*** End semester examination ***
*** Atoms molecules and radiation ***
40 marks, 2 Hours

State whether the following statements are true or false. Give a brief explanation in support of your answer. [10x1.5]

i). KE correction is diagonal in $|nlsm_lm_s\rangle$

False : Diagonal in Y_{lm} and χ_{sm_s} but not in n.

ii). Relativistic correction tends to weaken attraction of electrons to nucleus.

False : Net correction -ve : overbinds.

iii). Spin-orbit coupling increases with principal quantum number.

False : it has overall $1/n^2$ and $1/n$ dependence

iv). $\hat{\vec{L}}.\hat{\vec{S}}$ commutes with $\hat{\vec{L}}.\hat{\vec{L}}$ but not with $\hat{\vec{S}}.\hat{\vec{S}}$

False : Commutes with both

v). $\hat{\vec{L}}.\hat{\vec{S}}$ is diagonal in $|nlsm_lm_s\rangle \equiv |3,0,1/2,0,-1/2\rangle$

True : Does not impact $l=0$

vi). Relativistic correction to potential energy is more for $3s$ level than that of the $2s$ level.

False : Correction due to Darwin term decreases as the orbitals peak away from the nucleus.

vii). Number of observed emission lines generally decreases with increasing magnetic field.

True : Thinks of moderate to strong field

viii). Polarizability of a system of bound electrons in a potential $-Ae^{-\alpha x^2}$ will in general increase with decreasing α.

True : Decreasing α means broader potential well which implies lesser gap between levels and thus lower average ω

ix). The ground state of an H atom with an excess electron can only have $S=0$.

True : Space part will be necessarily symmetric

x). Ionization of C is more than Ne.

False : On average valence electrons of C feels a more spherically symmetric potential than the valence electrons of Ne since a valence electron of Ne finds more electrons in the same sub-shell(l) than that found by a valence electron of C.

2. Starting with a choice of $\vec{A}(\vec{r}) = \frac{-\mu_0}{4\pi}\left[\vec{\mu}_N \times \nabla(\frac{1}{r})\right]$ where $\vec{\mu}_N$ is the magnetic moment due to nuclear angular moment $\vec{I}$, show that correction due to interaction of the nuclear magnetic moment and the magnetic field due to the orbital motion of electron is proportional to $\langle\frac{\hat{\vec{L}}.\hat{\vec{I}}}{r^3}\rangle$. [2.5]

Hint: See the derivation of H_1' in hyperfine structure.

3. With $\vec{A} = \frac{1}{2}(\vec{B} \times \vec{r})$ show that $\langle nlsm_lm_s|\vec{A}.\hat{p}|nlsm_lm_s\rangle = Bm_l/2$ if $\vec{B} \parallel \hat{z}$. [2.5]

Hint : See Zeeman effect lectures : $(i\hbar q/m)\vec{A}.\nabla\psi = -(q/2m)\vec{B}.\hat{\vec{L}}\psi$

4. Show transitions among hyperfine levels with $n = 2$ of deuterium. [2.5]

Hint: Show transitions among (F=5/2,3/2,1/2 from $2p_{3/2}$),(F=3/2,1/2 from $2s_{1/2}$) and (F=3/2,1/2 from $2p_{1/2}$) as per selection rules.

5. Show transitions between $3d$ to $2p$ level in presence of magnetic field of strength much higher than that due to the relative motion on nucleus around the atoms.[2] (reduced from 2.5 to 1)

Already exactly done in notes! (did not realize)

Show how the transitions would evolve if the magnetic field is reduced to become comparable to the magnetic field due to the electronic motion. [3] (increased from 2.5 to 4)

Show transitions among (6 levels from $l = 2, j = 5/2$), (4 levels from $l = 2, j = 3/2$), (2 levels of $l = 2, j = 1/2$) and (4 levels from $l = 1, j = 3/2$) (2 levels of $l = 1, j = 1/2$). Be watchful that the spacings in each group will be different and need to be mentioned.

6. Show how would the $n = 3$ levels evolve under the action of a weak static electric field $E_0\hat{z}$ if $\langle n = 3, l = 0|r|n = 3, l = 1\rangle = R_{01}$, $\langle n = 3, l = 1|r|n = 3, l = 2\rangle = R_{12}$ and $\langle n = 3, l = 0|r|n = 3, l = 2\rangle = R_{02}$ with $R_{12} > R_{02} > R_{01}$. [5]

Hint: Find degenerate groups among which degeneracy to be lifted.(already told in class)
(n, l, m_l): [(3,0,0) (3,1,0) (3,2,0)] ; [(3,1,-1) (3,2,-1)] ; [(3,1,1) (3,2,1)] ; [(3,2,2)] ; [(3,,2,-2)]
Calculate $F(ll'm) = \langle l, m|\cos(\theta)|l', m\rangle$ for the required combinations (only major task!).

	3,0,0	3,1,,0	3,2,0	3,1,-1	3,2,-1	3,1,1	3,2,1	3,2,2	3,2,-2
3,0,0	$E_{3,0}$	R01F100	R02F200						
3,1,0	R01F010	$E_{3,1}$	R12F210						
3,2,0	R02F020	R12F120	$E_{3,2}$						
3,1,-1				$E_{3,1}$	R12F21-1				
3,2,-1				R12F12-1	$E_{3,2}$				
3,1,1						$E_{3,1}$	R12F121		
3,2,1						R12F211	$E_{3,2}$		
3,2,2								$E_{3,2}$	
3,2,-2									$E_{3,2}$

7. Write down the wave-functions of the 1^1S, 2^1S and 2^3S levels of He and arrange them ascending order of energy and give reason for your answer. [1.5x5]

$1^1S : (1/\sqrt{2})\psi_{1s}(1)\psi_{1s}(2)[\alpha(1)\beta(2) - \alpha(2)\beta(1)]$

$2^1S : (1/2)[\psi_{1s}(1)\psi_{2s}(2) + \psi_{1s}(2)\psi_{2s}(2)][\alpha(1)\beta(2) - \alpha(2)\beta(1)]$

$2^3S(M_S = 0) : (1/2)[\psi_{1s}(1)\psi_{2s}(2) - \psi_{1s}(2)\psi_{2s}(2)][\alpha(1)\beta(2) + \alpha(2)\beta(1)]$

$2^3S(M_S = 1) : (1/\sqrt{2})[\psi_{1s}(1)\psi_{2s}(2) - \psi_{1s}(2)\psi_{2s}(2)][\alpha(1)\alpha(2)]$

$2^3S(M_S = -1) : (1/\sqrt{2})[\psi_{1s}(1)\psi_{2s}(2) - \psi_{1s}(2)\psi_{2s}(2)][\beta(1)\beta(2)]$

$\alpha = \chi_{1/2,1/2}; \beta = \chi_{1/2,-1/2}$

Arrangement shown in notes.
Reason is exchange interaction.