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Institute for Theoretical Physics III, University of Stuttgart   WS 2024/25

Problem 4.1: Clebsch-Gordan coefficients and spin-orbit coupling   [Oral | 4 (+2 bonus) pt(s)]

ID: ex_clebsch_gordan_coefficients_spin_orbit_coupling:aqt2425

Learning objective

In this problem you will apply the angular momentum addition theorem. As an important use case, we consider the spin-orbit coupling in the hydrogen atom, which is the leading relativistic correction.

The spin-orbit coupling between the electron's spin $\boldsymbol{S}$ and the orbital angular momentum $\mathbf{L}$ for a hydrogen atom is given by the Hamiltonian

$$H_{\text{LS}} = f(r)\, \boldsymbol{L} \cdot \boldsymbol{S} = f(r) \sum_{\alpha=x,y,z} L_\alpha \otimes S_\alpha \,, \tag{1}$$

where $f(r) = e^2/2m_e^2 c^2 r^3$. The spin-orbit coupling can be seen as a perturbation to the non-relativistic Hamiltonian $H_0 = \boldsymbol{P}^2/2m - e^2/r$ of the hydrogen atom.

a) Define the total angular momentum operator as   **2**$^{\text{pt(s)}}$

$$\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S} = \boldsymbol{L} \otimes \mathbb{1} + \mathbb{1} \otimes \boldsymbol{S} \tag{2}$$

and show that $\boldsymbol{J}^2$ and J_z commute both with H_0 and H_{LS}.

b) Consider the subspace with orbital angular momentum ℓ and spin s. We can write the eigenstates   **2**$^{\text{pt(s)}}$
$|j, m\rangle$ of $\boldsymbol{J}^2$ and J_z as linear combinations of L_z- and S_z-eigenstates $|m_\ell, m_s\rangle = |\ell, m_\ell\rangle \otimes |s, m_s\rangle$,

$$|j, m\rangle = \sum_{m_\ell, m_s} c(m_\ell, m_s; j, m)\, |m_\ell, m_s\rangle \,. \tag{3}$$

The coefficients c are called *Clebsch-Gordan coefficients*. Due to their ubiquity in quantum physics there are comprehensive tables available, e.g.,

http://pdg.lbl.gov/2011/reviews/rpp2011-rev-clebsch-gordan-coefs.pdf.

Use this table to write down the change of basis (3) in the subspace with $\ell = 1$ and $s = 1/2$ explicitely.

*c) Derive the Clebsch-Gordan coefficients in b) by hand.   **+2**$^{\text{pt(s)}}$

Hint: Start with the *stretched state* $|j = 3/2, m_j = 3/2\rangle$ and use the ladder operator $J_- = J_x - iJ_y$ which acts as

$$J_- |j, m\rangle = \hbar\sqrt{j(j+1) - m(m-1)}\, |j, m-1\rangle \,. \tag{4}$$

Problem 4.2: Fine structure of the hydrogen atom   [Written | 4 (+1 bonus) pt(s)]

ID: ex_fine_structure_hydrogen_atom:aqt2425

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Learning objective

Here, we can apply the previously studied perturbation theory to derive the leading order energy corrections to the hydrogen atom due to spin-orbit coupling. This problem combines both topics, perturbation theory and addition of angular momenta, in one task.

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a) Calculate the energy corrections to the $2p$ levels of the hydrogen atom (with the principal quantum number $n = 2$ and orbital angular momentum $l = 1$) arising from the spin-orbit coupling within the first order of perturbation theory. **4**pt(s)

   Hint: Consider the coupling Hamiltonian H_{LS} from Problem 4.1 as a perturbation to the unperturbed Hamiltonian H_0 of the hydrogen atom such that $H = H_0 + H_{\text{LS}}$. Show that the states with total angular momentum J are eigenstates of $\mathbf{L} \cdot \mathbf{S}$. The first order energy corrections according to stationary perturbation theory can therefore in our case be calculated as

$$\Delta E^{(1)} = \langle \psi_{j,m} | H_{\text{LS}} | \psi_{j,m} \rangle. \tag{5}$$

   For the radial part of the matrix elements use $\langle \psi_{2,1,m} | 1/r^3 | \psi_{2,1,m} \rangle = 1/24a_0^3$, where $|\psi_{2,1,m}\rangle$ is an eigenfunction of H_0 and $a_0 = \hbar^2/m_e e^2$ is the Bohr radius.

*b) Derive the validity of equation (5) from the general perturbation theory. **+1**pt(s)

Problem 4.3: System of three interacting spin-1/2 particles [**Oral** | 4 pt(s)]

ID: ex_system_three_interacting_spin_one_half_particles:aqt2425

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Learning objective

In this exercise you will be going through an instructive example of a few particle spin system. The task is to show that using the theorem of addition of angular momentum, it is possible to analytically determine the ground state of three spins coupled antiferromagnetically.

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Let us consider a system composed of three spin-1/2 particles.

a) What is the dimension of the Hilbert space? **2**pt(s)

   The total spin operator can be defined as $\mathbf{S} = \sum_{i=1}^{3} \mathbf{S}^{(i)}$ and its z projection as $S_z = \sum_{i=1}^{3} S_z^{(i)}$. What are the eigenvalues and eigenstates of $\mathbf{S}^2$ and S_z? Express the states in the spin-1/2 basis $\left| S_z^{(1)}, S_z^{(2)}, S_z^{(3)} \right\rangle$.

b) The Hamiltonian of the system is **2**pt(s)

$$H = J \sum_{i=1}^{3} \mathbf{S}^{(i)} \cdot \mathbf{S}^{(i+1)}, \qquad J > 0.$$

   Here we assume a periodic system (for $i = 3$ take $i + 1 = 1$). Calculate the eigenstates and eigenenergies of this Hamiltonian.

   Hint: Rewrite H as a function of S^2 and $S^{(i)2}$.