Atoms and Molecules – Exam

January 28, 2025

Without explanation or calculation steps no points will be awarded to a sub-problem even if the answer is correct!

PROBLEM 1. Atomic Structure [15 points]

Manganese atoms have the following electronic configuration: $[Ar]4s^2 3d^5$

a) Following Hund's rules determine the ground level of Mn atoms
Explain your answer [6 pnts]

b) Mn atoms exhibit no fine structure splitting, why? Explain your answer [3 pnts]

c) The nuclear spin of Mn is 5/2. Determine the hyperfine structure quantum numbers F. Explain your answer [3 pnts]

d) How many hyperfine structure states does Mn have in its ground level? Explain your answer [3 pnts]

PROBLEM 2. Binding energies and Decay channels[20 points]

Consider C particles with an innershell hole in the 1s subshell. Neutral C has the following electronic configuration $1s^2 2s^2 2p^2$.

a) What are the two different types of decay that are possible [2 pnts]

b) For each of the two types of decay, indicate the final electronic configuration of the C particles after decay. Motivate your answer [4 pnts]

c) Which of the decay channels is most likely? Motivate your answer [2 pnts]

To calculate energies and wave functions of many-electron atoms several approximations are commonly made. Describe briefly (2 to 3 sentences) the main assumption(s) underlying:

d) The Independent Particle Model and indicate what this implies for the representation of the wave function. [3 pnts]

e) The Central-Field Approximation. [1 pnts]

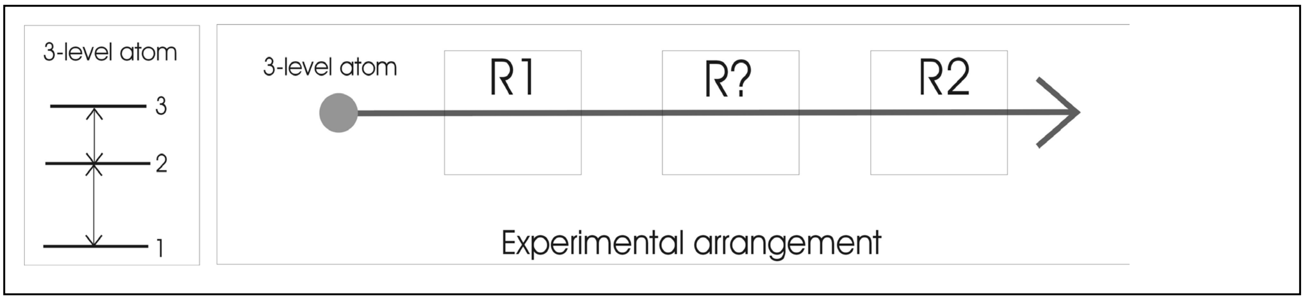
Consider an $O^{3+}(1s^2 3p^3)$. The $3p^3$ has a binding energy of 132.2 eV.

f) Calculate the effective charge experienced by each of the *3p* electrons. Explain your calculation steps. [3 pnts]

g) For such a *3p* electron how much of the nuclear charge is shielded by another *3p* electron. You may assume that the shielding by the $1s^2$ electrons is complete. Motivate your answer. [2 pnts]

h) How much energy does it take to remove one *3p* electron from a $O^{3+}(1s^2 3p^3)$ ion. Explain your answer [3 pnts]

PROBLEM 3. Non-destructive detection [15 points]



Consider a three-level atom which passes through two pulsed oscillating fields (labeled R1 and R2) of which the frequency is resonant with the transition between state $|1\rangle$ and $|2\rangle$. Between R1 and R2 the atom passes through an area R?, which might or might not contain an oscillating field of which the frequency is resonant with the transition between state $|2\rangle$ and $|3\rangle$. When the R? field is present its pulse length corresponds to a 2π pulse.

Initially the atom is in state $|1\rangle$ i.e., the atomic wavefunction is $\Psi = |1\rangle$.

a) The field in R1 corresponds to a $-\frac{\pi}{2}$ pulse. Determine the wave function after passage through R1. [4 pnts]

b) What is the atomic wave function after passage through R? if the field is on. Motivate your answer. [4 pnts]

c) What should be the pulse length of field R2 to determine whether R? was switched on or off? NB. Behind R2 a detector is positioned that can measure the population of states $|1\rangle$ and $|2\rangle$. Explain your answer. [7 pnts]

PROBLEM 4. Electron Capture [10 points]

The over-the-barrier model predicts that an electron can be captured from an atom B by an ion A^{q+} at an internuclear distance $R_c = \frac{1+2\sqrt{q}}{IP}$, with IP the ionization potential of the target. The formula is in a.u. (1 a.u. of length is 5×10^{-9} cm).

Consider a thermonuclear fusion reactor, like ITER, in which the core plasma is heated by injecting an energetic beam of neutral deuterium. D has an IP of 0.5 a.u. The core plasma consists of a mixture of D^+ and T^+ ions. The plasma ions can capture an electron from the neutral beam atoms and thus ionize them. When ionized, neutral-beam particles dump their kinetic energy in the plasma. Assume the core plasma to have a length of 4 m in the direction of the D heating beam.

a) Calculate the cross section for electron capture in D^+ - D collisions. [4 pnts]

b) For a plasma density of 10^{14} cm^{-3}, at which depth into the plasma is 90% of the neutral-beam particles ionized. Explain your answer [6 pnts]

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1a Hund's rule 1: consider partially fit l-shell.
$3d^5 \Longrightarrow$ 5 d electrons
Hund's rule 2: highest S possible.
with 5 electrons $(s = \frac{1}{2}, m_s = \frac{1}{2}, -\frac{1}{2})$.
highest $M_S = 5 \times (m_s = \frac{1}{2}) = \frac{5}{2} \Longrightarrow$ highest $S = \frac{5}{2}$.
Hund's rule 3: highest L value for highest S
highest L value defined by highest M_L
$M_L = \Sigma m_l$ for d electrons $l = 2$, thus
options for $m_l = -2, -1, 0, 1, 2$
all m_l values must differ, because for maximum M_S all 5 m_s values are the same.
$\Longrightarrow M_L = \Sigma m_l = 2 + 1 + 0 + (-1) + (-2) = 0$
$\Longrightarrow L$ max is 0.
Hund's rule 4: shell $\leq \frac{1}{2}$ filled lowest J.
shell $> \frac{1}{2}$ filled highest J.
$3d^5 \leq \frac{1}{2}$ filled lowest $J = |L - S| = \frac{5}{2}$

$\Longrightarrow$ ground level $^6S_{5/2}$

1b There is only one fine structure level (J level).
because $\bar{J} = \bar{L} + \bar{S}$ and as shown in 1a
$S = 0 \Longrightarrow J = L$

1c $J = \frac{5}{2}$, $I = \frac{5}{2}$. $\bar{F} = \bar{J} + \bar{I} \Longrightarrow F = 0, 1, 2, 3, 4, 5$

1d "states" means all m_F states
$$\# m_F = \sum_F (2m_F + 1) = 36$$

also possible via $(2I+1)(2J+1) = 36$
conservation of # of states.

2 C with configuration $1s2s^2 2p^2$.

2a: I radiative decay

II Auger decay.

2b: I $\Delta l = \pm 1$ $\Longrightarrow$ $1s2s^2 2p^2 \longrightarrow 1s^2 2s^2 2p$

II 2 el process one to lower level and another one emitted, preference for nearest continuum.

a. $1s2s^2 2p^2 \rightarrow 1s^2 2s 2p^2 + e$

b. $1s2s^2 2p^2 \rightarrow 1s^2 2s^2 2p + e$

a. preferred smallest change of energy "nearest continuum"

2c: for low Z elements, as C, Auger decay outbeats radiative decay, thus Auger!

2d. IPM:

1. el - el interaction approximated by an average potential of all other electrons
   no more cross terms
2. $H = h_1 + h_2 + h_3 + \ldots$ independent electrons.
   $E = E_1 + E_2 + E_3 + \ldots$
3. $\psi = \varphi_1 \cdot \varphi_2 \cdot \varphi_3 \cdots$

2e The potentials are spherical symmetric

$\bar{r} \rightarrow r$ or $V(\bar{r}) \rightarrow V(r)$.

2f 3 equivalent 3p electrons; together 132.2 eV.

44.1 eV/el $\quad E = 13.6 \dfrac{Z_{eff}^2}{n}$ $\quad (n=3)$.

$$\Longrightarrow Z_{eff} = 3\sqrt{\frac{E}{13.6}} = 5.4.$$

2g. $1s^2$ shielding complete, if there is no mutual shielding of the 3p electrons, one expects $Z_{eff} = 8 - 2 = 6$.

2f $\Longrightarrow Z_{eff} = 5.4$, $\Longrightarrow$ mutual shielding of the 3p electrons $\frac{6 - 5.4}{2} = 0.3$ (each 3p el. has 2 neighbours).

3 see tutorial excercise (with $\frac{\pi}{2}$ pulse).
identical

4 a capture distance

$$R_c = \frac{1+2\sqrt{q}}{IP}$$

$q = 1$

$IP = 0.5$

$\Rightarrow R_c = 6$ a.u. $= 3\times10^{-8}$ cm

cross sections $\sigma = \pi R_c^2 \simeq 28\times10^{-16}\,cm^2$.

b $N = N_0 e^{-n\sigma L}$

$n = 10^{14}\,cm^{-3}$

90% lost $\rightarrow$ 10% remaining

thus $N = 0.1 N_0$

$\Rightarrow 0.1 = e^{-n\sigma L}$

$$\Rightarrow L = \frac{\ln(0.1)}{-n\sigma} = 8.2\text{ cm}.$$