

## 4<sup>th</sup> Exercise sheet for Advanced Quantum Mechanics in WS16

### First-Order (Rayleigh–Schrödinger) Perturbation Theory

#### Exercise 10 *Review of first-order perturbation theory*

Let  $H$  be a Hamiltonian that consists of another Hamiltonian  $H_0$ , whose Schrödinger equation  $H_0|\Psi_a\rangle = E_a|\Psi_a\rangle$  we already solved, and a part that we will call *perturbation*  $H_1$ :

$$H = H_0 + \epsilon H_1. \quad (1)$$

In general we are not able to find exact solutions of the Schrödinger equation of  $H|\Psi'_a\rangle = E'_a|\Psi'_a\rangle$ . Instead we assume the  $\epsilon$  to be small compared to all relevant scales, such that we can hope to find an approximate spectrum, i.e. we make the *perturbative ansatz*

$$|\Psi'_a\rangle = |\Psi_a\rangle + |\delta\Psi_a\rangle, \quad |\delta\Psi_a\rangle = \sum_{n=1}^{\infty} \epsilon^n |\psi_{a,n}\rangle, \quad (2)$$

$$E'_a = E_a + \delta E_a, \quad \delta E_a = \sum_{n=1}^{\infty} \epsilon^n E_{a,n}. \quad (3)$$

- a) Write down the Schrödinger equation for  $H$  up to first-order in  $\epsilon$  and derive an expression for the energy shift  $E_{a,1}$ .

*Hint:* Make use of the orthonormality of the states, i.e.  $\langle\Psi_b|\Psi_a\rangle = \delta_{ba}$ , and the hermiticity of  $H_0$ .

- b) Now assume that some states  $a \neq b$  are degenerate. Show that this leads to

$$\langle\Psi_b|H_1|\Psi_a\rangle = 0, \quad (4)$$

and explain why this equation is not necessarily fulfilled. Argue why the derivation is wrong in general.

- c) We now relabel our unperturbed states as  $|\Psi_a^{(n)}\rangle$  where  $a$  denotes states belonging to different energies and  $n$  labels the degenerate states belonging to the same energy  $E_a$ . Show that the derivation in b) is correct if the eigenstates of  $H_0$  in the degenerate subspace are chosen as

$$|\Phi_a^{(n)}\rangle = \sum_m u_m^{(n)} |\Psi_a^{(m)}\rangle, \quad (5)$$

where  $u_m^{(n)}$  are the components of orthonormal eigenvectors  $\mathbf{u}^{(n)}$  satisfying

$$\sum_m A_{pm} u_m^{(n)} = E_{a,1}^{(n)} u_p^{(n)}, \quad A_{pm} = \langle\Psi_a^{(p)}|H_1|\Psi_a^{(m)}\rangle. \quad (6)$$

**Exercise 11**     *Application: Anomalous Zeeman effect and Paschen–Back effect*

An electron shall be described by the following Hamiltonian,

$$H = 2A\mathbf{L} \cdot \mathbf{S} + B(L_z + 2S_z), \quad (7)$$

where  $\mathbf{L}$  is the orbital angular momentum and  $\mathbf{S}$  the spin operator. The first term in  $H$  represents the spin-orbit interaction of the Hydrogen atom, once the  $\mathbf{r}$ -dependence of  $A$  is neglected, while the second term corresponds to the interaction with an external magnetic field along the  $z$ -axis.

- a) Consider the case  $A \ll B$ , which is known as the Paschen–Back effect, such that the first term in  $H$  can be considered as a perturbation of the second one. List the spectrum of the unperturbed states for the case  $l = 1$  and calculate the shifts of the energy due to the term  $2A\mathbf{L} \cdot \mathbf{S}$  in first-order perturbation theory.
- b) Consider the opposite case  $B \ll A$ , which is known as the anomalous Zeeman effect, such that the perturbation is now given by the term  $B(L_z + 2S_z)$ . List the spectrum of the unperturbed states for the case  $l = 1$  and calculate the shifts of the energy due to this term.

*Hint:* To calculate  $S_z|j, m_j\rangle$  make use of Clebsch–Gordan coefficients given on the next page.

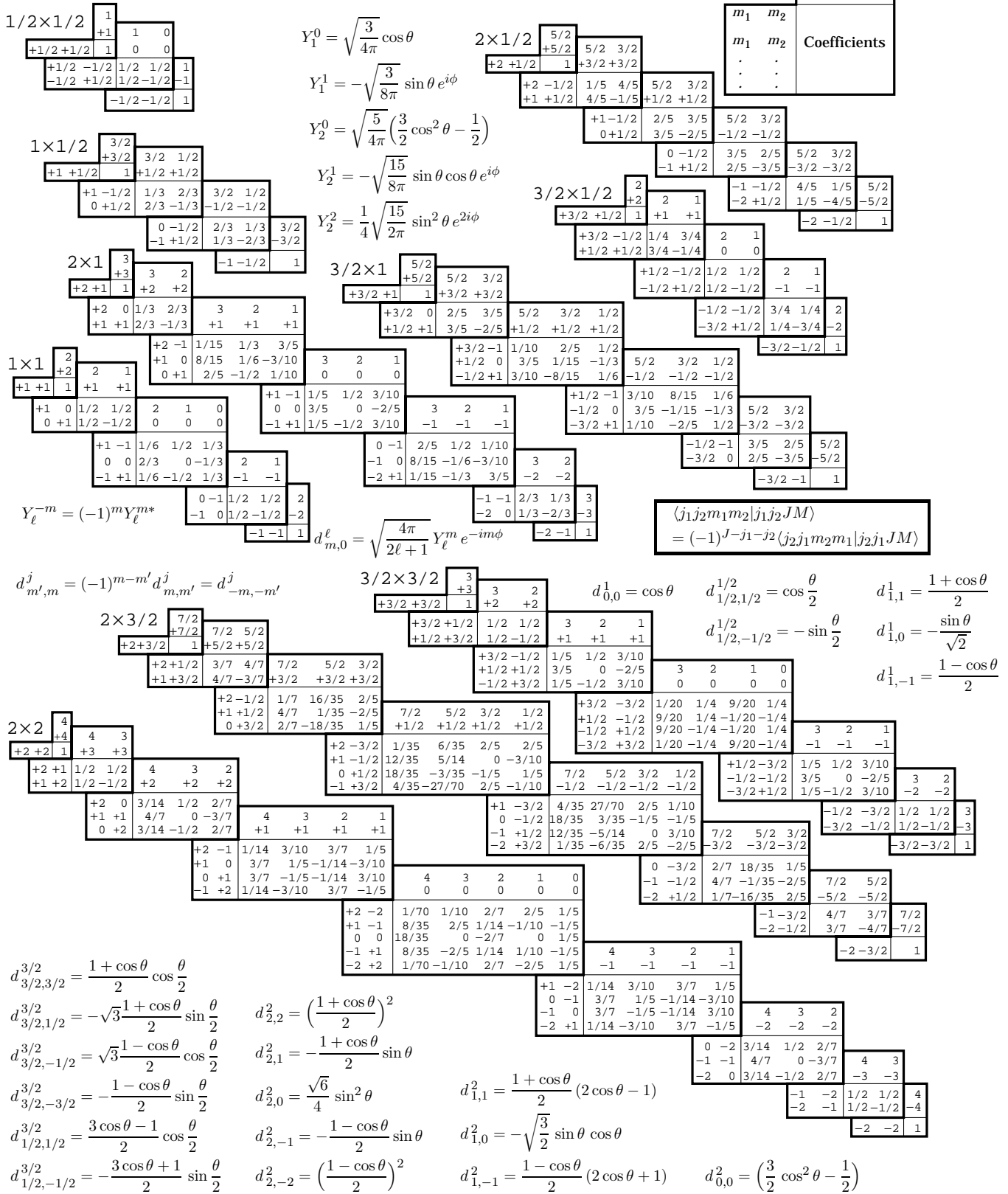
### 34. CLEBSCH-GORDAN COEFFICIENTS, SPHERICAL HARMONICS, AND $d$ FUNCTIONS

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

Notation:

	$J$	$J$	...
$m_1$	$m_2$	$M$	$M$
$m_1$	$m_2$	$M$	$M$
...	...	...	...
...	...	...	...

Coefficients



**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.