Advanced Quantum Mechanics

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Lecture #12

Quantum Mechanics of Many Particles

Systems with Many Particles

QM of one particle e.g.: Harmonic oscillator, single hydrogen atom etc.

QM of 2 particles e.g.: Scattering. Reduced to an effective 1-particle problem by going to COM and relative co-ordinates.

Most systems around us consist of many particles:

Jar of hydrogen gas, Electrons in a metal, Multi-electron Atoms, Nuclear matter

Many body quantum systems show interesting quantum effects:

Liquid Helium can flow without viscosity

The collapse of supernovae are arrested by Fermi pressure

Electrons in a metal can become superconducting

Many Particle systems can be in states that spontaneously break the symmetry of the underlying Hamiltonian

The whole is more than the sum of its parts

What is different in Many-Particle Systems?

3 big differences when we extend our understanding of single particle QM to many particles:

1) The most-obvious way to write the Hilbert space of many particle systems in terms of the Hilbert space of the constituent particles leads to unphysical states.

2) It is very hard to find eigenstates in a space with large no. of D.O.F., specially when constituents interact with each other.

3) In the N---> ∞ limit, we can have the phenomenon of spontaneous symmetry breaking with no analogue in 1 particle QM.

We will show how one can work in a formalism which automatically takes care of 1).

We will show some approximate techniques to deal with 2).

We will see an example of 3)

The Many-Particle Hilbert Space

Description of a system of N particles in CM: {q,p} ——> $\{q_i,p_i\}$ (a point in 6N dim. phase space).

1 particle QM: use |q> or |p> eigenstates as a basis to expand arbitrary states.

Many Particle QM

Naive guess: A Tensor product of Hilbert space for each particle

Let $\{|\alpha\rangle_i\}$ denote a complete set of basis states for the i^{th} particle.

$|\alpha\rangle = |\alpha\rangle_1 \otimes |\alpha\rangle_2 \otimes |\alpha\rangle_3 .... \otimes |\alpha\rangle_N$ can be used as a basis set

Example with momentum basis states: $|\alpha\rangle = |k_1\rangle_1 \otimes |k_2\rangle_2 \otimes |k_3\rangle_3 .... \otimes |k_N\rangle_N$

Particle 1 has momentum k_1, particle 2 has momentum k_2 .... particle N has momentum k_N

Example with position basis states: $|\alpha\rangle = |q_1\rangle_1 \otimes |q_2\rangle_2 \otimes |q_3\rangle_3 \otimes ... \otimes |q_N\rangle_N$

Particle 1 is at q_1, particle 2 is at q_2 .... particle N is at q_N

The Many-Particle Hilbert Space

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OK if we are dealing with distinguishable particles
e.g. A three particle system of an electron, a proton, and a neutron (Deuterium).

If we are trying to describe a system of many identical indistinguishable particles the Hilbert space spanned by the above basis states admits unphysical quantum many-body states.

To see this : $|\alpha\rangle = |x\rangle_1 \otimes |y\rangle_2 \otimes |z\rangle_3$ and $|\beta\rangle = |z\rangle_1 \otimes |y\rangle_2 \otimes |x\rangle_3$ are distinct states

- But if the particles are indistinguishable, the numbering 1,2,..N is superfluous
- We can only talk about a particle each at x,y,z, not about 1^{st} particle at x....
- So $|\alpha>$ and $|\beta>$ should be the same state (upto a phase)
- Using the tensor product basis thus overcounts the states

A Hint from classical probability

We have 2 distinguishable boxes and 2 distinguishable balls --- red and blue.
If all configurations are equally probable, what is the prob that box 2 has 2 balls?

Possible Config: {rb,0},{0,rb},{r,b},{b,r} Reqd. Probability: 1/4

2 distinguishable boxes and 2 indistinguishable balls — both red.
If all configurations are equally probable, what is the prob that box 2 has 2 balls?

Possible Config: {rr,0},{0,rr},{r,r} Reqd. Probability: 1/3

Tagged Balls: How to get the answer if we insist on tagging the balls (say 1^{st} and 2^{nd}) ?

Prescription: Count all config obtained by permuting the tagging index.
Divide by the number of permutations

{12,0},{0,12},{1,2},{2,1} ⟶ [{12,0}+{21,0}]/2!, [{0,12}+{0,21}]/2!, [{1,2}+{2,1}]/2!

Can we extend this prescription to QM states of many-particle systems?

Identical particles and Hilbert Space

In QM, we have to fix amplitudes while adding equivalent states. No analogue in classical probability

Example with 2 particles and 2 single particle states, $|\alpha>$ and $|\beta>$ $\quad |\alpha\rangle|\beta\rangle \longrightarrow e^{i\phi}|\beta\rangle|\alpha\rangle$

Need to figure out transf. of states under permutation of particles

$$P_{12}|\alpha\rangle_1|\beta\rangle_2 = e^{i\phi}|\beta\rangle_1|\alpha\rangle_2 \qquad P_{12}^2|\alpha\rangle_1|\beta\rangle_2 = e^{i2\phi}|\alpha\rangle_1|\beta\rangle_2$$

Since $P_{12}{}^2 = I$

$$e^{i2\phi} = 1 \Rightarrow e^{i\phi} = \pm 1$$

S_2: Permutation group of 2 objects (here the particles). This group has 2 1d irreps given by {1,−1}.

The particles whose states transform according to {+1} are called Bosons and particles whose states transform according to {−1} are called Fermions

For Bosons: $\frac{1}{\sqrt{2}}[|\alpha\rangle_1|\beta\rangle_2 + |\beta\rangle_1|\alpha\rangle_2]$ $\qquad$ For Fermions: $\frac{1}{\sqrt{2}}[|\alpha\rangle_1|\beta\rangle_2 - |\beta\rangle_1|\alpha\rangle_2]$

give valid states. However, arbitrary superpositions of tensor product states are not allowed

Spin and Exchange Statistics

Spin statistics theorem: Particles with half-integer spins behave like Fermions and those with integer spins behave like Bosons. The correlation between spin and statistics comes from relativistic field theories.

Some Consequences of Exchange Symmetry

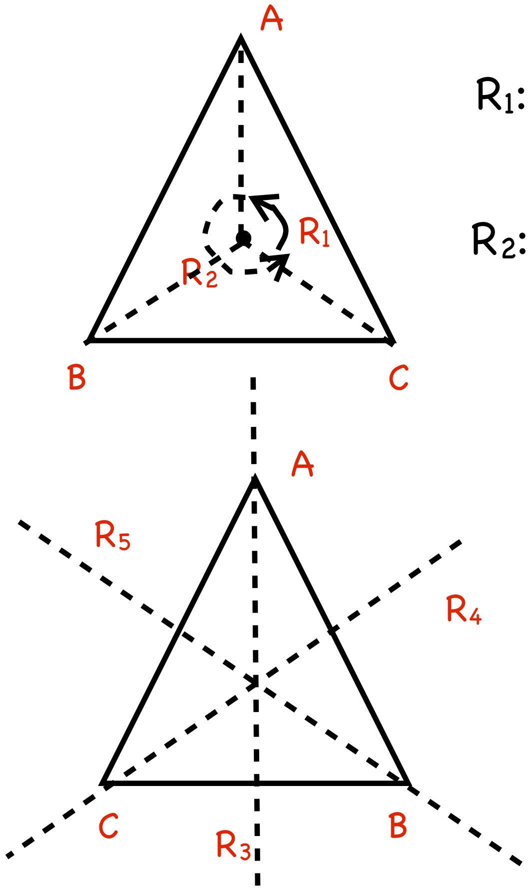
- The relative angular momentum of a spin 0 particle about another identical one is even
- Two fermions cannot occupy the same quantum state : Forms the basis for atomic structure, band theory etc.
- For 2 electrons, the spin triplet state needs to be spatially antisymmetric (odd angular mom.) while the singlet state needs to be spatially symmetric (even angular mom)
- Bosons can all occupy the lowest energy single-particle state: Bose Einstein Condensation

3 Identical Particles

Permutations of 3 objects : S_3

S_3 is isomorphic to D_3

	{E}	{R	{R
T	1	1	1
T	1	1	-1
T	2	-1	0



R_1: A –> B, B –> C, C –> A

R_2: A –> C, B –> A, C –> B

R_3: A –> A, B –> C, C –> B

R_4: A –> B, B –> A, C –> C

R_5: A –> C, B –> B, C –> A

S_3 is non-Abelian and has a 2d irrep

However, in nature we only get particles transforming acc. to $T^{(1)}$ and $T^{(2)}$

$T^{(1)}$ is the identity irrep. and corresponds to Bosons

$$|\psi_3^B\rangle = \frac{1}{\sqrt{3!}}\big[|x\rangle_1 \otimes |y\rangle_2 \otimes |z\rangle_3 + |x\rangle_1 \otimes |z\rangle_2 \otimes |y\rangle_3 + |y\rangle_1 \otimes |x\rangle_2 \otimes |z\rangle_3 + |y\rangle_1 \otimes |z\rangle_2 \otimes |x\rangle_3$$
$$+ |z\rangle_1 \otimes |x\rangle_2 \otimes |y\rangle_3 + |z\rangle_1 \otimes |y\rangle_2 \otimes |x\rangle_3\big]$$

3 Identical Particles

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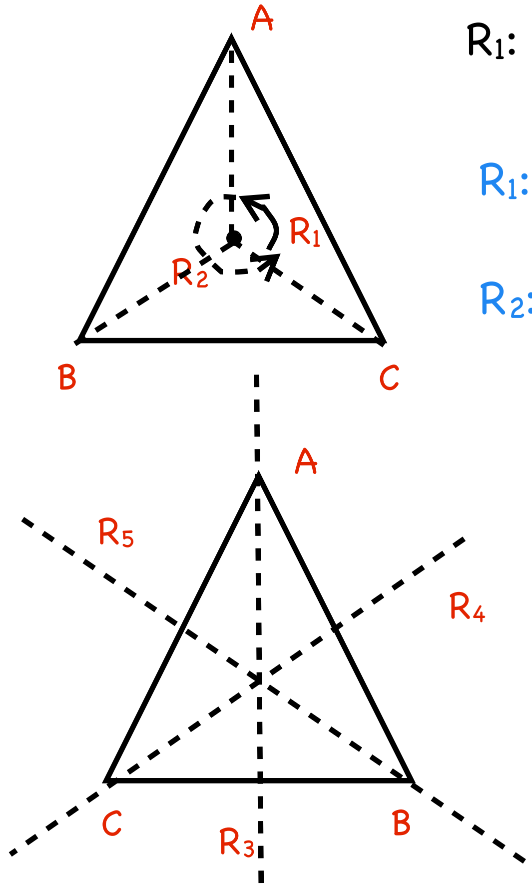


R_1: A –> B, B –> C, C –> A

R_1: A <–> B, then B <–> C

R_2: A <–> C, then B <–> A

R_3: A –> A, B –> C, C –> B

R_3: B <–> C

R_4: A <–> B

R_5: A <–> C

$T^{(2)}$ is the sign irrep. and corresponds to Fermions

Any permutation can be built up by many permutations of 2 objects at a time

For each such 2-perm put a – sign and keep multiplying the – signs. The ±1 that results is called the sign of the permutation.

$$|\psi_3^F\rangle = \frac{1}{\sqrt{3!}}[|x\rangle_1 \otimes |y\rangle_2 \otimes |z\rangle_3 - |x\rangle_1 \otimes |z\rangle_2 \otimes |y\rangle_3 + |y\rangle_1 \otimes |z\rangle_2 \otimes |x\rangle_3 - |y\rangle_1 \otimes |x\rangle_2 \otimes |z\rangle_3$$
$$+ |z\rangle_1 \otimes |x\rangle_2 \otimes |y\rangle_3 \quad - |z\rangle_1 \otimes |y\rangle_2 \otimes |x\rangle_3 \quad]$$

1,2,3..... N —> ∞

Let us now generalize the formalism to N particles

We want to write down a state where there are particles in the single particle states
$|\alpha_1>$, $|\alpha_2>$, $|\alpha_3>$,.... $|\alpha_N>$

For Bosons:

$$|\psi_B\rangle = \frac{1}{\sqrt{N!}} \sum_{P_N} P_N[|\alpha_1\rangle \times |\alpha_2\rangle .... \times |\alpha_N\rangle]$$

Start with $|\psi\rangle = |\alpha_1\rangle \times |\alpha_2\rangle .... \times |\alpha_N\rangle$

Take all permutations (P_N) of the particle no. index and add the states and normalize.

State symmetric under exchange of any 2 particles.

For Fermions:

$$|\psi_F\rangle = \frac{1}{\sqrt{N!}} \sum_{P_N} (-1)^{P_N} P_N[|\alpha_1\rangle \times |\alpha_2\rangle .... \times |\alpha_N\rangle]$$

Start with $|\psi\rangle = |\alpha_1\rangle \times |\alpha_2\rangle .... \times |\alpha_N\rangle$

Take all permutations (P_N) of the particle no. index and add the states with the sign of the permutation used to obtain it. Normalize.

State antisymmetric under exchange of any 2 particles.

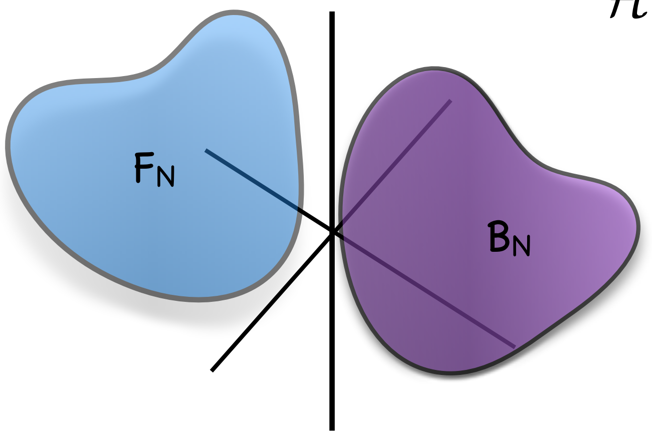
1,2,3..... N —> ∞

$\zeta = \pm 1$ for Bosons(Fermions)

Combined Notation: $$|\psi_{B(F)}\rangle = \frac{1}{\sqrt{N!}} \sum_{P_N} (\zeta)^{P_N} P_N [|\alpha_1\rangle \times |\alpha_2\rangle .... \times |\alpha_N\rangle]$$

Actual N particle Hilbert space is a subspace of the tensor product space

$$\mathcal{H}_N = \mathcal{H} \otimes \mathcal{H} \otimes .... \otimes \mathcal{H}$$ ⟶ Single Particle Hilbert Space



Need to Project onto the subspace of states which are completely (anti) symmetric w.r.t. exchange of particles to get the Hilbert space for N identical Bosons (Fermions)

$$\mathcal{B}_N = \mathcal{P}_B \mathcal{H}_N \qquad \mathcal{F}_N = \mathcal{P}_F \mathcal{H}_N$$

$$\mathcal{P}_{B(F)} |\alpha_1\rangle \times |\alpha_2\rangle .... \times |\alpha_N\rangle = \frac{1}{N!} \sum_{P_N} (\zeta)^{P_N} P_N [|\alpha_1\rangle \times |\alpha_2\rangle .... \times |\alpha_N\rangle]$$

Note: different normalization to make P a projection operator , $P^2 = P$

$$|\alpha_1, \alpha_2, ...\alpha_N\} = \sqrt{N!} \mathcal{P}_{B(F)} |\alpha_1, ...\alpha_n\rangle$$

If $|\alpha_1, ...\alpha_n\rangle$ is a complete basis set in $\mathcal{H}_N$, $|\alpha_1, \alpha_2, ...\alpha_N\}$ is a complete basis set in $\mathcal{B}_N(\mathcal{F}_N)$

Wavefunctions for Identical particles: 1,2,3..... ∞

We have constructed a basis set in the appropriate (anti)symmetric subspace of states

We can work with the tensor product basis and put the (anti)symmetry constraints on expansion co-efficients (wavefn.s)

Wavefunctions, Permanents and Determinants:

What is the wfn. of our (anti)symmetrized basis states in the original tensor product basis?

$$\langle \beta_1, ...\beta_N | \alpha_1, ...\alpha_N \rangle = \frac{1}{\sqrt{N! \prod_\alpha n_\alpha !}} S(\langle \beta_i | \alpha_j \rangle)$$

$$M_{ij} = \langle \beta_i | \alpha_j \rangle$$ is a matrix

$$S(M) = Perm(M)$$ for Bosons

$$S(M) = Det(M)$$ for Fermions

Using co-ord. basis for β and some single particle basis for α (say HO states) ,the wfn

$$\psi^{\{\alpha_i\}}(x_1, ...x_N) = \frac{1}{\sqrt{N! \prod_\alpha n_\alpha !}} S[\phi^{\alpha_i}(x_j)]$$

For Fermions, the Determinants are called Slater Determinants

Wavefunctions for Identical Bosons and Fermions

Example with 3 Bosons and Harmonic oscillator states:

A state where 1 boson occupies each of the states n=0,1,2

$$\psi_B(x_1, x_2, x_3) = \frac{1}{\sqrt{3!}} \text{Perm} \begin{pmatrix} \phi^0(x_1) & \phi^0(x_2) & \phi^0(x_3) \\ \phi^1(x_1) & \phi^1(x_2) & \phi^1(x_3) \\ \phi^2(x_1) & \phi^2(x_2) & \phi^2(x_3) \end{pmatrix}$$

A state where 2 bosons occupies n=0, and the third one is in n=1

$$\psi_B(x_1, x_2, x_3) = \frac{1}{\sqrt{3!2!}} \text{Perm} \begin{pmatrix} \phi^0(x_1) & \phi^0(x_2) & \phi^0(x_3) \\ \phi^0(x_1) & \phi^0(x_2) & \phi^0(x_3) \\ \phi^1(x_1) & \phi^1(x_2) & \phi^1(x_3) \end{pmatrix}$$

Example with 3 Fermions and Harmonic oscillator states:

A state where 1 fermion occupies each of the states n=0,1,2

$$\psi_F(x_1, x_2, x_3) = \frac{1}{\sqrt{3!}} \text{Det} \begin{pmatrix} \phi^0(x_1) & \phi^0(x_2) & \phi^0(x_3) \\ \phi^1(x_1) & \phi^1(x_2) & \phi^1(x_3) \\ \phi^2(x_1) & \phi^2(x_2) & \phi^2(x_3) \end{pmatrix}$$

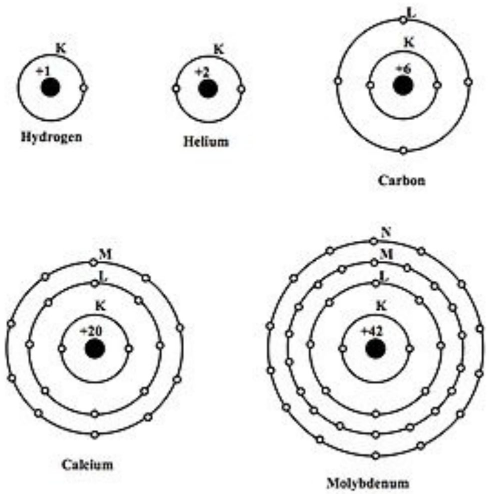
Is there a way around (some other basis), where the (anti)symmetrization is automatically taken care of and we do not have to deal with these cumbersome objects?

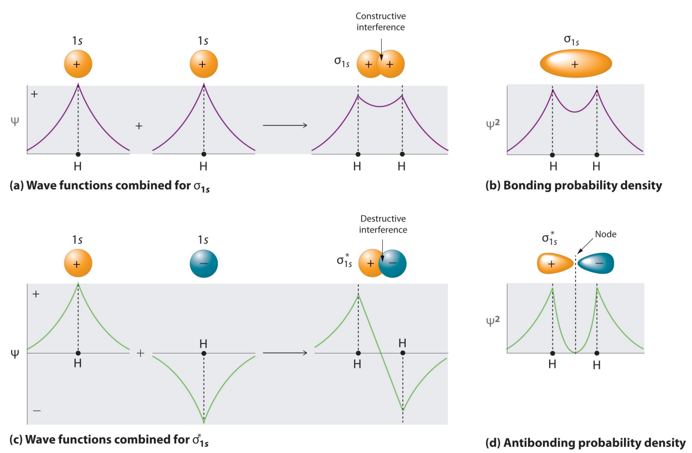
Fermions and Pauli Exclusion Principle

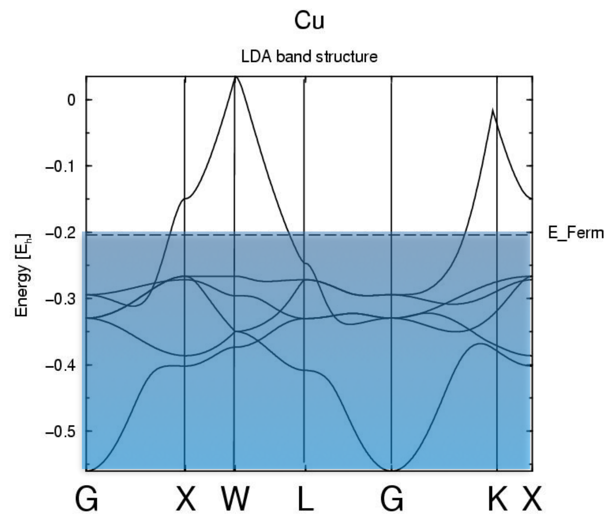
$$|\psi_{B(F)}\rangle = \frac{1}{\sqrt{N!}} \sum_{P_N} (\zeta)^{P_N} P_N [|\alpha_1\rangle \times |\alpha_2\rangle .... \times |\alpha_N\rangle]$$

For Bosons, the list $|\alpha_1>$, $|\alpha_2>$, $|\alpha_3>$,.... $|\alpha_N>$ can have repetitions, i.e. same SP state can appear many times. Many Bosons can occupy the same SP quantum state.

For Fermions, the list $|\alpha_1>$, $|\alpha_2>$, $|\alpha_3>$,.... $|\alpha_N>$ CANNOT have repetitions (due to antisymmetry)
2 Fermions cannot occupy the same SP quantum state —— Pauli Exclusion Principle







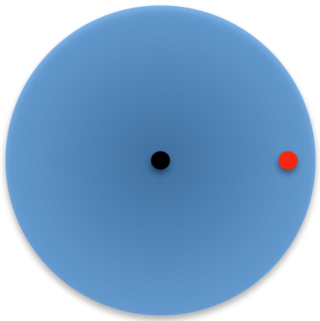
Fermions make atomic physics, chemistry and solid state physics so diverse

Atoms

The Basic Hamiltonian for electrons:

$$H = \sum_i \frac{p_i^2}{2m} - Ze^2 \sum_i \frac{1}{r_i} + \xi \sum_i \vec{L}_i \cdot \vec{S}_i + \sum_{ij}{}' \frac{e^2}{|r_i - r_j|}$$

Coulomb pot. of nucleus   Spin Orbit coupling   e-e repulsion



Part of e-e interaction can be absorbed into an effective screened potential from the nucleus

$$H = \sum_i \frac{p_i^2}{2m} - Ze^2 \sum_i \frac{1}{r_i} + \sum_i U(r_i) + \xi \sum_i \vec{L}_i \cdot \vec{S}_i + \sum_{ij}{}' \frac{e^2}{|r_i - r_j|} - \sum_{ij} U(r_i)\delta_{ij}$$

Screened Coulomb pot. Spin Orbit coupling   e-e repulsion

Hydrogen atom : No e-e interaction, no screening

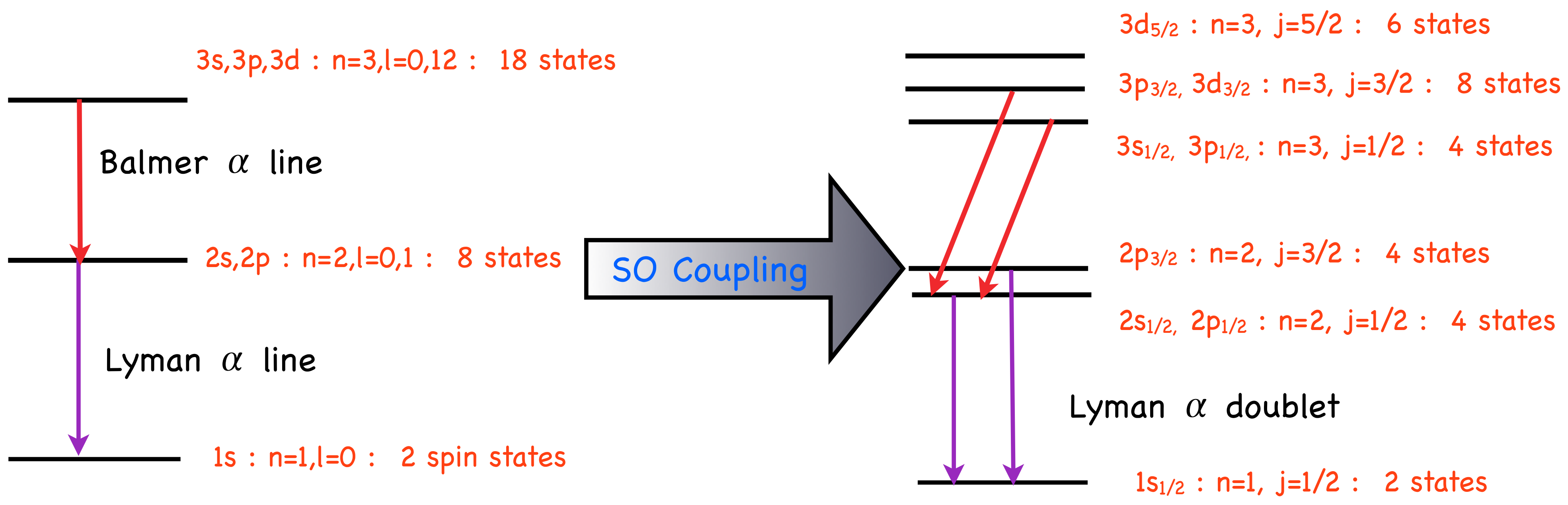
Fine Structure of Atomic Levels (H Atom)

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 $2p_{1/2}$ 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

Multi-Electron Atoms

$$H = \sum_i \frac{p_i^2}{2m} - Ze^2 \sum_i \frac{1}{r_i} + \sum_i U(r_i) + \xi \sum_i \vec{L}_i \cdot \vec{S}_i + \sum_{ij}{}' \frac{e^2}{|r_i - r_j|} - \sum_{ij} U(r_i)\delta_{ij}$$

Start with screened Coulomb potential : degeneracy of l levels are lifted

(n,l) levels are filled according to Pauli exclusion principle starting from lowest one

Stable electronic shells corresponding to filled orbitals.

What happens to atoms which have partially filled levels?

Think about electrons in the partially filled level only

Consider Carbon atom: 6 electrons

$1s^2\ 2s^2\ 2p^2$

n= 1, l=0 level will have 2 e with spin $\uparrow$ and $\downarrow$

n= 2, l=0 level will have 2 e with spin $\uparrow$ and $\downarrow$

n= 2, l=1 level will have 2 e

Which l orbitals would be occupied and what is the spin config of the 2p electrons?

Each electron can occupy 3 X 2 =6 states, so there are 36 states in all