

Today in Physics 237: state-vector symmetry, molecules, and atoms

- The exchange operator
- Molecular hydrogen's rotation and two-proton spin states
- H_2 's and helium's two-electron states
- Multi-electron atoms
 - L-S coupling
 - The periodic table

Periodic table of elements. Chlorine (Cl) is highlighted in yellow. Labels for Chlorine: Atomic Number 17, Name Chlorine, Symbol Cl, Chemical Group / Family Halogen.

1	2											13	14	15	16	17	18									
1 H Hydrogen Nonmetal												5 B Boron Metalloid	6 C Carbon Nonmetal	7 N Nitrogen Nonmetal	8 O Oxygen Nonmetal	9 F Fluorine Halogen	10 Ne Neon Noble Gas									
3 Li Lithium Alkali Metal	4 Be Beryllium Alkaline Earth Metal																									
11 Na Sodium Alkali Metal	12 Mg Magnesium Alkaline Earth Metal																									
19 K Potassium Alkali Metal	20 Ca Calcium Alkaline Earth Metal	21 Sc Scandium Transition Metal	22 Ti Titanium Transition Metal	23 V Vanadium Transition Metal	24 Cr Chromium Transition Metal	25 Mn Manganese Transition Metal	26 Fe Iron Transition Metal	27 Co Cobalt Transition Metal	28 Ni Nickel Transition Metal	29 Cu Copper Transition Metal	30 Zn Zinc Transition Metal	31 Ga Gallium Post-Transition Me...	32 Ge Germanium Metalloid	33 As Arsenic Metalloid	34 Se Selenium Nonmetal	35 Br Bromine Halogen	36 Kr Krypton Noble Gas									
37 Rb Rubidium Alkali Metal	38 Sr Strontium Alkaline Earth Metal	39 Y Yttrium Transition Metal	40 Zr Zirconium Transition Metal	41 Nb Niobium Transition Metal	42 Mo Molybdenum Transition Metal	43 Tc Technetium Transition Metal	44 Ru Ruthenium Transition Metal	45 Rh Rhodium Transition Metal	46 Pd Palladium Transition Metal	47 Ag Silver Transition Metal	48 Cd Cadmium Transition Metal	49 In Indium Post-Transition Me...	50 Sn Tin Post-Transition Me...	51 Sb Antimony Metalloid	52 Te Tellurium Metalloid	53 I Iodine Halogen	54 Xe Xenon Noble Gas									
55 Cs Cesium Alkali Metal	56 Ba Barium Alkaline Earth Metal											72 Hf Hafnium Transition Metal	73 Ta Tantalum Transition Metal	74 W Tungsten Transition Metal	75 Re Rhenium Transition Metal	76 Os Osmium Transition Metal	77 Ir Iridium Transition Metal	78 Pt Platinum Transition Metal	79 Au Gold Transition Metal	80 Hg Mercury Transition Metal	81 Tl Thallium Post-Transition Me...	82 Pb Lead Post-Transition Me...	83 Bi Bismuth Post-Transition Me...	84 Po Polonium Metalloid	85 At Astatine Halogen	86 Rn Radon Noble Gas
87 Fr Francium Alkali Metal	88 Ra Radium Alkaline Earth Metal											104 Rf Rutherfordium Transition Metal	105 Db Dubnium Transition Metal	106 Sg Seaborgium Transition Metal	107 Bh Bohrium Transition Metal	108 Hs Hassium Transition Metal	109 Mt Meitnerium Transition Metal	110 Ds Darmstadtium Transition Metal	111 Rg Roentgenium Transition Metal	112 Cn Copernicium Transition Metal	113 Nh Nihonium Post-Transition Me...	114 Fl Flerovium Post-Transition Me...	115 Mc Moscovium Post-Transition Me...	116 Lv Livermorium Post-Transition Me...	117 Ts Tennessine Halogen	118 Og Oganesson Noble Gas
		57 La Lanthanum Lanthanide	58 Ce Cerium Lanthanide	59 Pr Praseodymium Lanthanide	60 Nd Neodymium Lanthanide	61 Pm Promethium Lanthanide	62 Sm Samarium Lanthanide	63 Eu Europium Lanthanide	64 Gd Gadolinium Lanthanide	65 Tb Terbium Lanthanide	66 Dy Dysprosium Lanthanide	67 Ho Holmium Lanthanide	68 Er Erbium Lanthanide	69 Tm Thulium Lanthanide	70 Yb Ytterbium Lanthanide	71 Lu Lutetium Lanthanide										
		89 Ac Actinium Actinide	90 Th Thorium Actinide	91 Pa Protactinium Actinide	92 U Uranium Actinide	93 Np Neptunium Actinide	94 Pu Plutonium Actinide	95 Am Americium Actinide	96 Cm Curium Actinide	97 Bk Berkelium Actinide	98 Cf Californium Actinide	99 Es Einsteinium Actinide	100 Fm Fermium Actinide	101 Md Mendelevium Actinide	102 No Nobelium Actinide	103 Lr Lawrencium Actinide										

Symmetrization and the exchange operator

- We need to define an operator which can act on a two-quantum state vector and swap the quanta: can move quantum a from \mathbf{r}_1 to \mathbf{r}_2 , and simultaneously quantum b from \mathbf{r}_2 to \mathbf{r}_1 , while treating them as identical quanta.
- I guess we'll call it P :

$$\hat{P}|1,2\rangle = |2,1\rangle \quad ; \quad \hat{P}^2|1,2\rangle = |1,2\rangle \quad .$$

- This operator therefore acts on the two-quantum states we introduced on [Lecture 22](#) page 3, like this:

$$\begin{aligned} \hat{P}\psi_{\pm}(\mathbf{r}_1, \mathbf{r}_2) &= \hat{P}A(\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) \pm \psi_b(\mathbf{r}_1)\psi_a(\mathbf{r}_2)) = A(\psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1) \pm \psi_b(\mathbf{r}_2)\psi_a(\mathbf{r}_1)) \\ &= \pm A(\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) \pm \psi_b(\mathbf{r}_1)\psi_a(\mathbf{r}_2)) = (\pm 1)\psi_{\pm}(\mathbf{r}_1, \mathbf{r}_2) \quad ; \end{aligned}$$

$\psi_{\pm}(\mathbf{r}_1, \mathbf{r}_2)$ are eigenstates of \hat{P} , with eigenvalues ± 1 respectively.

Symmetrization and the exchange operator (continued)

- The Hamiltonian ([Lecture 21](#), p. 13), which is $\hat{H} = -\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + V(\mathbf{r}_1, \mathbf{r}_2, t)$, perforce treats identical quanta at locations 1 and 2 indistinguishably: $m_1 = m_2$, $V(\mathbf{r}_1, \mathbf{r}_2, t) = V(\mathbf{r}_2, \mathbf{r}_1, t)$.

- So \hat{P} and \hat{H} are compatible:

$$E|2,1\rangle = E|1,2\rangle = \hat{H}|1,2\rangle = \hat{H}|2,1\rangle = \hat{H}\hat{P}|1,2\rangle$$

$$\Rightarrow [\hat{H}, \hat{P}]|\psi\rangle = \hat{H}\hat{P}|\psi\rangle - \hat{P}\hat{H}|\psi\rangle = E|\psi\rangle - E|\psi\rangle = 0.$$

- According to the generalized Ehrenfest theorem ([Lecture 11](#), p. 5), therefore,

$$\frac{d}{dt}\langle P \rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{P}] \rangle + \left\langle \frac{\partial}{\partial t} \hat{P} \right\rangle = 0;$$

- That is, if a system starts off in an eigenstate of \hat{P} , symmetric or antisymmetric, it stays that way forever.

The hydrogen molecules

Example: molecular hydrogen and symmetrization.

- Consider H_2 to be a rigid rotor. Find its time-independent angular momentum eigenstates ψ and eigenvalues $J\hbar$. Then determine the symmetry of these states: that is, evaluate $\hat{P}|\psi\rangle$.
- Similarly, noting the protons in H_2 to be noninteracting identical fermions, find the properly symmetrized spin eigenstates χ and their eigenvalues $s(s+1)\hbar^2$ and $m\hbar$, and evaluate $\hat{P}|\chi\rangle$.
- Combine these states into states of angular momentum *and* spin, $|\psi\chi\rangle$. Evaluate $\hat{P}|\psi\chi\rangle$, and show that the joint states violate Fermi statistics unless certain combinations of ψ and χ are ruled out. Specifically: show that states with **even** angular momentum quantum number J combine only with **antisymmetric** spin states, and those of **odd** J combine only with **symmetric** spin states. And thus show that H_2 could be two separate molecular species, which we call para- H_2 and ortho- H_2 , respectively.

This is the simplest practical system for combining two spins with an orbital angular momentum. It's simple because the protons in H_2 do not interact significantly by electromagnetic forces/torques.

The hydrogen molecules (continued)

- a. You got started on this example in G&S problem 4.27 on assignment 9. Recap: you considered a diatomic molecule to be a rigid rotor: two masses separated by a fixed distance r and having moment of inertia I about their center of mass. You took the classical expression of energy of a rigid rotor with angular momentum of magnitude J ,

$$H = \frac{1}{2}I\omega^2 = \frac{1}{2I}(I\omega)^2 = \frac{J^2}{2I} ,$$

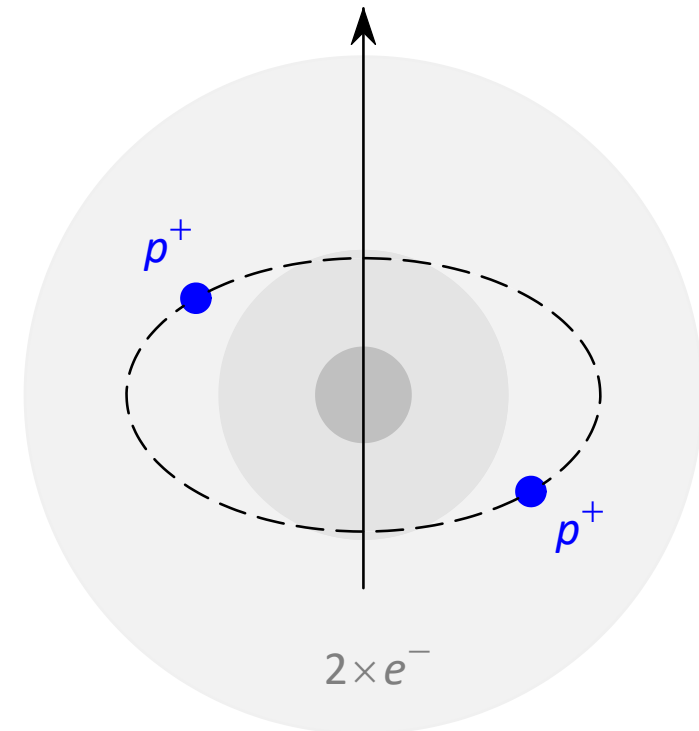
to correspond to the Hamiltonian, and found thereby that

$$\hat{H}\psi = \frac{1}{2I}\hat{j}^2 = E\psi = \frac{\hbar^2}{2I}J(J+1)\psi$$

$$\Rightarrow \boxed{\psi_{JM} = Y_J^M, \quad J=0,1,2,\dots \quad \text{and} \quad M=-J,-J+1,\dots,J} .$$

See also [Lecture 14](#).

- And thus the component \hat{j}_z has eigenvalues $J\hbar$.
- For H_2 , $I = m_H(r/2)^2$, with $r = 0.074$ nm.



The hydrogen molecules (continued)

- The angular momentum eigenfunctions are the spherical harmonics ([Lecture 14](#), pp. 8-12):

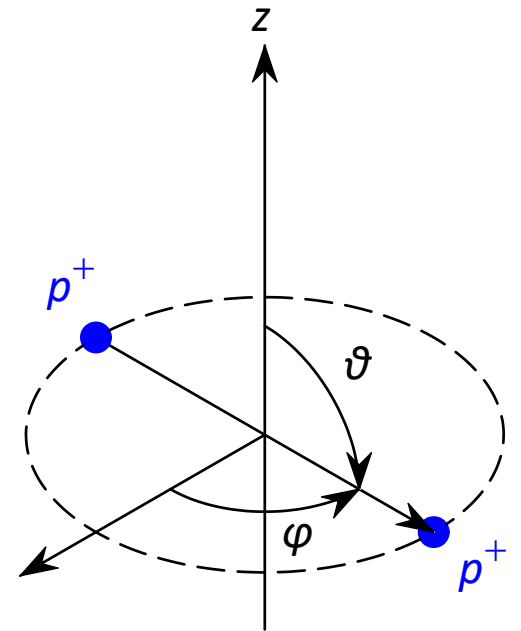
$$Y_J^M(\vartheta, \varphi) = \sqrt{\frac{2J+1}{4\pi} \frac{(J-M)!}{(J+M)!}} e^{iM\varphi} P_J^M(\cos\vartheta) \quad , \quad \text{where}$$

$$P_J^M(x) = \frac{(-1)^M (1-x^2)^{M/2}}{2^J J!} \left(\frac{d}{dx}\right)^M \left(\frac{d}{dx}\right)^J (x^2-1)^J \quad .$$

- In spherical coordinates: if one proton lies at $\mathbf{r}_1 = [r/2 \quad \vartheta \quad \varphi]$, the other lies at $\mathbf{r}_2 = [r/2 \quad \pi - \vartheta \quad \varphi + \pi]$.
- With $x = \cos\vartheta$: if one proton lies at x , the other lies at

$$\cos(\pi - \vartheta) = \cos\pi \cos\vartheta - \sin\pi \sin\vartheta = -\cos\vartheta = -x \quad \Rightarrow \quad \hat{P}|x, \varphi\rangle = |-x, \varphi + \pi\rangle \quad .$$

- And if $x \rightarrow -x$, then $\frac{d}{dx} \rightarrow \frac{d(-x)}{dx} \frac{d}{d(-x)} = -\frac{d}{d(-x)}$.



The hydrogen molecules (continued)

- This gives us

$$\begin{aligned}
 \hat{P}Y_J^M(x, \varphi) &= Y_J^M(-x, \varphi + \pi) = \sqrt{\frac{2J+1}{4\pi} \frac{(J-M)!}{(J+M)!}} e^{iM\varphi} [e^{iM\pi}] \frac{(-1)^M (1-[-x]^2)^{M/2}}{2^J J!} \left[\frac{d}{d(-x)} \right]^M \left[\frac{d}{d(-x)} \right]^J ([-x]^2 - 1)^J \\
 &= \sqrt{\frac{2J+1}{4\pi} \frac{(J-M)!}{(J+M)!}} e^{iM\varphi} [(-1)^M] \frac{(-1)^M (1-[x]^2)^{M/2}}{2^J J!} \left[(-1) \frac{d}{dx} \right]^M \left[(-1) \frac{d}{dx} \right]^J ([x]^2 - 1)^J \\
 &= [-1]^M [-1]^M [-1]^J \sqrt{\frac{2J+1}{4\pi} \frac{(J-M)!}{(J+M)!}} e^{iM\varphi} \frac{(-1)^M (1-x^2)^{M/2}}{2^J J!} \left(\frac{d}{dx} \right)^M \left(\frac{d}{dx} \right)^J (x^2 - 1)^J = (-1)^J Y_J^M(x, \varphi) .
 \end{aligned}$$

The hydrogen molecules (continued)

- b. Each proton has spin $\frac{1}{2}$, and (in good approximation) the spins don't exert forces or torques on each other, so the spin eigenstates are singlet and triplets, just like the pair of electrons considered in [Lecture 20](#), p. 4, so

$$\begin{aligned}
 |sm\rangle &= |11\rangle = |\uparrow\uparrow\rangle \\
 &= |10\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \quad \text{and} \quad |sm\rangle = |00\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \\
 &= |1-1\rangle = |\downarrow\downarrow\rangle \\
 \hat{P}|1m\rangle &= |1m\rangle = (-1)^{s+1}|1m\rangle \quad \hat{P}|00\rangle = -|00\rangle = (-1)^{s+1}|00\rangle .
 \end{aligned}$$

- for which

$$\begin{aligned}
 \hat{j}^2 |sm\rangle &= 2\hbar^2 |sm\rangle \text{ (triplet states) } , \quad = 0 \text{ (singlet state) } ; \\
 \hat{j}_z |sm\rangle &= \hbar m |sm\rangle \text{ (triplet states) } , \quad = 0 \text{ (singlet state) } .
 \end{aligned}$$

Here $s = 1$ and $m = 1, 0, -1$, for the triplet states.

The hydrogen molecules (continued)

c. So, for the complete state vector $|JMsm\rangle$,

$$\hat{P}|JMsm\rangle = (-1)^J (-1)^{s+1} |JMsm\rangle, \text{ and}$$

$= (-1)^J |JMsm\rangle$ because the nuclei being exchanged are identical fermions.

• So for

and for

$$\left. \begin{array}{l} s=0, \quad (-1)^J = 1 \Rightarrow J=2J' \\ s=1, \quad (-1)^J = -1 \Rightarrow J=2J'+1 \end{array} \right\} J' = 0, 1, 2, \dots$$

Even- J states have to be spin singlets (para- H_2) and odd- J states have to be spin triplets (ortho- H_2): two different subspecies of H_2 .

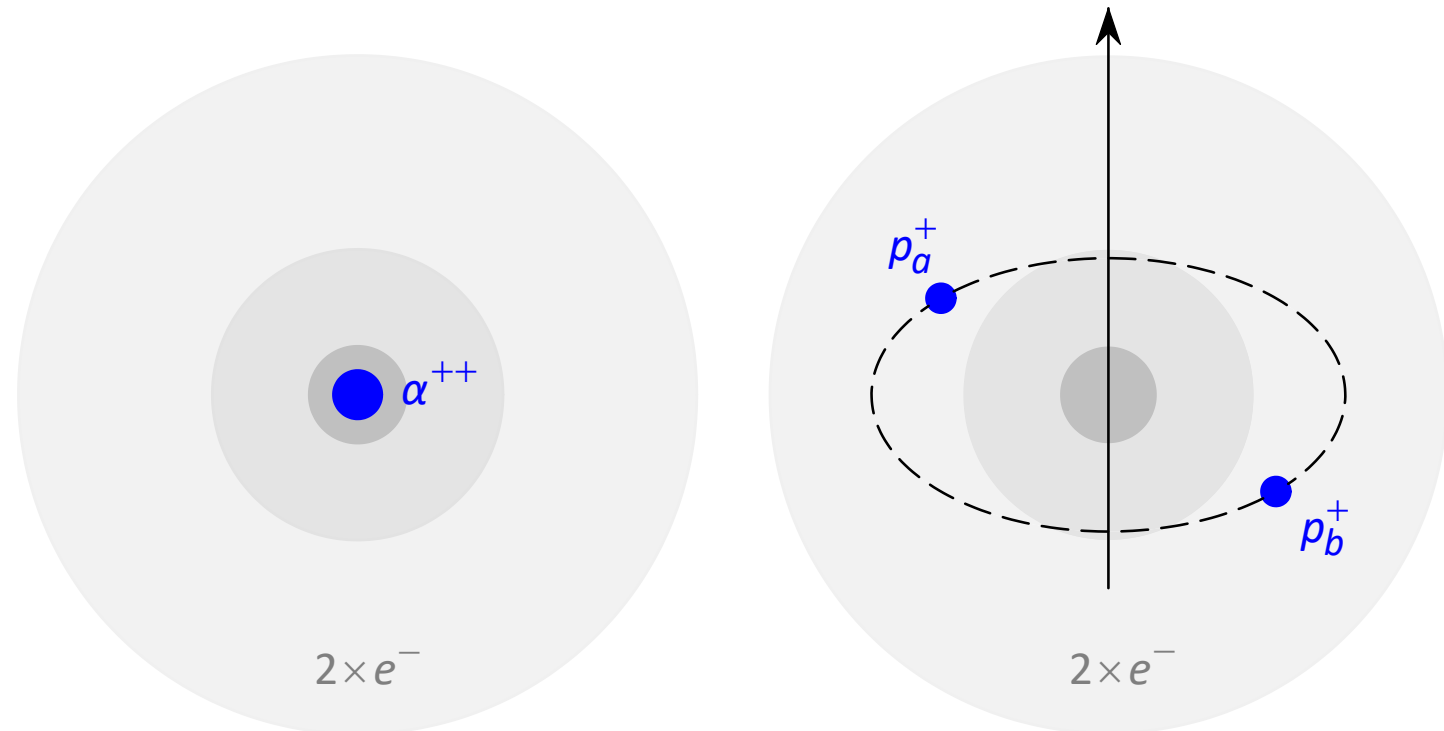
• It turns out that, because of the symmetry of the molecule, it is impossible for para- H_2 and ortho- H_2 to convert to one another, either by photon emission or by collisions at low or moderate speeds (Lecture). It takes chemical reactions to change one to the other. Thus in low temperature or low density environments (e.g. interstellar space), para- H_2 and ortho- H_2 really do behave like separate, independent species.

Spin symmetry of electrons in helium and molecular hydrogen

- The simplest systems in which to consider the state-vector symmetry of pairs of electrons are He and H₂.
- Neither can be solved analytically. For fixed proton or nuclear position, in cgs units,

$$\hat{H}_{\text{H}_2} = \left[-\frac{\hbar^2}{2m_e} \nabla_1^2 - \frac{\hbar^2}{2m_e} \nabla_2^2 \right] + \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} - e^2 \left(\frac{1}{|\mathbf{r}_1 - \mathbf{r}_a|} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_b|} + \frac{1}{|\mathbf{r}_2 - \mathbf{r}_a|} + \frac{1}{|\mathbf{r}_2 - \mathbf{r}_b|} \right),$$

$$\hat{H}_{\text{He}} = \left[-\frac{\hbar^2}{2m_e} \nabla_1^2 - \frac{\hbar^2}{2m_e} \nabla_2^2 \right] - e^2 \left(\frac{2}{r_1} + \frac{2}{r_2} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \right).$$



Spin symmetry of electrons in helium and molecular hydrogen (continued)

- But in the ground state, to good approximation, we can take the electrons to be **co-located** in both cases:
 - Mostly lying between the protons in H_2 , binding the protons together electrostatically.

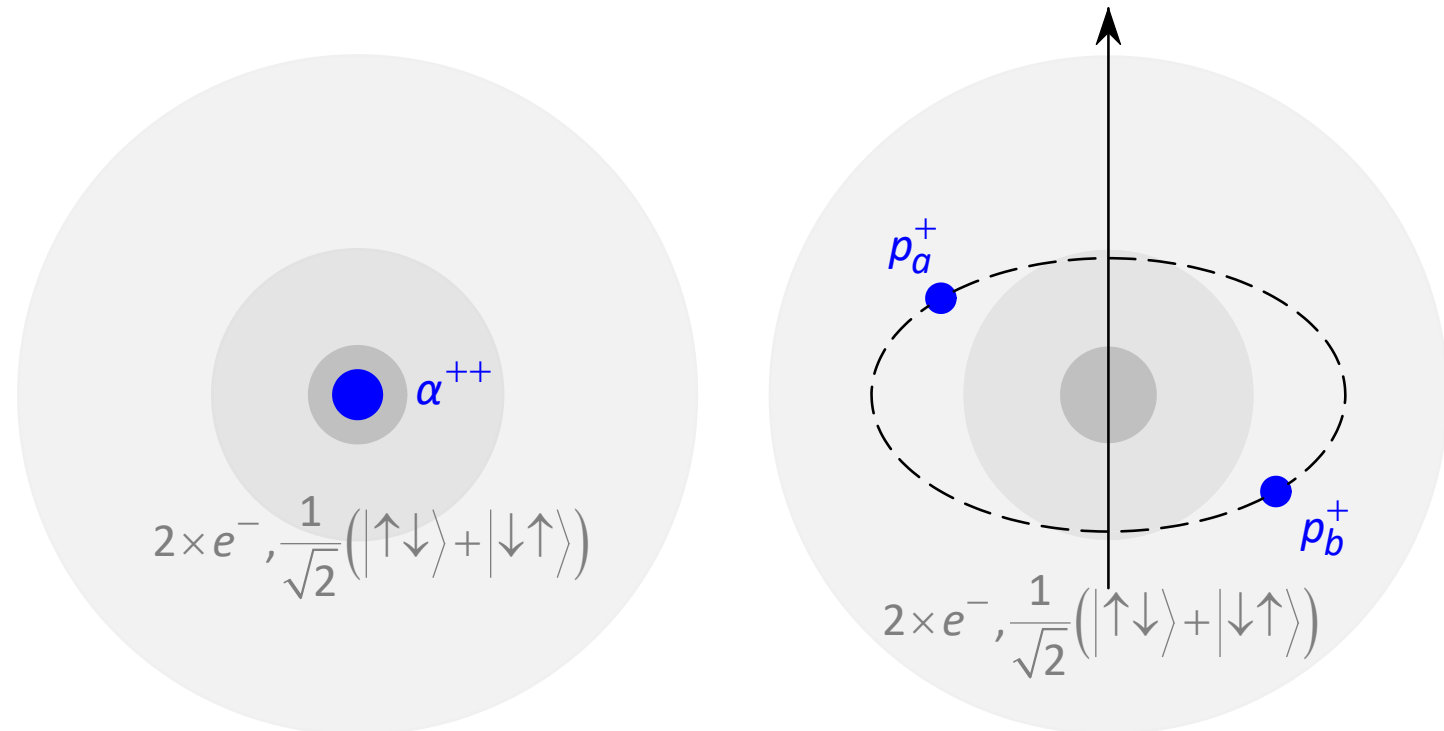
- For He, the first approximation would be a product of hydrogenic ground states, like $\psi \approx \psi_{n\ell m} \psi_{n'\ell' m'} = \psi_{100}^2$.

- Both have $\psi \sim (Y_0^0)^2$ in the ground state, so, as was the case for the proton part of the wavefunction in H_2 , the electron wavefunction apart from spin is **symmetric**: $\hat{P}|\psi\rangle = +1|\psi\rangle$.

- But electrons are fermions, so the complete wavefunction is antisymmetric:

$$\hat{P}|\psi\chi\rangle = -|\psi\chi\rangle \Rightarrow \hat{P}|\chi\rangle = -|\chi\rangle .$$

Electron spin singlets, in both cases.



Spin and symmetry in multielectronic atomic wavefunctions

- Considering electron symmetry in **atoms** with more than two electrons, one can proceed as follows, to at least decent approximation, to consider why atoms fill the period table the way they do.
 - As with He, consider the radial and angular part of the wavefunction, ψ , to be a product of hydrogenic wavefunctions $\psi_{n\ell m}$, one factor for each electron, and adjusting for the number of protons in the nucleus.
 - Consider the spin part of the wavefunction χ to factor out of the complete wavefunction. This is to ignore $\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}$ terms (**fine structure**) in the Hamiltonian, usually to good approximation.
 - Apply the symmetrization principle, used so far only for two quanta, to the whole list of electrons in the atom. That is, for the complete electron wavefunction

$$\hat{P}|\psi, \chi, j, i\rangle = -\hat{P}|\psi, \chi, i, j\rangle \quad ; \quad |0, 1, \dots, i, \dots, j, \dots, N\rangle = -|0, 1, \dots, j, \dots, i, \dots, N\rangle \quad .$$

- You can regard this as an axiom for now, but, because it is equivalent to the Pauli principle, it is an experimental fact.
- Remember that the angular parts of $\psi_{n\ell m}$ are either symmetric or asymmetric, as on pp. 6-7. So if a lone electron is in a symmetric ψ it has to be in an antisymmetric χ , and vice versa.

Spin and symmetry in multielectronic atomic wavefunctions (continued)

- Add some nomenclature: individual-electron parts of wavefunctions are referred by their values of n and ℓ , but the latter is encoded:

$$\ell = 0, 1, 2, 3, 4, \dots \Leftrightarrow s, p, d, f, g, \dots$$

- And the same for the sums of the atom's orbital, spin, and **total** angular momenta: they are referred to by their integer factors of \hbar , but by the capital letters L , S , and J .
 - Adding the orbital angular momenta and spin angular momenta separately, and then adding the results to produce the total, is called **LS**, or **Russell-Saunders**, coupling. It works pretty accurately for elements and ions of the first three rows of the periodic table.
- Reminiscent of the individual electrons, $L = 0, 1, 2, 3, \dots$ is encoded as S, P, D, F, \dots
- So electron **configurations** are given, for the example of carbon (element $N = 6$), as $1s^2 2s^2 2p^2$, and as we will see, the angular-momentum-and-symmetry **term** name is encoded in a hieroglyph:

$$^{2S+1}L_J.$$

Spin and symmetry in multielectronic atomic wavefunctions (continued)

- The ancient, prehistoric, empirical rules for how the configurations and terms go are called **Hund's Rules**, which go like this:
 1. Consistent with the Pauli principle, the state with largest total spin S has the lowest energy.
 2. For a given S , the state with the largest total orbital angular momentum L , consistent with overall antisymmetrization, has the lowest energy.
 3. If a subshell $n\ell$ is no more than half filled, then the lowest energy corresponds to $J = |L - S|$; if more than half filled, the lowest energy corresponds to $J = L + S$.

The period table

PubChem

1																	18										
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Atomic Number: 17

Name: Chlorine

Symbol: Cl

Chemical Group / Family: Halogen

The elements' ground states

- $N = 3$, lithium. The first two electrons go into the ground state as a spin singlet, same as He. The Pauli principle allows no state lower than $n = 2$. So the configuration is $1s^2 2s^1$ and the term is $^2S_{1/2}$.
- $N = 4$, beryllium. The extra electron can go into $2s$, as a spin singlet with the other one: $1s^2 2s^2$, 1S_0 .
- $N = 5$, boron. No room for another s , so it has $\ell = 1$, i.e. is a p : $1s^2 2s^2 2p^1$. Of the two J s, $\frac{1}{2}$ gives lower energy: $^2P_{1/2}$.
- $N = 6$, carbon. The sixth electron needs to be a p as well: $1s^2 2s^2 2p^2$. It can have m different from the first p electron, in which case their spins should be in a triplet. This makes $S = 1$ and J can be 0, 1, or 2. The lowest energy turns out to be $J = 0$: 3P_0 .
- $N = 7$, nitrogen, $1s^2 2s^2 2p^3$. Now all the values of m are used, making $L = 0$, so all the spins need to be up: $^4S_{3/2}$.
- $N = 8$, oxygen, $1s^2 2s^2 2p^4$. The next p electron joins with one of the others in ℓ and m , but their spins therefore have to be in a singlet. Turns out this time that the $J = 2$ is lower energy: 3P_2 .
- $N = 9$, fluorine. Only one unpaired p electron left, and again the larger J is the lower energy: $1s^2 2s^2 2p^5$, $^2P_{3/2}$.

And so on.