leftrightarrow ^2F_{7/2}$$

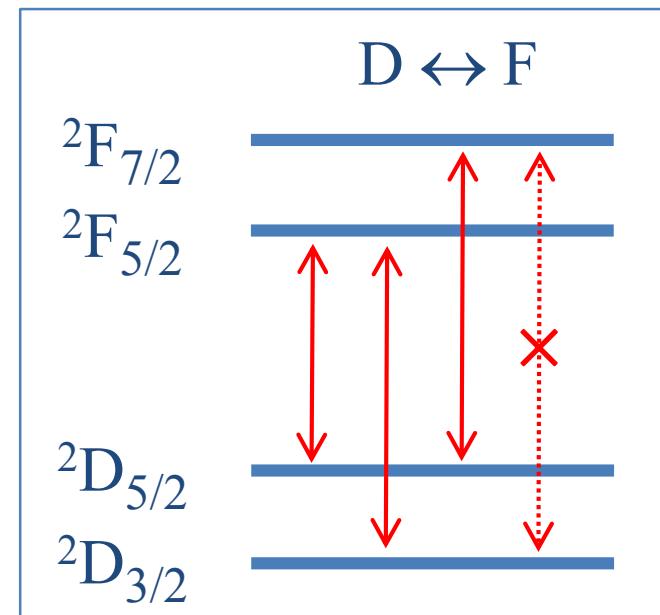
etc. etc., but *not*, for example :  $^2P_{1/2} \leftrightarrow ^2D_{5/2}$  (because  $|\Delta j| = 2$ )



(doublet)

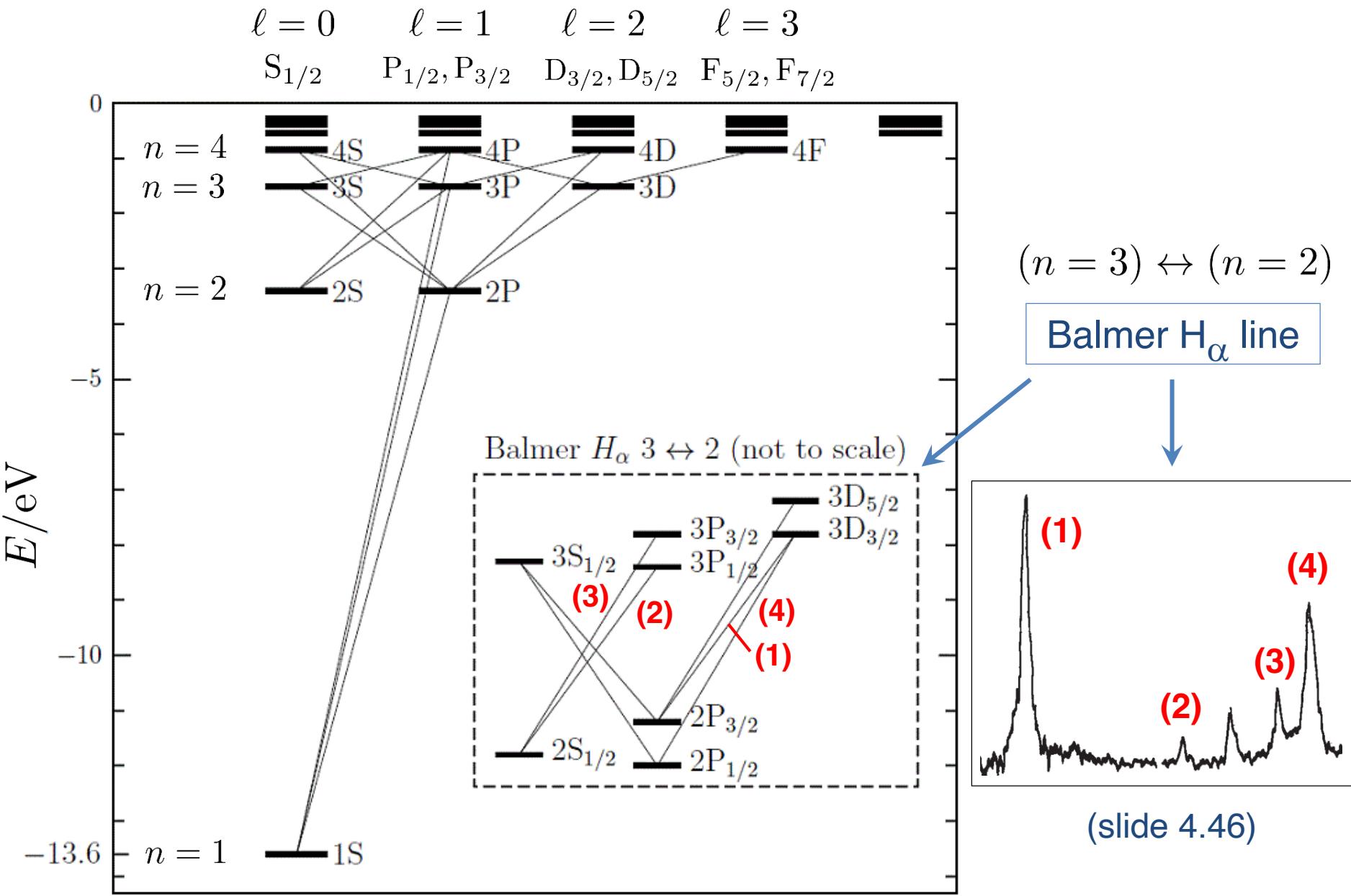


(triplet)



(triplet)

## Atomic transitions : hydrogen with fine structure (3)



## Atomic transitions : hydrogen with fine structure (4)

- Viewed on a large scale, the Grotrian diagram with fine structure included is indistinguishable from the zeroth-order diagram on slide 5.55

Viewed on a finer scale, however, the transitions are seen to be either doublets (for  $s \leftrightarrow p$ ) , or triplets (for all other transitions) (see slide 5.60)

- Transitions to the 1S ground state (the Lyman series) are all doublets  
All other  $n_1 \leftrightarrow n_2$  lines are built up from doublets and/or triplets, each of approximately the same energy
- The Balmer  $H_\alpha$  line,  $3 \leftrightarrow 2$ , for example, is a *septuplet*, built up from two doublets and a triplet (see inset diagram on previous slide)  
(only 7 of the  $5 \times 3 = 15$  possible transitions are allowed)

In practice, the  $H_\alpha$  line more typically appears as a *doublet* because the detailed structure is usually not resolved

Four peaks were clearly resolved in the “Lamb shift plot” on slide 4.46

## Atomic transitions : hydrogen with fine structure (5)

- Transitions between fine structure states lying within the same level  $n$  are allowed by the E1 selection rules

For example,  $2 \leftrightarrow 2$  transitions within the level  $n = 2$  are allowed :

$$2^2S_{1/2} \longleftrightarrow 2^2P_{1/2}; \quad 2^2S_{1/2} \longleftrightarrow 2^2P_{3/2}$$

But : such transitions have a very small energy  $\Delta E$ , and the E1 transition rate is proportional to  $(\Delta E)^3$

- the rates for E1 transitions  $n \leftrightarrow n$  within the same level are many orders of magnitude smaller than for transitions  $n_1 \leftrightarrow n_2$  between levels with different  $n_1, n_2$

## Atomic transitions : hydrogen with hyperfine structure

- Finally, “switch on” the proton spin and consider hyperfine structure :  
The strict selection rules for E1 transitions from Wigner-Eckart and parity now apply to the total angular momentum  $\mathbf{F} = \mathbf{L} + \mathbf{S} + \mathbf{I}$  :

$$\Delta F = 0, \pm 1 ; \quad F_1 + F_2 \geq 1 ; \quad \Delta m_F = 0, \pm 1$$

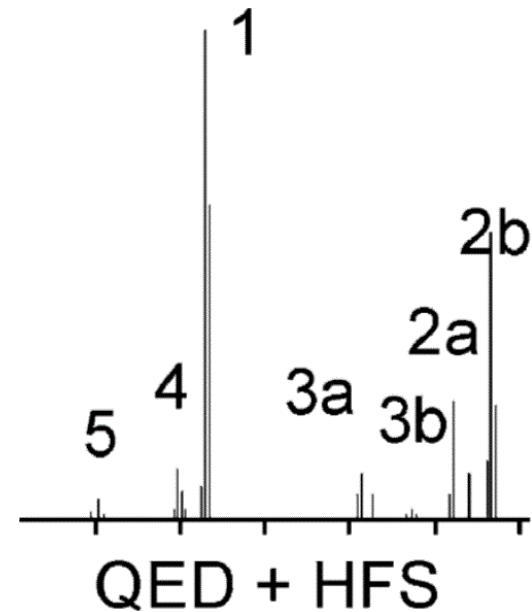
- In addition, the selection rules obtained above for zeroth-order and fine structure hydrogen continue to apply :

$$\Delta j = 0, \pm 1 ; \quad j_1 + j_2 \geq 1 ; \quad \Delta m_j = 0, \pm 1$$

$$\Delta \ell = \pm 1 ; \quad \Delta m_\ell = 0, \pm 1$$

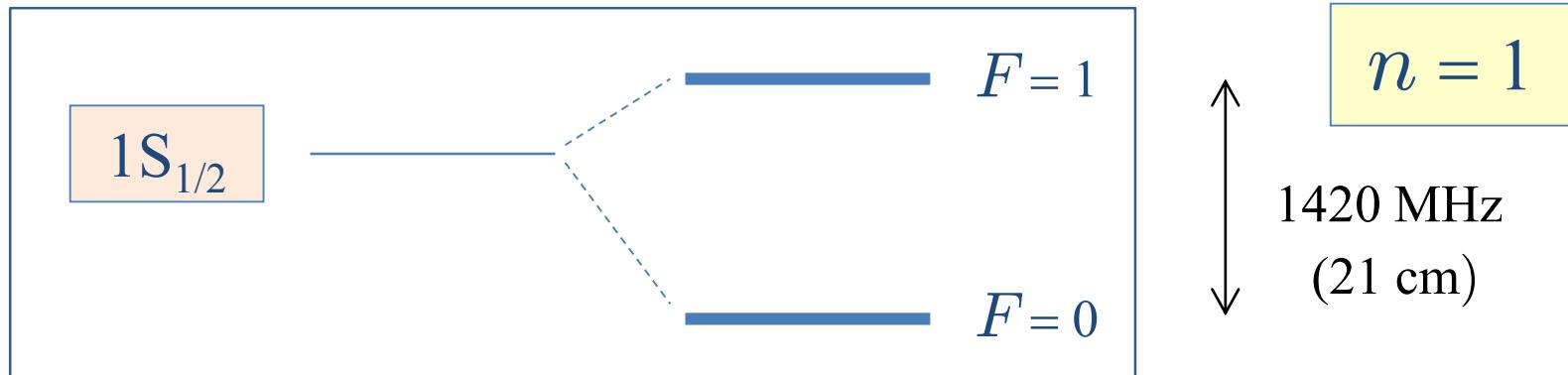
- With perfect resolution, the Balmer  $H_\alpha$  line, for example, would reveal itself to be a xxx-plet :

(only xxx of the  $10 \times 6 = 60$  possible transition energies are allowed by the selection rules above)



## Atomic transitions : hydrogen with hyperfine structure (2)

- The 21cm line of the hydrogen ground state is not an E1 transition :



It has  $|\Delta F| = 1$ ,  $\Delta j = 0$ , but also  $\Delta \ell = 0$  (i.e. it fails  $\Delta \ell = \pm 1$ )

(it is in fact a *magnetic dipole* M1 transition; these have transition rates several orders of magnitude smaller than for E1 transitions)

- Combined with the very small transition energy,

$$\Gamma \propto (\Delta E)^3, \quad \Delta E = 5.87 \times 10^{-6} \text{ eV}$$

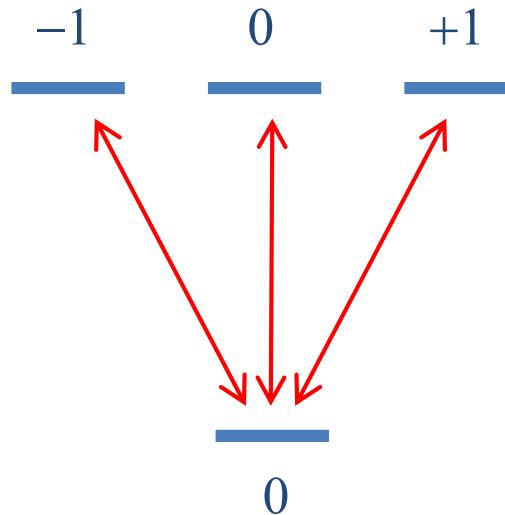
this explains the extremely low transition rate for 21cm photon emission compared to other transitions :

$$\Gamma = 2.8843 \times 10^{-15} \text{ s}^{-1} = (120 \text{ Myr})^{-1}$$

## Atomic transitions : $\Delta m$ selection rules

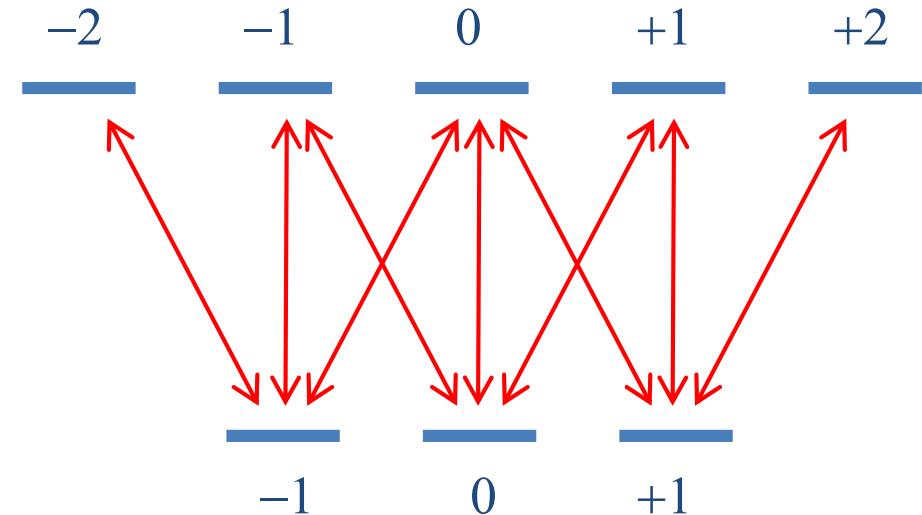
- A level with total angular momentum  $j$  has degeneracy  $g = 2j + 1$  (corresponding to the  $2j + 1$  possible values of  $m_j$ )  
The  $\Delta m_j$  selection rule restricts the possible transitions between initial and final degenerate sets of states; for example :

$$(j = 1) \leftrightarrow (j = 0)$$



No restrictions

$$(j = 2) \leftrightarrow (j = 1)$$



Forbids 6 of the 15 possible transitions

- The restrictions due to the  $\Delta m_j$  rule will become important later

## The Landé (Projection) Formula

- We now obtain a useful general expression for the matrix elements of a vector operator  $V$  between states of given  $j$  :
  - the *Landé projection formula*

The projection formula relates matrix elements of  $V$  to matrix elements of the total angular momentum operator  $J$   
(without reference to any Clebsch-Gordan coefficients)

- The projection formula will be used below to compute the magnetic dipole moments of the proton and neutron in the quark model
  - we can then understand why  $g = 2$  ( $g = 0$ ) fails so badly for p (n)

This requires knowing how to combine (add together) two or more individual magnetic dipole moments

- Later; the projection formula will be used to analyse the *Zeeman effect*

## The projection formula (2)

- The operator  $\mathbf{J}$  is a vector operator; applying the Wigner-Eckart theorem, slide 5.42, to the case  $\mathbf{V} = \mathbf{J}$  gives :

$$\langle \alpha'' j'' m'' | \hat{J}_m | \alpha' j' m' \rangle = \langle \alpha'' j'' | |\hat{\mathbf{J}}| | \alpha' j' \rangle \langle 1m; j' m' | j'' m'' \rangle$$

- The l.h.s. above vanishes unless  $j' = j''$ ; taking also  $\alpha'' = \alpha'$  then gives

$$\langle \alpha' j' m'' | \hat{V}_m | \alpha' j' m' \rangle = \langle \alpha' j' | |\hat{\mathbf{V}}| | \alpha' j' \rangle \langle 1m; j' m' | j'' m'' \rangle$$

$$\langle \alpha' j' m'' | \hat{J}_m | \alpha' j' m' \rangle = \langle \alpha' j' | |\hat{\mathbf{J}}| | \alpha' j' \rangle \langle 1m; j' m' | j'' m'' \rangle$$

- Eliminating the Clebsch-Gordan coefficient between the above equations then results in

$$\langle \alpha' j' m'' | \hat{V}_m | \alpha' j' m' \rangle = C(\alpha' j') \langle \alpha' j' m'' | \hat{J}_m | \alpha' j' m' \rangle$$

where  $C(\alpha' j')$  is a constant (the ratio of the two r.m.e's)

- We can now simplify the notation by dropping one prime throughout :

$$\langle \alpha j m' | \hat{V} | \alpha j m \rangle = C(\alpha j) \langle \alpha j m' | \hat{\mathbf{J}} | \alpha j m \rangle \quad (5.68.1)$$

## The projection formula (3)

-- Using the completeness relation (twice) :

$$\begin{aligned}
 \langle \alpha jm | \hat{\mathbf{V}} \cdot \hat{\mathbf{J}} | \alpha jm \rangle &= \sum_{k=1}^3 \langle \alpha jm | \underbrace{\hat{V}_k \hat{J}_k}_{\hat{I}} | \alpha jm \rangle \\
 &= \sum_{k,j',m'} \langle \alpha jm | \hat{V}_k | \alpha j'm' \rangle \langle \alpha j'm' | \hat{J}_k | \alpha jm \rangle \\
 &= \sum_{k,m'} \langle \alpha jm | \hat{V}_k | \alpha jm' \rangle \langle \alpha jm' | \hat{J}_k | \alpha jm \rangle \\
 &= C(\alpha j) \sum_{k,m'} \langle \alpha jm | \hat{J}_k | \alpha jm' \rangle \langle \alpha jm' | \hat{J}_k | \alpha jm \rangle \\
 &= C(\alpha j) \sum_{k,j',m'} \langle \alpha jm | \hat{J}_k | \alpha j'm' \rangle \underbrace{\langle \alpha j'm' | \hat{J}_k | \alpha jm \rangle}_{\sum_{j',m'} |j'm'\rangle\langle j'm'| = \hat{I}} \\
 &= C(\alpha j) \langle \alpha jm | \hat{\mathbf{J}}^2 | \alpha jm \rangle \\
 &= C(\alpha j) j(j+1)\hbar^2
 \end{aligned}$$

## The projection formula (4)

- For  $j > 0$ , the constant  $C(\alpha j)$  is therefore given by

$$C(\alpha j) = \frac{\langle \alpha jm | \hat{V} \cdot \hat{J} | \alpha jm \rangle}{j(j+1)\hbar^2}$$

- Substituting into equation (5.68.1), we obtain the *Landé projection formula* :

$$\langle \alpha jm' | \hat{V} | \alpha jm \rangle = \frac{\langle \alpha jm | \hat{V} \cdot \hat{J} | \alpha jm \rangle}{j(j+1)\hbar^2} \langle \alpha jm' | \hat{J} | \alpha jm \rangle$$

(5.70.1)

- In particular, for the  $z$  component  $V_z$ , this is

$$\langle \alpha jm' | \hat{V}_z | \alpha jm \rangle = \frac{\langle \alpha jm | \hat{V} \cdot \hat{J} | \alpha jm \rangle}{j(j+1)\hbar^2} m\hbar \delta_{m'm}$$

(5.70.2)

Setting  $m' = m$  above then shows that, for a given value of  $j$ , the matrix representation of  $V_z$  is diagonal with respect to  $m_j$  :

$$\langle \alpha jm' | \hat{V}_z | \alpha jm \rangle = \langle \alpha jm | \hat{V}_z | \alpha jm \rangle \delta_{m'm}$$

(5.70.3)

# Combining magnetic moments

- The projection formula allows us to combine (add together) two or more magnetic dipole moments; for example :
  - the orbital and/or spin magnetic moments of atomic electrons
  - ditto for protons and neutrons within a nucleus (nuclear shell model)
  - the spin magnetic moments of quarks in a proton (quark model)
- Orbital and spin magnetic dipole operators have the general form

$$\hat{\boldsymbol{\mu}}_L = \gamma_L \hat{\mathbf{L}} ; \quad \hat{\boldsymbol{\mu}}_S = \gamma_S \hat{\mathbf{S}}$$

- The combined effect of two dipoles of any origin in a magnetic field  $\mathbf{B}$  can be analysed generically by considering the Hamiltonian

$$\hat{H}_B = -\gamma_1 \hat{\mathbf{J}}_1 \cdot \mathbf{B} - \gamma_2 \hat{\mathbf{J}}_2 \cdot \mathbf{B}$$

or, equivalently,

$$\hat{H}_B = -\hat{\boldsymbol{\mu}} \cdot \mathbf{B} ; \quad \hat{\boldsymbol{\mu}} = \hat{\boldsymbol{\mu}}_1 + \hat{\boldsymbol{\mu}}_2 = \gamma_1 \hat{\mathbf{J}}_1 + \gamma_2 \hat{\mathbf{J}}_2$$

## Combining magnetic moments (3)

- Introduce the total angular momentum operator

$$\hat{\mathbf{J}} = \hat{\mathbf{J}}_1 + \hat{\mathbf{J}}_2$$

characterised by total angular momentum quantum numbers

$$j = j_1 \otimes j_2$$

- If the two gyromagnetic ratios are *equal* ( $\gamma_1 = \gamma_2$ ), then the total magnetic dipole operator is given simply by

$$\hat{\boldsymbol{\mu}} = \gamma \hat{\mathbf{J}} , \quad \hat{H}_B = -\gamma \hat{\mathbf{J}} \cdot \mathbf{B} , \quad \gamma = \gamma_1 = \gamma_2$$

If, however, the gyromagnetic ratios are *different* ( $\gamma_1 \neq \gamma_2$ ), then the total dipole and total angular momentum operators are no longer proportional :

$$\hat{\boldsymbol{\mu}} \neq \gamma \hat{\mathbf{J}} , \quad \hat{H}_B \neq -\gamma \hat{\mathbf{J}} \cdot \mathbf{B}$$

- However, for a *given value* of  $j$ , we now show that proportionality can be *effectively* restored using the Landé projection formula ...

## The Landé g-Factor

- Since  $\hat{\mu}$  is a vector operator, then, for  $j > 0$ , the projection formula of equation (5.70.1) gives

$$\langle \alpha jm' | \hat{\mu} | \alpha jm \rangle = \gamma_{\alpha j} \langle \alpha jm' | \hat{J} | \alpha jm \rangle$$

where

$$\gamma_{\alpha j} = \frac{\langle \alpha jm | \hat{\mu} \cdot \hat{J} | \alpha jm \rangle}{j(j+1)\hbar^2}$$

- The numerator above is

$$\langle \alpha jm | \hat{\mu} \cdot \hat{J} | \alpha jm \rangle = \langle \alpha jm | (\gamma_1 \hat{J}_1 \cdot \hat{J} + \gamma_2 \hat{J}_2 \cdot \hat{J}) | \alpha jm \rangle$$

- Squaring  $J_2 = J - J_1$  gives  $\hat{J}_1 \cdot \hat{J} = \frac{1}{2}(\hat{J}^2 + \hat{J}_1^2 - \hat{J}_2^2)$ , and hence

$$\langle \alpha jm | \hat{J}_1 \cdot \hat{J} | \alpha jm \rangle = \frac{\hbar^2}{2} [j(j+1) + j_1(j_1+1) - j_2(j_2+1)]$$

Similarly :

$$\langle \alpha jm | \hat{J}_2 \cdot \hat{J} | \alpha jm \rangle = \frac{\hbar^2}{2} [j(j+1) + j_2(j_2+1) - j_1(j_1+1)]$$

## The Landé g-Factor (2)

- Hence the constant  $\gamma_{\alpha j}$  is in fact independent of  $\alpha$  (and  $m$ ) and depends only on  $j$  (so  $\gamma_{\alpha j} \equiv \gamma_j$ ) : (5.74.1)

$$\gamma_j = \gamma_1 \frac{j(j+1) + j_1(j_1+1) - j_2(j_2+1)}{2j(j+1)} + \gamma_2 \frac{j(j+1) + j_2(j_2+1) - j_1(j_1+1)}{2j(j+1)}$$

- Thus, for each possible value of  $j$ , matrix elements of the total magnetic dipole moment operator  $\hat{\mu}$  are determined as

$$\langle \alpha jm' | \hat{\mu} | \alpha jm \rangle = \gamma_j \langle \alpha jm' | \hat{\mathbf{J}} | \alpha jm \rangle$$

i.e. magnetic dipoles combine as

$$\langle \alpha jm' | \gamma_1 \hat{\mathbf{J}}_1 + \gamma_2 \hat{\mathbf{J}}_2 | \alpha jm \rangle = \gamma_j \langle \alpha jm' | \hat{\mathbf{J}} | \alpha jm \rangle$$

- For a given value of  $j$ , we can effectively work with a total magnetic dipole operator

$$\hat{\mu} = \gamma_j \hat{\mathbf{J}}$$

where the *effective* gyromagnetic ratio  $\gamma_j$  is given by equation (5.74.1)

## The Landé g-Factor (3)

- Alternatively, the magnetic moments can be expressed in terms of the corresponding  $g$ -factors, as on slide 3.32 :

$$\hat{\mu}_1 = \gamma_1 \hat{J}_1 , \quad \hat{\mu}_2 = \gamma_2 \hat{J}_2 , \quad \hat{\mu} = \gamma_j \hat{J}$$
$$\gamma_1 = -g_1 \frac{\mu_B}{\hbar} , \quad \gamma_2 = -g_2 \frac{\mu_B}{\hbar} , \quad \gamma_j = -g_j \frac{\mu_B}{\hbar}$$

(or with the nuclear magneton  $\mu_N$  used throughout in place of  $\mu_B$ )

- Equation (5.74.1) then holds equivalently for  $g$ -factors :

$$g_j = g_1 \frac{j(j+1) + j_1(j_1+1) - j_2(j_2+1)}{2j(j+1)} + g_2 \frac{j(j+1) + j_2(j_2+1) - j_1(j_1+1)}{2j(j+1)}$$

**(5.75.1)**

## The Landé g-Factor : Summary

- In summary, when combining two magnetic dipole moments  $\mu_1$  and  $\mu_2$ ,

$$\hat{\mu} = \hat{\mu}_1 + \hat{\mu}_2 = \gamma_1 \hat{J}_1 + \gamma_2 \hat{J}_2$$

the Wigner-Eckart theorem shows that, in a state of total angular momentum  $j$ , we *effectively* have (in the sense that all matrix elements are given correctly)

$$\hat{\mu} = \gamma_j \hat{J}, \quad \hat{H}_B = -\gamma_j \hat{J} \cdot \mathbf{B} \quad (\hat{J} = \hat{J}_1 + \hat{J}_2)$$

where  $\gamma_j$  depends on  $j$  (for  $j > 0$ , and for given  $j_1, j_2$ ) as

$$\gamma_j = \gamma_1 \frac{j(j+1) + j_1(j_1+1) - j_2(j_2+1)}{2j(j+1)} + \gamma_2 \frac{j(j+1) + j_2(j_2+1) - j_1(j_1+1)}{2j(j+1)}$$

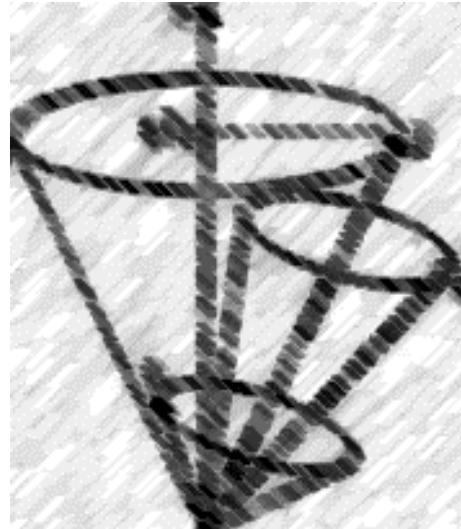
- For the case  $j = 0$  (see below) we obtain simply

$$\gamma_j = 0$$

- Thus each possible value of  $j = j_1 \otimes j_2$  has its own *effective* gyromagnetic ratio  $\gamma_j$ , or, equivalently, its own *effective* magnetic moment  $\mu_j$

## The vector model (of angular momentum)

- The results above are often obtained using the *vector model* of angular momentum, a pre-quantum relic which still lingers on ...



“ ... often explained in quantum mechanics textbooks as due to the rapid precession of the vectors  $\mathbf{S}$  and  $\mathbf{L}$  around the total angular momentum  $\mathbf{J}$ , but this odd blend of classical and quantum mechanical reasoning is quite unnecessary; ... ”

( S. Weinberg, “Lectures On Quantum Mechanics”, CUP, 2013 )

## The Landé g-Factor : particular cases

- For the case  $\gamma_1 = \gamma_2$ , or equivalently  $g_1 = g_2$ , equations (5.74.1) and (5.75.1) reduce, as expected, to (see slide 5.72)

$$\gamma_j = \gamma_1 = \gamma_2, \quad g_j = g_1 = g_2$$

- An important special case is the combination of two spin-half particles :

$$j = j_1 \otimes j_2 = 1/2 \otimes 1/2 = 0, 1$$

For a spin triplet, setting  $j_1 = 1/2, j_2 = 1/2, j = 1$  in equation (5.75.1) gives

$$g_j = \frac{1}{2}g_1 + \frac{1}{2}g_2 \quad (j = 1) \quad (5.78.1)$$

- The corresponding magnetic moments are

$$\mu_1 = \frac{1}{2}g_1\mu_B, \quad \mu_2 = \frac{1}{2}g_2\mu_B, \quad \mu_j = g_j\mu_B$$

Thus, for  $j = 1$ , the magnetic moments simply add linearly :

$$\mu_j = \mu_1 + \mu_2 \quad (j = 1)$$

## The Landé g-Factor : $j=0$

- For the spin *singlet* case, with total angular momentum  $j = 0$ , the Wigner-Eckart theorem (slide 5.42) immediately gives

$$\langle \alpha' 00 | \hat{\mu} | \alpha 00 \rangle = 0$$

→ in any state with zero total angular momentum, the magnetic moment vanishes :

$$\gamma_0 = \mu_0 = g_0 = 0 \quad (j = 0)$$

- This may seem an obvious result, but actually is not :

e.g. consider the ground state of hydrogen ( $\ell = 0$ ), with total angular momentum

$$F = S_e \otimes S_p = \frac{1}{2} \otimes \frac{1}{2} = 0, 1$$

For  $F = 1$  :  $g = \frac{1}{2}(g_e + g_p)$  ,  $\mu = \mu_e + \mu_p$

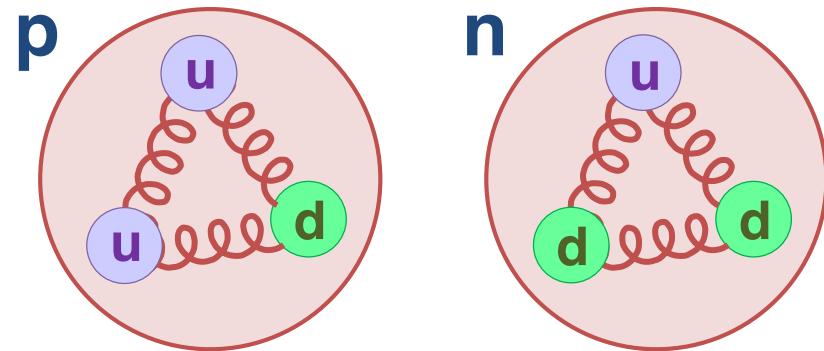
For  $F = 0$  :  $g = 0$  ,  $\mu = 0$

Since  $\mu_e \gg \mu_p$ , it is not easy to explain how the magnetic dipoles can sum to zero in a simple vector picture

# Proton and neutron magnetic moments

- The u ("up") and d ("down") quarks have fractional electric charges :

$$q_u = +\frac{2}{3}e ; \quad q_d = -\frac{1}{3}e$$



- Quarks are spin-half and pointlike, so their magnetic dipole moments are presumably as predicted by the Dirac equation :

$$\mu = \frac{q\hbar}{2m} \quad \Rightarrow \quad \mu_u = \frac{2}{3} \frac{e\hbar}{2m_u} ; \quad \mu_d = -\frac{1}{3} \frac{e\hbar}{2m_d} \quad (5.80.1)$$

- The proton is a bound state of (uud) quarks, with all orbital angular momenta zero, and with total angular momentum  $S_p = 1/2$  (the proton spin)

The two u quarks in the proton are in a state with  $S_{uu} = S_u \otimes S_u = 1$   
(a consequence of QCD colour symmetry : see next term)

*There are many other (uud) bound states, with non-zero orbital angular momentum and/or with  $S_{uu} = 0$ , but these are all unstable particles, and are not called protons*

## Proton and neutron magnetic moments (2)

- Since  $S_{uu} = 1$ , the two u quarks combine as in equation (5.78.1) :

$$g_{uu} = \frac{1}{2}g_u + \frac{1}{2}g_u = g_u$$

- Now add in the d quark; the proton has spin-half, so take  $j = S_p = 1/2$ ,  $j_1 = S_{uu} = 1$ ,  $j_2 = S_d = 1/2$  in equation (5.75.1) :

$$g_p = \frac{4}{3}g_{uu} - \frac{1}{3}g_d = \frac{4}{3}g_u - \frac{1}{3}g_d$$

- Now convert from  $g$ -factors to magnetic moments using

$$\mu_u = \frac{1}{2}g_u\mu_N ; \quad \mu_d = \frac{1}{2}g_d\mu_N ; \quad \mu_p = \frac{1}{2}g_p\mu_N$$

$$\Rightarrow \boxed{\mu_p = \frac{4}{3}\mu_u - \frac{1}{3}\mu_d}$$

- Similarly for the neutron (udd), with  $u \leftrightarrow d$  interchanged :

$$\boxed{\mu_n = \frac{4}{3}\mu_d - \frac{1}{3}\mu_u}$$

## Proton and neutron magnetic moments (3)

- Taking the u and d quark masses to be equal,  $m_u = m_d$ , equation (5.80.1) gives

$$\mu_u = -2\mu_d$$

Hence the quark model predicts the ratio of magnetic moments to be

$$\frac{\mu_p}{\mu_n} = -\frac{3}{2}$$

which is in (surprisingly?) good agreement with the measured ratio :

$$\frac{\mu_p}{\mu_n} \approx \frac{+2.793}{-1.913} \approx -1.460$$

- The proton and neutron magnetic moments are predicted to be

$$\mu_p = \frac{3}{2}\mu_u = \frac{e\hbar}{2m_u} = \frac{m_p}{m_u}\mu_N ; \quad \mu_n = -\frac{2}{3}\mu_p = -\frac{2}{3}\frac{m_p}{m_u}\mu_N$$

## Proton and neutron magnetic moments (4)

- Naïvely sharing the proton mass equally amongst the three quarks then gives magnetic moments which are in the right ballpark :

$$\mu_p = +3\mu_N ; \quad \mu_n = -2\mu_N$$

- Improved agreement with the measured moments is obtained by taking

$$m_u = m_d \approx \frac{m_p}{2.79} \approx 335 \text{ MeV}/c^2$$

These are *effective* quark masses ; the quarks have rest masses which are in fact much smaller :

$$m_u \approx m_d \approx 3 \text{ MeV}/c^2$$

(the proton rest mass is dominated by the energy stored in the gluon field responsible for binding the quarks together)