

Solved problems in quantum mechanics

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Abstract

This is a collection of solved problems in quantum mechanics. These exercises have been given to the students during the past examinations.¹

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¹Readers are kindly requested to report typos and mistakes to the authors

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1 Recommended books and resources

Lectures closely follow:

- *Cohen-Tannoudji, Diu, Laloe; Quantum Mechanics*
- *J.J. Sakurai; Modern Quantum Mechanics*
- *L.I. Schiff; Quantum Mechanics*

Other useful references:

- *"Quantum mechanics - a new introduction", K. Konishi and G. Pafuti. Oxford Univ. Press (2009).* An extremely useful textbook. Very strongly recommended. It contains detailed explanations and also some chapters that are not easy to find in other books. Remarkably, a very interesting collection of problems is included. The solutions to all the exercises are given in a CD but they can be found also in the website of Kenichi Konishi:
<http://www.df.unipi.it/~konishi/QMBook.html>.
- *"Lectures on quantum mechanics, 2nd edition", S. Weinberg. Cambridge Univ. Press.* An excellent book written by the famous Nobel laureate. This book can be considered the first of a set of books. Indeed, S. Weinberg wrote excellent books about quantum field theory, gravitation, cosmology and these lectures on quantum mechanics are basically the first step into the "particle-sector" of his books.
- *"I fondamenti concettuali e le implicazioni epistemologiche della meccanica quantistica", G.C. Ghirardi in Filosofia della fisica. Edizione Bruno Mondadori, Milano, 1997.* A very interesting paper about the conceptual foundations of quantum mechanics written by one of the masters of the subject. Very strongly recommended.
- *"Esercizi di meccanica quantistica elementare", C. Rossetti. 2-volumes. Levrotto e Bella - Torino.* All the exercises are solved step-by-step. It is a very useful collection of problems.
- *"Istituzioni di fisica teorica - 2nd edition", C. Rossetti. Levrotto-Bella Torino.* A classic textbook on the subject.

2 February 1, 2012

2.1 Exercise 1.1

We shall label as $|n, l, m\rangle$ the eigenstates of the hydrogen atom. Let χ be

$$\chi = \langle n = 3, l = 2, m = 2 | xy | n = 3, l = 0, m = 0 \rangle. \quad (1)$$

Compute, as a function of χ ,

$$\langle n = 3, l = 2, m | \mathcal{O}_j | n' = 3, l' = 0, m' = 0 \rangle$$

where $\mathcal{O}_j = xy, xz, yz, xx, yy, zz$.

Solution:

In this problem we must evaluate matrix elements for various operators. We will not follow the path of the direct evaluation. Indeed, we will exploit the Wigner-Eckart theorem over and over again.

First of all, let us analyze the transformation properties of the operators under rotation.

All the operators are components of a rank two cartesian tensor. Since the Wigner Eckart theorem applies to a spherical tensor, let's first recall how a rank two cartesian tensor is mapped into a spherical tensor. The cartesian tensor is symmetric therefore it decompose into a rank 0 spherical tensor

$$T^0 = (x^2 + y^2 + z^2) \quad (2)$$

and a rank 2 spherical tensor

$$T^2 = \begin{pmatrix} x^2 + 2ixy - y^2 \\ -2z(x + iy) \\ \frac{1}{\sqrt{6}}(-2x^2 - 2y^2 + 4z^2) \\ +2z(x - iy) \\ x^2 - 2ixy - y^2 \end{pmatrix} \quad (3)$$

Notice that the above definitions are unique up to two overall irrelevant constants: $T^r \rightarrow k_r T^r$, where r is the rank. The Wigner-Eckart theorem provides information about the ratio of matrix elements which is insensitive to these overall k_j constants.

According to the Wigner-Eckart theorem, we shall have (the Clebsch-Gordan is 1 because the composition of angular momenta is trivial)

$$\langle n = 3, l = 2, m | T_q^2 | n' = 3, l' = 0, m' = 0 \rangle = \lambda \delta_{mq} \quad (4)$$

$$\langle n = 3, l = 2, m | T^0 | n' = 3, l' = 0, m' = 0 \rangle = 0 \quad (5)$$

From eqn. 3

$$xy = \frac{i}{4}(T_{-2}^2 - T_2^2) \quad (6)$$

and from eqns. 1, 4 and 6 we have

$$\lambda = 4i\chi.$$

Indeed we can write

$$\chi = \langle 322 | xy | 300 \rangle = \langle 322 | [\frac{i}{4}(T_{-2}^2 - T_2^2)] | 300 \rangle = \langle 322 | [\frac{i}{4}(-T_2^2)] | 300 \rangle = -\frac{i}{4}\lambda.$$

where the compact notation

$$|n_0, l_0, m_0\rangle \equiv |n = n_0, l = l_0, m = m_0\rangle$$

has been used.

From eqns. 2.1, 5 and 6 we have

$$\langle n = 3, l = 2, m = -2 | xy | n' = 3, l' = 0, m' = 0 \rangle = -\chi$$

and all remaining matrix elements of xy vanish. Indeed, we can write

$$\langle 32-2 | xy | 300 \rangle = \frac{i}{4} \langle 32-2 | T_{-2}^2 | 300 \rangle = \frac{i}{4}\lambda = -\chi.$$

Analogously

$$xz = \frac{1}{4}(T_{-1}^2 - T_1^2)$$

which implies

$$\langle 321 | xz | 300 \rangle = \langle 321 | \frac{1}{4}(T_{-1}^2 - T_1^2) | 300 \rangle = \langle 321 | \frac{1}{4}(-T_1^2) | 300 \rangle = -\frac{\lambda}{4} = -i\chi$$

and

$$\langle 32-1 | xz | 300 \rangle = \langle 32-1 | \frac{1}{4}(T_{-1}^2 - T_1^2) | 300 \rangle = \langle 32-1 | \frac{1}{4}(T_{-1}^2) | 300 \rangle = \frac{\lambda}{4} = i\chi$$

with all other matrix elements of xz vanishing.

$$yz = \frac{i}{2}(T_{-1}^2 + T_1^2)$$

implies

$$\langle n = 3, l = 2, m = \pm 1 | yz | n' = 3, l' = 0, m' = 0 \rangle = -2\chi$$

with all other matrix elements of yz vanishing. Indeed we have

$$\langle 32 - 1 | yz | 300 \rangle = \langle 32 - 1 | \frac{i}{2}(T_{-1}^2 + T_1^2) | 300 \rangle = \langle 32 - 1 | \frac{i}{2}(T_{-1}^2) | 300 \rangle = \frac{i}{2}\lambda = -2\chi$$

and

$$\langle 321 | yz | 300 \rangle = \langle 321 | \frac{i}{2}(T_{-1}^2 + T_1^2) | 300 \rangle = \langle 321 | \frac{i}{2}(T_1^2) | 300 \rangle = \frac{i}{2}\lambda = -2\chi.$$

$$z^2 = \frac{1}{\sqrt{6}}T_0^2 + \frac{1}{3}T^0$$

which implies

$$\langle n = 3, l = 2, m = 0 | z^2 | n' = 3, l' = 0, m' = 0 \rangle = \langle 320 | \frac{1}{\sqrt{6}}T_0^2 | 300 \rangle = \frac{4i}{\sqrt{6}}\chi$$

with all other matrix elements of z^2 vanishing;

$$x^2 = -\frac{1}{2\sqrt{6}}T_0^2 + \frac{1}{4}(T_2^2 + T_{-2}^2) + \frac{1}{3}T_0^0$$

which implies

$$\begin{aligned} \langle n = 3, l = 2, m = \pm 2 | x^2 | n' = 3, l' = 0, m' = 0 \rangle &= i\chi \\ \langle n = 3, l = 2, m = 0 | x^2 | n' = 3, l' = 0, m' = 0 \rangle &= -i\sqrt{\frac{2}{3}}\chi \end{aligned}$$

with all other matrix elements of x^2 vanishing;

$$y^2 = -\frac{1}{2\sqrt{6}}T_0^2 - \frac{1}{4}(T_2^2 + T_{-2}^2) - \frac{1}{2}T_0^0$$

which implies

$$\begin{aligned} \langle n = 3, l = 2, m = \pm 2 | y^2 | n' = 3, l' = 0, m' = 0 \rangle &= -i\chi \\ \langle n = 3, l = 2, m = 0 | y^2 | n' = 3, l' = 0, m' = 0 \rangle &= -i\sqrt{\frac{2}{3}}\chi \end{aligned}$$

with all other matrix elements of y^2 vanishing.

Finally notice that the operators are the sum of two spherical tensors, namely T^0 and T^2 . Consequently, for generic matrix elements, we would need the evaluation of two distinct non zero matrix elements to use the Wigner-Eckart theorem to evaluate the remaining ones. In the present case, however, one of the two tensors (namely T^0) always vanishes and one matrix element is enough.

2.2 Exercise 1.2

We shall label as $|n, l, m\rangle$ the eigenstates of the hydrogen atom. Compute the matrix elements

$$a_{jk} = \langle n = 2, l = 1 | r_j p_k | n' = 3, l' = 0, m' = 0 \rangle,$$

where r_j and p_k are the j -th component of the position operator and the k -th component of the momentum operator, respectively.

Solution:

r_j and p_k are both parity-odd. Consequently, the operator $r_j p_k$ is parity-even and, therefore, it must connect states with the same parity. Since the parity of the wave functions is $(-1)^l$, all the matrix elements are vanishing.

2.3 Exercise 2.1

An hydrogen atom is subjected to a perturbation W

$$W = \lambda \mathbf{S} \cdot \mathbf{r}$$

Evaluate if and how the degeneracy of the $n = 2$ level is removed.

Solution:

We will neglect the fine-structure splitting. The degeneracy is 8: we have a degeneracy $n^2 = 4$ without spin and then we take into account the two possible spin states (up and down) in the basis $|L^2, S^2, L_z, S_z\rangle$.

Our intention is to use time-independent perturbation theory for the degenerate case. We must diagonalize the perturbation matrix (it is an 8×8 matrix).

The first step is to evaluate the matrix elements and, as usual, we impose the selection rules coming from parity and Wigner-Eckart theorem. Let us start with parity: the perturbation is parity-odd (it is a pseudo-scalar

operator). Hence the perturbation must connect states with opposite parity. In particular the matrix elements of the form $\langle 2s | W | 2s \rangle$ and $\langle 2p | W | 2p \rangle$ are all vanishing. We are left with $\langle 2s | W | 2p \rangle$ expectation values.

To diagonalize the matrix, it is better to change the basis. Let us further elaborate this point. The W operator is a *scalar* product of two *vector* operators, hence is a *scalar* under rotations and it commutes with the *total* angular momentum operators. This can be cross-checked verifying the commutation relationships $[J_k, W] = 0$. It is therefore convenient to move to the J, l, s, J_z basis. From the above consideration only matrix elements with $\Delta J = 0$, $\Delta J_z = 0$ and $\Delta l = \pm 1$ (parity) are non vanishing.

From the above constraints the only non vanishing matrix elements are

$$\langle j = 1/2, l = 0, s = 1/2, j_z = \pm 1/2 | W | j = 1/2, l = 1, s = 1/2, j_z = \pm 1/2 \rangle = \phi_{\pm}$$

and the hermitian conjugates. Taking into account the Wigner-Eckart theorem we have

$$\phi_+ = \phi_- = \phi$$

since the operator is a scalar (i.e. the Clebsch-Gordan coefficient is trivial).

We infer that the four $J = 3/2$ states don't receive any contribution. The $J = 1/2, j_z = \pm 1/2$ subspaces are invariant subspaces for the operator W . The matrix element restricted to these subspaces are (as discussed we have two identical such matrices, one for $j_z = 1/2$ and one for $j_z = -1/2$)

$$W_{J=1/2, j_z=\pm 1/2} = \begin{pmatrix} 0 & \phi \\ \phi^* & 0 \end{pmatrix}$$

with eigenvalues (energy shift)

$$\Delta E = \pm |\phi|$$

and (four) eigenvectors given by

$$\frac{1}{\sqrt{2}} (|j = 1/2, l = 1, j_z = 1/2\rangle \pm |j = 1/2, l = 0, j_z = 1/2\rangle)$$

and

$$\frac{1}{\sqrt{2}} (|j = 1/2, l = 1, j_z = -1/2\rangle \pm |j = 1/2, l = 0, j_z = -1/2\rangle)$$

Let us evaluate ϕ . To perform the calculation we move back to the l, s, l_z, s_z basis exploiting the Clebsch-Gordan coefficients. Indeed, we can write

$$|l = 0, s = 1/2, J = 1/2, J_z = 1/2\rangle = |l = 0, s = 1/2, l_z = 0, s_z = 1/2\rangle$$

and

$$|l = 1, s = 1/2, J = 1/2, J_z = 1/2\rangle = \sqrt{2/3} |l_z = 1, s_z = 1/2\rangle - \sqrt{1/3} |l_z = 0, s_z = 1/2\rangle.$$

Consequently, to evaluate

$$\phi = \langle l = 0, s = 1/2, J = 1/2, J_z = 1/2 | W | l = 1, s = 1/2, J = 1/2, J_z = 1/2 \rangle$$

we have to calculate two expectation values. Let us consider, for example, the direct evaluation of $\langle 2s+ | W | 2p_1- \rangle$. We have

$$\begin{aligned} \langle 2s+ | W | 2p_1- \rangle &= \langle 2s+ | \lambda \mathbf{S} \cdot \mathbf{r} | 2p_1- \rangle = \langle 2s+ | \lambda [S_x x + S_y y + S_z z] | 2p_1- \rangle = \\ &= \langle 2s+ | \lambda \left[\frac{S_+ + S_-}{2} x + \frac{S_+ - S_-}{2i} y + S_z z \right] | 2p_1- \rangle = \\ &= \langle 2s+ | \lambda \left[\frac{S_+}{2} x + \frac{S_+}{2i} y + S_z z \right] | 2p_1- \rangle = \\ &= \langle 2s+ | \lambda \left[\frac{x}{2} + \frac{y}{2i} \right] | 2p_1+ \rangle \end{aligned}$$

where in the last step we exploited the factorization of the wave function and the orthogonality of up and down states. Now only the orbital part remains and we write

$$\begin{aligned} \langle 2s | \lambda \left[\frac{x}{2} + \frac{y}{2i} \right] | 2p_1 \rangle &= \lambda R \int d\Omega (Y_0^0)^* \left[\frac{\cos\phi \sin\theta}{2} + \frac{\sin\phi \sin\theta}{2i} \right] Y_1^1 = \\ &= -\lambda R \int \int d\phi d\theta \sin^3\theta \frac{1}{\sqrt{4\pi}} \sqrt{\frac{3}{8\pi}} \frac{1}{2} = -\frac{2\lambda R}{3} \sqrt{3/8}, \end{aligned}$$

where R is the radial part of the integral and it is given by

$$R = \int_0^\infty dr r^2 R_{2s}^* r R_{2p} = r_B \int_0^\infty dx x^4 e^{-x} \frac{1}{4\sqrt{12}} (2-x).$$

In this formula we called $x = r/r_B$ and r_B is the Bohr radius. The integration over x can be easily performed exploiting the formulas in Appendix. The remaining expectation value can be calculated in a similar way.

2.4 Exercise 2.2

Let's consider a tridimensional isotropic oscillator.

- Determine the degeneracy of the first excited level.
- Assume that the particle is charged and placed into a uniform electric field of intensity E_0 . Evaluate the first non vanishing perturbative contribution to the energies of the first excited level.

Solution:

Question A

The degeneracy of the levels can be studied in various ways (see, for example, Konishi-Paffuti, p.142-143).

The simplest one is to observe that, mathematically, the problem is equivalent to a system of three identical oscillators. The energy levels are thus given by

$$E_{n_1 n_2 n_3} = \hbar \omega (3/2 + n_1 + n_2 + n_3) = \hbar \omega (3/2 + N)$$

and for a given energy level the degeneracy is provided by the set of n_1 , n_2 , and n_3 such that

$$N = n_1 + n_2 + n_3$$

For $N = 1$ it is readily found² that the level is three-fold degenerate.

Another possibility is to point out that the n -th energy eigenstates contain the angular momentum eigenstates up to $l = n$ and furthermore the given level has a definite parity. Summing the multiplicity $2l + 1$ over $l = 0, 2, \dots, n$ (n even) or $l = 1, 3, \dots, n$ (n odd), we obtain the degeneracy formula:

$$d(n) = (n + 2)(n + 1)/2.$$

Another strategy to obtain this formula is to point out that the hamiltonian is invariant under $SU(3)$ (this group acts on the three operators a_i of the oscillator). The degeneracy can be studied considering the totally symmetric irreducible representations of $SU(3)$. The calculation can be done exploiting Young tableaux. The result is the same found before.

²For a generic level the degeneracy D is $D = \sum_{j_1=0}^N \sum_{j_2=0}^{N-j_1} 1 = \sum_{j_1=0}^N (N - j_1 + 1) = \frac{1}{2}(N + 1)(N + 2)$. Indeed we can choose n_1 in $N + 1$ ways, then we are left with $N - n_1 + 1$ possibilities for n_2 and n_3 is fixed (to $N - n_1 - n_2$).

Question B

We must apply time independent perturbation theory. The perturbation can be written as

$$V = -qE_0z.$$

The first excited level has degeneracy factor 3. We must diagonalize V in this 3-dimensional subspace of degenerate states. V is odd under parity and, consequently, it must connect states with opposite parity. Hence at first order in perturbation theory the first excited level is not modified because all the states of the first excited level are odd under parity. We move to second order.

Formally our problem is to work out the result of *second order perturbation theory* for a system with degenerate levels when *the degeneracy of the levels is not removed at first order*. In general this is fairly involved and requires a careful adjustment of the eigenstates (see Sakurai, problem 12 chapter 5, for an example). In the present case, however, the symmetries of the potential simplify the issue. As discussed below the unperturbed potential is a scalar under rotation and the perturbation is a vectorial operator with magnetic quantum number 0. Thus the perturbation will be non vanishing only among states with the same l_z and, as shown below, this implies that we can treat the problem in analogy with a *one dimensional harmonic oscillator without any degeneracy*.

Our next task is to understand which states can be connected to the first excited level exploiting the perturbation. We will call the ground state 000, the three states of the first excited level (100, 010, 001) and the six states of the second excited level (200, 020, 002, 110, 101, 011). The selection rules are due to 1) parity and 2) Wigner-Eckart theorem. The Wigner-Eckart theorem corresponds formally to the composition of an angular momentum $l = 1$ (characterizing the first excited level) with another angular momentum $l = 1$ (characterizing the perturbation written in terms of Y_1^0). Consequently, we get an angular momentum characterizing the bra which can be 0, 1 or 2. Parity tells us that only 0 and 2 are allowed. Moreover the perturbation acts on the third cartesian factor of the wave function. All this symmetries are readily exhibited using the occupation number basis $|n_1, n_2, n_3\rangle$. The perturbation can be expressed as a combination of ladder operators

$$z = \frac{1}{\sqrt{2}}(a_3 + a_3^\dagger)$$

from which we have that its non vanishing matrix elements fulfill

$$\Delta n_1 = \Delta n_2 = 0 \quad \text{and} \quad \Delta n_3 = \pm 1$$

Thus any pair n_1, n_2 labels *an invariant subspace of the perturbation*. Within *an invariant subspace* n_3 labels *distinct energy levels* and non degenerate perturbation theory can be applied.

At second order the formula is (see for example the book by Weinberg, 2nd edition, chapter 5):

$$\delta_2 E_a = \sum_{b \neq a} \frac{|\langle \Psi_b, \delta H \Psi_a \rangle|^2}{E_a - E_b}.$$

We infer that the only matrix elements that we have to evaluate are: $A = \langle 000 | V | 001 \rangle$, $B = \langle 100 | V | 101 \rangle$, $C = \langle 002 | V | 001 \rangle$ and $D = \langle 010 | V | 011 \rangle$. The final formula becomes

$$\begin{aligned} \delta E_{100} &= |B|^2 / (E_{100} - E_{101}) \\ \delta E_{010} &= |D|^2 / (E_{010} - E_{011}) \\ \delta E_{001} &= \frac{|A|^2}{(E_{001} - E_{000})} + \frac{|C|^2}{(E_{001} - E_{002})}. \end{aligned}$$

The matrix elements can be readily evaluated using the results for the ladder operators. Alternatively, the integrals can be evaluated in cartesian coordinates. Even without the calculation we see that $A=B=D$ because we can obtain B from D simply exchanging $y \leftrightarrow x$ and the wave functions along the axes are normalized.

3 Exercise 1.1, February 22, 2012

Let $|j = 3/2, j_z\rangle$ label the simultaneous eigenvectors of the angular momentum operators J^2 and J_z . Evaluate

$$\langle j = 3/2, j'_z | J_m | j = 3/2, j_z \rangle, \quad m = x, y, z$$

and show that the results are in agreement with the Wigner-Eckart theorem.

Solution:

The angular momentum is $3/2$. Consequently we must consider a space with 4 states: $j_z = \pm 3/2, \pm 1/2$. We will proceed stepwise considering separately (1) the direct evaluation of the matrix elements and (2) the Wigner-Eckart theorem.

Before moving to the computation notice that J_m are the components of a *cartesian* vector. Since the Wigner-Eckart theorem applies to spherical tensor let's first move to a spherical tensor of rank one

$$V = (-J_+, \sqrt{2}J_z, J_-)$$

The matrix elements can be readily obtained from those of V with the appropriate linear combinations.

Direct evaluation:

Needless to say,

$$J_z |j = 3/2, j_z = m\rangle = m |j = 3/2, j_z = m\rangle,$$

where we have chosen $\hbar = 1$. Therefore the matrix is

$$\sqrt{2}J_z = \sqrt{2} \begin{pmatrix} 3/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & -3/2 \end{pmatrix}.$$

The evaluation of J_{\pm} on the eigenstates of angular momentum is

$$J_{\pm} |j, m\rangle = \sqrt{(j \mp m)(j \pm m + 1)} |j, m \pm 1\rangle$$

and therefore

$$\begin{aligned} J_+ |3/2, 3/2\rangle &= 0 \\ J_+ |3/2, 1/2\rangle &= \sqrt{3} |3/2, 3/2\rangle \\ J_+ |3/2, -1/2\rangle &= 2 |3/2, 1/2\rangle \\ J_+ |3/2, -3/2\rangle &= \sqrt{3} |3/2, -1/2\rangle \\ J_- |3/2, 3/2\rangle &= \sqrt{3} |3/2, 1/2\rangle \\ J_- |3/2, 1/2\rangle &= 2 |3/2, -1/2\rangle \\ J_- |3/2, -1/2\rangle &= \sqrt{3} |3/2, -3/2\rangle \\ J_- |3/2, -3/2\rangle &= 0. \end{aligned}$$

For the matrix elements V we have

$$-J_+ = \begin{pmatrix} 0 & -\sqrt{3} & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & -\sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

$$J_- = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}.$$

$$\sqrt{2}J_z = \sqrt{2} \begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}.$$

Wigner-Eckart theorem:

To check the Wigner-Eckart theorem is now sufficient to verify that the matrix elements computed above coincide *up to an overall constant* (the *reduced matrix element*) with the Clebsch-Gordon coefficients

$$\langle j_1 = 1, j_2 = 3/2; m_1, m_2 | j_1 = 1, j_2 = 3/2; j = 3/2, m \rangle$$

Using the short notation $\langle j_1 = 1, j_2 = 3/2; m_1, m_2 | j_1 = 1, j_2 = 3/2; j = 3/2, m \rangle = \langle m_1, m_2 | m \rangle$ we have

$$\begin{aligned} \left\langle 1, \frac{1}{2} \middle| \frac{3}{2} \right\rangle &= \sqrt{\frac{2}{5}} \\ \left\langle 1, -\frac{1}{2} \middle| \frac{1}{2} \right\rangle &= \sqrt{\frac{8}{15}} \\ \left\langle 1, -\frac{3}{2} \middle| -\frac{1}{2} \right\rangle &= \sqrt{\frac{2}{5}} \\ \left\langle 0, \frac{3}{2} \middle| \frac{3}{2} \right\rangle &= -\sqrt{\frac{3}{5}} \\ \left\langle 0, \frac{1}{2} \middle| \frac{1}{2} \right\rangle &= -\sqrt{\frac{1}{15}} \\ \left\langle 0, -\frac{1}{2} \middle| -\frac{1}{2} \right\rangle &= \sqrt{\frac{1}{15}} \end{aligned}$$

$$\begin{aligned}
\left\langle 0, -\frac{3}{2} \middle| -\frac{3}{2} \right\rangle &= \sqrt{\frac{3}{5}} \\
\left\langle -1, \frac{3}{2} \middle| \frac{1}{2} \right\rangle &= -\sqrt{\frac{2}{5}} \\
\left\langle -1, \frac{1}{2} \middle| -\frac{1}{2} \right\rangle &= -\sqrt{\frac{8}{15}} \\
\left\langle -1, -\frac{1}{2} \middle| -\frac{3}{2} \right\rangle &= -\sqrt{\frac{2}{5}}
\end{aligned}$$

With our choice for the normalization of the spherical tensor for the reduced matrix element we have

$$\langle j = 3/2 || V || j' = 3/2 \rangle = -\sqrt{\frac{15}{2}}$$

and multiplying the above Clebsch-Gordon coefficients for the reduced matrix element we obtain the matrix elements of the spherical tensor

$$V \equiv (-J_+, \sqrt{2}J_z, J_-)$$

3.1 Exercise 3.1

Let's consider a charged particle placed into an isotropic tridimensional harmonic oscillator potential of frequency ω_0 . Assume that the particle is placed into a time dependent and spatially uniform magnetic field $\mathbf{B} = B_0 \sin(\omega t)$.

- Establish, at first order in perturbation theory, the allowed transitions from the ground state. Discuss the conditions of validity of perturbation theory.
- Compute the corresponding transition probability per unit time. Discuss the conditions of validity of the result.

Solution:

Question A

We choose the frame with the z-axis parallel to the magnetic field:

$$\mathbf{B}(t) = B_0 \sin(\omega t) \mathbf{u}_z.$$

With this choice we have

$$H = H_0 - \frac{qB}{2mc}L_z + \mathcal{O}(B^2).$$

The ground state has $l=0$ and, therefore, $m=0$. Consequently, $L_z |ground\rangle = 0$ and no transition is induced at first order by the perturbation

$$V = -\frac{qB}{2mc}L_z.$$

We can consider the perturbation quadratic in the magnetic field, namely

$$V(t) = \frac{q^2}{8mc^2}B^2(x^2 + y^2).$$

The selection rules are, as usual, parity and Wigner-Eckart theorem. Parity tells us that the perturbation must connect states with the same parity. Since the ground state is even, the transition can take place only to even states. Let us study the transformation properties of the perturbation under rotation. We have³

$$\begin{aligned} x^2 + y^2 &= T_0^{(2)} + T_0^{(0)} \\ T_0^{(2)} &= \frac{1}{2}(x^2 + y^2 - z^2) \\ T_0^{(0)} &= \frac{1}{2}(x^2 + y^2 + z^2) \end{aligned}$$

We infer that this perturbation, at first order, can connect the ground state to the states with $l = 0$ or $l = 2$. If we work in cartesian coordinates we see that the allowed transitions are

$$\begin{aligned} (000) &\longmapsto (200) \\ (000) &\longmapsto (020) \end{aligned}$$

since

$$r_j^2 = \frac{1}{2}(a_j^2 + a_j^\dagger 2 + a_j a_j^\dagger + a_j^\dagger a_j)$$

³Recall that an overall normalization constant in the definition of the various $T^j \rightarrow k_j T_j$ is irrelevant to the extent that the Wigner-Eckart theorem is concerned and will result only into rescaling of the reduced matrix elements.

where we have used the compact notation

$$(n_x, n_y, n_z) \equiv |n_x, n_y, n_z\rangle = \frac{1}{\sqrt{n_x!n_y!n_z!}} a_x^{\dagger n_x} a_y^{\dagger n_y} a_z^{\dagger n_z} |0\rangle$$

Question B

Now we evaluate the transition probability per unit time for (000) \mapsto (200). The remaining transition, namely (000) \mapsto (020) can be evaluated in a similar way.

We apply time-dependent perturbation theory at first order. The main formula is

$$a^{(1)}(t) = -\frac{i}{\hbar} \int e^{i\omega_{ni}t'} V_{ni} dt'.$$

We have

$$V_{ni}(t') = \frac{q^2 B^2}{8mc^2} \langle 200 | (x^2 + y^2) | 000 \rangle.$$

We start with

$$\begin{aligned} \langle 200 | (x^2 + y^2) | 000 \rangle &= \int \psi_{x,2}^* x^2 \psi_{x,0} dx \int \psi_{y,0}^* \psi_{y,0} dy \int \psi_{z,0}^* \psi_{z,0} dz \\ &+ \int \psi_{x,2}^* \psi_{x,0} dx \int \psi_{y,0}^* y^2 \psi_{y,0} dy \int \psi_{z,0}^* \psi_{z,0} dz. \end{aligned}$$

Since the wave functions are orthonormal, we have

$$\langle 200 | (x^2 + y^2) | 000 \rangle = \int \psi_{x,2}^* x^2 \psi_{x,0} dx.$$

To proceed further, we exploit a formula valid in the case $m = n - 2$ (see Konishi-Paffuti p. 66) (or alternatively we directly evaluate the result substituting x^2 for the ladder operators)

$$(x^2)_{nm} = \frac{1}{\alpha^2} \sqrt{\frac{n(n-1)}{4}}$$

and we infer that

$$\langle 200 | (x^2 + y^2) | 000 \rangle = \frac{\hbar}{\sqrt{2m\omega_0}}.$$

Therefore we can write

$$a^{(1)}(t) = -\frac{i}{\hbar} \int e^{i\omega_{ni}t'} \frac{q^2 [B_0 \sin(\omega t')]^2}{8mc^2} \frac{\hbar}{\sqrt{2m\omega_0}} dt'.$$

To evaluate explicitly the integral, we point out that

$$\sin^2(\omega t') = \frac{\cos(2\omega t') - 1}{-2}$$

and hence

$$\int e^{i\omega_{ni}t'} \sin^2(\omega t') dt' = -\frac{1}{2} \int [e^{i(\omega_{ni}+2\omega)t'} + e^{i(\omega_{ni}-2\omega)t'} + e^{i\omega_{ni}t'}] dt'.$$

The amplitude becomes

$$a^{(1)}(t) = \frac{q^2 B_0^2}{16\sqrt{2}m^2 c^2 \omega_0^2} [e^{i\omega_{ni}t'} \left(\frac{e^{i2\omega t'}}{\omega_{ni} + 2\omega} + \frac{e^{-i2\omega t'}}{\omega_{ni} - 2\omega} + \frac{1}{\omega_{ni}} \right)]_{t_0}^t.$$

The probability is obtained by taking the modulus squared. The probability per unit time is dP/dt .

The validity of the above approximation requires $|a^1| \ll 1$, namely away from the resonant condition $\omega \simeq \omega_0 = 1/2\omega_{ni}$

$$\frac{q^2 B_0^2}{16\sqrt{2}m^2 c^2 \omega_0^2} \frac{1}{|\omega_{ni} - 2\omega|} \ll 1; \quad t > 0$$

whereas, near the resonant condition, the result is valid only for small t

$$a^1 \xrightarrow{\omega \rightarrow \omega_0} \frac{q^2 B_0^2}{16\sqrt{2}m^2 c^2 \omega_0^2} t \Rightarrow t \ll \frac{16\sqrt{2}m^2 c^2 \omega_0^2}{q^2 B_0^2}$$

4 Exercise 1.2, June 26, 2012

Let us consider a tridimensional harmonic isotropic oscillator.

- Determine the degeneracy of the second excited level.
- Tell if and how the degeneracy of the second excited level is removed by the following perturbations: $\mathcal{O}_1 = \lambda_1 |\mathbf{r}|^2$, $\mathcal{O}_2 = \lambda_2 \mathbf{r}$ and $\mathcal{O}_3 = \lambda_3 xy$.

Solution:

Question A

The degeneracy can be evaluated with the usual formula

$$d(n) = \frac{(n+2)(n+1)}{2},$$

and, consequently, the second excited level has 6 degenerate states.

Question B

We must use time-independent perturbation theory and, in particular, we must diagonalize the perturbation matrix. Let us discuss separately the various operators starting from $\mathcal{O}_1 = \lambda_1 |\mathbf{r}|^2$. The selection rules are, as usual, parity and Wigner-Eckart theorem. Parity does not give any information because the operator is parity-even and, therefore, it must connect states with the same parity. However, at the second excited level all the states are parity even and, hence, no information is obtained from parity considerations. The Wigner-Eckart theorem is more useful: the operator is a scalar and, consequently, it must connect states with the same l (and also with the same m). Hence the matrix is diagonal. We have 6 diagonal entries and, in the basis $|n = 2, l = 0, m = 0\rangle$, $|n = 2, l = 2, m = 2\rangle$, $|n = 2, l = 2, m = 1\rangle$, $|n = 2, l = 2, m = 0\rangle$, $|n = 2, l = 2, m = -1\rangle$, $|n = 2, l = 2, m = -2\rangle$, the eigenvalues are respectively A, B, B, B, B, B, where

$$A \equiv \langle n = 2, l = 0, m = 0 | \lambda_1 r^2 | n = 2, l = 0, m = 0 \rangle$$

and

$$B \equiv \langle n = 2, l = 2, m | \lambda_1 r^2 | n = 2, l = 2, m \rangle .$$

One remark is in order. We have 5 eigenvalues equal to B, because the quantum number m cannot modify the radial part of the integral and the spherical harmonics are normalized. The same result can be obtained exploiting the Wigner-Eckart theorem.

We can evaluate A and B directly and, for this purpose, the appendix will be useful. Indeed we have

$$A = \int_0^\infty dr \lambda_1 r^4 R_{20}^* R_{20} = \lambda_1 \frac{2}{3} \frac{1}{\sqrt{\pi}} \left(\frac{\hbar}{m\omega} \right)^{5/2} \int_0^\infty d\xi \xi^4 (4\xi^4 + 9 - 12\xi^2) e^{-\xi^2} ,$$

where $r \equiv \sqrt{\frac{\hbar}{m\omega}} \xi$. The integral can be easily evaluated with the formulas in Appendix.

Analogously, for the B coefficient we write

$$B = \int_0^\infty dr \lambda_1 r^4 R_{22}^* R_{22} = \left(\frac{\hbar}{m\omega} \right)^{5/2} \lambda_1 \frac{16}{15} \frac{1}{\sqrt{\pi}} I ,$$

where (see appendix)

$$I = \int_0^\infty d\xi \xi^8 e^{-\xi^2} = \frac{105}{32} \sqrt{\pi} .$$

We infer that the degeneration is partially lifted.

Now we move to the second operator, namely $\mathcal{O}_2 = \lambda_2 \mathbf{r}$. In this case the operator is odd and, therefore, it must connect states with opposite parity. We infer that the perturbation matrix is zero at first order.

Now we discuss the last operator, namely $\mathcal{O}_3 = \lambda_3 xy$. The problem is easier to deal with in the occupation number basis. The system is equivalent to a system of three identical uncoupled oscillators. Denoting by

$$a_j = \frac{1}{\sqrt{2}}(\sqrt{m}\omega r_j + i \frac{p_j}{\sqrt{m}})$$

the three destruction operators and by

$$N_j = a_j a_j^\dagger$$

the corresponding number operators. The unperturbed hamiltonian is

$$H = \sum_{j=1}^3 N_j + \frac{3}{2}\hbar$$

Let's denote by

$$|n_1, n_2, n_3\rangle \sim \prod_{j=1}^3 (a_j^\dagger)^{n_j} |0\rangle$$

the heigenstates of the unperturbed hamiltonian.

It is immediate to check that the perturbation $\lambda_3 r_1 r_2$ commutes with N_3 therefore n_3 labels the invariant subspaces of the perturbation namely it can have non zero matrix elements only between states with the same n_3 . The second excited stated is six-fold degenerate and its heigenstate are given by

$$\sum_{j=1}^3 n_j = 2$$

Within this energy level we have three invariant subspaces $n_3 = 0, 1, 2$. The perturbation can be written as

$$\lambda_3 xy = \frac{\lambda_3}{2}(a_1 + a_1^\dagger)(a_2 + a_2^\dagger) = \chi_3(a_1 a_2^\dagger + a_2 a_1^\dagger + \dots)$$

where the omitted terms don't contribute to first order perturbation theory since they vanish within the second excited state (they raise or lower the level by two units).

Taking into account the above consideration we now come to the evaluation of the matrix element of the perturbation among the states

$$|n_1, n_2, n_3\rangle; \quad n_1 + n_2 + n_3 = 2$$

The $n_3 = 2$ invariant subspace is non degenerate, we have

$$\langle 0, 0, 2 | (a_1 a_2^\dagger + a_2 a_1^\dagger) | 0, 0, 2 \rangle = 0$$

and thus $\delta E = 0$

For the $n_3 = 1$ invariant subspace the perturbation restricted to this subspace ($|1, 0, 1\rangle$ and $|0, 1, 1\rangle$) reads

$$\tilde{\mathcal{O}}_3^{(n_3=1)} = \chi_3 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

with eigenvalues

$$\delta E = \pm \chi_3$$

and eigenvectors

$$\frac{1}{\sqrt{2}}(|1, 0, 1\rangle \pm |0, 1, 1\rangle)$$

Finally for the $n_3 = 0$ invariant subspace ($|2, 0, 0\rangle, |0, 2, 0\rangle$ and $|1, 1, 0\rangle$) the perturbation reads

$$\tilde{\mathcal{O}}_3^{(n_3=0)} = \sqrt{2}\chi_3 \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

with eigenvalues

$$\delta E = 0, \pm 2\chi_3$$

and eigenvectors

$$\frac{1}{\sqrt{2}}(|2, 0, 0\rangle - |0, 2, 0\rangle)$$

$$\frac{1}{\sqrt{2}}|1, 1, 0\rangle \pm \frac{1}{2}(|2, 0, 0\rangle + |0, 2, 0\rangle)$$

4.1 Exercise 3.2

Let's consider a charged particle placed into an isotropic tridimensional harmonic oscillator potential of frequency ω_0 . Evaluate the decay probability per unit time of the first excited level.

Solution:

The hamiltonian is

$$H = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\omega_0^2 r^2.$$

The text does not mention any electromagnetic field but we know that the particle has a non-vanishing electric charge. The decay is consequently due to a spontaneous emission and we will evaluate the decay probability per unit time exploiting the dipole approximation. Let's briefly recall the arguments leading to the evaluation of spontaneous emission from an atomic system which apply here unchanged. Strictly speaking Schrödinger formalism doesn't apply to the present case. However with mild assumptions we can circumvent the issue. Our assumptions are

- our system consists of an *accelerated* charge particles and in analogy with classical physics we assume that the charged particle produces an electromagnetic wave and thus our final state will be

$$|\psi_f\rangle = \sum_{\epsilon} \int \frac{d\mathbf{k}}{(2\pi)^3} \epsilon A_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r} + i\omega t} |0\rangle$$

- the system is isolated: *energy is conserved*
- the system is isolated: *momentum is conserved*. The various fourier components of the radiation carry different momentum, thus the recoil of our system will be different for different values of \mathbf{k} . Different values of \mathbf{k} will point to *different final states* (to be more accurate in our previous formula we should trade $|0\rangle \rightarrow |0, \mathbf{p}(\mathbf{k})\rangle$ to account for the momentum of the bound system). Thus we evaluate the probability of the emission of a plane wave with wave vector \mathbf{k} and polarization ϵ and then *sum* over these probabilities⁴.

⁴This goes very much in the direction of quantizing the electromagnetic field and having \mathbf{k} as an additional quantum number to describe the final state.

We now apply time dependent perturbation theory, in presence of an harmonic perturbation induced by an electromagnetic plane wave. In view of the previous discussion our final state is a *continuum of final states labelled by \mathbf{k} and ϵ* and we can use the standard results which are appropriate in this limit. To assess conveniently the normalization for the emitted radiation we assume that it is bounded in a box of size L which we shall set to infinity at the very end.

The transition rate per unit time, the *decay width*, is

$$\Gamma = \frac{2\pi e^2}{\hbar m_e^2 c^2} \sum_{\mathbf{k}, \epsilon} |A_{\mathbf{k}}|^2 \sum_{\epsilon} \left| \langle 0 | e^{i\mathbf{k}\mathbf{r}} \boldsymbol{\epsilon} \mathbf{p} | 1 \rangle \right|^2 \delta(E_2 - E_1 - \hbar\omega)$$

Now

$$\omega = kc$$

thus the δ “function” ensures that $k = |\mathbf{k}|$ is nearly fixed. If we want the transition rate for a final state radiation with $k \in [k, k + \Delta k]$ and \mathbf{k} within a solid angle $\Delta\Omega$ the result of the sum will simply be an overall multiplicative factor $N(k, \Omega)$, namely the number of \mathbf{k} wave vector falling into the given volume $V(k, \Omega) = k^2 \Delta k \Delta\Omega$. The δ “function” finally ensures that the result vanishes unless k is tuned to reproduce the energy shift $\hbar\omega_0$.

With our boundary conditions \mathbf{k} can take only a discrete set of values

$$\mathbf{k} \equiv \frac{2\pi}{L} (n_1, n_2, n_3)$$

n_j being positive integers. Each of these wave vector will “sit” in the center of a cube of volume $\mathcal{V} = (2\pi/L)^3$ and thus, up to surface terms, $N(k, \Omega)$ will be the ratio among V and \mathcal{V}

$$N(k, \Omega) \Delta k \Delta\Omega = L^3 \frac{k^2}{(2\pi)^3} + \mathcal{O}(L^2) \Delta k \Delta\Omega$$

Thus

$$\Gamma = \frac{2\pi e^2}{\hbar m_e^2 c^2} \sum_{k, \Omega_k} N(k, \Omega_k) \Delta k \Delta\Omega_k |A_{\mathbf{k}}|^2 \sum_{\epsilon} \left| \langle 0 | e^{i\mathbf{k}\mathbf{r}} \boldsymbol{\epsilon} \mathbf{p} | 1 \rangle \right|^2 \delta(E_2 - E_1 - \hbar\omega)$$

Let's now fix $|A_{\mathbf{k}}|$. From the requirement of energy conservation, the radiation should carry away the energy lost by the particle $\hbar\omega_0$. For the electromagnetic field we have

$$\mathbf{E} = i \frac{A_{\mathbf{k}} \omega}{c} \boldsymbol{\epsilon} e^{i\omega t + \mathbf{k}\mathbf{r}} \quad \mathbf{B} = i \mathbf{k} \times \boldsymbol{\epsilon} e^{i\omega t + \mathbf{k}\mathbf{r}}$$

and the associated energy is

$$\tilde{E} = \frac{1}{4\pi} \int d\mathbf{r} \mathbf{E}\mathbf{E}^* + \mathbf{B}\mathbf{B}^* = 2L^3 \frac{|A_0|^2 \omega^2}{c^2 4\pi} \Rightarrow |A_0| = \sqrt{\frac{4\pi c^2 \tilde{E}}{2\omega^2 L^3}}$$

and thus with $\tilde{E} = \hbar \omega$

$$|A_{\omega/c}| = \sqrt{\frac{4\pi c^2 \hbar}{2\omega L^3}}$$

namely A is a function of $|\mathbf{k}|$ only.

We finally have

$$\Gamma = \frac{2\pi e^2}{\hbar m_e^2 c^2} \frac{c^2 \hbar}{4\pi^2} \int dk d\Omega_k \frac{k^2}{\omega} \sum_{\epsilon} |\langle 0 | e^{i\mathbf{k}\mathbf{r}} \boldsymbol{\epsilon} \mathbf{P} | 1 \rangle|^2 \delta(\hbar \omega_0 - \hbar kc)$$

where we have taken the limit $L \rightarrow \infty$ and traded $\Sigma \rightarrow f$. We have

$$\int dk \delta(\hbar \omega_0 - \hbar kc) g(k) = \int dk \delta(k - \omega_0/c) \frac{1}{\hbar c} g(k)$$

and thus

$$\Gamma = \frac{e^2 \omega_0}{2\pi m_e^2 \hbar c^3} \int d\Omega_k \sum_{\epsilon} |\langle 0 | e^{i\mathbf{k}\mathbf{r}} \boldsymbol{\epsilon} \mathbf{P} | 1 \rangle|^2$$

We now evaluate, in the dipole approximation, the matrix element

$$|\langle 0 | e^{i\mathbf{k}\mathbf{r}} \boldsymbol{\epsilon} \mathbf{P} | 1 \rangle|^2 \simeq \frac{m_e}{2} |\langle 0 | \boldsymbol{\epsilon} (\mathbf{a} + \mathbf{a}^\dagger) | 1 \rangle|^2$$

For convenience let's take angular momentum L_z eigenvectors

$$\begin{aligned} |1, m = 1\rangle &\equiv -\frac{1}{\sqrt{2}} (|n_x = 1, n_y = 0, n_z = 0\rangle + i |n_x = 0, n_y = 1, n_z = 0\rangle) \\ |1, m = 0\rangle &\equiv |n_x = 0, n_y = 0, n_z = 1\rangle \\ |1, m = -1\rangle &\equiv \frac{1}{\sqrt{2}} (|n_x = 1, n_y = 0, n_z = 0\rangle - i |n_x = 0, n_y = 1, n_z = 0\rangle) \end{aligned}$$

and thus we have

$$|\langle 0 | e^{i\mathbf{k}\mathbf{r}} \boldsymbol{\epsilon} \mathbf{P} | 1 \rangle|^2 \simeq \begin{cases} \frac{m_e}{4} (\epsilon_x^2 + \epsilon_y^2) & m = \pm 1 \\ \frac{m_e}{2} \epsilon_z^2 & m = 0 \end{cases}$$

so the width is

$$\Gamma_m = \frac{e^2 \omega_0}{4\pi m_e \hbar c^3} \int d\Omega_k \sum_{\epsilon} \mathcal{C}_m$$

where

$$\begin{aligned} \mathcal{C}_{\pm 1} &= \frac{1}{2}(\epsilon_x^2 + \epsilon_y^2) \\ \mathcal{C}_0 &= \epsilon_z^2 \end{aligned}$$

If we parametrize the wave vector direction \mathbf{u}_k as

$$\mathbf{u}_k = (\sin \theta_k \cos \phi_k, \sin \theta_k \sin \phi_k, \cos \theta_k)$$

We can choose the two polarization vectors as

$$\begin{aligned} \epsilon_1 &= (\sin \phi_k, -\cos \phi_k, 0) \\ \epsilon_2 &= (\cos \theta \cos \phi_k, \cos \theta \sin \phi_k, -\sin \theta) \end{aligned}$$

Notice that any two linear combination of $\epsilon_{1,2}$ are equivalent. We are dealing with “polarized atoms” thus the z axis is selected by the polarization of the initial atom. We have

$$\begin{aligned} d\Omega_k \sum_{\epsilon} |\mathcal{C}_1|^2 &= \int d\Omega_k 1 + \cos^2 \theta = 2\pi \int d\cos \theta 1 + \cos^2 \theta = \frac{8}{3}\pi \\ d\Omega_k \sum_{\epsilon} |\mathcal{C}_0|^2 &= 2 \int d\Omega_k \sin^2 \theta = 4\pi \int d\cos \theta \sin^2 \theta = \frac{8}{3}\pi \\ d\Omega_k \sum_{\epsilon} |\mathcal{C}_{-1}|^2 &= \int d\Omega_k 1 + \cos^2 \theta = 2\pi \int d\cos \theta 1 + \cos^2 \theta = \frac{8}{3}\pi \end{aligned}$$

and finally

$$\Gamma_m = \frac{2e^2 \omega_0}{3\pi m_e \hbar c^3}$$

independent from m , as expected since the choice of the z axis is arbitrary and it cannot have any impact on the physical result. Notice that our calculation contains more information than just the width of the excited state. The angular distribution of the radiation will be

$$\begin{aligned} \frac{d\Gamma_{\pm 1}}{d\Omega_k} &\sim 1 + \cos^2 \theta_k \\ \frac{d\Gamma_0}{d\Omega_k} &\sim \sin^2 \theta_k \end{aligned}$$

If we polarize the system (Stark or Zeeman effect for example) we then have a preferred direction (the polarization) and the angular distribution is not isotropic. We also gathered information about the polarization of the emitted light. From the above calculation we notice that for $m = 0$ the polarization is given directly from ϵ_1 since the transition amplitude to polarization ϵ_2 vanishes. Since the polarization vector is real the polarization is linear. For $m = \pm 1$ we need to introduce *complex polarization vectors* to describe the polarization of the emitted light. Defining

$$\epsilon_{\pm} = \frac{1}{\sqrt{1 + \cos^2 \theta_k}} (\cos \theta_k, \mp i \cos \theta_k, -\sin \theta_k e^{\mp i \phi_k})$$

which satisfies $\mathbf{u}_k \epsilon_{\pm}$, $\epsilon_{\pm} \epsilon_{\pm}^* = 1$ and $\epsilon_+ \epsilon_-^* = 0$. It's immediate to check that ϵ_{\pm} describe the polarization of the radiation emitted if $m = \pm 1$. Since the polarization vector is complex⁵ the emitted radiation will be elliptically polarized (in general).

4.2 Exercise 2.3

Consider a charged particle confined into a tridimensional box of length L . Compute the polarization of the light emitted in the decay of the first excited level (choose one specific wave function).

Solution:

We are considering the spontaneous emission of a photon and we will work in dipole approximation. We choose the initial state as

$$\psi = \left(\frac{2}{L}\right)^{3/2} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{\pi 2z}{L}\right).$$

With our choice of wave function,

$$\langle \psi | \mathbf{e}_r | 0 \rangle \sim \epsilon_z$$

indeed if the transition operator don't depend on z we shall have

$$\int dz \sin \frac{\pi}{L} z \sin \frac{2\pi}{L} z = 0$$

Let's denote with

$$\mathbf{u}_k \equiv (\sin \theta \cos \phi, \sin \theta \sin \phi)$$

⁵more precisely the condition to have elliptic polarization is $\epsilon = \mathbf{v}_1 + i\mathbf{v}_2$ with \mathbf{v}_j real and linearly independent; if the \mathbf{v}_j are linearly dependent the polarization is linear.

the direction of the wave vector. At a given angle, sufficiently far away from the system, it will point in the direction of the observer. Choosing as a basis for the polarization vector

$$\begin{aligned}\boldsymbol{\epsilon}_1 &= (\sin \phi_k, -\cos \phi_k, 0) \\ \boldsymbol{\epsilon}_2 &= (\cos \theta \cos \phi_k, \cos \theta \sin \phi_k, -\sin \theta)\end{aligned}$$

it is immediate to verify that the amplitude is non vanishing only for the polarization $\boldsymbol{\epsilon}_2$ which therefore is the polarization of the emitted radiation as a function of the emission angle with respect to the direction of the initial state “polarization”. Since $\boldsymbol{\epsilon}_2$ is real the polarization is linear.

4.3 Exercise 1.2

Consider a charged particle into a two dimensional well of infinite depth and width L . Evaluate the probability for the particle, initially into the ground state, to move to the first excited level due to a perturbing electromagnetic field time dependent and spatially isotropic:

$$\mathbf{E} = E_0 \cos(\omega t) \mathbf{u}_x$$

Specify the conditions under which first order time dependent perturbation theory is valid.

Solution:

We shall work with $\hbar = 1$.

The perturbing potential is

$$W = -qE_0 x \cos(\omega t)$$

To first order in perturbation theory the transition probability amplitude is given by

$$\begin{aligned}a_{01} &= -i \int_0^t \langle 1 | W | 0 \rangle e^{i\omega_{10}s} ds = \frac{iqE_0}{2} \langle 1 | x | 0 \rangle \int [e^{i(\omega_{10}+\omega)s} + (\omega \rightarrow -\omega)] ds \\ &= \frac{1}{2} \left\{ \frac{qE_0 \langle 1 | x | 0 \rangle}{\omega_{10} + \omega} [e^{i(\omega_{10}+\omega)t} - 1] + \frac{qE_0 \langle 1 | x | 0 \rangle}{\omega_{10} - \omega} [e^{i(\omega_{10}-\omega)t} - 1] \right\}\end{aligned}$$

We have

$$\langle 1 | x | 0 \rangle = \frac{2}{L} \int_0^L dx x \sin\left(\frac{\pi}{L}x\right) \sin\left(\frac{2\pi}{L}x\right) = -\frac{16L}{9\pi^2}$$

The transition probability is $\mathcal{P}_{01} = |a_{01}|^2$. Perturbation theory is valid provided the probability is small, namely either

$$\left| \frac{8qE_0L}{9\pi^2(\omega_{10} \pm \omega)} \right| \ll 1$$

or, in the case $\pm\omega \simeq \omega_{10}$, if

$$\frac{8qE_0Lt}{9\pi^2} \ll 1$$

which is obtained with a small t expansion.

4.4 Exercise 2

An hydrogen atom is in the ground state and is subjected to a time-dependent perturbation $W(t)$. Compute, in the dipole approximation, the transition probability to the $n = 2$ state if the perturbation is a monochromatic plane wave:

$$\mathbf{E} = E_0 \mathbf{u}_x \cos(\omega t - kz).$$

Solution:

The hamiltonian is

$$H = \frac{p^2}{2m} + e\phi - \frac{e}{mc} \mathbf{A} \cdot \mathbf{p}$$

where we neglected the A^2 -term because the electron and the proton form a bound state. The vector potential is

$$\mathbf{A} = 2A_0 \hat{\epsilon} \cos\left(\frac{\omega}{c} \mathbf{n} \cdot \mathbf{x} - \omega t\right),$$

where $\hat{\epsilon}$ is the polarization vector and we have

$$\mathbf{n} = (0, 0, 1)$$

$$\hat{\epsilon} = \mathbf{u}_x.$$

Therefore we can write

$$\mathbf{A} = A_0 [e^{i(kz - \omega t)} + e^{-i(kz - \omega t)}] \mathbf{u}_x.$$

The perturbing potential is

$$V(t) = -\frac{e}{mc} \mathbf{A} \cdot \mathbf{p}.$$

The next step is to use the dipole approximation. Hence we write

$$V(t) \simeq -\frac{e}{mc} A_0 \mathbf{u}_x \cdot \mathbf{p} = -\frac{e}{mc} A_0 \hat{\epsilon} \cdot \mathbf{p}.$$

Now we use time dependent perturbation theory. The relevant formula is

$$a_n^{(1)}(t) = -\frac{i}{\hbar} \int_{t_0}^t e^{i\omega_{ni}t'} V_{ni}(t') dt',$$

where

$$V_{ni}(t') = \langle n | V(t) | i \rangle = -\frac{eA_0}{mc} \langle n | p_x | i \rangle = -\frac{eA_0}{mc} im\omega_{ni} \langle n | x | i \rangle.$$

It is time to discuss selection rules. As usual they are due to (1) parity and (2) Wigner-Eckart theorem. Let us start from parity. The operator is parity-odd and consequently it must connect states with opposite parity. Therefore only the states with $n = 2$ and $l = 1$ can be our final states.

Now let us exploit the Wigner-Eckart theorem to obtain some more selection rule. The operator x is a vector operator and in general we can write

$$V_x = \frac{V_{-1}^{(1)} - V_1^{(1)}}{\sqrt{2}}.$$

Consequently, only the transitions with $\Delta m = \pm 1$ are allowed.

We infer that the only allowed transitions to $n = 2$ are $|n = 1, l = 0, m = 0\rangle \mapsto |n = 2, l = 1, m = -1\rangle$ and $|n = 1, l = 0, m = 0\rangle \mapsto |n = 2, l = 1, m = 1\rangle$. Let us start considering the first transition. We write

$$\langle 2, 1, -1 | x | 1, 0, 0 \rangle = \int dV \psi_{21-1}^* x \psi_{100} = \int dr r^3 R_{2,1} R_{1,0} \int d\Omega \sqrt{\frac{3}{8\pi}} \sin^2 \theta e^{i\phi} \cos \phi \frac{1}{\sqrt{4\pi}}.$$

We split the integration into a radial part and an angular part. The radial part (use the Appendix for the explicit calculation) is

$$\frac{1}{r_B^4 \sqrt{6}} \int_0^{+\infty} dr r^4 e^{-3r/(2r_B)} \equiv I_R,$$

where $r_B = \hbar^2/(me^2) \simeq 0.5 \times 10^{-8}$ cm is the Bohr radius and sets the scale of the problem. The angular part is

$$\int d\Omega \sqrt{3/(8\pi)} \sin^2\theta e^{i\phi} \cos\phi \frac{1}{\sqrt{4\pi}} = \frac{4}{3} \sqrt{3/32}.$$

Hence we can write

$$\langle 211 | x | 100 \rangle = I_R/\sqrt{6}.$$

Now we are ready to evaluate the transition probability to this particular state. We write the amplitude as

$$a_{21-1}^{(1)}(t) = -\frac{i}{\hbar} \int_{t_0}^t e^{i\omega_{ni}t'} \left[-\frac{eA_0}{mc} im\omega_{ni}(I_R/\sqrt{6}) \right] dt' = \frac{ieA_0I_R}{\hbar c\sqrt{6}} e^{i\omega_{ni}t_0} [e^{i\omega_{ni}(t-t_0)} - 1].$$

Therefore the transition probability to the state $|n = 2, l = 1, m = -1\rangle$ is

$$P_{21-1}(t) = |a_{21-1}^{(1)}(t)|^2 = \frac{e^2 A_0^2 I_R^2}{3\hbar^2 c^2} \{1 - \cos[\omega_{ni}(t - t_0)]\}.$$

In a completely analogous way we must calculate the transition probability to the remaining state $|211\rangle$. The final probability is given by the sum

$$P_{tot} = P_{21-1} + P_{211}.$$

4.5 Exercise 3

Consider three electrons subject to an harmonic oscillator tridimensional potential.

$$V = (1/2)m\omega^2|\mathbf{r}|^2.$$

Neglecting mutual interaction, evaluate the ground state energy, degeneracy, angular momentum and wave function.

Solution:

The problem for a single particle has a well-known solution with energy

$$E_n = \hbar\omega(n + 1/2).$$

When we "build" the ground state for three electrons, we must antisymmetrize the total wave function. Hence, we must fill the energy levels in harmony with the Pauli principle. We have two electrons with $n = 0$ and

opposite spin and one electron with $n = 1$ and arbitrary spin. Therefore, the energy of the ground state for three electrons is

$$E_{ground} = \frac{\hbar\omega}{2}2 + \frac{3}{2}\hbar\omega = \frac{5}{2}\hbar\omega.$$

To proceed further we analyze the degeneracy. The degeneracy is 6. Indeed the electron with $n = 1$ can be in a $n_x = 1, n_y = 0$ and $n_z = 0$ state or $n_y = 1$ or $n_z = 1$ and can have up or down spin. The orbital angular momentum is one (the two electrons in the ground state have zero angular momentum) whereas the total spin is $1/2$ since the two ground state electrons are in $S = 0$ antisymmetric state. The total angular momentum can be $1/2$ or $3/2$.

It seems worthwhile pointing out that the exchange degeneracy does not enter into the evaluation of the degeneracy. When the text mentions the degeneracy, it means "the degeneracy beyond the exchange one".

Now we discuss the wave function. We have six degenerate ground states with wave functions

$$A |n_{1x}, n_{1y}, n_{1z}, s_{1z}; n_{2x} = 0, n_{2y} = 0, n_{2z} = 0, s_{2z} = 1/2; n_{3x} = 0, n_{3y} = 0, n_{3z} = 0, s_{3z} = -1/2; \rangle$$

where s_{1z} is arbitrary, $n_{1x} + n_{1y} + n_{1z} = 1$ and A is the projector over the totally antisymmetric wave function space.

$$A = \frac{1}{\sqrt{6}} (P_{123} + P_{312} + P_{231} - P_{132} - P_{213} - P_{321})$$

4.6 Exercise 3

Two electrons are subjected to an harmonic oscillator potential

$$V = \frac{1}{2}m\omega^2(r_1^2 + r_2^2),$$

$\mathbf{r}_{1,2}$ being the position vectors of the two particles respectively. Let us denote by $\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2$ the total orbital angular momentum and by $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ the total spin of the system. Evaluate, to first order in perturbation theory, the energy level splitting induced by a spin-orbit $W = A\mathbf{S} \cdot \mathbf{L}$ for the first excited level.

Solution:

The first step is to discuss the unperturbed problem. The wave function for a single particle is

$$\psi^{(1)} = \psi_{n_1}(x)\psi_{n_2}(y)\psi_{n_3}(z),$$

where $\psi_n(x) = C_n H_n(\alpha x) e^{-\frac{1}{2}\alpha^2 x^2}$, $C_n = \sqrt{\frac{\alpha}{\pi^{1/2} 2^n n!}}$, $\alpha = (m\omega/\hbar)^{1/2}$ (see Konishi-Paffuti, p. 142). The energy is

$$E = \hbar\omega(n_1 + n_2 + n_3 + \frac{3}{2}).$$

It is also possible to analyze the problem with eigenstates of the angular momentum. In particular, the ground state for a single particle has $l = 0$ while the first excited level for a single particle has $l = 1, m = 0, \pm 1$.

For a system with two particles the wave function is of the form

$$\psi^{(2)}(\mathbf{x}_1, \mathbf{x}_2) = \sum_{i,j} C_{ij} \psi_i(\mathbf{x}_1) \psi_j(\mathbf{x}_2)$$

where i, j are multi-indexes.

Let us study the ground state. We have two electrons and, therefore, the total wave function must be antisymmetric. For the ground state we take a singlet of spin (which is antisymmetric) and a symmetric orbital part. The wave function for the two electrons has this orbital part:

$$\psi^{(2)}(\mathbf{x}_1, \mathbf{x}_2) = \left(\sqrt{\frac{\alpha}{\sqrt{\pi}}}\right)^3 e^{-\frac{m\omega}{2\hbar}r_1^2} \left(\sqrt{\frac{\alpha}{\sqrt{\pi}}}\right)^3 e^{-\frac{m\omega}{2\hbar}r_2^2},$$

where, as we see, both electrons are in a state $n = 0$. The unperturbed energy is

$$E = 2[3\hbar\omega/2] = 3\hbar\omega.$$

To proceed further, let us analyze the first excited level: now we have one electron in the ground state of single particle and another electron in the first excited level of single particle. Therefore, the orbital part of the wave function is given by

$$\psi_m^{(2)}(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{\sqrt{2}} [\psi_{1,ground}(\mathbf{x}_1) \psi_{2,m}(\mathbf{x}_2) \pm \psi_{1,m}(\mathbf{x}_1) \psi_{2,ground}(\mathbf{x}_2)],$$

where $m = 0, \pm 1$ (it is the magnetic quantum number of $l = 1$ states), while the $+$ ($-$) must be used when the spinorial part of the wave function is a

spin singlet (triplet). Indeed, here our guideline is to antisymmetrize the total wave function of the two particles. The energy of the first excited level is

$$E = \hbar\omega(3/2 + 5/2) = 4\hbar\omega.$$

Now the unperturbed problem is solved. We can consider the perturbation exploiting time-independent perturbation theory. The perturbation is a spin-orbit interaction and, therefore, when we compose the spin with the orbital angular momentum, we will use the basis $|L^2, S^2, J^2, J_z\rangle$. It is better to write the perturbation as

$$W = AS \cdot \mathbf{L} = A \frac{J^2 - S^2 - L^2}{2}.$$

We must diagonalize the perturbation matrix. Indeed, at the first excited level we have degeneracy and the energy corrections at first order are given by the eigenvalues of the matrix. We start considering the case $m = 1$, but our argument must be repeated analogously also for $m = -1$ and $m = 0$. We have $l = 1$ while the spin can be zero or one. Consequently, we have the following degenerate states for $m = 1$ (remember that the third component of the angular momentum is additive):

$$\begin{aligned} &|l = 1, s = 0, j = 1, m_j = 1\rangle, \\ &|l = 1, s = 1, j = 0, m_j = 0\rangle, \\ &|l = 1, s = 1, j = 1, m_j = 1\rangle, \\ &|l = 1, s = 1, j = 1, m_j = 0\rangle, \\ &|l = 1, s = 1, j = 2, m_j = 2\rangle, \\ &|l = 1, s = 1, j = 2, m_j = 1\rangle, \\ &|l = 1, s = 1, j = 2, m_j = 0\rangle. \end{aligned}$$

For $m = 0$ we have the following degenerate states:

$$\begin{aligned} &|l = 1, s = 0, j = 1, m_j = 0\rangle, \\ &|l = 1, s = 1, j = 0, m_j = 0\rangle, \\ &|l = 1, s = 1, j = 1, m_j = 1\rangle, \\ &|l = 1, s = 1, j = 1, m_j = 0\rangle, \\ &|l = 1, s = 1, j = 1, m_j = -1\rangle, \\ &|l = 1, s = 1, j = 2, m_j = 1\rangle, \\ &|l = 1, s = 1, j = 2, m_j = 0\rangle, \\ &|l = 1, s = 1, j = 2, m_j = -1\rangle. \end{aligned}$$

For $m = -1$ we have the following degenerate states:

$$\begin{aligned} &|l = 1, s = 0, j = 1, m_j = -1\rangle, \\ &|l = 1, s = 1, j = 0, m_j = 0\rangle, \\ &|l = 1, s = 1, j = 1, m_j = 0\rangle, \\ &|l = 1, s = 1, j = 1, m_j = -1\rangle, \\ &|l = 1, s = 1, j = 2, m_j = -2\rangle, \\ &|l = 1, s = 1, j = 2, m_j = 0\rangle, \\ &|l = 1, s = 1, j = 2, m_j = -1\rangle. \end{aligned}$$

We have a total of 22 degenerate states at the first excited level but, happily, the perturbation matrix in this basis is already diagonal. For $m = 1$ we have the eigenvalues: 0, -2A, -A, -A, A, A, A. The cases $m = 0, -1$ can be discussed in a similar way.

4.7 Exercise 4

Two identical particles of spin one are subjected to a potential

$$V = \frac{1}{2}m\omega^2(r_1^2 + r_2^2).$$

Establish the degeneracy of the first excited state. Evaluate the energy shift of the levels of the first excited state induced by a perturbation

$$W = \lambda(2x_1 + 3y_1 + 4z_1)(2x_2 + 3y_2 + 4z_2).$$

Solution:

Let us start considering the unperturbed problem. The ground state is defined by the condition of minimum energy and, hence, both particles have $n_x = n_y = n_z = 0$ and the energy of the ground state is:

$$E_{ground} = 2\hbar\omega\frac{3}{2} = 3\hbar\omega.$$

In the first excited state, one of the particles has $n_x = n_y = n_z = 0$ and the other one has $n_x = 1, n_y = n_z = 0$ or $n_x = 0, n_y = 1, n_z = 0$ or $n_x = n_y = 0, n_z = 1$. Hence the energy of the first excited state is

$$E_1 = \hbar\omega\frac{3}{2} + \hbar\omega(1 + \frac{3}{2}) = 4\hbar\omega.$$

Now it is time to write the wave function. The two particles are identical bosons and, hence, the total wave function must be symmetric under particle exchange. As usual, since the hamiltonian does not depend on spin operators, we factorize the total wave function in a spatial part times a spinorial part. In order to obtain the symmetry properties of the spinorial part under particle permutation, we can use the Clebsch-Gordan coefficients (table 1 \times 1). The composition of a spin 1 with another spin 1 can give us a total spin 0, 1 or 2. The Clebsch-Gordan coefficients tell us that the spin 0 state is symmetric, the spin 1 states are three antisymmetric states and the five spin 2 states are symmetric.

As far as the spatial part of the wave function is concerned, we have

$$\psi_{space} = \frac{\psi_{1,ground}(\mathbf{r}_1)\psi_{2,first}(\mathbf{r}_2) \pm \psi_{1,first}(\mathbf{r}_1)\psi_{2,ground}(\mathbf{r}_2)}{\sqrt{2}},$$

where the minus sign must be used with (total) spin 1 states, while the plus sign must be used with (total) spin 0 and spin 2 states. Since ψ_{first} can correspond to the three cases $n_x = 1, n_y = n_z = 0$ or $n_x = 0, n_y = 1, n_z = 0$ or $n_x = n_y = 0, n_z = 1$ we have a total of $9 \times 3 = 27$ unperturbed degenerate states with energy $E_1 = 4\hbar\omega$.

Now a brute force calculation would lead to a highly cumbersome calculation. The perturbation is made out of nine terms each one having non zero matrix elements between different states. However observe that the perturbation can be written as

$$\begin{aligned} W &= 29\lambda(\mathbf{r}_1\mathbf{u})(\mathbf{r}_2\mathbf{u}) \\ \mathbf{u} &\equiv \frac{1}{\sqrt{29}}(2, 3, 4) \end{aligned}$$

The energy shift cannot depend on our choiche of reference frame and we can choose the z axis along the direction of \mathbf{u} . In this frame

$$W = \lambda'z'_1z'_2$$

from now on we shall omit the prime to simplify notazion but it is always assumed that the we are working in this new reference frame. The perturbation doesn't depend on the spin of the particle therefore $|S, S_z\rangle$ will label nine invariant subspaces six even and three odd under particle spin exchange. We shall denote by

$$|\mathcal{P}_1 : n'_x, n'_y, n'_z\rangle \quad |\mathcal{P}_2 : n'_x, n'_y, n'_z\rangle$$

the spatial part of the eigenfunctions. The potential raise/lower by one unit n'_z and therefore only the exchange integral contribute

$$\begin{aligned}
\delta E &= \pm \frac{\lambda'}{2} \sqrt{\frac{\hbar}{m\omega}} \left(\langle \mathcal{P}_1 : 0, 0, 1 | a_{z_1}^\dagger | \mathcal{P}_1 : 0, 0, 0 \rangle \langle \mathcal{P}_2 : 0, 0, 0 | a_{z_2} | \mathcal{P}_2 : 0, 0, 1 \rangle + \right. \\
&\quad \left. \langle \mathcal{P}_1 : 0, 0, 0 | a_{z_1} | \mathcal{P}_1 : 0, 0, 1 \rangle \langle \mathcal{P}_2 : 0, 0, 1 | a_{z_2}^\dagger | \mathcal{P}_2 : 0, 0, 0 \rangle \right) \\
&= \pm \lambda' \sqrt{\frac{\hbar}{m\omega}}
\end{aligned}$$

where plus sign apply to symmetric spin states $S = 0, 2$ and minus sign to antisymmetric one $S = 1$. All other matrix elements vanish. We thus have eighteen levels whose energy is left unchanged, three which receive a negative energy shift and nine which receive a positive energy shift. The degeneracy is only partially lifted.