

Advanced Quantum Mechanics

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Lecture #8

Symmetries and Quantum Mechanics

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

The Many-Particle Hilbert Space

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

1 particle QM: use $|q\rangle$ or $|p\rangle$ 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.

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

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

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

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

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

The Many-Particle Hilbert Space

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

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

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 1st particle at x....
- So $|\alpha\rangle$ and $|\beta\rangle$ should be the same state (upto a phase)
- Using the tensor product basis thus overcounts the states

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, $|\alpha\rangle$ and $|\beta\rangle$ $|\alpha\rangle|\beta\rangle \longrightarrow e^{i\phi}|\beta\rangle|\alpha\rangle$

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

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

Since $P_{12}^2 = I$

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

S₂: 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: $\frac{1}{\sqrt{2}}[|\alpha\rangle_1|\beta\rangle_2 + |\beta\rangle_1|\alpha\rangle_2]$

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

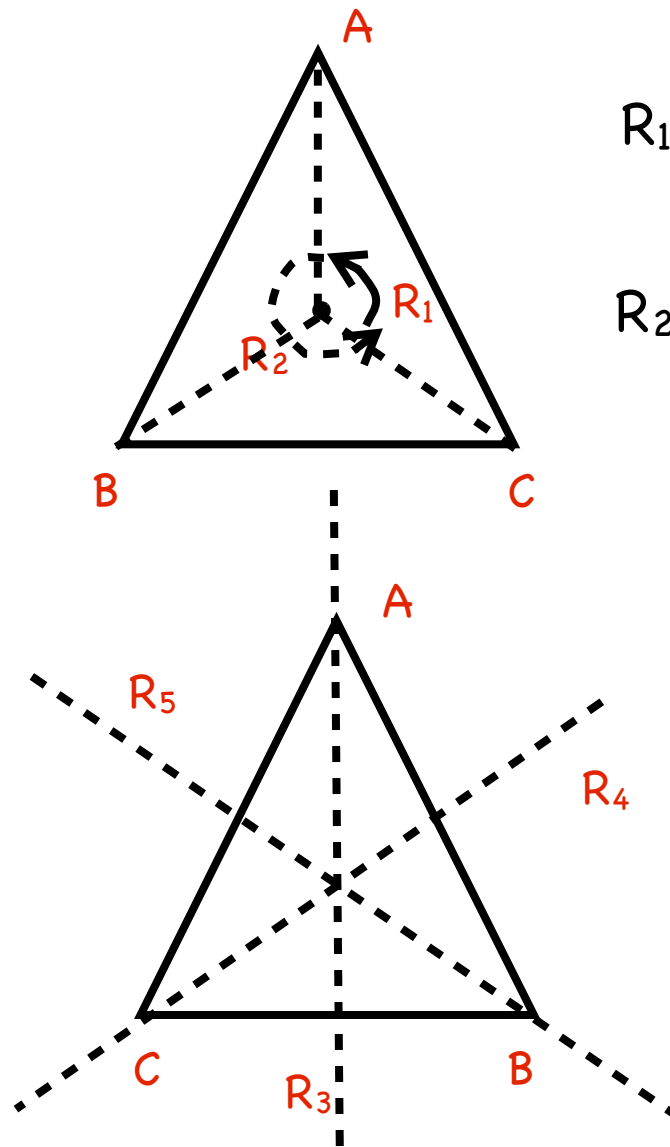
3 Identical Particles

Permutations of 3 objects : S_3

S_3 is isomorphic to D_3

	$\{E\}$	$\{R_1, R_2\}$	$\{R_3, R_4, R_5\}$
$T^{(1)}$	1	1	1
$T^{(2)}$	1	1	-1
$T^{(3)}$	2	-1	0

S_3 is non-Abelian and has a 2d irrep



$$R_1: A \rightarrow B, B \rightarrow C, C \rightarrow A$$

$$R_2: A \rightarrow C, B \rightarrow A, C \rightarrow B$$

$$R_3: A \rightarrow A, B \rightarrow C, C \rightarrow B$$

$$R_4: A \rightarrow B, B \rightarrow A, C \rightarrow C$$

$$R_5: A \rightarrow C, B \rightarrow B, C \rightarrow A$$

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

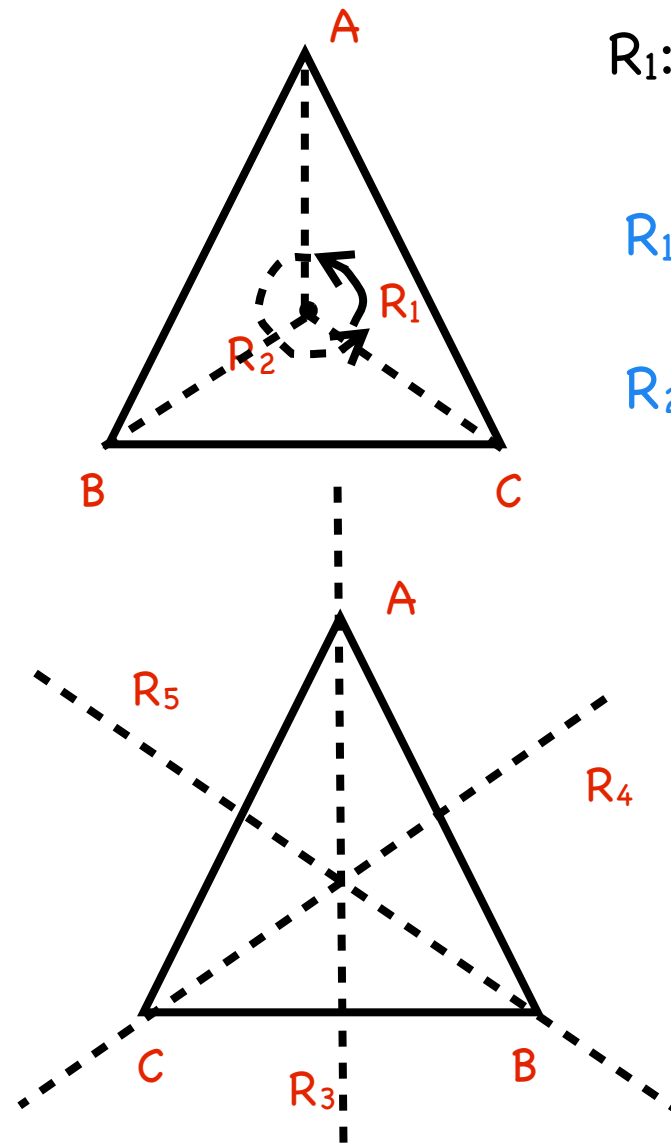
$$|\psi_3^B\rangle = \frac{1}{\sqrt{3!}} [|x\rangle_1 \otimes |y\rangle_2 \otimes |z\rangle_3 + |x\rangle_1 \otimes |z\rangle_2 \otimes |y\rangle_3 + |y\rangle_1 \otimes |x\rangle_2 \otimes |z\rangle_3 + |y\rangle_1 \otimes |z\rangle_2 \otimes |x\rangle_3 + |z\rangle_1 \otimes |x\rangle_2 \otimes |y\rangle_3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

3 Identical Particles

Permutations of 3 objects : S_3

S_3 is isomorphic to D_3

	$\{E\}$	$\{R_1, R_2\}$	$\{R_3, R_4, R_5\}$
$T^{(1)}$	1	1	1
$T^{(2)}$	1	1	-1
$T^{(3)}$	2	-1	0



$$R_1: A \rightarrow B, B \rightarrow C, C \rightarrow A$$

$$R_1: A \leftrightarrow B, \text{ then } B \leftrightarrow C$$

$$R_2: A \leftrightarrow C, \text{ then } B \leftrightarrow A$$

$$R_3: A \rightarrow A, B \rightarrow C, C \rightarrow B$$

$$R_3: B \leftrightarrow C$$

$$R_4: A \leftrightarrow B$$

$$R_5: A \leftrightarrow C$$

$T^{(2)}$ 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.

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

1,2,3..... N $\longrightarrow$ ∞

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 $|\alpha_1\rangle, |\alpha_2\rangle, |\alpha_3\rangle, \dots, |\alpha_N\rangle$

For Bosons:

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

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

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:

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

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

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.

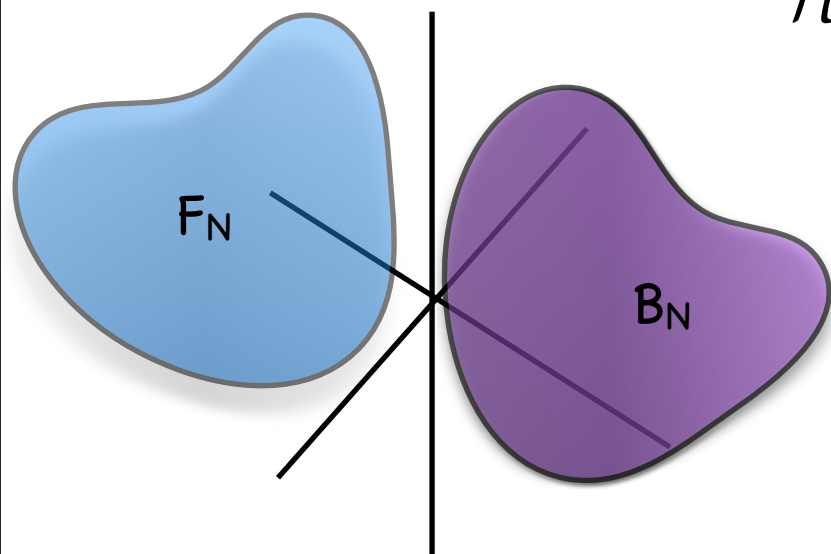
1,2,3..... N $\longrightarrow$ ∞

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

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

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

$$\mathcal{H}_N = \mathcal{H} \otimes \mathcal{H} \otimes \dots \otimes \mathcal{H} \longrightarrow \text{Single Particle Hilbert Space}$$



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)

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

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

Note: different normalization to make $\mathcal{P}$ a projection operator, $\mathcal{P}^2 = \mathcal{P}$

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

If $|\alpha_1, \dots, \alpha_n\rangle$ is a complete basis set in $\mathcal{H}_N$, $|\alpha_1, \alpha_2, \dots, \alpha_N\rangle$ 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?

$$\langle \beta_1, \dots, \beta_N | \alpha_1, \dots, \alpha_N \rangle = \frac{1}{\sqrt{N! \prod_{\alpha} n_{\alpha}!}} S(\langle \beta_i | \alpha_j \rangle) \quad M_{ij} = \langle \beta_i | \alpha_j \rangle \quad \text{is a matrix}$$

$$S(M) = \text{Perm}(M) \quad \text{for Bosons} \quad S(M) = \text{Det}(M) \quad \text{for Fermions}$$

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

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

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 $n=0,1,2$

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

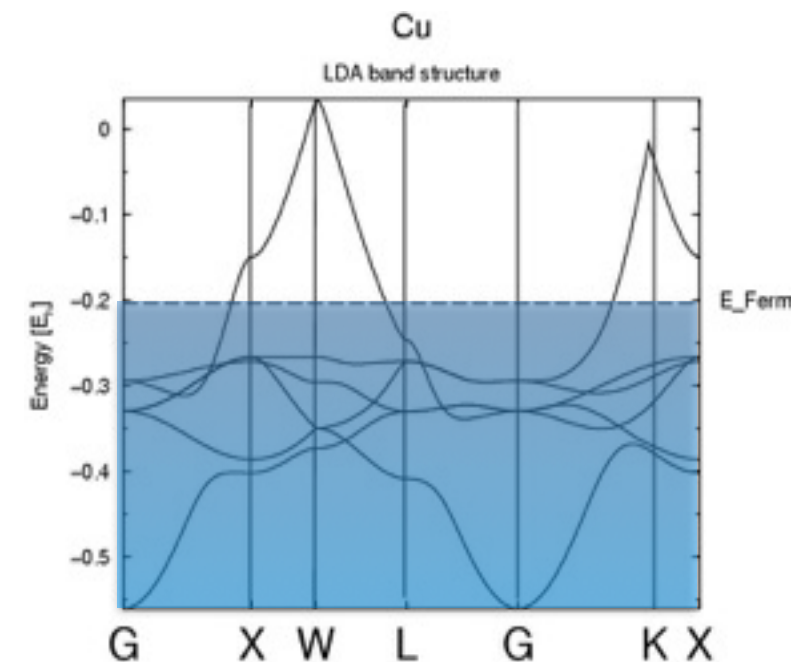
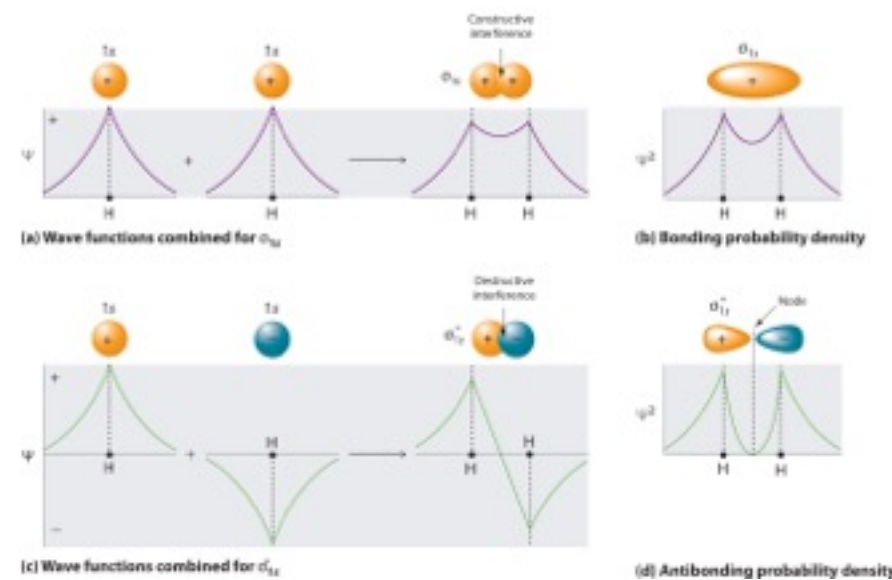
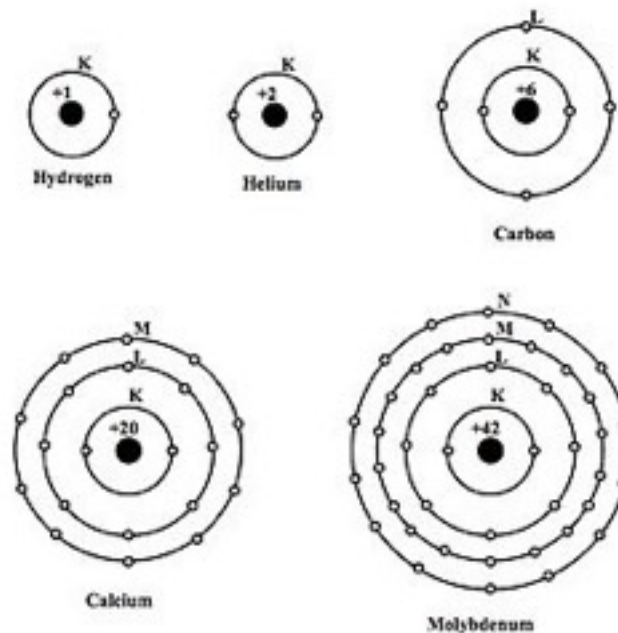
Is there a way around (some other basis), where the (anti)symmetrization is automatically taken care of and we do not have to deal with these cumbersome objects?

Fermions and Pauli Exclusion Principle

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

For Bosons, the list $|\alpha_1\rangle, |\alpha_2\rangle, |\alpha_3\rangle, \dots, |\alpha_N\rangle$ 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 $|\alpha_1\rangle, |\alpha_2\rangle, |\alpha_3\rangle, \dots, |\alpha_N\rangle$ **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

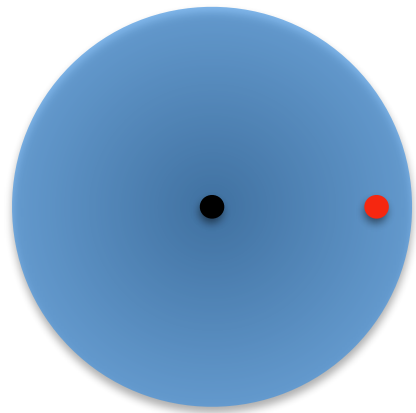
The Basic Hamiltonian for electrons:

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

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)

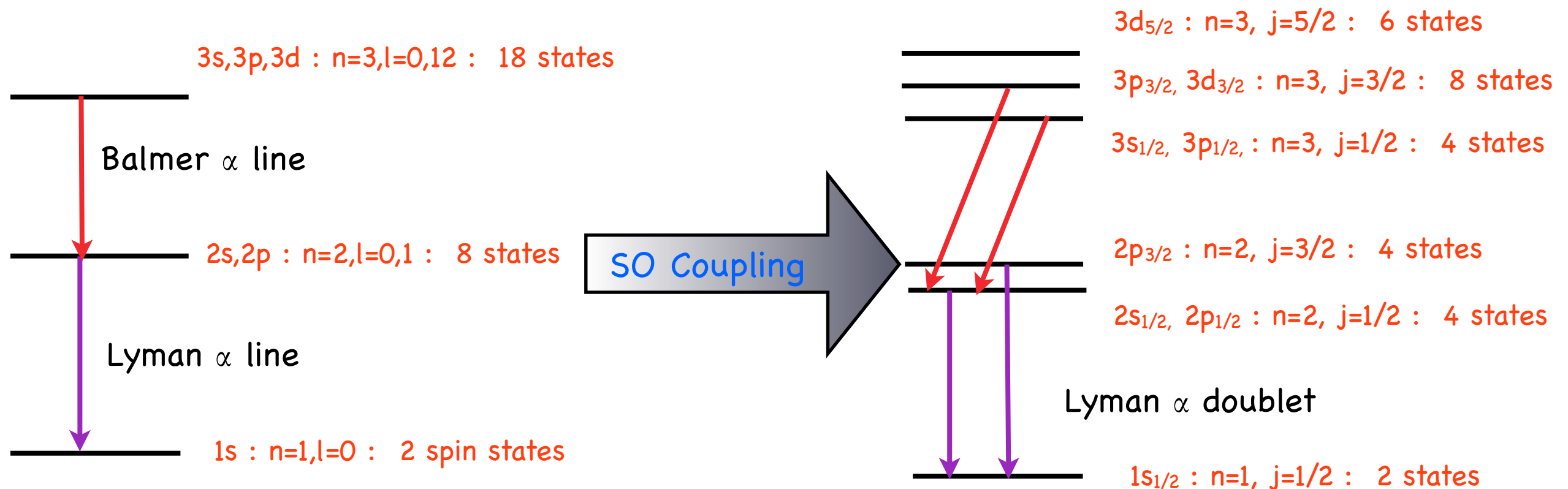
The Coulomb problem has a large symmetry group [$O(4)$ for the spatial part]

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

Total Degeneracy $2n^2$

- Each n level has n fold l degeneracy of $l=0,1,\dots,n-1$ (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

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

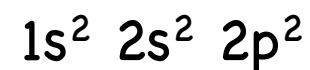
Start with screened Coulomb potential : degeneracy of l levels are lifted

(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 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 $3 \times 2 = 6$ states, so there are 36 states in all

Multi-Electron Atoms

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

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

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The Case of Carbon

The wavefunction of two non-interacting atoms occupying state m and n (given by both L_z and S_z)

$$\psi_F(x_1, x_2) = \begin{pmatrix} \phi_m(x_1) & \phi_m(x_2) \\ \phi_n(x_1) & \phi_n(x_2) \end{pmatrix}$$

The Slater determinant implies that there are actually 15 states consistent with Fermi statistics

You simply choose 2 out of the 6 states, making sure that they are different.

What are the quantum numbers of these 15 states?

If SO coupling is neglected, spin and orbital part can be treated separately

$$\psi_F(x_1, x_2) = \chi(s_1, s_2)\phi(x_1, x_2)$$

Spin states of 2 spin 1/2 particles : $S = S_1 + S_2$

Triplet States

$$|1/2, 1/2\rangle = \frac{1}{\sqrt{2}}(|1/2, -1/2\rangle + |-1/2, 1/2\rangle) \quad |-1/2, -1/2\rangle$$

Symmetric under exchange

Singlet States

$$\frac{1}{\sqrt{2}}(|1/2, -1/2\rangle - |-1/2, 1/2\rangle)$$

Anti-symmetric under exchange

The Case of Carbon

Orbital states of 2 $l=1$ particles $L=L_1+L_2$ (Eigenstates of total angular momentum)

$L=2, 1, 0$ states Consider $L=L_1+L_2$, where L_1 and L_2 transform according to the l irrep

States with $L=2l$ are symmetric under exchange of 2 particles

$$|2l, 2l\rangle = |l\rangle|l\rangle \quad \text{is symmetric under } 1 \rightleftharpoons 2$$

$$|j, m\rangle \quad |m_1, m_2\rangle \quad |j=2l, m\rangle \text{ is obtained from } |j=2l, m=2l\rangle \text{ by acting with } L^- = L_1^- + L_2^-$$

Since L^- is symmetric under $1 \rightleftharpoons 2$, $|j=2l, m\rangle$ is symmetric under $1 \rightleftharpoons 2$

States with $L=2l-1$ are anti symmetric under exchange of 2 particles

$$\begin{aligned} |2l-1, 2l-1\rangle &= a|l-1\rangle|l\rangle + b|l\rangle|l-1\rangle \\ &= [ac_l L_1^{-1} + bc_l L_2^-] |l\rangle|l\rangle = c_l \left[\frac{a+b}{2} (L_1^{-1} + L_2^-) + \frac{a-b}{2} (L_1^{-1} - L_2^-) \right] |l\rangle|l\rangle \\ &= c_l \frac{(a+b)}{2} |2l, 2l-1\rangle + c_l \frac{(a-b)}{2} (L_1^{-1} - L_2^-) |l\rangle|l\rangle \end{aligned}$$

$$\text{Since } \langle 2l, 2l-1 | 2l-1, 2l-1 \rangle = 0, \quad a = -b \longrightarrow |2l-1, 2l-1\rangle = ac_l (L_1^{-1} - L_2^-) |l\rangle|l\rangle$$

$|j=2l-1, m\rangle$ is obtained from $|j=2l-1, m=2l-1\rangle$ by acting with $L^- = L_1^- + L_2^- \longrightarrow$ Antisymmetric

The Case of Carbon

Similarly $|2l-2, 2l-2\rangle$ can be written in terms of $|l, l\rangle$ and same orthogonality arguments show it to be symmetric under $1 \rightleftharpoons 2$

Thus $2l$, $2l-2$, $2l-4$ etc are symmetric under exchange, while $2l-1$, $2l-3$ etc are antisymmetric

For half-integer valued l , $2l$ is odd, so odd irreps are symmetric while even irreps are antisymmetric

$S=1$ is symmetric, $S=0$ is antisymmetric

For integer valued l , $2l$ is even, so even irreps are symmetric while odd irreps are antisymmetric

$L=2, 0$ is symmetric, $L=1$ is antisymmetric

Since the wavefn (orbital + spin part) needs to be antisymmetric, possible combinations are

$L=0 \ S=0 \longrightarrow {}^1s$ $L=2 \ S=0 \longrightarrow {}^1d$ $L=1 \ S=1 \longrightarrow {}^3p$ ${}^{2S+1}L$ Spectroscopic terms

9 states

$L=1 \ S=1 \longrightarrow {}^3p$

1 state

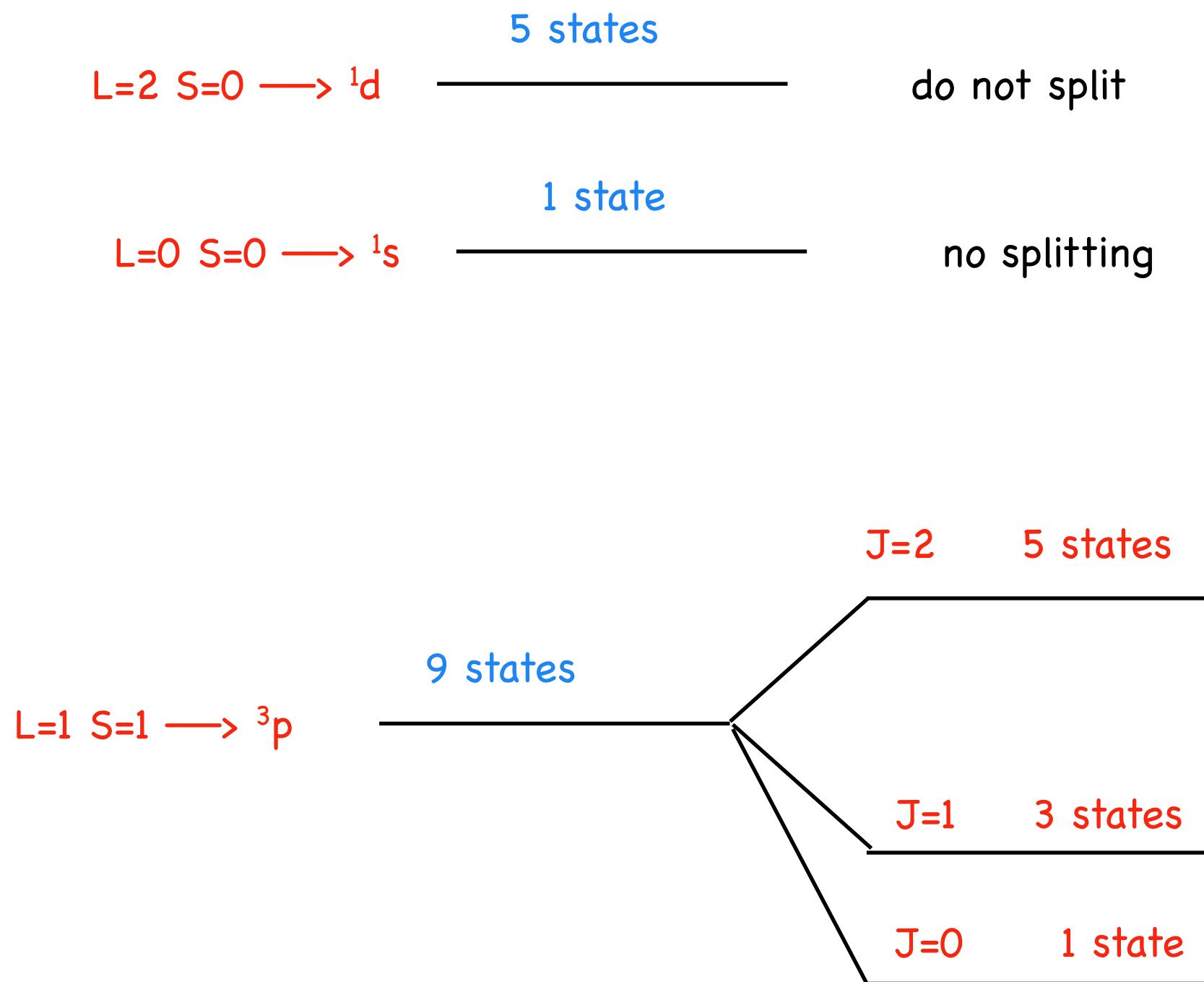
$L=0 \ S=0 \longrightarrow {}^1s$

5 states

$L=2 \ S=0 \longrightarrow {}^1d$

The Case of Carbon: Spin Orbit Coupling

Splitting of the terms



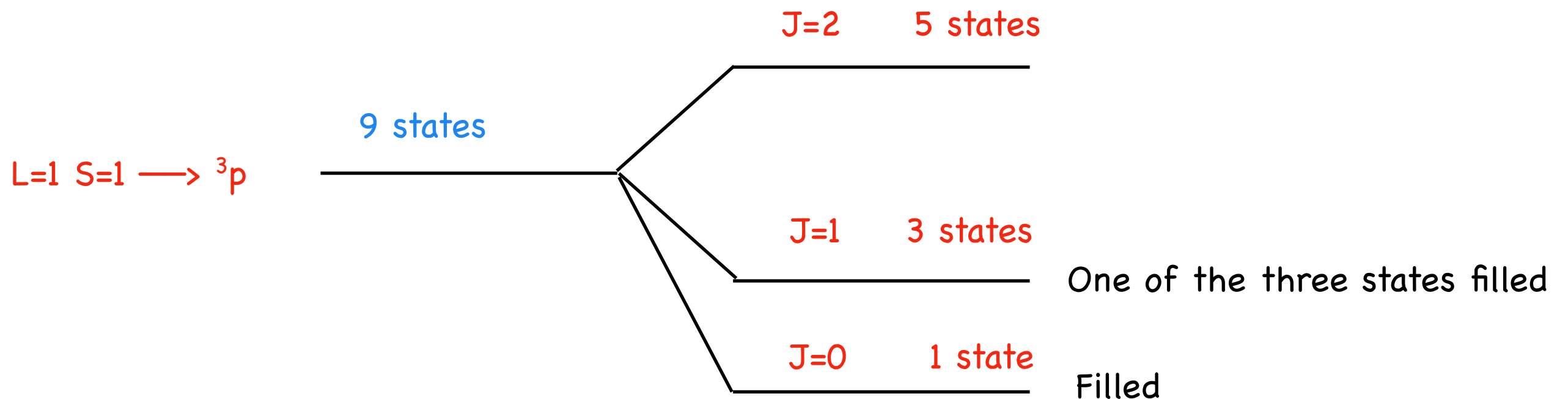
The Case of Carbon: Hund's Rule

Hund's Rule: State with largest multiplicity (largest spin) makes atoms more stable (lower energy)

In Antisymmetric orbital wavefunctions, the probability of two electrons occupying same pos. is 0

Electrons interact with repulsive Coulomb repulsion $\sim 1/r$. They can minimize this energy by staying as far apart, subject to other constraints (read other contribution to energy). So, anti-symmetric orbital wavefunctions and hence symmetric spin wfn.s are preferred. For 2 electrons $S=1$, $L=1$ would be preferred from Hund's coupling

Effective active degree of freedom : $L=1, S=1$ object



The Case of Nitrogen: 3 valence Electron

One can extend similar analysis to 3 valence electrons (N has 7 electrons $1s^2 2s^2 2p^3$)

The permutation symmetry group is S_3

Note that the full wfn (spin + orbital part) should transform according to $T^{(a)}$, but the orbital and the spin parts can individually transform according to any irrep including $T^{(m)}$ which is a mixed irrep (neither symmetric nor antisymmetric)

	$\{E\}$	$\{R_1, R_2\}$	$\{R_3, R_4, R_5\}$
$T^{(s)}$	1	1	1
$T^{(a)}$	1	1	-1
$T^{(m)}$	2	-1	0

S_3 is non-Abelian and has a 2d irrep

$T^{(a)}$ occurs in the reduction of $T^{(a)} \times T^{(s)}$

$$T^{(s)} \times T^{(a)}$$

So, any of these are possibilities

$$T^{(m)} \times T^{(m)}$$

Note, in the last case the two irreps correspond to orbital and spin states, so no symmetrization is required

Details to be worked out in HW

Time Reversal Symmetry



Can you tell me if the video is running forward or backward?

If you cannot the motion is time-reversal symmetric



More precisely, if the reversed motion is a valid motion of the system, the system has TR invariance

If you deduced the laws of motion from the forward and the reversed video, would you get the same laws of motion?

TR for Classical Hamiltonian System

$$H = H(\vec{x}, \vec{p}) \quad \dot{x} = \frac{\partial H}{\partial p} \quad \dot{p} = -\frac{\partial H}{\partial x}$$

Under TR $\vec{x} \rightarrow \vec{x}, \quad \vec{p} \rightarrow -\vec{p}, \quad t \rightarrow -t$ **Note that this is not a canonical transformation**

If $H(\vec{x}, \vec{p}) = H(\vec{x}, -\vec{p})$ Eqn. of motion is TR invariant

Eg: $H(x, p) = \frac{p^2}{2m} + V(x)$ Eqn. of motion is TR invariant

$$H(x, p) = \frac{(p - eA)^2}{2m} + V(x)$$

Eqn. of motion is not TR invariant for fixed A. If you consider source of A and apply TR transformation on them as well, A will change sign and EOM will be TR invariant.

Problem: A pendulum is given just enough velocity when it is in vertically downward position, so that it comes to rest at the vertically upward position. Find the time taken to reach this position.

If the time was finite, TR invariance would mean that the pendulum can start with 0 velocity in the upward position and come down. Do you think that is a valid motion?

TR for QM

Start with defn. from CM Under TR $\vec{x} \rightarrow \vec{x}, \quad \vec{p} \rightarrow -\vec{p}, \quad t \rightarrow -t$

QM equivalent: $\hat{x}' = \mathcal{T} \hat{x} \mathcal{T}^{-1} = \hat{x}$ $\hat{p}' = \mathcal{T} \hat{p} \mathcal{T}^{-1} = -\hat{p}$

Does not preserve $[\hat{x}, \hat{p}] = i$ Not a canonical transformation

TR is an anti-unitary operator (takes i to $-i$ and solves above problem)

$$\mathcal{T} = UK$$

Unitary Operator

Complex conjugation

$$\mathcal{T} \hat{O} \mathcal{T}^{-1} = UK \hat{O} K U^\dagger = U \hat{O}^* U^\dagger$$

$$\mathcal{T} c \mathcal{T}^{-1} = c^*$$

TR is an anti-linear operator $\mathcal{T}(\alpha|\psi_1\rangle + \beta|\psi_2\rangle) = \alpha^* \mathcal{T}|\psi_1\rangle + \beta^* \mathcal{T}|\psi_2\rangle$

Action of TR on a state: Choose a basis and expand, apply cc to co-eff, then apply unitary operator on the state.

Under TR, inner product of quantum states is not conserved

$$\mathcal{T}|\psi_1\rangle = U|\psi_1^*\rangle \quad \mathcal{T}|\psi_2\rangle = U|\psi_2^*\rangle \quad \langle \mathcal{T}\psi_1 | \mathcal{T}\psi_2 \rangle = \langle \psi_1^* | U^\dagger U | \psi_2^* \rangle = (\langle \psi_1 | \psi_2 \rangle)^*$$

Representations of TR

TR looks like a Z_2 symmetry, but is $T^2 = 1$?

One dimensional representation $\mathcal{T}|\psi\rangle = e^{i\theta}|\psi\rangle$

$$\mathcal{T}^2|\psi\rangle = \mathcal{T}e^{i\theta}|\psi\rangle = e^{-i\theta}\mathcal{T}|\psi\rangle = |\psi\rangle \quad \mathcal{T}^2 = 1$$

QM: states are same upto a phase

$$|\psi'\rangle = e^{i\alpha}|\psi\rangle \quad \mathcal{T}|\psi'\rangle = e^{-i\alpha}e^{i\theta}|\psi\rangle$$

α is a choice which can be used to get rid of θ . There is thus 1 1-d representation of T

Representations of TR

2D representation and spin 1/2

Spin, being angular momentum, should change sign under TR.

$$\mathcal{T}\sigma_x\mathcal{T}^{-1} = -\sigma_x \quad \mathcal{T}\sigma_y\mathcal{T}^{-1} = -\sigma_y \quad \mathcal{T}\sigma_z\mathcal{T}^{-1} = -\sigma_z$$

Use $\mathcal{T} = UK$ and $K\sigma_x K = \sigma_x \quad K\sigma_y K = -\sigma_y \quad K\sigma_z K = \sigma_z$

$$U\sigma_x U^\dagger = -\sigma_x \quad U\sigma_y U^\dagger = \sigma_y \quad U\sigma_z U^\dagger = -\sigma_z$$

The matrix $e^{i\phi}\sigma_y$ would do the job. It is the only matrix which will do it — show !!

φ is arbitrary, choose $\varphi=\pi/2$ to make U real $U = i\sigma_y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \mathcal{T} = i\sigma_y K$

$$\mathcal{T}^2 = i\sigma_y K (i\sigma_y) K = i(-i)\sigma_y(-\sigma_y)K^2 = -1$$

Projective representation — upto a - sign saw similar situation for the spin 1/2 representation of rotation group.

Nature (Fermions) are not classical, get used to it !!

$T^2 = -1$ and Kramer's degeneracy

In a TR invariant system, if $T^2 = -1$, all energy eigenstates must be doubly degenerate

It is clear that for a TR invariant system, if $H|\Psi\rangle = E|\Psi\rangle$, $H T|\Psi\rangle = E T|\Psi\rangle$

However, one needs to show that $|\Psi\rangle$ and $T|\Psi\rangle$ are different states for this to count as a degeneracy of eigenstates.

Assume that $|\Psi\rangle$ and $T|\Psi\rangle$ are the same state, i.e. $\mathcal{T}|\psi\rangle = e^{i\theta}|\psi\rangle$

$$\text{Then } \mathcal{T}^2|\psi\rangle = \mathcal{T}e^{i\theta}|\psi\rangle = e^{-i\theta}\mathcal{T}|\psi\rangle = |\psi\rangle \quad \mathcal{T}^2 = 1$$

This contradicts our assumption that $T^2 = -1$

So, for $T^2 = -1$ $\mathcal{T}|\psi\rangle \neq e^{i\theta}|\psi\rangle$ and this proves Kramer's degeneracy theorem

E.g.: True for : single electron, odd no of electrons, odd no of Fermions in general