Spektroskopi och materiens kvantmekaniska beskrivning FYST20
VT 2012

Hand-in exercise 2: Spectroscopy on atoms

The number of electrons (Z) in an atom is essential to determine the dominant interaction term beyond the central field approximation. The other terms are thereafter treated as a perturbation of the Hamiltonian H_0, which includes the central field approximation and the dominant term. The good quantum numbers, given by a set of operators that commutes with H_0, define the basis set that is used to describe the fine structure of the atom.

a) For many electron atoms, coupling schemes such as the LS- coupling or JJ-coupling are well adapted to describe the fine structure of light or heavy atoms. Give the fine structure (spectroscopic terms) of the excited electronic state:

- 2p3s in carbon (C)
- 6p7s in lead (Pb)

b) There are important consequences of the Pauli principle in finding the atomic fine structure, namely:
- two electrons that have the same m_l and m_s must be excluded
- two electrons are indistinguishable, i.e. two pairs (m_{l1},m_{s1}) and (m_{l2},m_{s2}) which differ only by the electron label (1 or 2) only give one state.
Using the LS coupling scheme, determine the spectroscopic terms for two equivalent electrons in the s-shell (ns^2) and in the p-shell (np^2).

c) We consider now the ionization of rare gas atoms in valence shell with an electronic state $|\gamma np^6[^1S_0]>$ (with n≥2). The absorption of one photon promotes one electron in another outer shell, or in the continuum of ionization with an orbital momentum ($\vec{l}$). The j_cl-coupling scheme becomes a good approximation to describe the fine structure since the spin of the optical electron ($\vec{s}$) can be decoupled from the others. Electronic states in this basis are written as $|\gamma np^5[^2P_{jc}]ml[K]_J>$, where $\vec{j_c}$ is the total angular momentum of the core electrons, $\vec{K} = \vec{j_c} + \vec{l}$ defines the total orbital momentum and $\vec{J} = \vec{K} + \vec{s}$ the total kinetic momentum. Give the spectroscopic terms of the electronic configuration np^5md.