Quantum Mechanics and Atomic Physics 750:361

Prof. Sean Oh, Fall 2011

HW #12

Due date: **Wednesday, Dec. 7**, 2011, at the beginning of class: no late HW will be accepted.

5. Reed, Prob. 8-8

Problem 8-8

Classify the following neutral atoms as to whether they will be fermions or bosons: ${}^{29}_{14}\mathrm{Si}$, ${}^{40}_{20}\mathrm{Ca}$, ${}^{69}_{31}\mathrm{Ga}$, ${}^{105}_{46}\mathrm{Pd}$, ${}^{137}_{55}\mathrm{Cs}$, ${}^{235}_{92}\mathrm{U}$.

For a neutral species of the form ${}^{A}_{Z}\mathrm{X}$ the total number of protons, neutrons, and electrons is A+Z. For the cases given these are 43, 60, 100, 151, 192 and 327. These constituents are all spin-1/2; if the total is even we have a boson and if it is odd we have a fermion. Hence we have F,B,B,F,B,F.

6. Reed, Prob. 8-9

Problem 8-9

In Problem 4-16 it was remarked that early in the history of nuclear physics the electrically neutral mass of nuclei now attributed to neutrons was considered to arise from neutral particles composed of combinations of protons and electrons (as opposed neutrons in their own right as fundamental particles). That problem explored the implications of the uncertainty principle for that theory. Here we have a look at the spin statistics of the situation. Consider a nitrogen-14 (${}^{14}_{7}\mathrm{N}$) nucleus. If the "protons + electrons" model were correct, would you predict N-14 to be a spin-1/2 or spin-1 system? What about in the case of the "protons + neutrons" model? Spectroscopic evidence indicates that N-14 is a spin-1 system: which model does this support?

In the "protons + electrons" model the total number of particles is 21: 14 protons plus 7 electrons, for a net positive charge of 7. This would be a spin-1/2 system. In the "protons + neutrons" model the number of constituents is 14, hence a spin-1 system. The spectroscopic evidence favors the neutrons + protons model, as does the uncertainty principle argument.

1. For two electrons in an infinite potential well ($0<x<L$), construct total wavefunctions of the first excited states, ignoring the electron-electron Coulomb potential. For this problem, use the following notation. $\psi_n(x_1)$ ($\psi_n(x_2)$) implies the first (second) electron occupying the n'th energy eigenfunction of the infinite potential well problem. χ_S (χ_T) represents the singlet (triplet) spin state.

2. In the above problem, ignoring the electron-electron interaction, find the energy of the system in terms of E_1, where E_1 represents the lowest energy of a single electron occupying the infinite potential well.

3. In the above problem, still ignoring the electron-electron interaction, find the probability density of both electrons occupying $x=L/4$ if the electrons are in the triplet spin state.

4. In the above problem, if you include electron-electron Coulomb interaction, which state will have a lower energy: the triplet or the singlet state? Is this energy higher or lower than the value you obtained in Prob. 2 above.

7. "Tb" in periodic table has 65 electrons. Using the rules discussed in class, figure out its most likely electron configuration (starting with 1*s* all the way up to the highest energy subshell with the number of electrons in each subshell, as done in class: e. g. Al(Z=13) has its electron configuration of $1s^2 2s^2 2s^6 3s^2 3p^1$). Also find each of the angular momentum quantum numbers and the spectroscopic notation of the ground state electron configuration.

HW #12

Note Title 12/7/2011

1. The total wavefns should be antisymmetric w.r.t. the exchange of two particles.

χ_S is antisymmetric and χ_T is symmetric. Therefore, the spatial wave ftns should be symmetric for χ_S and antisymmetric for χ_T.

The first excited state will have one electron in ψ_1 state and the 2nd electron in ψ_2 state.

Therefore,

$$\Psi_{total,\,singlet} = \frac{1}{\sqrt{2}}\Big(\psi_1(x_1)\psi_2(x_2) + \psi_1(x_2)\psi_2(x_1)\Big)\cdot\chi_S$$

$$\Psi_{total,\,triplet} = \frac{1}{\sqrt{2}}\Big(\psi_1(x_1)\psi_2(x_2) - \psi_1(x_2)\psi_2(x_1)\Big)\chi_T$$

Both of these states have the same energy if we ignore electron-electron interaction

2. $E_1 = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2$, $E_2 = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 = 4E_1$

$$E_{total} = E_1 + E_2 = 5E_1$$

3. $\Psi_{total,\ triplet}\left(x_1 = \frac{L}{4}, x_2 = \frac{L}{4}\right)$

$= \frac{1}{\sqrt{2}}\left(\psi_1\left(\frac{L}{4}\right) \psi_2\left(\frac{L}{4}\right) - \psi_1\left(\frac{L}{4}\right) \psi_2\left(\frac{L}{4}\right) \right) \chi_T$

$= 0$

$\therefore$ The probability density of both electrons occupying $\frac{L}{4}$ is zero

4. electron-electron coulomb interaction is repulsive, and thus has positive potential energy ($P.E. = \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$)

Electrons in the triplet state are tend to be more away from each other than in the singlet state.

Because $P.E. \propto \frac{1}{r}$, electrons further away from each other has lower energy.

Thus Triplet state has lower energy

Because coulomb interaction has positive potential energy between electrons, this new energy will be higher than the one without any electron

-electron Interaction.

7.
1s
2s 2p
3s 3p 3d
4s 4p 4d 4f
5s 5p 5d 5f
6s 6p 6d 6f

$1s^2\, 2s^2\, 2p^6\, 3s^2\, 3p^6\, 4s^2\, 3d^{10}\, 4p^6\, 5s^2$
$4d^{10}\, 5p^6\, 6s^2\, 4f^9$; total of "65"

Let's look at only 4f orbital

-3	-2	-1	0	1	2	3
$\uparrow$	$\uparrow$	$\uparrow$	$\uparrow$	$\uparrow$	$\uparrow\downarrow$	$\uparrow\downarrow$

$$S = \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + 0 + 0 = \frac{5}{2}$$

$$L = -3\times1 + -2\times1 + -1\times1 + 0\times1 + 1\times1 + 2\times2 + 2\times3$$

$$= -3 - 2 - 1 + 1 + 4 + 6 = 5$$

Less than half-filled $\Rightarrow J = L - S = \frac{5}{2}$

$\therefore\ {}^{2S+1}L_J \Rightarrow {}^{6}H_{\frac{5}{2}}$

[$L = 5 \Rightarrow H$ symbol]

S, P, D, F, G, H
0 1 2 3 4 5