10390-716(8) Atomic Physics (1½l, 1½p)

2014

Course summary:

Multi-electron atoms, exclusion principle, electrostatic interaction and exchange degeneracy, Hartree model, angular momentum coupling: L-S and j-j coupling, transition probability and selection rules.

Outcomes of course:

The student is equipped with a basic working knowledge of atomic physics. As this course serves as general basis for all Atomic Physics modules in the Hons course, the approach is rather towards theoretical description of atomic structure, than experimental techniques.

Lecturer:

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Course content:

A. RADIATIVE TRANSITIONS

1. Einstein's A and B coefficients
2. Transition Probabilities
3. The electric dipole approximation
4. Selection rules
5. Higher order radiation

B. THE HYDROGEN ATOM : FINE STRUCTURE

1. Electron spin
2. The interaction terms
3. The vector model
4. The Lamb shift
5. Summary of the Hydrogen spectrum

C. TWO ELECTRON ATOMS

1. Introduction
2. An infinite set of products of hydrogen-like single electron eigenfunctions, known as electron configurations is obtained when solving the Schrödinger equation and considering only the Coulomb potential between the nucleus and two independent electrons. Indistinguishability of the two electrons leads to a discrepancy with the Heisenberg uncertainty principle for certain configurations.
3. Electrostatic electron-electron Coulomb interaction is considered as a first order perturbation in the potential term and leads to the lifting of the exchange degeneracy.
4. The formulation of the direct- (J), and exchange- (K) integrals as indicators of the energy level shift and splitting caused by the electron- electron Coulomb interaction.
5. The ground state of helium.
6. Excited states of helium.
7. Gross energy level scheme of helium-like atoms and the formation of singulet and triplet terms.
8. Electron spin functions and the Pauli exclusion principle.
9. Anti-symmetric eigenstates for systems with bound identical fermions.
10. Determinantal product functions.
11. The occupation of electron configurations and the classification of elements in the periodic system.

D. THE CENTRAL FIELD APPROXIMATION FOR MULTI-ELECTRON ATOMS

1. Introduction.
2. Schrödinger equation for a multi-electron atom with a mean central potential.
3. The Hartree technique.
4. Self consistent mean field calculational techniques.
5. The formation of shells and sub-shells and the maximal filling thereof caused by the Pauli exclusion principle.
6. The role of the valence-electrons and electrons in the filled shells and subshells. Chemical properties, optical and X-ray transitions.
7. Effective nuclear charge, screening by underlying filled shells and subshells.
8. Penetration of higher eigenstates into other states caused by the difference in radial probability distribution of s, p, d etc. states.
9. Competition between the different states for the lower energy of the ground state.
10. Order of filling of the ground state electron configuration in subshells with increasing Z number in the periodic table.
11. The Thomas-Fermi potential.
12. The gross structure of the alkaline elements.
13. s-Electron penetration into the filled core of noble gas-like electrons.
14. The Rydberg formula.
15. Quantum defect, and effective quantum number.

E. ANGULAR MOMENTUM COUPLING IN MULTI-ELECTRON ATOMS

1. Introduction.
2. The residual Coulomb field (non-radial component of the electron- electron electrostatic interactions) as first order perturbation, in the potential term of the Schrödinger equation for the central field approximation.
3. The spin-orbital interaction of the individual electrons as first order perturbation in the potential term of the Schrödinger equation for the central field approximation.
4. Configuration mixing of the base eigenfunctions caused by perturbations in the potential.
5. Diagonality of the perturbation in the base function representation.
6. Commutation of the perturbation with the different angular momentum operators.
7. The LS-coupling approximation.
8. Relative size of the Coulomb residual field perturbation compared to the spin-orbital perturbation and applicable atom/ion states.
9. Commutation of the perturbation.
10. Appropriate single electron eigenfunction representations in which the perturbation is diagonal.
11. Splitting of the gross structure energy eigenvalues derived from the central field approximation in terms caused by the Coulomb residual potential as perturbation.
12. Allowed terms in LS coupling.
13. Allowed terms for non-equivalent electrons in LS coupling.
14. Allowed terms for equivalent electrons when taking the Pauli exclusion principle into consideration.
    - I. Examples of the allowed terms in two and three valence electron systems.
    - II. The use of up- and down- ladder operators to find the linear combinations of base functions constituting the eigenfunction belonging to a specific term's energy eigenvalue.
15. Hund's rule as regards the groundstate term in LS coupling.
16. Examples of the groundstate term for the different periods in the periodic table.
17. The half-filled subshell symmetry property, equivalency of electrons and vacancies.
18. Formulation of the direct and exchange integrals.
19. Example of the energy splitting of a single electron configuration in terms for the groundstate of Si and comparison of the theoretical result as predicted by means of the Slater integrals with the experimental values.
20. Fine structure in LS coupling.
21. Considering the spin-orbital interaction, with a small first order perturbation in the eigenfunction of the term retaining the LS coupling approximation and L and S as "good" quantum numbers.
22. The splitting of LS coupled terms into fine structure or multiplets caused by spin-orbital interaction.

23. The relationship between the single electron spin-orbital strength parameter and the effective spin-orbital strength parameter for the term.
24. The origination of the interval rule and its use for testing the validity of the LS coupling approximation for specific terms.
25. The origination of normal and inverted multiplets and the half filled subshell symmetry.
26. The fine structure splitting in the alkaline elements and helium as examples.
27. Relative intensities in LS coupling.
28. The statistical population of allowed states for an ensemble of identical free atoms and its relationship with radiational intensities.
29. Relationship between spectral intensity and the square of the matrix element of the radiational operator.
30. Selection rules for parity, electrical dipole, magnetic dipole and electrical quadrupole single photon transitions.
31. The polarization properties of specific radiational transition types.
32. Breaking down of the selection rule at inter-combination lines where LS coupling's validity starts to fail.
33. Tables of Clebsch-Gordon coefficients as well as 3j and 6j symbol tables containing the angular factors in the radiational transition probabilities.
34. Summary of the results derived from the angular factors in terms of D J and D L; L changes during radiational transitions.
35. The Ornstein-Burger-Dorgelo sum rule for intensities in a LS coupled multiplet transition.
36. Example in applying the interval rule and the sum rule to analyse a set of spectral lines of Ca with the purpose of determining the appropriate energy eigenvalues and term classification thereof, and testing the validity of the LS coupling approximation to the specific terms.
37. The j-j coupling approximation
38. Perturbation theory approximation in which the spin-orbital interaction is much larger than the Coulomb residual field perturbation.
39. Appropriate single electron configuration in which the perturbation is diagonal.
40. Classification of states originating from the lifting of the degeneracy in the configuration caused by spin-orbital interaction.
41. Lifting of the J degeneracy by introducing the Coulomb residual field as the next smaller perturbation.
42. Applicable domain of j-j coupled states and examples thereof.
43. Other coupling schemes.
44. Coupling mechanism in the noble gas like excited states.

Practical (Tutorials):

Study material:

Elementary Atomic Structure, 2nd Edition, G.K. Woodgate, Clarendon Press, Oxford.

Learning opportunities:

Lectures and tutorials as indicated on time tables

Assessment:

Methods of Assessments
Two tests and tutorial problems.

Venue and time of assessment opportunities
In the Merensky Physics Building as discussed with the students.

Calculation of final mark for the module:
45% weight of 1st test,
45% weight of 2nd test,
10% weight of tutotorial problems