PHY2202F PHYSICS OF ATOMS & MOLECULES Final Exam 2013

Take-home: 15 December 2013, 5 pm – 16 December 2013, 5 pm (hand in to staff in MP1109, or else under my office door; keep a copy)

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Restrictions: You may not cooperate with or take help from anyone else in answering these questions. You may consult any 'passive' reference (books, online references), and use computer-based aids. Please note in your answers any aid you take from Wolfram Alpha, and credit any other sources.

General: Be precise and careful in your written answers, identifying assumptions and giving all logical steps. Give references for any sources you use.

ANSWER ALL FIVE QUESTIONS

- [20] 1. Terms, Definitions, Concepts Define & explain each of the following terms or phrases, and describe the <u>significance</u> of each in the context of atomic physics. Use formulæ wherever appropriate, diagrams if needed, and answers of roughly 3-4 sentences. Because this is a take-home exam, this question will be marked to a high standard of how well you meet the requirements above.
 - a) configurations, terms, levels, states
 - b) the exchange interaction (and why if B=0 and no spin-dependent terms in the Hamiltonian, does it look like spin-spin coupling?)
 - c) g-factor generally, and the Landé g-factor
 - d) central-field approximation
 - e) the Hartree-Fock method

[10] 2. *Correcting heuristics*

Neglecting relativistic and other small effects, the energies of the s, p, d... states of hydrogen for a given value of the principle quantum number n are the same. They have the same potential energy, and the same kinetic energy. However, say a student argues as follows: "Compared with high-angular-momentum states of the same n, the low-angular-momentum states have a higher probability of being near the nucleus, so their potential energy must be more negative. Their low angular momentum means they have lower kinetic energy also. So the low-angular-momentum states should lie deeper in energy."

Give an explanation for the student about what is wrong with this argument.

[20] 3. Interpretation of quantized nature

Consider a particle of mass μ and its arbitrary, normalised wavefunction $\Psi(\vec{r},t)$.

a) Provide the physical interpretation (significance, meaning) of the probability density $\rho(\vec{r},t)$, where $\rho(\vec{r},t) = |\Psi(\vec{r},t)|^2$, and the probability current density $\vec{J}(\vec{r},t)$,

$$\vec{J}(\vec{r},t) = \frac{\hbar}{2\mu i} \left[\Psi^*(\vec{r},t) \nabla \Psi(\vec{r},t) - \Psi(\vec{r},t) \nabla \Psi^*(\vec{r},t) \right]$$

and explain their relation

$$\frac{\partial \rho(\vec{r},t)}{\partial t} = -\overline{\nabla} \cdot \vec{J}(\vec{r},t)$$

b) Let
$$\Psi(\mathbf{r}, \mathbf{t}) = \Psi(\vec{r}, t) = \sqrt{\rho(\vec{r}, t)} e^{i\alpha(\vec{r}, t)}$$
, where α is a real function of r . Show that

$$\vec{J}(\vec{r},t) = \frac{h}{\mu} \rho(\vec{r},t) \nabla \alpha(\vec{r},t)$$

The normalised energy eigenfunction of the hydrogen atom can be written as

$$\varphi_{n,l,m}(\vec{r}) = R_{n,l}(r)Y_l^m(\theta,\phi)$$

The radial function $R_{n,l}(r)$ is real, and the spherical harmonic $Y_l^m(\theta,\phi)$ can be written as the product of the real function $P_l^m(\theta)$ and $\exp(im\phi)$.

c) Use spherical polar coordinates to show that the only non-vanishing component of the probability current density is

$$J_{\phi} = \frac{\hbar m}{\mu r \sin \theta} \left| \varphi_{n,l,m}(\vec{r}) \right|^2$$

d) The eigenvalue $m\hbar$ of the z-component of the angular momentum can be viewed as resulting from the rotational motion of the probability fluid around the z-axis. What is the contribution of the current at the infinitesimal volume element dV, situated at point \vec{r} , to the z-component of the angular momentum? How do you obtain $m\hbar$?

e) Sketch the current in the xy plane for the 2p state of the hydrogen atom in the cases $m = \pm 1$ and m = 0. Provide a physical interpretation of the result.

[25] 4. Atomic Transitions

a) What do the quantum numbers L, S, J, M_J signify in the LS coupling model of multielectron atoms? State and give a simple justification of the electric dipole selection rules in atomic spectroscopy which apply in the LS coupling scheme. Suggest a simple physical reason why a transition between two levels both having $M_J = 0$ is forbidden for the case $\Delta J = 0$.

b) Give reasons why the following transitions obey or disobey electric dipole selection rules:

$$\frac{1s^{2}2p^{2}P_{1/2} - 1s^{2}3d^{2}D_{5/2}}{1s^{2}2s2p^{1}P_{1} - 1s^{2}2p3p^{1}P_{1}}$$
$$\frac{1s^{2}2s^{2}{}^{1}S_{0} - 1s^{2}2p^{2}{}^{3}P_{1}}{1s^{2}2s^{2}{}^{1}S_{0} - 1s^{2}2p^{2}{}^{3}P_{1}}$$

Because two 'families' of levels were identified to exist, with transitions within each family but without transitions between them, early on it was supposed that helium existed in two distinct forms, *orthohelium* and *parahelium*. However, under certain conditions such *intercombination lines* are permitted.

c) Explain the prohibition of intercombination lines, and the circumstances under which such lines can be observed.

d) These intercombination lines can be used as a diagnostic of density. Use your accounts on FLYCHK to illustrate this behaviour for helium-like Al ions (ionized until only two bound electrons remain) in a hot plasma of $k_B T_e = 400 \text{ eV}$ with zero opacity.

Calculate in non-LTE for a range of electron densities $10^{18}-10^{24}$ cm⁻³, in decade steps, and for this range roughly plot the ratio w/y between the resonance line 'w' $(1s^{2} {}^{1}S_{0} - 1s2p {}^{1}P_{1})$ and the group of lines including the intercombination line 'y' $(1s^{2} {}^{1}S_{0} - 1s2p {}^{3}P_{1})$. (For this, do not worry about integrating the whole-line intensity, just describe your reasonable estimation)

e) Why is this ratio sensitive to density? What sensitivity do you expect for this ratio versus temperature?



[25] 5. Zeeman Effect

a) For the magnesium atom (Mg) in a weak magnetic field, state all the interactions and approximations that are important for describing its atomic structure and in what order they should be considered.

b) When a weak magnetic field is applied to an atom, a spectral line splits into several components (Zeeman effect). Draw a level diagram indicating the allowed transitions for each of the following:

i) ${}^{1}P_{1} - {}^{1}D_{2}$ spectral line in Mg

ii) ${}^{2}P_{3/2} - {}^{2}S_{1/2}$ spectral line in Na

For each of these two spectral lines, find and sketch the relative spacing between the components observed perpedicular to the direction of a weak magnetic field. Indicate on each of your sketches which components will be observed when viewed parallel to the magnetic field. Explain why.

c) Explain briefly the role of the Landé *g*-factor, given by

$$g_J = \frac{3J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}$$

in describing the weak-field Zeeman effect (no formal derivation required).

d) The weak-field Zeeman splitting pattern of a transition from an upper level *known* to be ³D to a lower level of *unknown* L, S, J values is shown in the line spectrum below. The spectrum shows all possible components of the transition. Find the J value of the upper level and the L, S, J values of the lower level.



[100] TOTAL MARKS