Prof. Dr. Hans-Peter Büchler

Institute for Theoretical Physics III, University of Stuttgart

February 1st, 2022

WS 2021/22

Problem 14.1: Clebsch-Gordan coefficients and spin-orbit coupling   [Oral] (4 pts.)

↪ ID: ex_clebsch_gordan_coefficients_spin_orbit_coupling:qm2122

> **Learning objective**
>
> In this problem you 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. In particular, you practice the construction of the new basis states for a fixed total angular momentum.

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

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

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

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

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 $|j, m\rangle$ 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 $s = \frac{1}{2}$ explicitly.

c) The spin-orbit coupling Eq. (1) lifts the degeneracy of the $n = 2$ manifold of the hydrogen atom; this manifold is spanned by the two states of the $2s$-orbital

$$\left|n = 2, \ell = 0, m_\ell = 0;\, s = \tfrac{1}{2}, m_s \in \{-\tfrac{1}{2}, +\tfrac{1}{2}\}\right\rangle \tag{4}$$

and the 6 states of the $2p$-orbitals

$$\left|n = 2, \ell = 1, m_\ell \in \{-1, 0, +1\};\, s = \tfrac{1}{2}, m_s \in \{-\tfrac{1}{2}, +\tfrac{1}{2}\}\right\rangle \,. \tag{5}$$

Use the addition of angular momentum to derive a basis $|n, \ell, s, j, m_j\rangle$ of the $n = 2$ manifold such that the spin-orbit coupling term $\boldsymbol{L} \cdot \boldsymbol{S}$ in Eq. (1) is diagonal.

Hint: Rewrite the Hamiltonian in terms of $\boldsymbol{J}^2$, $\boldsymbol{L}^2$ and $\boldsymbol{S}^2$.

d) Finally, combine your results from b) and c) to determine the energy shifts due to Eq. (1) explicitly in first order perturbation theory. Show that the degeneracy of the $n = 2$ manifold of H_0 is lifted into three non-degenerate energies and determine the remaining degeneracy in each subspace.

Explain why you have to use perturbation theory although you diagonalized $\boldsymbol{L} \cdot \boldsymbol{S}$ successfully.

Hint: To evaluate the radial part of the matrix elements, use

$$\langle 2, 1, m_\ell | \frac{1}{r^3} | 2, 1, m_\ell \rangle_{n\ell m_\ell} = \frac{1}{24a_0^3} \tag{6}$$

where $a_0 = \hbar^2 / m_e e^2$ is the Bohr radius.

Problem 14.2: Identical fermions in a potential well [Oral] (3 pts.)
↪ ID: ex_identical_fermions_potential_well:qm2122

> **Learning objective**
>
> In the lecture you learned that the wave function of multiple fermions must be antisymmetric under the exchange of particles. Here you study the consequences of this rule by means of a simple toy model. In particular, you elaborate on the consequences of the antisymmetry in the presence of interactions between the fermions.

We consider two identical spin-$\frac{1}{2}$ fermions in a one-dimensional potential given by

$$V(x) = \begin{cases} 0 & |x| \leq 1 \\ \infty & \text{otherwise} . \end{cases} \tag{7}$$

The (dimensionless) single-particle Hamiltonian for the ith particle is given by

$$H^{(i)} = -\frac{1}{2}\partial_{x_i}^2 + V(x_i) . \tag{8}$$

a) Explain why we can treat the spatial motion and the spin dynamics separately, that is, explain why we can write the single-particle eigenstates as a product of spatial- and spin wave functions.

Write down the spatial wave functions and eigenenergies of the two single-particle eigenstates that are lowest in energy.

b) Determine the ground state and the ground state energy of a two-fermion system with Hamiltonian $H = \sum_{i=1}^2 H^{(i)}$ in the following two cases:

   i. For a spin state that is *antisymmetric* under exchange of the two fermions, i.e., the singlet state $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$.

   ii. For a spin state that is *symmetric* under exchange of the two fermions, i.e., one of the triplet states $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$ or $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$.

c) Examine the influence of a contact-interaction between the two fermions which is described by the interaction potential $\lambda\,\delta(x_1 - x_2)$ with strength $\lambda \in \mathbb{R}$. To this end, calculate the energy correction in first order perturbation theory (assuming $|\lambda| \ll 1$) for both the singlet state and the triplet states.

Explain why the perturbative result for the triplet states is correct for arbitrary λ.