Advanced Quantum Theory
WS 13/14

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Problem Set 8 (due Monday, 09.12.2013 in the lecture)

QUESTIONS

(Q1) Which atom is bigger, hydrogen or uranium?

(Q2) Which element has the highest, which one has the lowest ionization potential, and why?

(8.1) A CARBON CONFIGURATION *(3 points)*

Let us consider the excited-state carbon configuration

$$(1\mathrm{s})^2\ (2\mathrm{s})^2\ (2\mathrm{p})\ (3\mathrm{d}).$$

(i) Show that the possible terms ${}^{2S+1}\mathrm{L}$ are

$$^1\mathrm{P},\ ^3\mathrm{P},\ ^1\mathrm{D},\ ^3\mathrm{D},\ ^1\mathrm{F},\ ^3\mathrm{F}$$

and determine their degeneracies.

(ii) Determine the fine-structure multiplet ${}^{2S+1}\mathrm{L}_J$ for the ${}^3\mathrm{P}$-term above and specify the degeneracy of each fine-structure term.

(8.2) GOOD QUANTUM NUMBERS WITH SPIN-ORBIT COUPLING *(3 points)*

In the lecture, it has been claimed that with spin-orbit coupling present, M_L and M_S are no good quantum numbers anymore but J and M_J are. In order to check this assertion show exemplarily that

(a) $[\hat{H}_2, \hat{L}_z] \neq 0,$

(b) $[\hat{H}_2, \hat{J}_z] = 0.$

Moreover, show that

(c) $[\hat{H}_2', \hat{\boldsymbol{L}}^2] = 0.$

Here, as usual,

$$\hat{\boldsymbol{L}} = \sum_{i=1}^{N} \hat{\boldsymbol{l}}_i, \quad \hat{L}_z = \boldsymbol{e}_z \cdot \hat{\boldsymbol{L}}, \quad \hat{\boldsymbol{J}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}, \quad \hat{\boldsymbol{S}} = \sum_{i=1}^{N} \hat{\boldsymbol{s}}_i, \quad \hat{J}_z = \boldsymbol{e}_z \cdot \hat{\boldsymbol{J}},$$

and (cf. lecture notes, section 3.7)

$$\hat{H}_2 = \sum_{i=1}^{N} \xi_i \hat{\boldsymbol{l}}_i \cdot \hat{\boldsymbol{s}}_i, \qquad \hat{H}_2' = A\ \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{S}}$$

are the two spin-orbit Hamiltonians discussed in the lecture.

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(8.3) SPIN-ORBIT COUPLING IN ATOMIC HYDROGEN *(4 points)*

Consider hydrogenic states $|n\ell m_\ell s m_s\rangle$. With spin-orbit coupling $\hat{\boldsymbol{\ell}} \cdot \hat{\boldsymbol{s}}$ present, the good quantum numbers are n, j, m_j, ℓ, s, with $\hat{\boldsymbol{j}} = \hat{\boldsymbol{\ell}} + \hat{\boldsymbol{s}}$. For a given n one may switch from the uncoupled basis $|\ell m_\ell s m_s\rangle$ to the coupled basis $|j m_j \ell s\rangle$,

$$|j m_j \ell s\rangle = \sum_{m_\ell} \sum_{m_s} |\ell m_\ell s m_s\rangle \langle \ell m_\ell s m_s | j m_j\rangle .$$

Using spherical harmonics $Y_\ell^m(\Omega)$ and spinors $\chi_{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $\chi_{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ this change of basis may be written as

$$\mathcal{Y}_{j\ell}^{m_j}(\Omega) := \langle \Omega | j m_j \ell s\rangle = \sum_{m_\ell} \sum_{m_s} Y_\ell^m(\Omega) \chi_{m_s} \langle \ell m_\ell s m_s | j m_j\rangle$$

where the spinors $\mathcal{Y}_{j\ell}^{m_j}(\Omega)$ are called *generalized spherical harmonics*, and $\langle \ell m_\ell s m_s | j m_j\rangle$ are Clebsch-Gordan coefficients.[1]

Determine the $\mathcal{Y}_{j\ell}^{m_j}(\Omega)$, show that they are eigenfunctions of the operator $\hat{\boldsymbol{\ell}} \cdot \hat{\boldsymbol{s}}$, and calculate their eigenvalues.

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[1] In general, the Clebsch-Gordan coefficient $\langle a\alpha \tfrac{1}{2}\beta | c\gamma\rangle$ is non-vanishing only for $\alpha + \beta = \gamma$. For $c = a + \frac{1}{2}$ and $\beta = \pm\frac{1}{2}$ it is given by $\left(\dfrac{c \pm \gamma}{2c}\right)^{1/2}$. For $c = a - \frac{1}{2}$ and $\beta = \pm\frac{1}{2}$ it is given by $\mp \left(\dfrac{c \mp \gamma + 1}{2c+2}\right)^{1/2}$.