Advanced Quantum Mechanics

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Lecture #7

Symmetries and Quantum Mechanics

Recap of Last Class

- Irreps of Lie Groups and Orthogonality
- Characters, Orthogonality and Reduction for Rotation Group
- Addition of Angular Momentum: Spin-Orbit coupling, Hyperfine coupling
- Different Basis and Basis Transformation: Clebsch Gordan Co-efficients
- Irreducible set of Operators : Scalar & Vector Operators
- Cartesian Tensors and their reduction: Spherical Tensors

Matrix Elements and Selection Rules

If $\hat{O}_i^{(\alpha)}$ is an irreducible operator, $\hat{O}_i^{(\alpha)}|\phi_j^{(\beta)}\rangle$ transforms according to ij row of $T^{(\alpha\times\beta)} = \oplus_\gamma m^{(\gamma)} T^{(\gamma)}$

- Then matrix element of $\hat{O}^{(\alpha)}$ between $\phi^{(\beta)}$ and $\phi^{(\gamma)}$ is non-zero only if $m^{(\gamma)} \neq 0$

Specifically $\langle\phi_k^{(\gamma)}|\hat{O}_i^{(\alpha)}|\phi_j^{(\beta)}\rangle = C^*(\alpha,\beta,\gamma;i,j,k)\langle\gamma||\hat{O}^{(\alpha)}||\beta\rangle$ → Indep. of i,j,k

Wigner-Eckart Theorem:

Example: Dipole Selection Rules

The dipole moment is a vector operator which transforms according to j=1 irrep

Considering |n,l,m> atomic states, the dipole operator connects states with Δl =0 or 1 or -1 only. l=0 to l=0 transition is forbidden.

The dipole operator connects states with Δm =0 or 1 or -1 only

Example: Selection Rules for spherical tensors

$T_q^{(k)}|j,m\rangle$ transform according to qm row $\mathcal{D}^{(j\times k)}$

$$T_q^{(k)}|j,m\rangle = \sum_{lm} C(j,k,l;m,q,m')|l,m'\rangle \qquad \langle n'j'm'|T_q^{(k)}|n,j,m\rangle = C(j,k,j';m,q,m')\langle n'|\tilde{T}_q^{(k)}|n\rangle$$

Wigner-Eckart Theorem:

Selection Rules: |j-k| <= l <= j+k, m′ = m+q

Example: Wigner Eckart Theorem

Consider a set of vector operators r_i, p_i, d_i, V_i etc

$$\langle j,m|V_i|j,n\rangle = C(j,1,j;m,i,n)\langle j||V||j\rangle \qquad \langle j,m|J_i|j,n\rangle = C(j,1,j;m,i,n)\langle j||J||j\rangle$$

$$\langle j,m|V_i|j,n\rangle = \langle j,m|J_i|j,n\rangle \frac{\langle j||V||j\rangle}{\langle j||J||j\rangle}$$

True for any set of vector operators

Concrete Example: Calculation of dipole moment in spin-orbit coupled states

Method #1: Write the state in terms of Y^l_m s using Clebsch Gordon coeff.
Work out integrals involving r in each of these states

Method #2: Use total matrix elements of total angular momentum operator
How to get the prop constant? —— HW

This implies $$\frac{\langle j,m|V_i|j,n\rangle}{\langle j,k|V_q|j,l\rangle} = \frac{\langle j,m|J_i|j,n\rangle}{\langle j,k|J_q|j,l\rangle}$$

very useful in calculating ratios of matrix Elements

Used (within FGR) to calculate ratio of intensity of different transitions

Used to calculate branching ratios for different decay processes.

Proper and Improper Rotations

Define a set of transformations of the Cartesian co-ordinates which keeps $r^2 = x_i x_i$ invariant.

$$x_i' = R_{ij} x_j \qquad x_i' x_i' = R_{ik} R_{ij} x_k x_j = R^T_{ki} R_{ij} x_k x_j = (R^T R)_{kj} x_k x_j = x_i x_i$$

So, $R^T R = 1$, i.e. transformations correspond to group of 3 dimensional Orthogonal matrices O(3)

It is obvious that $[\text{Det } R]^2 = 1$, so $[\text{Det } R] = \pm 1$

Rotations are continuously connected to the identity matrix and hence correspond to $[\text{Det } R] = 1$

Corresponding group : SO(3)

What about the set of orthogonal R with [Det R]= -1 ?

They do not form a group by themselves, but together with rotn. forms the O(3) group

Corresponding transformations are called improper rotations. Product of a "proper" rotation and spatial inversion

Inversion and Pseudovectors

Scalar Operator : $\mathcal{D}^\dagger \hat{A} \mathcal{D} = \hat{A}$ Invariant under rotation

Vector Operator: A set D operators in D dim which transform according to $\mathcal{D}^\dagger \hat{A}_i \mathcal{D} = R_{ij} \hat{A}_j$

Let us now include spatial inversion (parity) transformations into the mix.

Vector Operator: The vector operators change sign under inversion. e.g $\vec{r} \longrightarrow -\vec{r}$

Pseudovector Operator: A set D operators in D dim which transform according to $\mathcal{D}^\dagger \hat{A}_i \mathcal{D} = R_{ij} \hat{A}_j$ but does not change sign under inversion

E.g.: Angular Momentum L, Spin S etc

Scalar Operator : Invariant under both rotation and inversion

Pseudoscalar Operator : Invariant under rotation but changes sign under inversion

E.g.: p.S etc

Back to vibrations of NH_3

To take out contribution of the modes corresponding to translation and rotation of center of mass to the characters in our 12 D representation we used

Character contribution of the translation and rotation modes:

For translation modes, $\chi_t(R_\theta) = (2\cos\theta + 1)$ $\chi_t(S_\theta) = (2\cos\theta - 1)$ $\chi_t(E) = 3$

For rotation modes, $\chi_r(R_\theta) = (2\cos\theta + 1)$ $\chi_r(S_\theta) = -(2\cos\theta - 1)$ $\chi_r(E) = 3$

Components of translation of C.O.M. form a set of vector operators.

So under (proper and improper) rotation, it transforms in a way similar to any 3-coord. This explains the character contribution of translation modes.

A Rotation, under a proper rotation transforms in the same way as translation modes.

But under inversion, it gets additional - sign (wrt vectors), To see this, note that infinitesimal rotations correspond to cross product n X r, which is a pseudovector.

U(1) Symmetry

Already encountered in the form of 2D rotations R_2

(x,y) ⟶ u=(x+ iy)

$R_z(\theta)$ [(x,y)] = (x cosθ+y sinθ, -x sinθ+y cosθ)

$R_z(\theta)$ [u] = u $e^{-i\theta}$ ⟶ U(1)

Group Combination Rule: $\theta_c = \theta_a + \theta_b$ $\rho(\theta) = 1$ $V = \int_0^{2\pi} d\theta = 2\pi$

Abelian Group --> 1D irreps $T(a)T(b) = T(a+b) \Rightarrow T(a)T^{'}(0) = T^{'}(a) \Rightarrow T(a) = exp[T^{'}(0)a]$

Single Valued Representation $T(a+2\pi) = T(a) \Rightarrow T^{'}(0) = im \quad m = 0, \pm 1, \pm 2... \quad T(\theta) = e^{im\theta}$

The Fourier Expansion $\psi(r,\theta) = \sum_m \psi_m(r) e^{im\theta}$ is reduction of a function into irreducible components

Direct Product Representation: $T^{(m\times n)}(\theta) = T^{(m)}(\theta)T^{(n)}(\theta) = T^{(m+n)}(\theta)$

1D SHO and U(1)

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \longrightarrow \frac{\hat{H}}{\omega} = \frac{1}{2}(\hat{k}^2 + \hat{y}^2)$$

$$\hat{k} = \hat{p}/\sqrt{m\omega} \qquad \hat{y} = \hat{x}\sqrt{m\omega}$$

$$[\hat{y}, \hat{k}] = i$$

Classical Phase Trajectories corresponding to fixed E : circle ⟶ R_2 ⟶ U(1)

(x,y) ⟶ u=(x+ iy) (y,k) ⟶ u=(y+ ik)

QM Equivalent: $a^\dagger = \frac{1}{\sqrt{2}}[\hat{y} + i\hat{k}]$ $a = \frac{1}{\sqrt{2}}[\hat{y} - i\hat{k}]$ $\hat{H} = \omega\left(a^\dagger a + \frac{1}{2}\right)$

U(1) Transformation: Rotation (phase shift) operator: $e^{-ia^\dagger a\theta}$

$$a^\dagger \to e^{ia^\dagger a\theta} a^\dagger e^{-ia^\dagger a\theta} = a^\dagger e^{i\theta}$$

H is invariant under this, so the system has U(1) symmetry

Eigenstates labeled by integer valued eigenvalues of $a^\dagger a$

$$|n\rangle \sim (a^\dagger)^n|0\rangle \qquad |n\rangle \to e^{in\theta}|n\rangle$$

U(1) Gauge Transformations and EM

Consider a system with the following symmetry: The observables are unchanged under a space-time dependent phase rotation of the wavefunction [U(1) gauge symmetry]

$$i\partial_t\psi(x,t) = [-\frac{\nabla^2}{2m} + V(x)]\psi(x,t) \qquad \psi^{'}(x,t) = e^{i\Lambda(x,t)}\psi(x,t)$$

Under this transf.
the momentum operator

$$p = -i\nabla \rightarrow -ie^{i\Lambda(x,t)}\nabla e^{-i\Lambda(x,t)} = -i\nabla - \nabla\Lambda(x,t) = p - \nabla\Lambda(x,t)$$

and the Energy operator

$$i\partial_t \rightarrow ie^{i\Lambda(x,t)}\partial_t e^{-i\Lambda(x,t)} = i\partial_t + \partial_t\Lambda(x,t)$$

So

$$i\partial_t\psi^{'}(x,t) = \left[\frac{(p-\nabla\Lambda)^2}{2m} + V(x) - \partial_t\Lambda\right]\psi^{'}(x,t)$$

we recover the std Hamiltonian
of a charged particle in em field.

$$i\partial_t\psi(x,t) = \left[\frac{(p-\frac{e}{c}A)^2}{2m} + e\phi(x)\right]\psi(x,t)$$

with

$$\nabla\Lambda(x,t) = \frac{e}{c}\vec{A} \qquad \text{and} \qquad e\phi = -\partial_t\Lambda(x,t)$$

U(1) Gauge Transformations and EM

Consider now a system which already has charged particle interacting with EM field

$$i\partial_t \psi(x,t) = \left[\frac{(p - \frac{e}{c}A)^2}{2m} + e\phi(x)\right]\psi(x,t)$$

A Gauge transformation of the form $\psi^{'}(x,t) = e^{i\Lambda(x,t)}\psi(x,t)$

simply leads to an equation of motion of the form

$$i\partial_t \psi(x,t) = \left[\frac{(p - \frac{e}{c}A)^2}{2m} + e\phi(x)\right]\psi(x,t)$$

$A \to A + \nabla\Lambda \qquad \phi \to \phi - \frac{1}{c}\partial_t\Lambda$ which leaves

$E = -\nabla\phi - \frac{1}{c}\partial_t A$ and $B = \nabla \times A$ invariant.

SU(2) and its generators

Arbitrary 2D Unitary Matrix $\hat{U} = e^{i\hat{H}}$, where H is a Hermitian matrix (4 real numbers). with Det[U]=1, which means H is traceless. Hence 3 indep. parameters

3 parameter Non-Abelian Lie Group

Arbitrary Traceless 2 X 2 matrix $a_x\sigma_x + a_y\sigma_y + a_z\sigma_z = \vec{a}.\vec{\sigma}$

$$U = e^{i\vec{a}\cdot\vec{\sigma}} = \cos(a/2) + i\vec{\sigma}\cdot\hat{a}\sin(a/2)$$

Pauli Matrices $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0^* \end{pmatrix}$ $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$\vec{a} = 0$ is the identity

Pauli Matrices provide a set of generators, so the Lie Algebra is $[J_i, J_j] = i\epsilon_{ijk}J_k$

The Lie Algebra is same as that of rotation group [R3 or SO(3)]. In fact everything about irreps, basis fn.s etc which can be obtained from the Lie Algebra can be translated.

In SU(2) the angle of rotation a goes from 0 to 4π, while angle of rotation goes from 0 to 2π for SO(3)

2 rotations in SU(2) by θ and $\theta+2\pi$, correspond to the same rotation by θ for SO(3).
This is a 2 to 1 map.

2D Harmonic Oscillator

$$H = \frac{p_1^2 + p_2^2}{2m} + \frac{1}{2}m\omega_0^2(x_1^2 + x_2^2) \qquad [x_i, p_j] = i\hbar\delta_{ij} \qquad [x_i, x_j] = [p_i, p_j] = 0$$

$$H = \frac{1}{2}\hbar\omega_0(k_1^2 + k_2^2 + x_1^2 + x_2^2) \qquad a = \frac{1}{\sqrt{2}}(\hat{x} + i\hat{k}) \qquad a^\dagger = \frac{1}{\sqrt{2}}(\hat{x} - i\hat{k})$$

$$[a_i, a_j^\dagger] = \delta_{ij} \qquad [a_i^\dagger, a_j^\dagger] = [a_i, a_j] = 0$$

1 and 2 denote indep. Harmonic oscillators. Eigenstates are labelled by occupancy of 1&2 modes

$$E(n_1, n_2) = \hbar\omega_0[n_1 + n_2 + 1]$$

Note the N+1 fold degeneracy ($N=n_1+n_2$).

N=1 ---- (1,0) and (0,1) , N=2 ---- (2,0), (1,1),(0,2) N=3 ---- (3,0),(2,1),(1,2),(0,3)

Symmetries : Inversion, 2D rotation, U(1) X U(1) ..... Abelian symmetries. No degeneracy expected.

This is either "accidental" or due to some symmetry we have not thought about

2D SHO and SU(2)

Consider N=1 sector (1,0) and (0,1).

Any 2 orthogonal linear combination of (1,0) and (0,1) can be used as eigenstates. The physics should be independent of this choice.

The symmetry corresponds to arbitrary rotations in the 2D complex vector space (upto a phase) spanned by this two states. This is simply the symmetry group SU(2).

Degenerate states for generic N : (N,0), (N-1,1) ... (0,N) 2N+1 fold degeneracy

Work with new variables $\{n_1,n_2\}$ -----> $\{(n_1+n_2)/2, (n_1-n_2)/2\}$

[(N,0), (N-1,1), ...(0,N)] -------> [(N/2,N/2),(N/2,N/2-1), ...(N/2,-N/2)]

Looks like angular momentum eigenstates with $(n_1+n_2)/2$ --> j and $(n_1-n_2)/2$ ---> m

$$\frac{1}{2}(a_1^\dagger a_1 - a_2^\dagger a_2) \to L_z \qquad a_1^\dagger a_2 \to L^+ \qquad a_2^\dagger a_1 \to L^-$$

These operators obey the standard angular momentum commutation relations

Check Explicitly !!

Schwinger Bosons

Note that the 2D nature of the system is not imp. (only need 2 indep. Harmonic Oscillator)

$$[a_i, a_j^\dagger] = \delta_{ij} \qquad [a_i^\dagger, a_j^\dagger] = [a_i, a_j] = 0 \qquad \text{i,j =1,2}$$

Schwinger Bosons

All of rotation and angular momentum can be worked out if you know Harmonic Oscillators

with the replacement $\frac{1}{2}(a_1^\dagger a_1 - a_2^\dagger a_2) \to L_z \qquad a_1^\dagger a_2 \to L^+ \qquad a_2^\dagger a_1 \to L^-$

$$L^2|j,m\rangle = (n_1+n_2)^2/4 + (n_1+n_2)/2|j,m\rangle = j(j+1)|j,m\rangle \qquad |j,m\rangle = \frac{(a_1^\dagger)^{j+m}(a_2^\dagger)^{j-m}}{\sqrt{j+m}\sqrt{j-m}}|0\rangle$$

$$\mathcal{D}^{(j)}_{mm'}(\alpha,\beta,\gamma) = \langle j,m'|e^{-iL_z\alpha}e^{-iL_y\beta}e^{-iL_z\gamma}|j,m\rangle = e^{-i(m'\alpha+m\gamma)}\underline{\langle j,m'|e^{-iL_y\beta}|j,m\rangle}$$

$$d^{(j)}_{mm'}(\beta)$$

$$d^{(j)}_{m'm}(\beta) = \sum_k (-1)^{k-m+m'} \frac{\sqrt{(j+m)!(j-m)!(j+m')!(j-m')!}}{(j+m-k)!k!(j-k-m')!(k-m+m')!} \cos^{2j-2k+m-m'}(\beta/2)\sin^{2k-m+m'}(\beta/2)$$

Show This !!

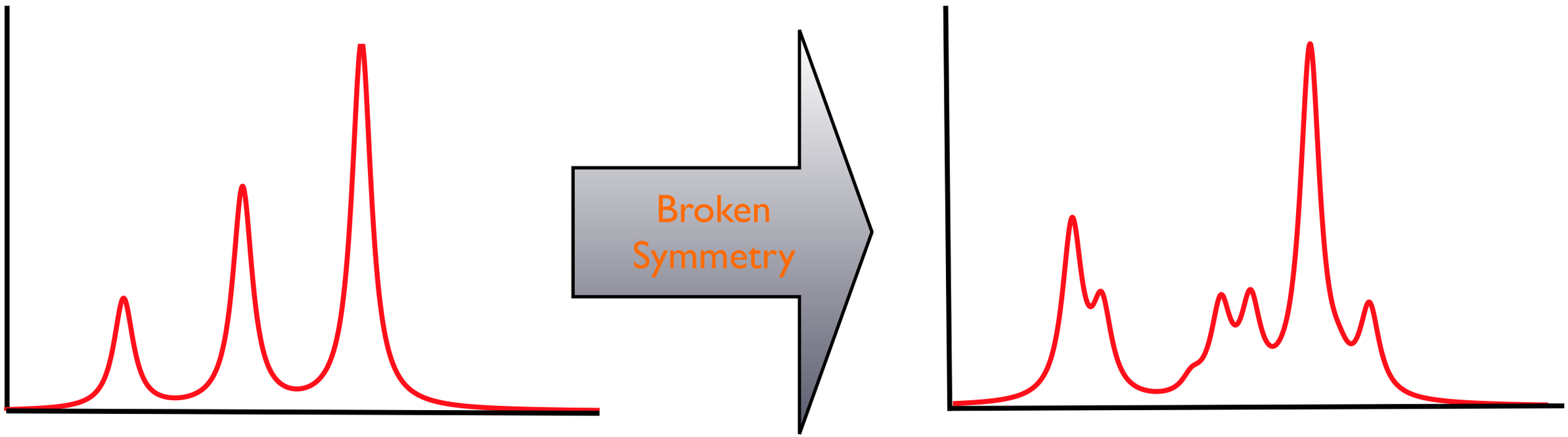
Symmetry Breaking and Splitting of degeneracy

We have till now considered the consequences of symmetry on various aspects of QM problems

Symmetries, however correspond to non-observables. It is often by breaking symmetry and studying the consequences (when we can) that we ascertain aspects of symmetry.

E.g.: Symmetries lead to degeneracies. However, it is hard to experimentally determine how many degenerate states one is looking at. Usually spectroscopic methods tell us the energy levels, but unless it is a simple enough problem where we know various matrix elements exactly, it is hard to predict how many states one is looking at.

By breaking symmetries in specific ways, we can split the degenerate levels. The specific manner of splitting of the degenerate levels give us a handle over various aspects of both the symmetric and symmetry broken system.



Splitting of degeneracies as seen in typical spectroscopic data

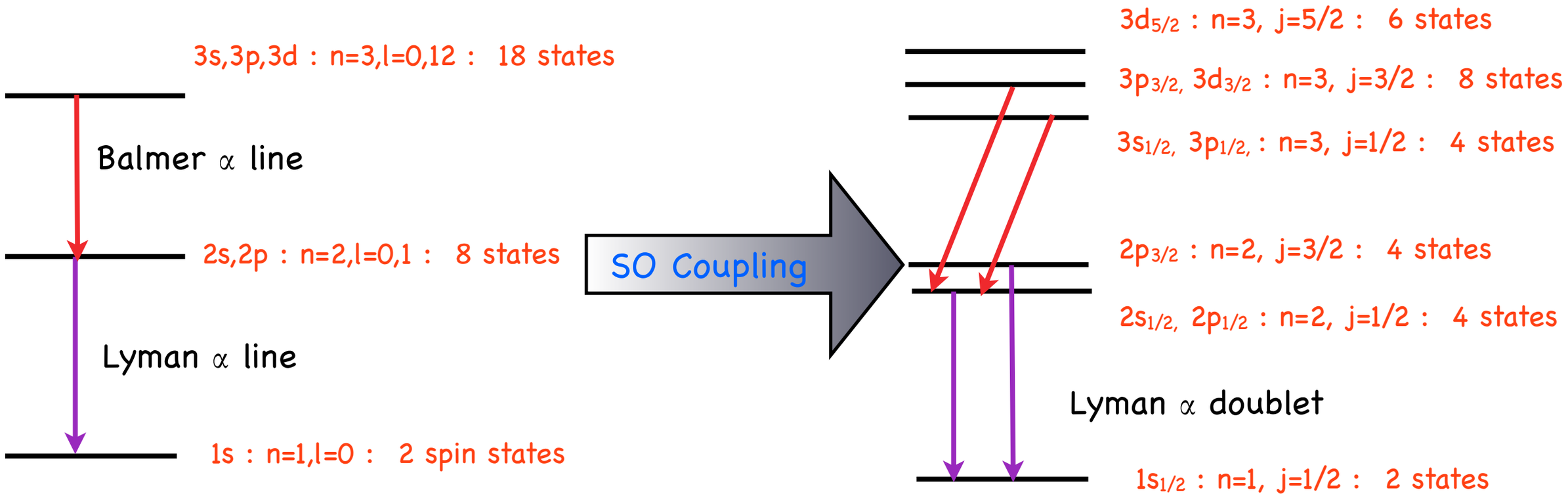
Fine Structure of Atomic Levels (H Atom)

The Coulomb problem has a large symmetry group [O(4) for the spatial part]

Energy Levels $E_n \sim 1/n^2$ Total Degeneracy $2n^2$

- Each n level has n fold l degeneracy of l=0,1,..n-1 (Coulomb special, nothing to do with rotn.)
- Each l level is 2l+1 fold degenerate (m states) due to rotational symmetry.
- In addition there is 2 fold degeneracy due to rotational symmetry in spin 1/2 space

Hydrogen Atom



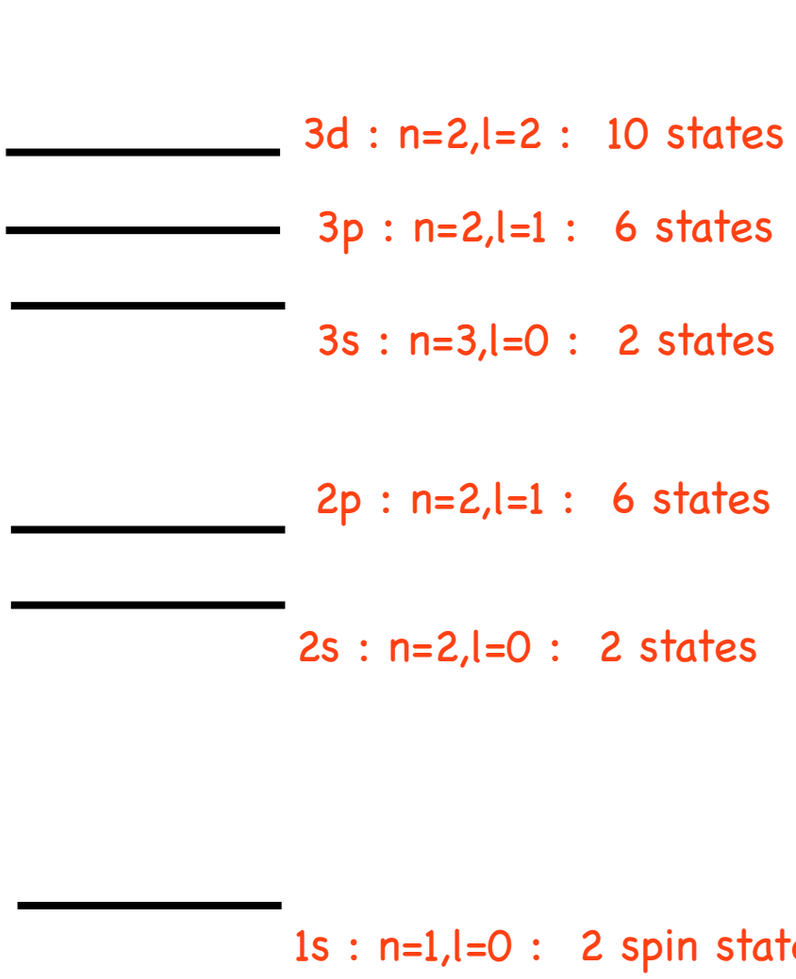
In Hydrogen, the $2s_{1/2}$ and 2p1/2 states are split due to interaction with vacuum polarization of QED. This shift, called Lamb shift, was calculated to a very high precision using QFT

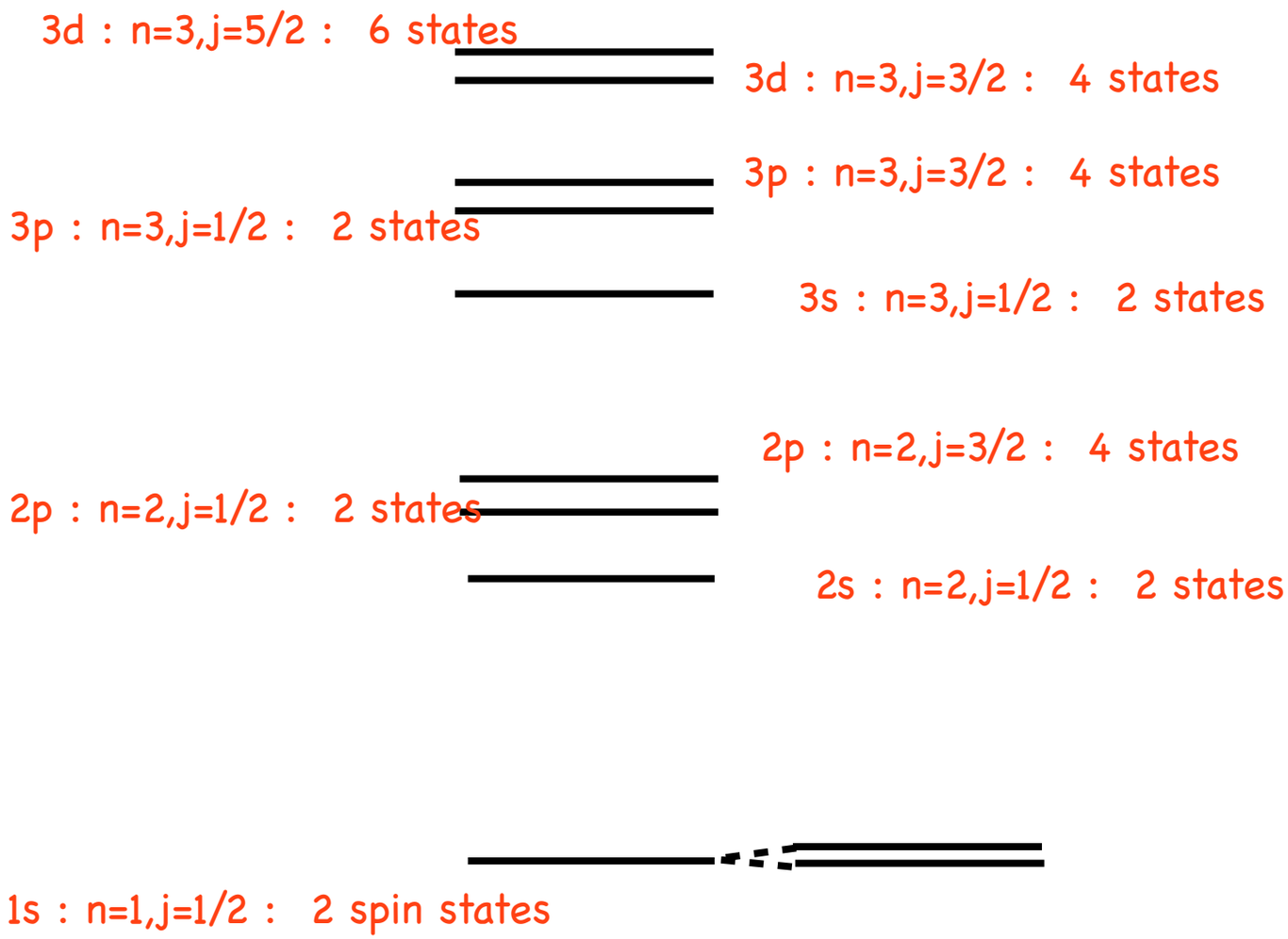
Fine Structure of Atomic Levels (Beyond H atom)

In multi-electron atoms, the outer electrons "see" the nuclear charge through a fog of charges due to inner electrons. This results in an effectively screened interaction .

$$V(r) \sim e^{-\mu r}/r$$

This splits the different l levels. We have 2(2l+1) fold degenerate states due to rotation symmetry.





Hyperfine splitting