

Additional exercises

Quantum Physics 2

Exercises 1-3 belong to Chapter 4.4

Exercise 4 belongs to Chapter 6.3

Exercise 5 belongs to Chapter 6.5

Exercise 6 belongs to Chapter 6.4

Exercise 7 belongs to Chapter 7

Exercise 8 belongs to Chapter 9.1

Exercise 1: **addition of angular momentum**

- a) Explicitly construct the states of total spin for a system of two spin- $\frac{1}{2}$ particles
- b) Use the table (given below) to verify the Clebsch-Gordan coefficients
- c) Construct the $|l_1, l_2; l, m\rangle = |1, 1; 0, 0\rangle$ state explicitly and by using the table

Table 1: Clebsch-Gordan coefficients $\langle j_1, \frac{1}{2}; m_1, m_2 | jm \rangle$

j	$m_2 = \frac{1}{2}$	$m_2 = -\frac{1}{2}$
$j_1 + \frac{1}{2}$	$\left(\frac{j_1 + m + \frac{1}{2}}{2j_1 + 1} \right)^{\frac{1}{2}}$	$\left(\frac{j_1 - m + \frac{1}{2}}{2j_1 + 1} \right)^{\frac{1}{2}}$
$j_1 - \frac{1}{2}$	$-\left(\frac{j_1 - m + \frac{1}{2}}{2j_1 + 1} \right)^{\frac{1}{2}}$	$\left(\frac{j_1 + m + \frac{1}{2}}{2j_1 + 1} \right)^{\frac{1}{2}}$

Table 2: Clebsch-Gordan coefficients $\langle j_1, 1; m_1, m_2 | jm \rangle$

j	$m_2 = 1$	$m_2 = 0$	$m_2 = -1$
$j_1 + 1$	$\left[\frac{(j_1 + m)(j_1 + m + 1)}{(2j_1 + 1)(2j_1 + 2)} \right]^{\frac{1}{2}}$	$\left[\frac{(j_1 - m + 1)(j_1 + m + 1)}{(2j_1 + 1)(j_1 + 1)} \right]^{\frac{1}{2}}$	$\left[\frac{(j_1 - m)(j_1 - m + 1)}{(2j_1 + 1)(2j_1 + 2)} \right]^{\frac{1}{2}}$
j_1	$-\left[\frac{(j_1 + m)(j_1 - m + 1)}{2j_1(j_1 + 1)} \right]^{\frac{1}{2}}$	$\frac{m}{[j_1(j_1 + 1)]^{\frac{1}{2}}}$	$\left[\frac{(j_1 - m)(j_1 + m + 1)}{2j_1(j_1 + 1)} \right]^{\frac{1}{2}}$
$j_1 - 1$	$\left[\frac{(j_1 - m)(j_1 - m + 1)}{2j_1(2j_1 + 1)} \right]^{\frac{1}{2}}$	$-\left[\frac{(j_1 - m)(j_1 + m)}{j_1(2j_1 + 1)} \right]^{\frac{1}{2}}$	$\left[\frac{(j_1 + m)(j_1 + m + 1)}{2j_1(2j_1 + 1)} \right]^{\frac{1}{2}}$

Exercise 2: **Clebsch-Gordan coefficients (CGC)**

- a) The CGC possess the symmetry property

$$\langle l_1, l_2; m_1, m_2 | l, m \rangle = (-1)^{l-l_1-l_2} \langle l_2, l_1; m_2, m_1 | l, m \rangle. \quad (1)$$

Use this property to show that for two electrons in equivalent orbitals the total orbital angular momentum quantum number l must have even values for singlet (spin) states and odd values for triplet states.

- b) Prove the recurrence relation

$$\langle l_1, l_2; m_1 - 1, m_2 + 1 | l, l \rangle = -\sqrt{\frac{l_2(l_2 + 1) - m_2(m_2 + 1)}{l_1(l_1 + 1) - m_1(m_1 - 1)}} \langle l_1, l_2; m_1, m_2 | l, l \rangle \quad (2)$$

- c) Verify this recurrence relation explicitly for the coefficient $\langle l_1, l_2; m_1, m_2 | l, l \rangle = \langle 1, \frac{1}{2}; 1, -\frac{1}{2} | \frac{1}{2}, \frac{1}{2} \rangle$ using the table on the next page.

34. CLEBSCH-GORDAN COEFFICIENTS, SPHERICAL HARMONICS, AND d FUNCTIONS

Note: A square-root sign is to be understood over *every* coefficient, e.g., for $-8/15$ read $-\sqrt{8/15}$.

Notation:

J	J	...
M	M	...
m_1	m_2	
m_1	m_2	Coefficients
.	.	
.	.	

$1/2 \times 1/2$
 $Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos \theta$
 $2 \times 1/2$
 $Y_1^1 = -\sqrt{\frac{3}{8\pi}} \sin \theta e^{i\phi}$
 $1 \times 1/2$
 $Y_2^0 = \sqrt{\frac{5}{4\pi}} \left(\frac{3}{2} \cos^2 \theta - \frac{1}{2} \right)$
 $1 \times 1/2$
 $Y_2^1 = -\sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{i\phi}$
 2×1
 $Y_2^2 = \frac{1}{4} \sqrt{\frac{15}{2\pi}} \sin^2 \theta e^{2i\phi}$
 $3/2 \times 1/2$
 $Y_\ell^m = (-1)^m Y_\ell^{m*}$
 $d_{m,0}^\ell = \sqrt{\frac{4\pi}{2\ell+1}} Y_\ell^m e^{-im\phi}$
 $d_{m',m}^j = (-1)^{m-m'} d_{m,m'}^j = d_{-m,-m'}^j$
 $3/2 \times 3/2$
 $d_{0,0}^1 = \cos \theta$
 $d_{1/2,1/2}^{1/2} = \cos \frac{\theta}{2}$
 $d_{1,1}^1 = \frac{1 + \cos \theta}{2}$
 $d_{1/2,-1/2}^{1/2} = -\sin \frac{\theta}{2}$
 $d_{1,0}^1 = -\frac{\sin \theta}{\sqrt{2}}$
 $d_{1,-1}^1 = \frac{1 - \cos \theta}{2}$
 2×2
 $d_{3/2,3/2}^{3/2} = \frac{1 + \cos \theta}{2} \cos \frac{\theta}{2}$
 $d_{3/2,1/2}^{3/2} = -\sqrt{3} \frac{1 + \cos \theta}{2} \sin \frac{\theta}{2}$
 $d_{3/2,-1/2}^{3/2} = \sqrt{3} \frac{1 - \cos \theta}{2} \cos \frac{\theta}{2}$
 $d_{3/2,-3/2}^{3/2} = -\frac{1 - \cos \theta}{2} \sin \frac{\theta}{2}$
 $d_{1/2,1/2}^{3/2} = \frac{3 \cos \theta - 1}{2} \cos \frac{\theta}{2}$
 $d_{1/2,-1/2}^{3/2} = -\frac{3 \cos \theta + 1}{2} \sin \frac{\theta}{2}$
 $d_{2,2}^2 = \left(\frac{1 + \cos \theta}{2} \right)^2$
 $d_{2,1}^2 = -\frac{1 + \cos \theta}{2} \sin \theta$
 $d_{2,0}^2 = \frac{\sqrt{6}}{4} \sin^2 \theta$
 $d_{2,-1}^2 = -\frac{1 - \cos \theta}{2} \sin \theta$
 $d_{2,-2}^2 = \left(\frac{1 - \cos \theta}{2} \right)^2$
 $d_{1,1}^2 = \frac{1 + \cos \theta}{2} (2 \cos \theta - 1)$
 $d_{1,0}^2 = -\sqrt{\frac{3}{2}} \sin \theta \cos \theta$
 $d_{1,-1}^2 = \frac{1 - \cos \theta}{2} (2 \cos \theta + 1)$
 $d_{0,0}^2 = \left(\frac{3}{2} \cos^2 \theta - \frac{1}{2} \right)$

Figure 34.1: The sign convention is that of Wigner (*Group Theory*, Academic Press, New York, 1959), also used by Condon and Shortley (*The Theory of Atomic Spectra*, Cambridge Univ. Press, New York, 1953), Rose (*Elementary Theory of Angular Momentum*, Wiley, New York, 1957), and Cohen (*Tables of the Clebsch-Gordan Coefficients*, North American Rockwell Science Center, Thousand Oaks, Calif., 1974). The coefficients here have been calculated using computer programs written independently by Cohen and at LBNL.

Exercise 3: spin operators

- a) Write down the spin operators $\mathbf{S}^2, S_x, S_y, S_z$ in matrix representation, i.e. using the basis $|s, m\rangle$, for the case of spin- $\frac{1}{2}$ and spin- $\frac{3}{2}$
- b) Check the commutation relations for $[S_x, S_y]$ and $s = \frac{3}{2}$.
- c) Construct spin- $\frac{1}{2}$ states that have $\langle \mathbf{S} \cdot \hat{\mathbf{n}} \rangle = \pm \frac{\hbar}{2}$ for arbitrary direction $\hat{\mathbf{n}}$ (see also problem 4.30 of the book)

Exercise 4: Fine structure of hydrogenic atoms

- a) Consider a Hamiltonian $H = H_0 + \lambda H'$, with $\lambda H'$ a small perturbation. Show that in (non-degenerate) perturbation theory the first order correction to the unperturbed, discrete energy level $E_n^{(0)}$ ($H_0|\phi_n^{(0)}\rangle = E_n^{(0)}|\phi_n^{(0)}\rangle$) is given by

$$E_n^{(1)} = \langle \phi_n^{(0)} | H' | \phi_n^{(0)} \rangle$$

and the second order by

$$E_n^{(2)} = \sum_{m \neq n} \frac{|H'_{mn}|^2}{E_n^{(0)} - E_m^{(0)}}$$

where $H'_{mn} = \langle \phi_m^{(0)} | H' | \phi_n^{(0)} \rangle$.

- b) Apply this to evaluate the first order corrections to the energy levels (the so-called fine structure) of a hydrogenic atom, that arise due to relativistic corrections. Confirm that the answer for the total first order correction is

$$E_n^{(1)} = E_n^{(0)} \frac{(Z\alpha)^2}{n^2} \left(\frac{n}{j + \frac{1}{2}} - \frac{3}{4} \right)$$

where $\alpha = e^2/(4\pi\epsilon_0\hbar c)$.

The Hamiltonian is written in this case as (taking $\mu = m$):

$$\begin{aligned} H_0 &= \frac{\mathbf{p}^2}{2m} + V(r) \\ V(r) &= -\frac{Ze^2}{(4\pi\epsilon_0)r} \\ H' &= H'_1 + H'_2 + H'_3 \\ H'_1 &= -\frac{\mathbf{p}^4}{8m^3c^2} \\ H'_2 &= \frac{1}{2m^2c^2} \frac{1}{r} \frac{dV(r)}{dr} \mathbf{L} \cdot \mathbf{S} \\ H'_3 &= \frac{\pi\hbar^2}{2m^2c^2} \frac{Ze^2}{4\pi\epsilon_0} \delta(\mathbf{r}) \end{aligned}$$

(continued on next page)

One can use the following results:

$$\begin{aligned}
E_n^{(0)} &= -\frac{Z^2 e^2}{4\pi\epsilon_0 a_0} \frac{1}{2n^2} \\
a_0 &= \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2} \\
\langle \phi_{nlm}^{(0)} | \frac{1}{r} | \phi_{nlm}^{(0)} \rangle &= \frac{Z}{n^2 a_0} \\
\langle \phi_{nlm}^{(0)} | \frac{1}{r^2} | \phi_{nlm}^{(0)} \rangle &= \frac{Z^2}{n^3 a_0^2 (l + \frac{1}{2})} \\
\langle \phi_{nlm}^{(0)} | \frac{1}{r^3} | \phi_{nlm}^{(0)} \rangle &= \frac{Z^3}{n^3 a_0^3 l(l + \frac{1}{2})(l + 1)} \quad (l \neq 0) \\
|\phi_{n00}^{(0)}(\mathbf{r} = 0)|^2 &= \frac{Z^3}{\pi a_0^3 n^3}
\end{aligned}$$

Estimate the order of magnitude of the corrections.

Exercise 5: Hyperfine structure

The hyperfine structure of the hydrogen atom is due to the interactions of the magnetic moments of the electron and the proton: $\boldsymbol{\mu}_e = -g_s e \mathbf{S} / (2m_e)$ and $\boldsymbol{\mu}_p = g_p e \mathbf{I} / (2M_p)$, where $g_s = 2$, $g_p = 5.5883$ and \mathbf{I} is the nuclear spin. The interaction term for s -waves is given by:

$$W_{hf} = -\frac{2}{3\epsilon_0 c^2} \boldsymbol{\mu}_e \cdot \boldsymbol{\mu}_p \delta^3(\mathbf{r}).$$

a) Show that the energy shift caused by this W_{hf} , in first order perturbation theory, is given by

$$E_{hf}^{(1)} = |E_n^{(0)}| \frac{4\alpha^2}{3n} g_p \frac{m_e}{M_p} [F(F+1) - S(S+1) - I(I+1)],$$

where the total angular momentum is $\mathbf{F} = \mathbf{J} + \mathbf{I}$, $\alpha = e^2 / (4\pi\epsilon_0 \hbar c)$ and

$$\begin{aligned}
E_n^{(0)} &= -\frac{m_e \alpha^2 c^2}{2n^2}, \\
|\phi_{n00}^{(0)}(\mathbf{r} = 0)|^2 &= \frac{1}{\pi} \left(\frac{m_e \alpha c}{n \hbar} \right)^3.
\end{aligned}$$

b) Consider the ground state. How many levels are there? What is the degeneracy of each level?

Recall that the fine structure energy shift is given in first order by:

$$E_f^{(1)} = E_n^{(0)} \left(\frac{\alpha}{n} \right)^2 \left(\frac{n}{j + \frac{1}{2}} - \frac{3}{4} \right).$$

c) Compare the magnitudes of the hyperfine *splitting* of the ground state and the fine *splitting* of the $n = 2$ states. What is the main reason that the hyperfine splitting is smaller than the fine splitting? Give an order of magnitude estimate of their ratio.

Exercise 6: Hyperfine structure and Zeeman splitting

Taking into account the nuclear spin leads to the hyperfine splitting. If a constant, uniform magnetic field ($|\mathbf{B}| = B$) is applied in the \hat{z} direction, then because of the nuclear spin an additional Zeeman interaction term W_Z is added to the standard Zeeman term in the Hamiltonian, which becomes:

$$W_Z = \frac{e}{2m_e}(L_z + 2S_z - g_p \frac{m_e}{M_p} I_z)B.$$

This additional term due to the nuclear spin can however be neglected, such that for the ground state

$$W_Z \approx \frac{eS_z B}{m_e}.$$

Despite its approximate independence of the nuclear spin, W_z can affect the various hyperfine structure levels differently. Determine the energy shifts of the hyperfine structure levels of the ground state for an arbitrary magnetic field magnitude and check the limits of weak and strong magnetic field against their perturbation theory expectations.

Exercise 7: Variational principle and hydrogen atom

- a) Variational method: show that $E[\phi_T] = \langle \phi_T | H | \phi_T \rangle / \langle \phi_T | \phi_T \rangle$ yields an upper bound to the exact ground state energy E_0 for any trial wave function ϕ_T .
- b) Apply the variational method to the ground state of the hydrogen atom (without relativistic corrections), using as trial function $\phi_T = Ce^{-\alpha r}$ and compare it to the result of problem 7.13 of the book.
- c) The variational method can also be applied to excited states, by taking care of orthogonality with respect to lower energy states. Can one be sure again that one will obtain an upper bound to the energy of the excited state? Explain how symmetry can be exploited in this case.

Exercise 8: Time dependence of a two-level system

Consider a two-level system with stationary states a and b with unperturbed energies $E_a^{(0)}$ and $E_b^{(0)}$ and corresponding eigenfunctions $\phi_a^{(0)}$ and $\phi_b^{(0)}$, respectively. Assume $E_b^{(0)} > E_a^{(0)}$, such that the Bohr angular frequency $\omega_{ba} \equiv (E_b^{(0)} - E_a^{(0)})/\hbar$ is positive. A time-independent perturbation V is switched on at time $t = 0$.

a) Write down the coupled set of equations for the coefficients $c_a(t)$ and $c_b(t)$ of the wave function of the system:

$$\psi(t) = c_a(t)\psi_a^{(0)} \exp(-iE_a^{(0)}t/\hbar) + c_b(t)\psi_b^{(0)} \exp(-iE_b^{(0)}t/\hbar).$$

Note that we have suppressed any spatial coordinate dependence for simplicity.

b) Show that these equations are solved exactly under the initial condition that the system is in the ground state for $t < 0$, by

$$\begin{aligned} c_a(t) &= e^{-i\alpha t} \left(\cos \beta t + i \frac{\gamma}{\beta} \sin \beta t \right), \\ c_b(t) &= -i \frac{V_{ba}}{\hbar \beta} e^{-i(\alpha - \omega_{ba})t} \sin \beta t, \end{aligned}$$

where

$$\begin{aligned} \alpha &= \frac{1}{2\hbar} (V_{aa} + V_{bb} + \hbar\omega_{ba}), \\ \beta &= \frac{1}{\hbar} \left[\frac{1}{4} (V_{bb} - V_{aa} + \hbar\omega_{ba})^2 + |V_{ba}|^2 \right]^{\frac{1}{2}}, \\ \gamma &= \alpha - \frac{V_{aa}}{\hbar}, \end{aligned}$$

and $V_{ij} = \langle \psi_i^{(0)} | V | \psi_j^{(0)} \rangle$ for $i, j = a, b$.

c) Compare this exact solution to the first-order perturbation theory result.

d) Consider the degenerate case $E = E_b^{(0)} = E_a^{(0)}$ for the simplified case in which $V_{aa} = 0 = V_{bb}$, and interpret the result.

e) Consider again the nondegenerate case $E_b^{(0)} > E_a^{(0)}$ and now a periodic perturbation of the form:

$$V(t) = A e^{i\omega t} + A^\dagger e^{-i\omega t},$$

with A time independent. Solve for $c_a(t)$ and $c_b(t)$ in the rotating wave approximation, which means dropping all terms that oscillate with frequencies larger than $\Delta\omega = \omega - \omega_{ba}$, assuming $\Delta\omega \ll \omega, \omega_{ba}$.

f) Compare this answer to the first-order perturbation theory result.

g) Consider the degenerate case $E = E_b^{(0)} = E_a^{(0)}$ and compare the result with that of question d.