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Tutorial Advanced Quantum Mechanics

Winter semester 2021/2022 — Tübingen, 6th December 2021

Problem Set 8

Problem 24 (Periodic system) (2 points)

a. (1 point) What determines the period and the group of an element?

b. (1 point) The electronic configuration of potassium ($Z = 19$) is $1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,4s^1 = [Ar]\,4s^1$ and not $[Ar]\,3d^1$ as one might expect. Can you explain why?

Problem 25 (Hund's rules) (4 points)

As an example of Hund's rules we treat the outer shell of a titanium atom, whose electron configuration is $[Ar]\,4s^2\,3d^2$. Since the 4s subshell is filled up, the relevant electrons are the two occupying the 3d subshell.

a. (2 points) How many states are there in a d shell? What is the degeneracy of the configuration d^2? How do the Hilbert spaces of the total spin ($\mathcal{H}_S$) and of the total orbital angular momentum ($\mathcal{H}_L$) decompose? Which are the antisymmetric states for the product Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_L$? What are the multiplet representations ${}^{2S+1}L$ of these states?

b. (1 point) Which of these states is the ground state according to the first two Hund rules?

c. (1 point) Take the spin-orbit interaction into consideration, and find the corresponding L–S multiplets ${}^{2S+1}L_J$. What is the ground state according to the third Hund rule?

Problem 26 (Landé projection theorem) (3 points)

Let $\mathbf{A}$ be an arbitrary vector operator, i.e. a set of three operators A_i satisfying the commutation relations $[J_i, A_j] = \mathrm{i}\hbar\varepsilon_{ijk}A_k$ with the total angular momentum $\mathbf{J}$.

a. (1 point) Retrace the steps performed in Problem 20 and prove the equation

$$[\mathbf{J}^2, [\mathbf{J}^2, A_i]] = 2\hbar^2(\mathbf{J}^2 A_i + A_i\,\mathbf{J}^2) - 4\hbar^2\mathbf{A}\cdot\mathbf{J}\,J_i.$$

b. (2 points) Show the identity

$$\langle j, m|A_i|j, m'\rangle = \frac{\langle j, m|\mathbf{A}\cdot\mathbf{J}\,J_i|j, m'\rangle}{\hbar^2 j(j+1)}.$$

Problem 27 (Magnetic dipole moment of deuteron) (14 points)

The deuteron ^{2}H (i.e. the nucleus of a deuterium atom) is a bound state of a proton and a neutron (each being a particle with spin 1/2). The total spin **I** of deuteron is hence the sum of the two spins $\mathbf{S}_\mathrm{p}$ and $\mathbf{S}_\mathrm{n}$ and of the relative orbital angular momentum **L**:

$$\mathbf{I} = \mathbf{S}_\mathrm{p} + \mathbf{S}_\mathrm{n} + \mathbf{L}.$$

a. (3 points) The deuteron has spin $i = 1$ and positive parity. Couple the proton's and neutron's spins $\mathbf{S}_\mathrm{p}$ and $\mathbf{S}_\mathrm{n}$ to $\mathbf{S} = \mathbf{S}_\mathrm{p} + \mathbf{S}_\mathrm{n}$, and then couple **S** to the orbital angular momentum **L**. Give all possible multiplets $^{2S+1}L_1$ and show that the most general state vector of the deuteron can be written as

$$|^2\mathrm{H}\rangle = \alpha_s|^3S_1\rangle + \alpha_d|^3D_1\rangle, \qquad |\alpha_s|^2 + |\alpha_d|^2 = 1.$$

Of which angular momentum operators is this state an eigenstate?

Hint: Because of parity only *even* values of ℓ are allowed.

The nuclear magnetic moment is defined as the expectation value

$$\mu = \langle i, m_i = i|\mu_3|i, m_i = i\rangle$$

of the z component of the magnetic moment operator

$$\boldsymbol{\mu} = \frac{\mathbf{L}}{2\hbar}\,\mu_\mathrm{N} + g_\mathrm{p}\frac{\mathbf{S}_\mathrm{p}}{\hbar}\,\mu_\mathrm{N} + g_\mathrm{n}\frac{\mathbf{S}_\mathrm{n}}{\hbar}\,\mu_\mathrm{N},$$

where $\mu_\mathrm{N} = e\hbar/(2m_\mathrm{p}) = 31{,}5\,\mathrm{neV/T}$ is the nuclear magneton, and the g-factors of proton and neutron are $g_\mathrm{p} = 5{,}5857$ and $g_\mathrm{n} = -3{,}8261$.

b. (2 points) Show that the deuteron's magnetic moment can be written as

$$\mu = \frac{1}{2\hbar}\,\langle^2\mathrm{H}|\boldsymbol{\mu}\cdot\mathbf{I}|^2\mathrm{H}\rangle \equiv \frac{1}{2\hbar}\,\langle\boldsymbol{\mu}\cdot\mathbf{I}\rangle.$$

(From now on we will use the notation $\langle ... \rangle$ to represent expectation values $\langle^2\mathrm{H}|\,...\,|^2\mathrm{H}\rangle$.)

c. (2 points) Use the explicit definition of the operator $\boldsymbol{\mu}$ and bring the result of part **b.** into the form

$$\frac{\mu}{\mu_\mathrm{N}} = \frac{1}{4\hbar^2}\Big[(g_\mathrm{p}+g_\mathrm{n})\langle\mathbf{I}\cdot\mathbf{S}\rangle + \langle\mathbf{I}\cdot\mathbf{L}\rangle + (g_\mathrm{p}-g_\mathrm{n})\langle\mathbf{I}\cdot(\mathbf{S}_\mathrm{p}-\mathbf{S}_\mathrm{n})\rangle\Big].$$

d. (3 points) Rewrite the products $\mathbf{I}\cdot\mathbf{S}$ and $\mathbf{I}\cdot\mathbf{L}$ as suitable combinations of $\mathbf{I}^2$, $\mathbf{S}^2$ and $\mathbf{L}^2$, and show

$$\frac{\mu}{\mu_\mathrm{N}} = \frac{g_\mathrm{p}+g_\mathrm{n}}{2} + \frac{1-g_\mathrm{p}-g_\mathrm{n}}{8\hbar^2}\langle\mathbf{L}^2\rangle + \frac{g_\mathrm{p}-g_\mathrm{n}}{4\hbar^2}\langle\mathbf{I}\cdot(\mathbf{S}_\mathrm{p}-\mathbf{S}_\mathrm{n})\rangle.$$

e. (3 points) Explain (without calculations) why the term $\langle\mathbf{I}\cdot(\mathbf{S}_\mathrm{p}-\mathbf{S}_\mathrm{n})\rangle$ vanishes. Work out the remaining expectation value and show

$$\frac{\mu}{\mu_\mathrm{N}} = \frac{g_\mathrm{p}+g_\mathrm{n}}{2} + \frac{3}{4}\,|\alpha_d|^2(1-g_\mathrm{p}-g_\mathrm{n}).$$

f. (1 point) Compare the result for the magnetic moment to the experimental value $0.85744\,\mu_\mathrm{N}$ and determine $|\alpha_d|^2$.