Answers to Exam IIa (Nov. 2005)

Prob 1

LS coupling

For LS coupling of identical particles, we have the restriction L+S is even. As a first step, couple two particles
(2s2s) $\rightarrow$ ^{1}S (even parity)
(2s2p) $\rightarrow$ ^{1}P, ^{3}P (odd-parity)
(2p2p)$\rightarrow$^{1}S, ^{3}P, ^{1}D (even-parity)

For an even parity 3-particle state couple two 2p states (2p2p)
then couple the resulting state with the 2s (2p2p)[LS]2s
The possible combinations are
(2p2p) [^{1}S]2s ^{2}S 2×1 substates
(2p2p) [^{3}P]2s ^{2}P 2×3 substates
(2p2p) [^{3}P]2s ^{4}P 4×3 substates
(2p2p) [^{1}D]2s ^{2}D 2×5 substates
Total number of substates = 2+6+12+10=30

jj coupling

For jj coupling of identical particles J is even. The (2p2p) states are
$(3p_{1/2}\ 3p_{1/2}) \rightarrow [0]$
$(3p_{1/2}\ 3p_{3/2}) \rightarrow [1], [2]$
$(3p_{3/2}\ 3p_{3/2}) \rightarrow [0], [2]$

Combining these with a 2s state leads to

$[(\ 3p_{1/2}\ 3p_{1/2})\ [0]2s_{1/2}]$	[1/2]	2	substates
$[(\ 3p_{1/2}\ 3p_{3/2})\ [1]2s_{1/2}]$	[1/2] & [3/2]	2 + 4 = 6	substates
$[(\ 3p_{1/2}\ 3p_{3/2})\ [2]2s_{1/2}]$	[3/2] & [5/2]	4 + 6 = 10	substates
$[(\ 3p_{1/2}\ 3p_{3/2})\ [0]2s_{1/2}]$	[1/2]	2	substates
$[(\ 3p_{1/2}\ 3p_{3/2})\ [2]2s_{1/2}]$	[3/2] & [5/2]	4 + 6 = 10	substates

Total number of substates = 2+6+10+2+10=30

Prob 2

The energy of the (1s3p) state is
E[(1s3p) ^{3}P] = $\epsilon_{1s}+\epsilon_{3p}$ + R_0(1s3p1s3p) - $\frac{1}{3}R_1$(1s3p3p1s) - $U_{\rm 3p3p}$
where U = $\frac{1}{r}$ accounts for the screening of the 3p (or 2s) electron.

The energy of the (1s2s) state is

E[(1s2s) ^{3}S] = $\epsilon_{1s}+\epsilon_{2s}$ + R_0(1s2s1s2s) - R_0(1s2s2s1s) - $U_{\rm 2s2s}$.

As a first step we need lowest order energies and Coulomb wave functions:

$\boldsymbol{\epsilon}$**1s = −*Z*^2/2**

$-\frac{Z^2}{2}$

Let Zs = Z-1 be the screened charge.

$\boldsymbol{\epsilon}$**2s = −Zs^2/(22^2)**

$-\frac{\text{Zs}^2}{8}$

$\boldsymbol{\epsilon}$**3p = −Zs^2/(23^2)**

$-\frac{\text{Zs}^2}{18}$

P1s[r_]:=2*Z*^(3/2)*r*Exp[−*Zr*]

P2s[r_]:=(Zs^(3/2)/Sqrt[2])*r*(1 − Zs*r*/2)Exp[−Zs*r*/2]

P3p[r_]:=8Zs^(5/2)/(27Sqrt[6])*r*^2(1 − Zs*r*/6)Exp[−Zs*r*/3]

Now evaluate the screening potentials and Slater Integrals

v01s[r_]:= Integrate[P1s[*x*]^2, {*x*, 0, *r*}, Assumptions → *Z* > 0]/*r*+ Integrate[P1s[*x*]^2/*x*, {*x*, *r*, Infinity}, Assumptions → *Z* > 0]

v01s2s[r_]:= Integrate[P1s[*x*]P2s[*x*], {*x*, 0, *r*}, Assumptions → {*Z* > 0, Zs > 0}]/*r*+ Integrate[P1s[*x*]P2s[*x*]/*x*, {*x*, *r*, Infinity}, Assumptions → {*Z* > 0, Zs > 0}]

v11s3p[r_]:= Integrate[P1s[*x*]P3p[*x*]*x*, {*x*, 0, *r*}, Assumptions → {*Z* > 0, Zs > 0}]/*r*^2+ *r*Integrate[P1s[*x*]P3p[*x*]/*x*^2, {*x*, *r*, Infinity}, Assumptions → {*Z* > 0, Zs > 0}]

G01s2s:=Integrate[P2s[*r*]^2v01s[*r*], {*r*, 0, Infinity}, Assumptions → {*Z* > 0, Zs > 0}]

G01s3p:=Integrate[P3p[*r*]^2v01s[*r*], {*r*, 0, Infinity}, Assumptions → {*Z* > 0, Zs > 0}]

F01s2s:=Integrate[P2s[*r*]P1s[*r*]v01s2s[*r*], {*r*, 0, Infinity}, Assumptions → {*Z* > 0, Zs > 0}]

F11s3p:=Integrate[P3p[*r*]P1s[*r*]v11s3p[*r*], {*r*, 0, Infinity}, Assumptions → {*Z* > 0, Zs > 0}]

Now evaluate the background potentials

U2s:=Integrate[P2s[*r*]^2/*r*, {*r*, 0, Infinity}, Assumptions → Zs > 0]

U3p:=Integrate[P3p[*r*]^2/*r*, {*r*, 0, Infinity}, Assumptions → Zs > 0]

Put things together: E[(1s3p) ^{3}P] = $\epsilon_{1s}+\epsilon_{3p}$ + R_0(1s3p1s3p) - $\frac{1}{3}R_1$(1s3p3p1s) - $U_{\rm 3p3p}$

e1s3p = $\boldsymbol{\epsilon}$**1s +** $\boldsymbol{\epsilon}$**3p + G01s3p − F11s3p/3 − U3p**

$$-\frac{Z^2}{2}-\frac{\text{Zs}}{9}-\frac{\text{Zs}^2}{18}-\frac{36Z^3\text{Zs}^5\left(56Z^2-28Z\text{Zs}+5\text{Zs}^2\right)}{(3Z+\text{Zs})^9}+\frac{Z\text{Zs}\left(243Z^6+567Z^5\text{Zs}+567Z^4\text{Zs}^2+315Z^3\text{Zs}^3+69Z^2\text{Zs}^4+21Z\text{Zs}^5+\text{Zs}^6\right)}{(3Z+\text{Zs})^7}$$

e1s3p = e1s3p/.{*Z* → 5, Zs → 4}//*N*

−13.4073

E[(1s2s) ^{3}S] = $\epsilon_{1s}+\epsilon_{2s}$ + R_0(1s2s1s2s) - R_0(1s2s2s1s) - $U_{\rm 2s2s}$.

e1s2s = $\boldsymbol{\epsilon}$**1s +** $\boldsymbol{\epsilon}$**2s + G01s2s − F01s2s − U2s**

$-\frac{Z^2}{2}-\frac{\text{Zs}}{4}-\frac{\text{Zs}^2}{8}-\frac{16Z^3\text{Zs}^3(20Z^2-30Z\text{Zs}+13\text{Zs}^2)}{(2Z+\text{Zs})^7}+$
$\frac{Z\text{Zs}(8Z^4+20Z^3\text{Zs}+12Z^2\text{Zs}^2+10Z\text{Zs}^3+\text{Zs}^4)}{(2Z+\text{Zs})^5}$

e1s2s = e1s2s/.{$Z \to 5$, Zs $\to$ 4}//N

-14.7663

ΔE = e1s3p − e1s2s

1.35901

Energy in cm^{-1}

decm = 219474.62ΔE

298268.

Wavelength in Angstrom

$\lambda = 10^8$/decm

335.269

The NIST table gives 337.07 Angstrom so the difference with NIST is only 0.5 %

Prob 3

The reduced matrix element R_{E1} =¡(1s2s) ^{2}S —— r —— (1s3p) ^{3}P¿ = $\sqrt{3}$ ¡0 ——C1——1¿ R_{1s3p} , where
$R_{1s2p} = \int P_{2p}(\text{r})\ \text{r}\ P_{1s}(\text{r})\ \text{dr}$ is the radial dipole integral.

Rsp = Integrate[P3p[r]rP2s[r], {r, 0, Infinity}, Assumptions → Zs > 0]

$\frac{27648\sqrt{3}}{15625\text{Zs}}$

Let cps = ¡0 ——C1——1¿

cps = Sqrt[3]ThreeJSymbol[{0, 0}, {1, 0}, {1, 0}]

-1

Then, we find that the reduced matrix element is:

RE1 = Sqrt[3]cpsRsp

$-\frac{82944}{15625\text{Zs}}$

The associated line strength is

SE1 = RE1^2

$\frac{6879707136}{244140625\text{Zs}^2}$

The transition rate is A = $\frac{2.0261310^{18}}{\lambda^3}\ \frac{\text{SE1}}{g_a}$ in 1/s, where g_a is the initial state degeneracy (9 for a triplet P state) and λ= 335.269 from previous problem

$A = \frac{2.0261310^{18}}{\lambda^3}\frac{\text{SE1}}{g_a}$**/.{Zs → 2, g_a → 9}**

4.20839×10^{10}

Prob 4

5$d_{5/2}$

This state decays to the ground state by M1 emission
λ = 62374 Angstrom

$4f_{5/2}$ & $4f_{7/2}$

These states decay by E1 emission to the 5d levels
$4f_{5/2} \to 5d_{3/2}$ $\lambda = 13898$ Angstrom
$4f_{5/2} \to 5d_{5/2}$ $\lambda = 17883$ Angstrom
$4f_{7/2} \to 5d_{5/2}$ $\lambda = 14100$ Angstrom

$6s_{1/2}$

The 6s decays to the lower 5d levels b E2 emission
$6s_{1/2} \to 5d_{3/2}$ $\lambda = 7358$ Angstrom
$6s_{1/2} \to 5d_{5/2}$ $\lambda = 8342$ Angstrom

Prob 5

The only lower state in Be is the $^1S_0$ ground state.

The J=0 sublevel cannot decay by single-photon emission since the angular momentum triangle relations require —0-0— ≤ J ≤ 0+0 and there is no multipole with J=0!.

The J=1 sublevel could decay to the ground state by E1 emission; however, for this transition $S_F \neq S_I$ so the transition is forbidden nonrelativistically.

The J=2 sublevel could decay by M2 emission. As above, $S_F \neq S_I$, so the transition is forbidden nonrelativistically.