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"Angular momentum and tensor operators", 5p
Hand-in exercises

Define all symbols used and explain your calculations in detail. You are encouraged to discuss the problems together. Each individual should hand-in a complete (and "unique") set of solutions. Please do not hesitate to contact me if you have questions or get "stuck". Good luck!

E-mail your solutions (scan and make pdf/jpg/gif...) to
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1. When evaluating $\langle l' || Y_k || l \rangle$ we used

$$Y_{lm}(0\phi) = \sqrt{\frac{[l]}{4\pi}}\delta_{m0}$$

a) Show the above relation.
b) Evaluate (in detail) $\langle l' || C^{(k)} || l \rangle$. Describe each step.
c) Evaluate (in detail) $\langle l'm' | C^{(k)}_q | lm \rangle$. Describe each step.

2. Starting from the relation
$|j_1 = 1, j_2 = 3, J = 4, M = 4\rangle = |j_1 = 1, j_2 = 3, m_1 = 1, m_2 = 3\rangle$
(*c.f.* phase conventions of Condon & Shortley),
a) calculate the Clebsch-Gordan coefficients:
$\langle 1312|1343\rangle$, $\langle 1303|1343\rangle$,
$\langle 1312|1333\rangle$ and $\langle 1303|1333\rangle$.
b) Verify the results by comparing to tabulated values of $3j$-symbols.
Hint: Use Wigner's definition of $3j$-symbols.

3. An f-electron ($l = 3$) is placed in an octaedrical crystal field.
a) Consider the spin-orbit interaction neglectable and calculate the crystal field matrix in lm_l-representation.
b) Show that three energy levels are obtained with the degeneracy 3,3 and 1, respectively. Give these three energies in terms of $A_4^0\langle r^4\rangle$.
Hint: Arrange the matrix according to m_l =0, 2, -2, 3, -1, -3 ,1.

4. Derive the complete electric quadrupole matrix (Im_I-representation, $|Im_I\rangle$ is an angular momentum eigenstate), where $I = 3/2$ and the electric quadrupole operator K_Q is given by

$$K_Q = \frac{4\pi}{5}\sum_q (-1)^q Q_q^{(2)} V_{-q}^{(2)}$$

$Q^{(2)}$ is the nuclear quadrupole operator and $V^{(2)}$ represent the electric field gradient

$$\begin{aligned} V_0^{(2)} &= \frac{1}{4}\sqrt{\frac{5}{\pi}}V_{zz} \\ V_{\pm 1}^{(2)} &= 0 \\ V_{\pm 2}^{(2)} &= \frac{1}{4}\sqrt{\frac{5}{6\pi}}\eta V_{zz} \end{aligned}$$

V_{zz} and η are constants.
Hint:

$$\langle Im_I'|Q_q^{(2)}|Im_I\rangle = \frac{Q}{2}\frac{\begin{pmatrix} I & 2 & I \\ -m_I' & 1 & m_I \end{pmatrix}(-1)^{I-m_I'}}{\begin{pmatrix} I & 2 & I \\ -I & 0 & I \end{pmatrix}}$$

where Q is another constant.

5. The matrix element $\langle\gamma SLJM|L_z + g_S S_z|\gamma SLJ+1M\rangle$ is the main element that has to be considered when the Lande factor g_J is corrected due the the Zeeman split. This follows because only the E_{j+1} level is close to E_J in a free atom or ion. Give an explicit expression for this matrix element in terms of S, L, J and M.

6. It can be shown that the average of the electric field gradient is zero for a d-electron in an octaedrical crystal field. However, quadrupole splitting can be obtained if the crystal is placed in a strong external magnetic field at a low temperature. The different m-states will then be weighted according to:

$$W_m = \exp\left(-E_m/kT\right) = \exp\left(\mu_B gBm/kT\right) = e^{mx}$$

Give an expression for $\langle \partial^2 V/\partial z^2 \rangle$ as a function of $x = \mu_B gB/kT$.
Hints: The eigenfunctions for a d-electron in an octaedrical crystal field can be written:

$$\alpha|21\rangle + \beta|2-1\rangle + \gamma\frac{1}{\sqrt{2}}[|22\rangle - |2-2\rangle]$$

where $\alpha,\ \beta,\ \gamma$ are given by W_m.

$$\langle \partial^2 V/\partial z^2 \rangle = -\frac{2e}{3 \cdot 4\pi\epsilon_0}\frac{1}{N^2}\langle rlm'|C_0^{(2)}|rlm\rangle$$

Also note that $e^x + e^{-x} = 2\cosh\left(x\right)$

7. $\bar{x}$ and $\bar{y}$ are two vectors. It is well known that also the vectorial product $\bar{z} = \bar{x} \times \bar{y}$ is a vector. Express the spherical components of $\bar{z}$ in terms of the spherical components of $\bar{x}$ and $\bar{y}$.

8. An exchange field in a ferromagnetic material acts only on the electrons spin. Calculate in the case of LS-coupling the splitting between the different $|SLJM\rangle$-states in terms of the Lande factor g_J. The Hamiltonian is given by

$$H = -\mu_B(g_J B_z^{ext} J_z + g_S B_z^{exch} S_z)$$

B^{ext} acts on J and B^{exch} on S and the fields are parallel.

9. a) Derive the Zeeman splitting in the two jj-coupled two electron states: $(s_{1/2}p_{1/2})_{J=1}$ and $(s_{1/2}p_{3/2})_{J=1}$.

Hint: Consider

$$\langle (l_1 s_1) j_1 (l_2 s_2) j_2 J' M' | H | (l_1 s_1) j_1 (l_2 s_2) j_2 J M \rangle$$

where

$$H = -\mu \cdot B = \mu_B (l_{1z} + l_{2z} + 2s_{1z} + 2s_{2z}) = \mu_B (L_z + 2S_z)$$

Arrive at

$$g_J = 1 + \frac{\langle j_1 j_2 J' || s_1 || j_1 j_2 J \rangle \langle j_1 j_2 J' || s_2 || j_1 j_2 J \rangle}{\sqrt{J(J+1)(2J+1)}}$$

where the operator equivalent $H'_m = -g_J \mu_B B J_z = -g_J \mu_B B \cdot J$ has been used. This is true within a multiplet where the elements are proportional to M. In evaluating g_J it is good to know

$$\langle l_1 s_1 j_1 || s_1 || l_1 s_1 j_1 \rangle = \frac{1}{2} \sqrt{\frac{2j_1 + 1}{j_1(j_1+1)}} [j_1(j_1+1) + s_1(s_1+1) - l_1(l_1+1)]$$

b) Verify (for this case) the g sum rule, *i.e.* the sum of the g-values for the states within a configuration with the same J is independent of the coupling between the electrons.
Hint: Start from g_J for the individual electrons.

10. Show that the one electron state $|nsljm\rangle$ with $j = 1/2$ has a spherically symmetric charge distribution.
Hint: Change to $m_l m_s$-representation and work with spherical harmonics.