ANGULAR MOMENTUM THEORY

by

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Abstract

Discussion of angular momentum revolved around two basic classes, of orbiting and spinning. Quantum mechanics successfully presented this two very distinct characteristics of angular momentum in detail and even more to add them up in coupling schemes. Of course, angular momentum has played a major role in cradling the more advanced physics theories, especially the development of the atomic and nuclear physics today. From the point of view of a mathematical model, it is always a happy moment to accept the fact that calculations agree to a close proximity of experimental data. This is what happened to the theory of angular momentum, as we see in examples such as the fine and hyperfine splitting of hydrogen, Hund's rules, nuclear shell model and Heisenberg isospin. These models more or less are the fundamental respect of most of the higher level physics.

Abstrak

Perbincangan mengenai momentum sudut berkisar dalam 2 kelas asas,mengorbit dan berputar. Mekanik kuantum telah berjaya menyampaikan 2 ciri-ciri momentum sudut yang sangat berbeza ini dengan lebih terperinci dan lebih lagi untuk menambah mereka dalam gandingan skim. Sudah tentu,momentum telah memainkan peranan utama dalam asas teori fizik yang lebih sofiskated,terutamanya pembangunan fizik atom dan nuclear hari ini. Dari sudut pandangan model matematik, hakikat pengiraan akhir sangat hampir dengan data eksperimen merupakan hakikat yang memuaskan. Ini adalah apa yang berlaku kepada teori momentum sudut seperti yang kita lihat dalam contoh-contoh seperti ne dan hipern memisahkan hydrogen, peraturan Hund, model petala nuclear dan isopin Heisenberg. Model ini lebih kurang adalah berkenaan asas yang paling fizik di peringkat yang lebih tinggi.

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Thank God for giving me this opportunity to expose to the studies of Angular Momentum. Along the completion of this project, I have been receiving a lot of helps from various people.

First of all, as a team we would like to express our most sincere appreciation to our supervisors, Dr. Myo Thaik, and Dr. Yoon Tiem Leong. We have two supervisors because Dr. Myo left his teaching position during the second semester of the project. Both lecturers were excellent and creative in encouraging us to learn more and work more. In my opinion, Dr. Myo is a great and knowledgeable theorist in Quantum Mechanics, and he has guided us through lots of mathematical difficulties. He has led us through the weekly presentation as well. On the other hand, Dr. Yoon is a great young man, passionate in teachings and physics. For the project, he had supply a lot of information with regard to atomic and nuclear physics. Not to forget he also provided us with some computational suggestions, especially for the preparation of this report itself, which we were exposed to "LaTeX". We really learnt a lot during the presentation sessions under the guidance of both supervisors.

Next, personally I would like to express my deepest gratitude to my project partner, Miss Lee Chou Yueh, whom I have cooperated with the most throughout the project. She is equiped with skilled english, which is absolutely important in our method as communication come first when we try to teach each other. We manage to share ideas and achieve mutual understanding as a team. Not only did we come to know deeper the physics of angular momentum, but we have learnt a lot through our plans.

Lastly, to my family, friends and course mates as well, I am really thankful for their advice and support.

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Chapter 1

Introduction

Beside its importance in the conservation principle, angular momentum plays a major role in quantum mechanics, enabling us to study the dynamics of a system that involves any kind of spherical symmetry. Its usage is exceptionally essential when dealing with atomic and nuclear physics calculations. As in classical mechanics, we embed the pictures of angular motions, either revolving or spinning, in vectors. This, however does not imply the real physical structure in the microscopic world, as the vector states follow exactly all formalisms of quantum mechanics. At first, it is interesting to know that angular momentum theory fits quite well onto the hydrogen atom, since spherical harmonics describes it exactly. However, as we encounter more complicated systems, angular momentum starts to limit the accuracy of structures.

To be exact, this project is a more suitably termed study as it is in an all-rounded theoretical work. It is not a study of a new theory, but of an old profile, covering what has not been taught to USM physics undergraduates. This project first outlines some mathematical backgrounds of orbital angular momentum, L and spin angular momentum, S separately. The content of first two chapters are referred directly from Griffiths' Introduction to Quantum Mechanics. [4] In addition to the reference text content, we added exact step-by-step mathematical tools and procedures, which were omitted in the reference text. Only certain helpful parts of the reference text were picked, particularly the results and the theoretical explanations. The choices of symbols and characters are slightly edited to be coherent with the overall structure of this report.

The major outcome of this study is in the next two chapters, which encompasses self study methods and teaching experience. This is done by studying different topics separately between us, followed by attempts to teach each other on a weekly basis. In this report, we have divided part of the chapters, with which Chapter 4 was done by myself while my partner covered the Chapter 5. We believe through this way, we will be able to cover more ground in this study. Besides that, a weekly presentation with our supervisor was scheduled while either one of us present a topic for discussion and sharing. Through this method, we not only gained a clearer understanding about the topic but at the same time, acquire experiences of impromptu presentation.

Chapter 4 talks about the addition of angular momentum, also known as total angular momentum. Some simple examples and case studies of angular momentum usage that move towards the scale of atomic physics is explained here. The hydrogen model was used as a starting model, as it is the least complicated among the elements. The concept explanation is an adaptation from Griffiths' text with extensions of selective topics which were fundamentally required: Hund's rules and Clebsch-Gordan coefficients. The main idea of the theory is dissected and presented in this chapter while some further case studies that stress total angular momentum implementation is shown in the Appendix.

On the other hand, Chapter 5 explains nuclear properties such as structural details, spin, iso-spin, and nuclear shell model. These are included because at this particular moment, these are some of the remaining simple applications of angular momentum in nuclear physics.

The results are all presented mathematically in detail in the following chapters.

Chapter 2

Orbital Angular Momentum

This chapter is an adaptation from Section 6.3 of Introduction to Quantum Mechanics (2nd ed.) by Griffiths, page 160-166.

2.1 Introduction

In classical mechanics, angular momentum is defined with respect to the origin as:

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} \tag{2.1}$$

which gives the components:

$$L_x = yp_z - zp_y \tag{2.2}$$

$$L_y = zp_x - xp_z \tag{2.3}$$

$$L_z = xp_y - yp_x. \tag{2.4}$$

These relations are used in obtaining the operators, eigenvalues and eigenfunction.

2.2 Eigenvalues

The commutation relation between L_x and L_y is:

$$\begin{aligned}
[L_x, L_y] &= [yp_z - zp_y, zp_x - xp_z] \\
&= [yp_z, zp_x] - [yp_z, xp_z] - [zp_y, zp_x] + [zp_y, xp_z] \\
&= yp_z zp_x - zp_x yp_z + (-yp_z xp_z + xp_z yp_z) + (-zp_y zp_x + zp_x zp_y) \\
&\quad + zp_y xp_z - xp_z zp_y \\
&= yp_x(p_z z - zp_z) + xp_y(zp_z - p_z z) \\
&= yp_x[p_z, z] + xp_y[z, p_z] \\
&= [z, p_z](xp_y - yp_x) \\
&= i\hbar L_z
\end{aligned} \tag{2.5}$$

where the commutation relations of position and momentum are known to be:

$$[r_i, p_j] = -[p_i, r_j] = i\hbar\delta_{ij}. \tag{2.6}$$

Notice the cyclic permutation of x, y and z, the following relations can be directly written:

$$[L_z, L_x] = i\hbar L_y \tag{2.7}$$

$$[L_y, L_z] = i\hbar L_x. \tag{2.8}$$

Equivalently in vector form, these relation can readily be compiled as:

$$\begin{aligned}
\mathbf{L} \times \mathbf{L} &= \begin{vmatrix} \hat{\imath} & \hat{\imath} & \hat{k} \\ L_x & L_y & L_z \\ L_x & L_y & L_z \end{vmatrix} \\
&= (L_y L_z - L_z L_y)\hat{\imath} - (L_x L_z - L_z L_x)\hat{\jmath} + (L_x L_y - L_y L_x)\hat{k} \\
&= i\hbar(L_x\hat{\imath} + L_y\hat{\jmath} + L_z\hat{k}) \\
&= i\hbar\mathbf{L}.
\end{aligned} \tag{2.9}$$

Now, since L_x, L_y, L_z are incompatible observables, they should obey the uncertainty relation:

$$\begin{aligned} \sigma_{L_x}^2 \sigma_{L_y}^2 &\geq (\frac{1}{2i}\langle [L_x, L_y] \rangle)^2 \\ &= (\frac{1}{2i}\langle i\hbar L_z \rangle)^2 \\ &= \frac{\hbar^2}{4}\langle L_z \rangle^2 \end{aligned} \tag{2.10}$$

and

$$\sigma_{L_x}\sigma_{L_y} \geq \frac{\hbar}{2}\left|\langle L_z \rangle\right|. \tag{2.11}$$

Which means the common eigenstates never exist, since they are not simultaneously measurable.

On the other hand,

$$\mathbf{L}^2 = L^2 = L_x^2 + L_y^2 + L_z^2 \tag{2.12}$$

commute with each component, say for L_x,

$$\begin{aligned} [L^2, L_x] &= [L_x^2, L_x] + [L_y^2, L_x] + [L_z^2, L_x] \\ &= L_y[L_y, L_x] + [L_y, L_x]L_y + L_z[L_z, L_x] + [L_z, L_x]L_z \\ &= L_y(-i\hbar L_z) + (-i\hbar L_z)L_y + L_z(i\hbar L_y) + (i\hbar L_y)L_z \\ &= 0 \end{aligned} \tag{2.13}$$

where the simplifications are based on the fact that any operator commutes with itself and followed the relation:

$$\begin{aligned} [AB, C] &= ABC - CAB - ACB + ACB \\ &= A[B, C] + [A, C]B. \end{aligned} \tag{2.14}$$

This is applied for the other cases as well:

$$[L^2, L_y] = 0 \tag{2.15}$$

and

$$[L^2, L_z] = 0 \tag{2.16}$$

or even more compactly,

$$[L^2, \mathbf{L}] = 0. \tag{2.17}$$

However, notice that simultaneous eigenstates of L^2 and L_z can be found, let

$$L^2 f = \lambda f \tag{2.18}$$

and

$$L_z f = \mu f. \tag{2.19}$$

By using the ladder operator technique, which is:

$$L_\pm = L_x \pm i L_y \tag{2.20}$$

and of course, commutation is maintained for:

$$[L^2, L_\pm] = 0. \tag{2.21}$$

They possess yet another set of common eigenstate, or $L_\pm f$ can actually be taken as eigenfunction of L^2, as be seen in:

$$L^2(L_\pm f) = L_\pm(L^2 f) = L_\pm(\lambda f) = \lambda(L_\pm f) \tag{2.22}$$

with the same eigenvalue λ. While the commutator with L_z is:

$$\begin{aligned} [L_z, L_\pm] &= [L_z, L_x] \pm i[L_z, L_y] \\ &= i\hbar L_y \pm i(-i\hbar L_x) \\ &= \pm(\hbar L_x \pm i\hbar L_y) \\ &= \pm\hbar L_\pm. \end{aligned} \tag{2.23}$$

As in the case of L^2,

$$\begin{aligned} L_z(L_\pm f) &= (L_z L_\pm - L_\pm L_z) f + L_\pm L_z f \\ &= \pm\hbar L_\pm f + \mu L_\pm f \\ &= (\mu \pm \hbar)(L_\pm f). \end{aligned} \tag{2.24}$$

Equation 2.24 shown that $L_\pm f$ is also an eigenfunction of L_z with the new eigenvalue $\mu \pm \hbar$. The L_+ is being labeled as 'raising' operator while L_- is 'lowering' operator. However, when L_z approaches $|\mathbf{L}|$, for $L_z \leq |\mathbf{L}|$ there must exist a maximum eigenstate f_{max}, where L_+ have no more effect on it, says:

$$L_+ f_{max} = 0. \tag{2.25}$$

The eigenvalue of L_z at this state is being defined as $\hbar l$,

$$L_z f_{max} = \hbar l f_{max} \tag{2.26}$$

$$L^2 f_{max} = \lambda f_{max}. \tag{2.27}$$

To establish a relation between l and λ by means of ladder operator, the following product relates their operators:

$$\begin{aligned} L_{\pm}L_{\mp} &= (L_x \pm iL_y)(L_x \mp iL_y) \\ &= L_x^2 \mp iL_xL_y \pm iL_yL_x + L_y^2 + L_z^2 - L_z^2 \\ &= L^2 - L_z^2 \pm i(L_yL_x - L_xL_y) \\ &= L^2 - L_z^2 \pm i(-i\hbar L_z) \\ &= L^2 - L_z^2 \pm \hbar L_z \end{aligned} \tag{2.28}$$

or

$$L^2 = L_{\pm}L_{\mp} + L_z^2 \mp \hbar L_z. \tag{2.29}$$

It follows that:

$$\begin{aligned} L^2 f_{max} &= (L_{\pm}L_{\mp} + L_z^2 \mp \hbar L_z) f_{max} \\ &= (L_{-}L_{+} + L_z^2 + \hbar L_z) f_{max} \\ &= (0 + \hbar^2 l^2 + \hbar^2 l) f_{max} \\ &= \hbar^2 l(l+1) f_{max} \end{aligned} \tag{2.30}$$

which gives

$$\lambda = \hbar^2 l(l+1) \tag{2.31}$$

so that the magnitude of the angular momentum is given by $\sqrt{\lambda} = \hbar\sqrt{l(l+1)}$ and is governed by l.

Meanwhile, by the same reason for the minimum state, f_{min} such that

$$L_{-} f_{min} = 0 \tag{2.32}$$

and by putting $\hbar\bar{l}$ as the eigenvalue of L_z at this state,

$$L_z f_{min} = \hbar\bar{l} f_{min} \tag{2.33}$$

$$L^2 f_{min} = \lambda f_{min}. \tag{2.34}$$

Still using the same equation and same approach,

$$\begin{aligned} L^2 f_{min} &= (L_+L_- + L_z^2 - \hbar L_z) f_{min} \\ &= (0 + \hbar^2 \bar{l}^2 + \hbar^2 \bar{l}) f_{min} \\ &= \hbar^2 \bar{l}(\bar{l} - 1) f_{min} \end{aligned} \tag{2.35}$$

and thus,

$$\lambda = \hbar^2 \bar{l}(\bar{l} - 1) \tag{2.36}$$

leads to:

$$l(l+1) = \bar{l}(\bar{l} - 1). \tag{2.37}$$

For one of the possible solution is rejected, $\bar{l} = l + 1$ since $\bar{l} < l$, the correct solution is $\bar{l} = -l$.

Now, the eigenvalues of L_z is replaced as $m\hbar$ where m goes from $-l$ to l in N-integer steps. In particular, it follows that $l = -l + N$, and hence $l = \frac{N}{2}$ which makes l either an integer or half-integer. The eigenfunctions [1] are characterized by the number l and m:

$$L^2 f_l^m = \hbar^2 l(l+1) f_l^m \tag{2.38}$$

$$L_z f_l^m = \hbar m f_l^m \tag{2.39}$$

where $l = 0, 1/2, 1, 3/2, \ldots$; $m = -l, -l+1, \ldots, l-1, l$. For any l, there are $2l+1$ different values of m.

The eigenfunction, f_l^m is nothing else but the spherical harmonics, Y_l^m.[2] This statement is shown in details in appendix A.3.

2.3 Chapter Summary

Of all the derivatives lead in the end to equation 2.38 and 2.39, which are the most mathematical representation of orbital angular momentum. These two equation explain the orbital behavior of particles for each states of l, m.

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[1] Besides L^2 and L_z, the role of L_x and Ly in this configuration lies within $L_\pm$, with $L_\pm f_l^m = \hbar\sqrt{l(l+1) - m(m \pm 1)} f_l^{m\pm1}$. This is shown in Appendix A.1.

[2] The wave function of hydrogen is spitted into radial part (radial equation) and angular part (spherical harmonics). The spherical harmonics is worked out in Appendix A.2.

Chapter 3

Spin

This chapter is an adaptation from Section 4.4 of Introduction to Quantum Mechanics (2nd ed.) by Griffiths, page 171-188.

3.1 Introduction

The algebraic theory of spin is exactly like the orbital angular momentum:

$$[S_i, S_j] = i\hbar S_k \tag{3.1}$$

where $i, j, k =$ cyclic permutation of x, y, z. Also: [1]

$$\begin{aligned} S^2 \left|s\, m_s\right\rangle &= \hbar^2 s(s+1) \left|s\, m_s\right\rangle && (3.2) \\ S_z \left|s\, m_s\right\rangle &= \hbar m_s \left|s\, m_s\right\rangle && (3.3) \\ \text{and} \qquad S_\pm \left|s\, m_s\right\rangle &= \hbar\sqrt{s(s+1) - m_s(m_s \pm 1)} \left|s\, m_s \pm 1\right\rangle && (3.4) \end{aligned}$$

where $S_\pm = S_x \pm iS_y$, and $s = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$, $m_s = -s, -s+1, \ldots, s-1, s$.

3.2 Spin $\frac{1}{2}$

This is an important class, since electrons, protons and neutrons are all spin $\frac{1}{2}$. $s = \frac{1}{2}$, $m_s = \pm\frac{1}{2}$ which allow only 2 possible states, the state $\left|\frac{1}{2}\, \frac{1}{2}\right\rangle$ is called spin up and the

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[1] For spin, the eigenstate are not spherical harmonics, or in other words not a function. Therefore, the vector state are scoped to be presented in “ket” notation.

state $\left|\frac{1}{2}\ -\frac{1}{2}\right\rangle$ is called spin down. In this part, the use of spinor is introduced:

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a\chi_+ + b\chi_- \tag{3.5}$$

with $\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ representing spin up, and $\chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ representing spin down.
It is clear from matrix mechanics, that the operators are 2 × 2 matrices. First, for the case of:

$$S^2\chi_\pm = \hbar^2\frac{1}{2}(\frac{1}{2}+1)\chi_\pm = \frac{3}{4}\hbar^2\chi_\pm. \tag{3.6}$$

The entries of S^2 is figured out by comparing $S^2 = \begin{pmatrix} c & d \\ e & f \end{pmatrix}$ with each cases of spinors,
$\begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} c \\ e \end{pmatrix} = \frac{3}{4}\hbar^2\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, so $c = \frac{3}{4}\hbar^2$ and $e = 0$.
$\begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} d \\ f \end{pmatrix} = \frac{3}{4}\hbar^2\begin{pmatrix} 0 \\ 1 \end{pmatrix}$, that $d = 0$ and $f = \frac{3}{4}\hbar^2$.
Thus,

$$S^2 = \frac{3}{4}\hbar^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{3.7}$$

The rest of operators are traced in similar manners:

$$S_z\chi_+ = \frac{\hbar}{2}\chi_+ \tag{3.8}$$

$$S_z\chi_- = -\frac{\hbar}{2}\chi_- \tag{3.9}$$

let $S_z = \begin{pmatrix} c' & d' \\ e' & f' \end{pmatrix}$,
$\begin{pmatrix} c' & d' \\ e' & f' \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} c' \\ e' \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, gives $c' = \frac{\hbar}{2}$, $e' = 0$.
$\begin{pmatrix} c' & d' \\ e' & f' \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} d' \\ f' \end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$, gives $d' = 0$, $f' = -\frac{\hbar}{2}$.
So,

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{3.10}$$

Also for ladder operators:

$$S_+\chi_- = \hbar\chi_+ \tag{3.11}$$

$$S_-\chi_+ = \hbar\chi_- \tag{3.12}$$

$$S_+\chi_+ = S_-\chi_- = 0. \tag{3.13}$$

It is assumed that $S_+ = \begin{pmatrix} c_+ & d_+ \\ e_+ & f_+ \end{pmatrix}$, $S_- = \begin{pmatrix} c_- & d_- \\ e_- & f_- \end{pmatrix}$, which give
$\begin{pmatrix} c_+ & d_+ \\ e_+ & f_+ \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} d_+ \\ f_+ \end{pmatrix} = \hbar\begin{pmatrix} 1 \\ 0 \end{pmatrix}$; $\begin{pmatrix} c_+ & d_+ \\ e_+ & f_+ \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} c_+ \\ e_+ \end{pmatrix} = 0$, $d_+ = \hbar$,
with $c_+ = e_+ = f_+ = 0$.
$\begin{pmatrix} c_- & d_- \\ e_- & f_- \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} c_- \\ e_- \end{pmatrix} = \hbar\begin{pmatrix} 0 \\ 1 \end{pmatrix}$; $\begin{pmatrix} c_- & d_- \\ e_- & f_- \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} d_- \\ f_- \end{pmatrix} = 0$, $e_- = \hbar$,
such that $c_- = d_- = f_- = 0$.
Hence,

$$S_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, S_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{3.14}$$

From $S_\pm = S_x \pm iS_y$, $S_x = \frac{1}{2}(S_+ + S_-)$, $S_y = \frac{1}{2i}(S_+ - S_-)$, it is clear that,

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{3.15}$$

$$S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{3.16}$$

To tidy up, denote $\mathbf{S} = (\frac{\hbar}{2})\hat{\sigma}$, where

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3.17}$$

are known as Pauli spin matrices. The characteristics of an observable for any operator is that the operator itself being hermitian, so S_x, S_y, S_z, S^2 are observables, but $S_\pm$ not.

Next, to locate the eigenspinor as the generic form $\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a\chi_+ + b\chi_-$, the normalization state have:

$$|a|^2 + |b|^2 = 1. \tag{3.18}$$

For the case S_z is straight forward, since

$$\begin{aligned} S_z\chi &= aS_z\chi_+ + bS_z\chi_- \\ &= a\frac{\hbar}{2}\chi_+ - b\frac{\hbar}{2}\chi_- \end{aligned} \tag{3.19}$$

this can be interpret as the probability of getting $+\frac{\hbar}{2}$ is $|a|^2$ while the probability of getting $-\frac{\hbar}{2}$ is $|b|^2$. However, it is not the same for the case of S_x,

$$\begin{aligned} S_x\chi &= aS_x\chi_+ + bS_x\chi_- \\ &= a\frac{\hbar}{2}\chi_- + b\frac{\hbar}{2}\chi_+. \end{aligned} \tag{3.20}$$

Here is a twist at the inconsistency in eigenvalues, a new set of eigenspinors must be introduced as a linear combination that will give the same χ. Let $S_x\chi_x = \lambda\chi_x$, $(S_x - \lambda\hat{I})\chi_x = 0$, this equation is valid when $\det(S_x - \lambda\hat{I}) = 0$ since it allows no inverse,

$$\begin{vmatrix} -\lambda & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\lambda \end{vmatrix} = 0 \rightarrow \lambda^2 = (\frac{\hbar}{2})^2, \lambda = \pm\frac{\hbar}{2}. \tag{3.21}$$

Take

$$\chi_x = \begin{pmatrix} a_x \\ b_x \end{pmatrix} \tag{3.22}$$

$$S_x\chi_x = \pm\frac{\hbar}{2}\begin{pmatrix} a_x \\ b_x \end{pmatrix} \equiv \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a_x \\ b_x \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} b_x \\ a_x \end{pmatrix} \tag{3.23}$$

gives $\pm a_x = b_x$ or equivalently, $a_x = \pm b_x$. Evidently in linear combination,

$$\begin{aligned} \chi_x &= \begin{pmatrix} a_x \\ \pm a_x \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} a_x \\ a_x \end{pmatrix} + \frac{1}{\sqrt{2}}\begin{pmatrix} a_x \\ -a_x \end{pmatrix} \quad \text{, being equally possible} \\ &\equiv a_x\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} + b_x\begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = a_x\chi_{x+} + b_x\chi_{x-}. \end{aligned} \tag{3.24}$$

In order for $\chi_x = \chi$ in generic form, $\frac{1}{\sqrt{2}}a_x + \frac{1}{\sqrt{2}}b_x = a$ and $\frac{1}{\sqrt{2}}a_x - \frac{1}{\sqrt{2}}b_x = b$. The solutions are:

$$a_x = \frac{a+b}{\sqrt{2}} \text{ and } b_x = \frac{a-b}{\sqrt{2}} \tag{3.25}$$

gives χ_x finally as:

$$\chi = \chi_x = \frac{a+b}{\sqrt{2}}\chi_{x+} + \frac{a-b}{\sqrt{2}}\chi_{x-}. \tag{3.26}$$

Now, S_x is applied again to the newly constructed χ:

$$\begin{aligned} S_x\chi &= \frac{a+b}{\sqrt{2}} S_x \chi_{x+} + \frac{a-b}{\sqrt{2}} S_x \chi_{x-} \\ &= \frac{a+b}{\sqrt{2}} \frac{\hbar}{2} \chi_{x+} + \frac{a-b}{\sqrt{2}} (-\frac{\hbar}{2}) \chi_{x-} \end{aligned} \tag{3.27}$$

which gives the statistical details for probability of getting $\frac{\hbar}{2}$ being $\frac{1}{2}\left|a+b\right|^2$ while for $-\frac{\hbar}{2}$ is $\frac{1}{2}\left|a-b\right|^2$.

3.3 Addition of Angular Momentum for Two Spin Half Particles

A simple case of this would be hydrogen atom at its ground state, since both electron and proton are spin $\frac{1}{2}$. Each can either in spin up or spin down state, giving 4 possible combinations:

$$\uparrow\uparrow, \uparrow\downarrow, \downarrow\uparrow, \downarrow\downarrow .$$

Let the first particle be labeled as 1 and second particle 2. Their total spin take the form $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ and $S_z = S_{z1} + S_{z2}$. So,

$$\begin{aligned} S_z \chi_1 \chi_2 &= (S_{z1} + S_{z2}) \chi_1 \chi_2 \\ &= (S_{z1} \chi 1) \chi_2 + \chi_1 (S_{z2} \chi_2) \\ &= \hbar m_{s1} \chi_1 \chi_2 + \chi_1 \hbar m_{s2} \chi_2 \\ &= \hbar (m_{s1} + m_{s2}) \chi_1 \chi_2 \end{aligned} \tag{3.28}$$

so that, $m_s = m_{s1} + m_{s2}$ with m_s denotes magnetic spin quantum number of composite system. The method of operators here might not seem familiar at the moment. It is introduced in later part as tensor product.

In comparison, each m_s corresponds to:

$$\begin{array}{lcccc} \text{states:} & \uparrow\uparrow, & \uparrow\downarrow, & \downarrow\uparrow, & \downarrow\downarrow \\ m_s: & 1, & 0, & 0, & -1 \end{array} .$$

There exists an extra state with $m_s = 0$. From mathematics' point of view, applying lowering operator $S_- = S_{1-} + S_{2-}$ to $\uparrow\uparrow$ gives:

$$\begin{aligned} S_-(\uparrow\uparrow) &= (S_{1-}\uparrow)\uparrow + \uparrow(S_{2-}\uparrow) \\ &= \hbar\downarrow\uparrow + \uparrow\hbar\downarrow \\ &= \hbar(\uparrow\downarrow + \downarrow\uparrow) \end{aligned} \tag{3.29}$$

where $S_- \uparrow \equiv S_- \left|\frac{1}{2}\,\frac{1}{2}\right\rangle = \hbar\sqrt{\frac{1}{2}(\frac{1}{2}+1) - \frac{1}{2}(\frac{1}{2}-1)}\left|\frac{1}{2}\,-\frac{1}{2}\right\rangle = \hbar\downarrow$.
So far, the identity of s is yet to mention, but since $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$, $s = s_1 + s_2 = \frac{1}{2} + \frac{1}{2} = 1$. The three possible states in notation $|s\,m_s\rangle$ is thus:

$$\left.\begin{array}{l} |1\,1\rangle = \uparrow\uparrow \\ |1\,0\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) \\ |1\,-1\rangle = \downarrow\downarrow \end{array}\right\} s = 1 \tag{3.30}$$

These are called the triplet states. The constant $\frac{1}{\sqrt{2}}$ in $|1\,0\rangle$ states is the normalization constant.
Now, if $\mathbf{S} = \mathbf{S}_1 - \mathbf{S}_2$, $s = s_1 - s_2 = \frac{1}{2} - \frac{1}{2} = 0$, the only allowed value of m_s is $m_s = 0$ since for given s, $m_s = -s, -s+1, \ldots, s-1, s$. So, the singlet state is:

$$\left.|0\,0\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)\right\} s = 0. \tag{3.31}$$

3.4 Chapter Summary

In $|s\,m_s\rangle$ notation, all previous four results can be written as:

$$|s\,m_s\rangle = \sum_{m_{s1}+m_{s2}=m_s} C^{s_1\ \ s_2\ \ s_3}_{m_{s1}\,m_{s2}\,m_{s3}}\,|s_1\,m_{s1}\rangle\,|s_2\,m_{s2}\rangle \tag{3.32}$$

The addition of angular momentum $|s\,m_s\rangle$ is linear combination of composite states $|s_1\,m_{s1}\rangle\,|s_2\,m_{s2}\rangle$ with $C^{s_1\ \ s_2\ \ s_3}_{m_{s1}\,m_{s2}\,m_{s3}}$ are called Clebsch-Gordan coefficients. The details of its usefulness will be discussed in the later section.

Chapter 4

Total Angular Momentum

4.1 Introduction

In both atomic and nuclear structure it is important to know how the interaction energy between particles depends on the orientation of their angular momenta. Two different coupling schemes: *j*-*j* coupling and *L*-*S* coupling represent extreme cases. However, the real situation is a deviation from both pictures, see Elementary Theory of Angular Momentum, Rose, p. 187 [5] The effect of each scheme depends largely on the size of atom, which influences the relative strength of coupling interaction. In the absent of strong external magnetic field, electron spins interact strongly. The same goes to the orbital angular momentum. Stronger external magnetic field causes the two momenta to be decoupled. This happen wisely in light atom, heavier nucleus gives rise to a bigger nuclear charge, causing the spin-orbit interactions to be larger than previous *L*-*S* interaction. This situation favors a self-combination of l_i and s_i to give j_i to be coupled up in *j*-*j* coupling.

Before going further into known cases, two particles with intrinsic spin s_1 and s_2 and their orbital angular momentum l_1 and l_2 are considered. The general picture in matrix form: [1]

$$\begin{bmatrix} s_1 & l_1 & j_1 \\ s_2 & l_2 & j_2 \\ S & L & J \end{bmatrix}$$

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[1] See Elementary theory of Angular Momentum by Rose,[5] page 187-192 for further explanations.

j-*j* coupling is described by:

$$j_1 = l_1 + s_1 \tag{4.1}$$
$$j_2 = l_2 + s_2 \tag{4.2}$$
$$J = j_1 + j_2 \tag{4.3}$$

apparently there is a strong coupling between l_i and s_i. Besides s_1^2, s_2^2, l_1^2 and l_2^2, the constants of motion are:

$$J^2, J_z, j_1^2, j_2^2$$

with their respective eigenvalues as $\hbar^2 J(J+1)$, m_J, $\hbar^2 j_1(j_1+1)$, $\hbar^2 j_2(j_2+1)$.
Meanwhile, *L*-*S* coupling is described by:

$$L = l_1 + l_2 \tag{4.4}$$
$$S = s_1 + s_2 \tag{4.5}$$
$$J = L + S \tag{4.6}$$

there is a strong coupling among l_i or among s_i. Similarly, other than s_1^2, s_2^2, l_1^2 and l_2^2, the constants of motion are:

$$J^2, J_z, L^2, S^2$$

The respective eigenvalues are $\hbar^2 J(J+1)$, m_J, $\hbar^2 l(l+1)$, $\hbar^2 s(s+1)$. [5]

4.2 The Fine Structure of Hydrogen

This is an adaptation from Section 6.3 of Introduction to Quantum Mechanics (2nd ed.) by Griffiths, page 266-275.
In the hydrogen atom the Hamiltonian is:

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r} \tag{4.7}$$

fine structure is a tiny perturbation [2] , smaller by a factor of α^2 as compared to Bohr energies, where

$$\alpha \equiv \frac{e^2}{4\pi\epsilon_0\hbar c} \cong \frac{1}{137.036} \tag{4.8}$$

is the famous fine structure constant.

The sole purpose of this section is to find out how the energy spectrum of hydrogen

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[2] To find the first order correction, non-degenerate perturbation theory will be used, as introduced in Appendix B.1

atom is influenced by the fine structure. There are two major contributors to the fine structure formula:
a) the relativistic correction, [3]

$$E_r^1 = -\frac{E_n^2}{2mc^2}[\frac{4n}{l+1/2} - 3] \tag{4.9}$$

b) the spin-orbit coupling correction, [4]

$$E_{SO}^1 = \frac{E_n^2}{mc^2}\{\frac{n[j(j+1) - l(l+1) - 3/4]}{l(l+1/2)(l+1)}\} \tag{4.10}$$

Adding them together is the complete fine-structure formula:

$$E_{fs}^1 = E_r^1 + E_{SO}^1 \tag{4.11}$$

since $j = l + s = l + \frac{1}{2}$, the case here is $l = j - \frac{1}{2}$; $l + 1 = j + \frac{1}{2}$,

$$\begin{aligned} E_{SO}^1 &= \frac{E_n^2}{mc^2}\{\frac{n[j^2 + j - (j-1/2)(j+1/2) - 3/4]}{j(j-1/2)(j+1/2)}\} \\ &= \frac{E_n^2}{mc^2}\{\frac{n[j^2 + j - j^2 + 1/4 - 3/4]}{j(j-1/2)(j+1/2)}\} \\ &= \frac{E_n^2}{mc^2}\frac{n(j-1/2)}{j(j-1/2)(j+1/2)} \\ &= \frac{E_n^2}{mc^2}\frac{n}{j(j+1/2)} \end{aligned} \tag{4.12}$$

hence

$$\begin{aligned} E_{fs}^1 &= \frac{E_n^2}{2mc^2}[\frac{2n}{j(j+1/2)} - \frac{4n}{j} + 3] \\ &= \frac{E_n^2}{2mc^2}[3 + \frac{2n - 4n(j+1/2)}{j(j+1/2)}] \\ &= \frac{E_n^2}{2mc^2}[3 + \frac{2n - 4nj - 2n)}{j(j+1/2)}] \\ &= \frac{E_n^2}{2mc^2}[3 - \frac{4n}{j+1/2}]. \end{aligned} \tag{4.13}$$

Now,

$$E_1 = -\frac{m}{2\hbar^2}(\frac{e^2}{4\pi\epsilon_0})^2 = -\frac{m\hbar^2c^2}{2\hbar^2}(\frac{e^2}{4\pi\epsilon_0\hbar c})^2 = -\frac{mc^2\alpha^2}{2} \tag{4.14}$$

---

[3] Refer Appendix B.2 for details in obtaining E_r^1.

[4] Refer Appendix B.3 for derivation of E_{SO}^1.

where $\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c}$ the fine structure constant, and the Bohr formula, $E_n = \frac{E_1}{n^2}$. Combining the Bohr formula with the fine structure correction in terms of fine structure constant,

$$\begin{aligned} E_{nj} &= E_n + E^1_{fs} = E_n + \frac{E_n^2}{2mc^2}[3 - \frac{4n}{j+1/2}] \\ &= E_n[1 + \frac{E_n}{2mc^2}(3 - \frac{4n}{j+1/2})] \\ &= \frac{E_1}{n^2}[1 + \frac{E_n}{2mc^2n^2}(3 - \frac{4n}{j+1/2})] \\ &= \frac{E_1}{n^2}[1 - \frac{mc^2\alpha^2}{4mc^2n^2}(3 - \frac{4n}{j+1/2})] \\ &= \frac{E_1}{n^2}[1 + \frac{\alpha^2}{n^2}(\frac{n}{j+1/2} - \frac{3}{4})]. \end{aligned} \tag{4.15}$$

Fine structure breaks the degeneracy in l, but it still preserves degeneracy in j. The z-component eigenvalues for orbital and spin angular momentum (m_l and m_s) are no longer "good" quantum number - the stationary state are linear combination of state, with different values of these quantities, the "good" quantum numbers are n, l, s, j and m_j, see page 266-275 of Griffiths, Introduction to Quantum Mechanics. [4]

4.3 Hyperfine splitting

This is an adaptation from Section 6.5 of Introduction to Quantum Mechanics (2nd ed.) by Griffiths, page 283-285.

The proton itself constitutes a magnetic dipole, though its dipole moment is much smaller than the electron's because of the mass in the denominator:

$$\vec{\mu}_p = \frac{g_p e}{2m_p}\mathbf{S}_p \; , \; \vec{\mu}_e = -\frac{e}{m_e}\mathbf{S}_e \tag{4.16}$$

where g_p = g-factor whose value is measured to be 5.59, as opposed to electron's 2.00, due to proton being a composite structure.

According to classical electrodynamics, a dipole $\vec{\mu}$ sets up a magnetic field: [5]

$$\mathbf{B} = \frac{\mu_0}{4\pi r^3}[3(\vec{\mu}\cdot\mathbf{r})\hat{r} - \vec{\mu}] + \frac{2\mu_0}{3}\vec{\mu}\delta^3(\mathbf{r}). \tag{4.17}$$

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[5] Refer Introduction to Electrodynamics, 3rd ed. Griffiths, problem 5.59, page 253-254. [6]

So, the Hamiltonian of the electron, in the magnetic field due to the proton's magnetic dipole moment, is

$$\begin{aligned} H &= -\vec{\mu}\cdot\mathbf{B} = -\vec{\mu}_e\cdot\mathbf{B}_p \\ &= -\frac{\mu_0}{4\pi r^3}[3(\vec{\mu}_e\cdot\hat{r})(\vec{\mu}_p\cdot\hat{r}) - \vec{\mu}_e\cdot\vec{\mu}_p] - \frac{2\mu_0}{3}(\vec{\mu}_e\cdot\vec{\mu}_p)\delta^3(\mathbf{r}) \qquad (4.18) \\ H'_{hf} &= \frac{\mu_0 g_p e^2}{8\pi m_p m_e}\frac{[3(\mathbf{S}_p\cdot\hat{r})(\mathbf{S}_e\cdot\hat{r}) - \mathbf{S}_p\cdot\mathbf{S}_e]}{r^3} + \frac{\mu_0 g_p e^2}{3m_p m_e}\mathbf{S}_p\cdot\mathbf{S}_e\delta^3(\mathbf{r}). \qquad (4.19) \end{aligned}$$

According to the perturbation theory, the first-order correction to the energy: $E^1_n = \left\langle\psi^0_n|H'_{hf}|\psi^0_n\right\rangle$ is the expectation value of the perturbing Hamiltonian:

$$E^1_n = \frac{\mu_0 g_p e^2}{8\pi m_p m_e}\left\langle\frac{3(\mathbf{S}_p\cdot\hat{r})(\mathbf{S}_e\cdot\hat{r}) - \mathbf{S}_p\cdot\mathbf{S}_e}{r^3}\right\rangle + \frac{\mu_0 g_p e^2}{3m_p m_e}\left\langle\mathbf{S}_p\cdot\mathbf{S}_e\right\rangle\left\langle\psi^0_n\delta^3(\mathbf{r})|\psi^0_n\right\rangle. \qquad (4.20)$$

Dirac delta function:

$$\begin{aligned} \langle\psi^0_n\delta^3(\mathbf{r})|\psi^0_n\rangle &= \textstyle\int|\psi^0_n(\mathbf{r})|^2\delta^3(\mathbf{r}-0)d^3\mathbf{r} = |\psi^0_n(0)|^2 \qquad (4.21) \\ E^1_n &= \tfrac{\mu_0 g_p e^2}{8\pi m_p m_e}\left\langle\tfrac{3(\mathbf{S}_p\cdot\hat{r})(\mathbf{S}_e\cdot\hat{r})-\mathbf{S}_p\cdot\mathbf{S}_e}{r^3}\right\rangle + \tfrac{\mu_0 g_p e^2}{3m_p m_e}\left\langle\mathbf{S}_p\cdot\mathbf{S}_e\right\rangle|\psi^0_n(0)|^2. \qquad (4.22) \end{aligned}$$

In the ground state (or any other state for which $l = 0$) the wave function is spherical symmetrical, and the first expectation value vanishes.

$$\left\langle\frac{3(\mathbf{S}_p\cdot\hat{r})(\mathbf{S}_e\cdot\hat{r}) - \mathbf{S}_p\cdot\mathbf{S}_e}{r^3}\right\rangle = 0. \qquad (4.23)$$

Meanwhile, from ground state hydrogen wave function, [6]

$$\begin{aligned} \psi_{100}(r,\theta,\phi) &= \frac{1}{\sqrt{\pi a^3}}e^{-r/a} \qquad (4.24) \\ \psi_{100}(0) &= \frac{1}{\sqrt{\pi a^3}} \qquad (4.25) \\ |\psi_{100}(0)|^2 &= \frac{1}{\pi a^3}. \qquad (4.26) \end{aligned}$$

So,

$$E^1_{hf} = \frac{\mu_0 g_p e^2}{3\pi m_p m_e a^3}\left\langle\mathbf{S}_p\cdot\mathbf{S}_e\right\rangle \qquad (4.27)$$

in the ground state. This is called spin-spin coupling, because it involves the dot product of two spins. In the presence of spin-spin coupling, the individual spin angular momenta

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[6] These results are outlined by Griffiths himself in the text, [4]

are no longer conserved; the "good" states are eigenvectors of the total spin.

$$\mathbf{S} = \mathbf{S}_e + \mathbf{S}_p. \tag{4.28}$$

As before, the square of equation 4.28 gives:

$$S^2 = S_e^2 + S_p^2 + 2\mathbf{S}_e \cdot \mathbf{S}_p \tag{4.29}$$

$$\mathbf{S}_e \cdot \mathbf{S}_p = \frac{1}{2}(S^2 - S_e^2 - S_p^2). \tag{4.30}$$

But the electron and proton have spin $\frac{1}{2}$, so

$$S_e^2 = S_p^2 = s(s+1)\hbar^2 = \frac{3}{4}\hbar^2. \tag{4.31}$$

In the triplet state (spin "parallel") the total spin S is 1: $S_p + S_e = \frac{1}{2} + \frac{1}{2} = 1$, and hence

$$\mathbf{S} = \mathbf{S}_p + \mathbf{S}_e\ ,\ S^2 = S(S+1)\hbar^2 = 2\hbar^2. \tag{4.32}$$

In the singlet state, (spin "anti parallel") the total spin S is 0:

$$S = S_p + S_e = \frac{1}{2} - \frac{1}{2} = 0\ ,\ \text{and}\ \ S^2 = 0 \tag{4.33}$$

thus for the triplet state:

$$\mathbf{S}_p \cdot \mathbf{S}_e = \frac{1}{2}(2\hbar^2 - \frac{3}{4}\hbar^2 - \frac{3}{4}\hbar^2) = \frac{1}{2}(\frac{2}{4}\hbar^2) = \frac{1}{4}\hbar^2 \tag{4.34}$$

and for the singlet state:

$$\mathbf{S}_p \cdot \mathbf{S}_e = \frac{1}{2}(0 - \frac{3}{4}\hbar^2 - \frac{3}{4}\hbar^2) = \frac{1}{2}(-\frac{6}{4}\hbar^2) = -\frac{3}{4}\hbar^2 \tag{4.35}$$

$$E_{hf}^1 = \frac{\mu_0 g_p e^2 \hbar^2}{3\pi m_p m_e a^3} \left\{ \begin{array}{ll} +\frac{1}{4} & \text{triplet} \\ -\frac{3}{4} & \text{singlet} \end{array} \right. \tag{4.36}$$

multiply by $\frac{4\epsilon_0 m_e \hbar^2}{4\epsilon_0 m_e \hbar^2}$,

$$E_{hf}^1 = \frac{4\mu_0 \epsilon_0 g_p \hbar^4}{3 m_p m_e^2 a^3}(\frac{m_e e^2}{4\pi\epsilon_0 \hbar^2}) \left\{ \begin{array}{l} +\frac{1}{4} \\ -\frac{3}{4} \end{array} \right. \tag{4.37}$$

using $\frac{1}{a} = \frac{me^2}{4\pi\epsilon_0\hbar^2}$; $\mu_0\epsilon_0 = \frac{1}{c^2}$, then

$$E_{hf}^1 = \frac{4 g_p \hbar^4}{3 m_p m_e^2 a^4 c^2} \left\{ \begin{array}{ll} +\frac{1}{4} & \text{triplet} \\ -\frac{3}{4} & \text{singlet} \end{array} \right. . \tag{4.38}$$

Spin-spin coupling breaks the spin degeneracy of the ground state, lifting the triplet configuration and depressing the singlet. The energy gap is:

$$\begin{aligned} \Delta E &= \frac{4g_p\hbar^4}{3m_p m_e^2 a^4 c^2}[\frac{1}{4} - (-\frac{3}{4})] \\ &= 5.88 \times 10^{-6}\text{eV}. \end{aligned} \tag{4.39}$$

The corresponding wavelength of the photon emitted in a transition from the triplet to the singlet state is:

$$\lambda = \frac{hc}{\Delta E} \cong 21\text{cm} \tag{4.40}$$

which falls in the microwave region. This famous 21 centimeter is among the ubiquitous forms of radiation in the universe, as recorded by Griffiths, Introduction to Quantum Mechanics, pp. 283-285. [4]

4.4 Bosons and Fermions

Consider 2 identical non-interaction particles, the composite of the system can be described by:

$$\psi(1,2) = \psi(1)\psi(2) \tag{4.41}$$

the probability density $|\psi|^2$ of the system when the particles exchange should remain the same:

$$|\psi|^2(1,2) = |\psi|^2(2,1) \tag{4.42}$$

or in other words, being equally possible,

$$\psi(1,2) = \psi_a(1)\psi_b(2) \tag{4.43}$$

$$\psi(2,1) = \psi_a(2)\psi_b(1). \tag{4.44}$$

They can be rewritten in linear combination:

$$\psi_S(1,2) = \frac{1}{\sqrt{2}}[\psi_a(1)\psi_b(2) + \psi_a(2)\psi_b(1)] \tag{4.45}$$

representing the symmetric wave function of bosons;

$$\psi_A(1,2) = \frac{1}{\sqrt{2}}[\psi_a(1)\psi_b(2) - \psi_a(2)\psi_b(1)] \tag{4.46}$$

representing the anti-symmetric wave function of fermions. See Tipler, Modern Physics pp. 295-297. [7]

To see what happen if two identical fermions are in the same state:

$$\psi_A(1,2) = \frac{1}{\sqrt{2}}[\psi_a(1)\psi_a(2) - \psi_a(2)\psi_a(1)] = 0 \tag{4.47}$$

which completely nullify the existence of the composite system, since $|\psi|^2$ give the probability density. This account for Pauli exclusion principle for fermions [8]:
"No more than one Fermion may occupy a given quantum state specified by particular set of quantum numbers."

A second important feature to be noted about Bosons and Fermions are their respective spin. Bosons carry an integer spin, $S = +Z\hbar$ where Z stand for integers. While Fermions carry half-integer spin, $S = +\frac{Z}{2}\hbar$. [4]

4.5 Spectroscopy Notation / Term Symbol

An electron configuration is a listing of the number of electrons in each sub-shell and shows the occupational scheme of atomic orbitals, according to a set of pre-defined quantum numbers. LS-coupling scheme is used here as L and S are good quantum numbers, the angular momentum of individual electrons combined to the total orbital angular momentum, L and total spin S of the atom. For atom with large atomic number Z, the jj-coupling scheme is more appropriate where each l_i and s_i of every electron are first combined to the total angular momentum j_i of the electron so that L and S lose their meaning. The different schemes of treatment is due to the relative strength of Coulombic interaction term and Spin-Orbit interaction term in the total Hamiltonian operator.

$$H = H_o + H_{ee} + H_{SO}. \tag{4.48}$$

For $H_{ee} > H_{SO}$, LS-coupling, H_{SO} is treated as a perturbation and applies to light atoms. While for case where $H_{ee} < H_{SO}$, jj-coupling, H_{ee} is treated as a perturbation and applies to heavy atoms, as written in D.Fluri, Molecular Universe, pp.4-8. [9]

Now, the spectroscopy notation says, [10]

$$^{2S+1}\mathcal{L}_J$$

where

$$\begin{aligned}
S &= s_1 + s_2 + \ldots = \sum_i s_i && (4.49)\\
L &= l_1 + l_2 + \ldots = \sum_i l_i && (4.50)\\
J &= j_1 + j_2 + \ldots = \sum_i j_i && (4.51)\\
\text{and also } J &\equiv L + S && (4.52)
\end{aligned}$$

are capital letters to emphasize these are quantum number for an ensemble of electrons. Also, $\mathcal{L}$ are capital letters correspond to:

$$\begin{array}{rcccccccc}
L &=& 0 & 1 & 2 & 3 & 4 & \cdots \\
\mathcal{L} &=& S & P & D & F & G & \cdots
\end{array}$$

The number $2S + 1$ is called the multiplicity of the term because it determines the number of levels in a term with $L \geq S$. The multiplicity of term $1, 2, 3, \ldots$ is read as singlet, doublet, triplet, ... These names are traditionally kept for $2S + 1$ even though when $L < S$, the term contains $2L+1$ levels. Hund's rules is used to predict the notation for ground state of a given atom, in consistent with the Pauli exclusion principle. It has some special cases such as Cr, Cu whereby the stability of electronic ground state is affected by some other factors.

Hund's Rules

1. Other things being equal, the lowest energy state of atomic electrons is the state with the highest S.
2. For a given total spin S, the lowest energy state is the state with the largest L.
3. For a given total S and L, if the valence level is not more than half filled, the lowest energy state has the minimum $J = |L - S|$; if the shell is more than half filled, the lowest energy state has $J = L + S$.

For a clearer picture, two examples are described, one of C-12 and another Ni-28 in Appendix B.4.

4.6 Clebsch-Gordan Coefficient

4.6.1 Coupled and Uncoupled Representation

Let's consider a composite system consisting of two subsystems which can either be two particles or the orbital angular momentum and the spin of a particle. The angular momentum are $\mathbf{J}_1$ and $\mathbf{J}_2$ with z-components m_1 and m_2. The states of angular momentum for this system can be represented with either one of two sets of quantum numbers, namely the coupled representation and uncoupled representation, correspond to the eigenstates $|j\, m\,;\, j_1\, j_2\rangle$ and $|j_1\, m_1\,;\, j_2\, m_2\rangle$. Here, the total z-component is:

$$m = m_1 + m_2 \tag{4.53}$$

while the total angular momentum is:

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2 = \sqrt{j(j+1)}\hbar\hat{J}. \tag{4.54}$$

An intuitive explanation for the range of allowed values of j follows from vector additions [1] as in the following figure:

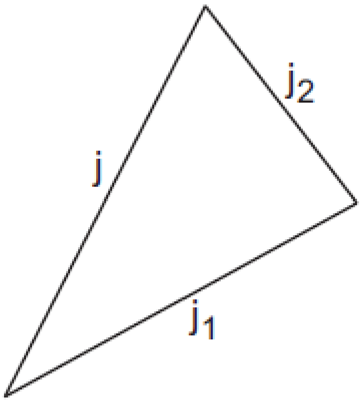

Figure 4.1: Triangle of vectors addition j, j_1, j_2 in arbitrary directions [1]

Without specifying a definite direction for each vector, the vectors required that

$$\begin{aligned} j &\leq j_1 + j_2 && (4.55)\\ j_1 &\leq j_2 + j && (4.56)\\ j_2 &\leq j_1 + j. && (4.57)\end{aligned}$$

The second and third condition can be rewritten as $j \geq j_1 - j_2$ and $j \geq j_2 - j_1$ which can be combined to give $j \geq |j_1 - j_2|$. Together with the first condition, the following range is obtained:

$$|j_1 - j_2| \leq j \leq j_1 + j_2. \tag{4.58}$$

As mentioned earlier, for the coupled representation, the total angular momentum are important, J^2, J_z along with J_1^2 and J_2^2 are specified. While in uncoupled representation, the z-component and magnitude of angular momentum of all subsystem remain specified, that is J_1^2, J_{1z}, J_2^2 and J_{2z}. See Introductory Quantum Mechanics, Liboff, pp. 347-349. [11]

4.6.2 Clebsch-Gordan Coefficient

The eigenstates in both representation are constructed from the tensor products of the eigenstates $|j_1\, m_1\rangle$ and $|j_2\, m_2\rangle$. First, for uncoupled basis,

$$|j_1\, m_1\, ;\, j_2\, m_2\rangle = |j_1\, m_1\rangle \otimes |j_2\, m_2\rangle \tag{4.59}$$

with $\sum_{|j_1-j_2|}^{j_1+j_2}(2j+1) = (2j_1+1)(2j_2+1)$ linearly independent states. To write the representation in coupled basis, the discrete completeness closure operator $\hat{I}$ for unitary transformation is applied:

$$\begin{aligned} |j\, m\, ;\, j_1\, j_2\rangle &= \hat{I}\, |j\, m\, ;\, j_1\, j_2\rangle \\ &= \sum_m |j_1\, m_1\, ;\, j_2\, m_2\rangle \, \langle j_1\, m_1\, ;\, j_2\, m_2 | j\, m\, ;\, j_1\, j_2\rangle \\ &= \sum_m C^{j_1\; j_2\; j}_{m_1\, m_2\, m}\, |j_1\, m_1\, ;\, j_2\, m_2\rangle \\ &= \sum_m C^{j_1\; j_2\; j}_{m_1\, m_2\, m}\, |j_1\, m_1\rangle \otimes |j_2\, m_2\rangle \end{aligned} \tag{4.60}$$

where $m = m_1 + m_2$ constraints the summation and $C^{j_1\; j_2\; j}_{m_1\, m_2\, m}$ are the Clebsch-Gordan coefficients. [7]

The significance of Clebsch-Gordan coefficients as explain by Liboff in his text [11] is:

$|C^{j_1\; j_2\; j}_{m_1\, m_2\, m}|^2 =$ probability that measurement finds one electron with $J_{1z} = m_1\hbar$ and the other electron with $J_{2z} = m_2\hbar$.

---

[7] Every even-numbered years, Particle Data Group (PDG) will publish lists of reviews, tables, and plots summarizing particle physics, as well as related areas of cosmology and astrophysics. Worth mentioning here is that Clebsh-Gordan coefficients tables are publish under category "mathematical tools", refer "http://pdg.lbl.gov/index.html". The latest page is included in section 4.6.3 of this report.

Now, since the transformation are unitary, the inverse is taken by multiplying $C^{j_1\,j_2\,j}_{m_1\,m_2\,m}{}^*$ from the left:

$$\begin{aligned} C^{j_1\,j_2\,j}_{m_1\,m_2\,m}{}^* \left|j\,m\,;\,j_1\,j_2\right\rangle &= \sum_m \left|C^{j_1\,j_2\,j}_{m_1\,m_2\,m}\right|^2 \left|j_1\,m_1\,;\,j_2\,m_2\right\rangle \\ &= \left|j_1\,m_1\,;\,j_2\,m_2\right\rangle \end{aligned} \tag{4.61}$$

and rearranging it gives:

$$\left|j_1\,m_1\,;\,j_2\,m_2\right\rangle = \sum_m \left\langle j\,m\,;\,j_1\,j_2\middle|j_1\,m_1\,;\,j_2\,m_2\right\rangle \left|j\,m\,;\,j_1\,j_2\right\rangle \tag{4.62}$$

where $C^{j_1\,j_2\,j}_{m_1\,m_2\,m}{}^* = \left\langle j\,m\,;\,j_1\,j_2\middle|j_1\,m_1\,;\,j_2\,m_2\right\rangle$. As it turned out, the Clebsch-Gordan coefficients can always be chosen to be real, so that the conjugate symbol may be dropped here. This is explained by Tristan Hbsch in Addition of Angular Momenta, pp.2-4. [12]

4.6.3 Table of Clebsch-Gordan Coefficients

As a conclusion to this chapter, an input of the original copy of 2011 web edition of Clebsch-Gordan coefficient tables are attached in the following page. [13] These tables are computer generated rather than calculate analytically.[8]

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[8] In Appendix B.5, the two simplest tables are worked out, with reference to Perkins, Introduction to High Energy Physics, pp.386-390. [14]

36. 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	...
m₁	m₂	Coefficients		
m₁	m₂			
.	.			
.	.			

1/2×1/2

		1
		+1
+1/2	+1/2	1

		1	0
		0	0
+1/2	−1/2	1/2	1/2
−1/2	+1/2	1/2	−1/2

		1
		−1
−1/2	−1/2	1

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}$$

$$Y_2^0 = \sqrt{\frac{5}{4\pi}}\Big(\frac{3}{2}\cos^2\theta - \frac{1}{2}\Big)$$

$$Y_2^1 = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{i\phi}$$

$$Y_2^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{2i\phi}$$

2×1/2

		5/2
		+5/2
+2	+1/2	1

		5/2	3/2
		+3/2	+3/2
+2	−1/2	1/5	4/5
+1	+1/2	4/5	−1/5

		5/2	3/2
		+1/2	+1/2
+1	−1/2	2/5	3/5
0	+1/2	3/5	−2/5

		5/2	3/2
		−1/2	−1/2
0	−1/2	3/5	2/5
−1	+1/2	2/5	−3/5

		5/2	3/2
		−3/2	−3/2
−1	−1/2	4/5	1/5
−2	+1/2	1/5	−4/5

		5/2
		−5/2
−2	−1/2	1

1×1/2

		3/2
		+3/2
+1	+1/2	1

		3/2	1/2
		+1/2	+1/2
+1	−1/2	1/3	2/3
0	+1/2	2/3	−1/3

		3/2	1/2
		−1/2	−1/2
0	−1/2	2/3	1/3
−1	+1/2	1/3	−2/3

		3/2
		−3/2
−1	−1/2	1

3/2×1/2

		2
		+2
+3/2	+1/2	1

		2	1
		+1	+1
+3/2	−1/2	1/4	3/4
+1/2	+1/2	3/4	−1/4

		2	1
		0	0
+1/2	−1/2	1/2	1/2
−1/2	+1/2	1/2	−1/2

		2	1
		−1	−1
−1/2	−1/2	3/4	1/4
−3/2	+1/2	1/4	−3/4

		2
		−2
−3/2	−1/2	1

2×1

		3
		+3
+2	+1	1

		3	2
		+2	+2
+2	0	1/3	2/3
+1	+1	2/3	−1/3

		3	2	1
		+1	+1	+1
+2	−1	1/15	1/3	3/5
+1	0	8/15	1/6	−3/10
0	+1	2/5	−1/2	1/10

		3	2	1
		0	0	0
+1	−1	1/5	1/2	3/10
0	0	3/5	0	−2/5
−1	+1	1/5	−1/2	3/10

		3	2	1
		−1	−1	−1
0	−1	2/5	1/2	1/10
−1	0	8/15	−1/6	−3/10
−2	+1	1/15	−1/3	3/5

		3	2
		−2	−2
−1	−1	2/3	1/3
−2	0	1/3	−2/3

		3
		−3
−2	−1	1

3/2×1

		5/2
		+5/2
+3/2	+1	1

		5/2	3/2
		+3/2	+3/2
+3/2	0	2/5	3/5
+1/2	+1	3/5	−2/5

		5/2	3/2	1/2
		+1/2	+1/2	+1/2
+3/2	−1	1/10	2/5	1/2
+1/2	0	3/5	1/15	−1/3
−1/2	+1	3/10	−8/15	1/6

		5/2	3/2	1/2
		−1/2	−1/2	−1/2
+1/2	−1	3/10	8/15	1/6
−1/2	0	3/5	−1/15	−1/3
−3/2	+1	1/10	−2/5	1/2

		5/2	3/2
		−3/2	−3/2
−1/2	−1	3/5	2/5
−3/2	0	2/5	−3/5

		5/2
		−5/2
−3/2	−1	1

1×1

		2
		+2
+1	+1	1

		2	1
		+1	+1
+1	0	1/2	1/2
0	+1	1/2	−1/2

		2	1	0
		0	0	0
+1	−1	1/6	1/2	1/3
0	0	2/3	0	−1/3
−1	+1	1/6	−1/2	1/3

		2	1
		−1	−1
0	−1	1/2	1/2
−1	0	1/2	−1/2

		2
		−2
−1	−1	1

$$Y_\ell^{-m} = (-1)^m Y_\ell^{m*}$$

$$d^{\,\ell}_{m,0} = \sqrt{\frac{4\pi}{2\ell+1}}\, Y_\ell^m\, e^{-im\phi}$$

$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 J M\rangle = (-1)^{J-j_1-j_2}\langle j_2 j_1 m_2 m_1 | j_2 j_1 J M\rangle$$

$$d^{\,j}_{m',m} = (-1)^{m-m'} d^{\,j}_{m,m'} = d^{\,j}_{-m,-m'}$$

3/2×3/2

		3
		+3
+3/2	+3/2	1

		3	2
		+2	+2
+3/2	+1/2	1/2	1/2
+1/2	+3/2	1/2	−1/2

		3	2	1
		+1	+1	+1
+3/2	−1/2	1/5	1/2	3/10
+1/2	+1/2	3/5	0	−2/5
−1/2	+3/2	1/5	−1/2	3/10

		3	2	1	0
		0	0	0	0
+3/2	−3/2	1/20	1/4	9/20	1/4
+1/2	−1/2	9/20	1/4	−1/20	−1/4
−1/2	+1/2	9/20	−1/4	−1/20	1/4
−3/2	+3/2	1/20	−1/4	9/20	−1/4

		3	2	1
		−1	−1	−1
+1/2	−3/2	1/5	1/2	3/10
−1/2	−1/2	3/5	0	−2/5
−3/2	+1/2	1/5	−1/2	3/10

		3	2
		−2	−2
−1/2	−3/2	1/2	1/2
−3/2	−1/2	1/2	−1/2

		3
		−3
−3/2	−3/2	1

$$d^{\,1}_{0,0} = \cos\theta \qquad d^{\,1/2}_{1/2,1/2} = \cos\frac{\theta}{2} \qquad d^{\,1}_{1,1} = \frac{1+\cos\theta}{2}$$

$$d^{\,1/2}_{1/2,-1/2} = -\sin\frac{\theta}{2} \qquad d^{\,1}_{1,0} = -\frac{\sin\theta}{\sqrt{2}}$$

$$d^{\,1}_{1,-1} = \frac{1-\cos\theta}{2}$$

2×3/2

		7/2
		+7/2
+2	+3/2	1

		7/2	5/2
		+5/2	+5/2
+2	+1/2	3/7	4/7
+1	+3/2	4/7	−3/7

		7/2	5/2	3/2
		+3/2	+3/2	+3/2
+2	−1/2	1/7	16/35	2/5
+1	+1/2	4/7	1/35	−2/5
0	+3/2	2/7	−18/35	1/5

		7/2	5/2	3/2	1/2
		+1/2	+1/2	+1/2	+1/2
+2	−3/2	1/35	6/35	2/5	2/5
+1	−1/2	12/35	5/14	0	−3/10
0	+1/2	18/35	−3/35	−1/5	1/5
−1	+3/2	4/35	−27/70	2/5	−1/10

		7/2	5/2	3/2	1/2
		−1/2	−1/2	−1/2	−1/2
+1	−3/2	4/35	27/70	2/5	1/10
0	−1/2	18/35	3/35	−1/5	−1/5
−1	+1/2	12/35	−5/14	0	3/10
−2	+3/2	1/35	−6/35	2/5	−2/5

		7/2	5/2	3/2
		−3/2	−3/2	−3/2
0	−3/2	2/7	18/35	1/5
−1	−1/2	4/7	−1/35	−2/5
−2	+1/2	1/7	−16/35	2/5

		7/2	5/2
		−5/2	−5/2
−1	−3/2	4/7	3/7
−2	−1/2	3/7	−4/7

		7/2
		−7/2
−2	−3/2	1

2×2

		4
		+4
+2	+2	1

		4	3
		+3	+3
+2	+1	1/2	1/2
+1	+2	1/2	−1/2

		4	3	2
		+2	+2	+2
+2	0	3/14	1/2	2/7
+1	+1	4/7	0	−3/7
0	+2	3/14	−1/2	2/7

		4	3	2	1
		+1	+1	+1	+1
+2	−1	1/14	3/10	3/7	1/5
+1	0	3/7	1/5	−1/14	−3/10
0	+1	3/7	−1/5	−1/14	3/10
−1	+2	1/14	−3/10	3/7	−1/5

		4	3	2	1	0
		0	0	0	0	0
+2	−2	1/70	1/10	2/7	2/5	1/5
+1	−1	8/35	2/5	1/14	−1/10	−1/5
0	0	18/35	0	−2/7	0	1/5
−1	+1	8/35	−2/5	1/14	1/10	−1/5
−2	+2	1/70	−1/10	2/7	−2/5	1/5

		4	3	2	1
		−1	−1	−1	−1
+1	−2	1/14	3/10	3/7	1/5
0	−1	3/7	1/5	−1/14	−3/10
−1	0	3/7	−1/5	−1/14	3/10
−2	+1	1/14	−3/10	3/7	−1/5

		4	3	2
		−2	−2	−2
0	−2	3/14	1/2	2/7
−1	−1	4/7	0	−3/7
−2	0	3/14	−1/2	2/7

		4	3
		−3	−3
−1	−2	1/2	1/2
−2	−1	1/2	−1/2

		4
		−4
−2	−2	1

$$d^{\,3/2}_{3/2,3/2} = \frac{1+\cos\theta}{2}\cos\frac{\theta}{2}$$

$$d^{\,3/2}_{3/2,1/2} = -\sqrt{3}\,\frac{1+\cos\theta}{2}\sin\frac{\theta}{2} \qquad d^{\,2}_{2,2} = \Big(\frac{1+\cos\theta}{2}\Big)^2$$

$$d^{\,3/2}_{3/2,-1/2} = \sqrt{3}\,\frac{1-\cos\theta}{2}\cos\frac{\theta}{2} \qquad d^{\,2}_{2,1} = -\frac{1+\cos\theta}{2}\sin\theta$$

$$d^{\,3/2}_{3/2,-3/2} = -\frac{1-\cos\theta}{2}\sin\frac{\theta}{2} \qquad d^{\,2}_{2,0} = \frac{\sqrt{6}}{4}\sin^2\theta \qquad d^{\,2}_{1,1} = \frac{1+\cos\theta}{2}(2\cos\theta-1)$$

$$d^{\,3/2}_{1/2,1/2} = \frac{3\cos\theta-1}{2}\cos\frac{\theta}{2} \qquad d^{\,2}_{2,-1} = -\frac{1-\cos\theta}{2}\sin\theta \qquad d^{\,2}_{1,0} = -\sqrt{\frac{3}{2}}\sin\theta\cos\theta$$

$$d^{\,3/2}_{1/2,-1/2} = -\frac{3\cos\theta+1}{2}\sin\frac{\theta}{2} \qquad d^{\,2}_{2,-2} = \Big(\frac{1-\cos\theta}{2}\Big)^2 \qquad d^{\,2}_{1,-1} = \frac{1-\cos\theta}{2}(2\cos\theta+1) \qquad d^{\,2}_{0,0} = \Big(\frac{3}{2}\cos^2\theta - \frac{1}{2}\Big)$$

Figure 36.1: 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).

Chapter 5

Nuclear spin

5.1 Introduction

The spin quantum number for nucleon is $s = \frac{1}{2}$. A nucleon moving in a central potential with orbital angular momentum l and spin s has a total angular momentum given by [15] :

$$j = l + s. \tag{5.1}$$

This total angular momentum j is behaving in the same way as l and s,

$$\begin{aligned} \left\langle j^2 \right\rangle &= \hbar^2 j\,(j+1) & (5.2)\\ \langle j_z \rangle &= \langle l_z + s_z \rangle = \hbar m_j & (5.3) \end{aligned}$$

where $m_j = -j, -j+1, \ldots, j-1, j$ and j is the total angular momentum quantum number. Since

$$\begin{aligned} \langle l_z \rangle &= \hbar m_l \\ \langle s_z \rangle &= \hbar m_s \\ \langle j_z \rangle &= \langle l_z + s_z \rangle = \hbar m_j \end{aligned}$$

thus

$$m_j = m_l + m_s = m_l \pm \frac{1}{2}.$$

Recall that m_s is always a half-integer and m_l is an integer which makes m_j half integer $\left(\pm\frac{1}{2}, \pm\frac{3}{2}, \pm\frac{5}{2}, \cdots\right)$ and thus, so do j. Vector coupling suggests only two possible values for j, which is $j = j + \frac{1}{2}$ or $j = l - \frac{1}{2}$.

In spectroscopic notation, j value is indicated as a subscript. Therefore, there are two possible j values for $l = 1$ (p states), $l + \frac{1}{2} = \frac{3}{2}$ and $l - \frac{1}{2} = \frac{1}{2}$.

These states are written as $p_{\frac{3}{2}}$ and $p_{\frac{1}{2}}$. A principle quantum number n is added and the states are indicated as $2p_{\frac{3}{2}}$, $3p_{\frac{3}{2}}$ instead.

Each nucleon possess a total angular momentum of $j = l \pm s$ and the total spin of the nucleus, I is the sum of the nucleon spins $I = \sum j$. [15] Since j is always a half-integer, nuclides with odd number of nucleons or odd A must have half-integer value, or odd I; While those with even A must have even I. The nucleon always pair, so even number of protons yield 0 net spin. Same goes to even number of neutrons.

The total angular momentum of a nucleus containing A nucleons (protons + neutrons) would then be the vector sum of the angular momenta of all the nucleons. This total angular momentum is called nuclear spin and is represented by the symbol I, with the following properties:

$$\mathbf{I}^2 = \hbar^2 I\,(I+1) \tag{5.4}$$

$$I_z = m\hbar \quad (-I \leq m \leq I)\,. \tag{5.5}$$

The nucleus behave as if it were a single entity with an instrinsic angular momentum of I. For this reason, the spin $\mathbf{I}$ and the corresponding spin quantum number I are used to describe nuclear states.

To avoid confusion, the I is denoted as the nuclear spin while j will be used to represent the total angular momentum of a single nucleon.

One important restriction on the allowed values of I comes from considering the possible z components of the total angular momentum of the individual nucleons. Each j must be half integer and thus its only possible z components are likewise half-integer. If an even number of nucleons (A) is given, there will be an even number of half-integer components, with the result that the z component of the total I can take only integer values. This requires that I itself be an integer. If the number of nucleons is odd, the total z component must be half-integral and so must be total I. We thereof required the following rules:

(a) In nuclei containing an even number of nucleons, the nuclear spin quantum number, I, is an integer
(b) In nuclei containing an odd number of nucleons, the nuclear spin quantum number, I, is a half-integer.
(c) In almost all nuclei containing an even number of both protons and neutrons (even-even), the nuclear spin quantum number $I = 0$.

These results suggest that the protons and neutrons in a nucleus tend to pair their angular momentum in opposite direction. The measured values of the nuclear spin can tell us a great deal about the nuclear structure. For example, of the hundred known even-Z, even-N nuclei, all have spin 0 ground states.

5.2 Parity

Parity or space reflection, transformation is the operation whereby all three coordinate axes in the Cartesian system change sign. Given the location of a point in space denoted by coordinates (x, y, z) in a particular system, if the system undergo a parity transformation P, the coordinates of the same point in a system related to the original are $(-x, -y, -z)$.

$$(x, y, z) \to (-x, -y, -z).$$

Such a reflection of the axes changes a right-handed coordinate system to a left-handed one.

In quantum mechanics, the probability of finding a particle at location r is given by $|\varphi(r)|^2$. Since the probability is an observable, it cannot change its value simply because we have switched from using a right-handed coordinate system to a left-handed one, or vice-versa. The wave function itself, however, may change under a parity transformation, subject to the following two conditions. The first is that $|\varphi(r)|^2$ must remain invariant, as above. The second is that the two successive parity operations must bring the system back to its original state, with $P^2 = 1$. As a result, the wave function $\varphi(r)$ can change at most by a sign. States whose wave functions do not change sign under a parity transformation,

$$P\psi(r) = \psi(-r) = +\psi(r)$$

are called positive-parity state, and those whose wave functions change sign

$$P\psi(r) = \psi(-r) = -\psi(r)$$

are negative-parity states. A wave function that does not fall into either one of these categories does not have a definite parity.

In terms of spherical polar coordinates, the radial distance r is not affected by a parity transformation. The only changes are in the angular variables,

$$(r, \theta, \phi) \to (r, \pi - \theta, \pi + \phi).$$

Hence, for a state with definite orbital angular momentum (l, m), the wave function is decomposed into a product of radial and angular parts,

$$\psi(r) = R_{nl}(r) Y_l^m(\theta, \phi)$$

where n and m are the principal and magnetic quantum numbers and $Y_l^m(\theta, \phi)$ is spherical harmonic. From equation 5.6, it can be shown that

$$Y_l^m(\theta, \phi) \to Y_l^m(\pi - \theta, \pi + \phi) = (-)^l Y_l^m(\theta, \phi). \tag{5.6}$$

Central potentials, which depend only on the magnitude of $\mathbf{r}$, are thus invariant with respect to parity, and their wave functions have definite parity, odd if l is odd, and even if l is even. See Krane, Introductory Nuclear Physics, p. 38. [15] The wave function for a system of many particles is formed from the product of the wave functions for the individual particles. The parity of the combined wave function will be even if the combined wave function represents any number of even-parity particles or an even number of odd-parity particles; it will be odd if there is an odd number of odd-parity particles. Thus nuclear states can be assigned a definite parity, odd or even.

On the other hand, if a system given for which $|\psi(\mathbf{r})|^2 \neq |\psi(-\mathbf{r})|^2$, then it is concluded that $V(\mathbf{r}) \neq V(-\mathbf{r})$; that is, the system is not invariant with respect to parity. In 1957 it was discovered that certain nuclear processes (β decays) gave observable quantities whose measured values did not obey the parity symmetry. Moreover, there is no evidence yet that either the strong nuclear interaction or the electromagnetic interaction violate parity. The establishment of parity violation in β decay was one of the most dramatic discoveries in nuclear physics and has had profound influences on the development of theories of fundamental interactions between particles.

Along with the nuclear spin, the parity is also used to label nuclear states, denoted by a $\pi = +$ or $\pi = -$ superscript to the nuclear spin, as I^{π}.

5.3 Nuclear Energy Level

The nucleus also has discrete energy levels whose location and properties are governed by the rules of quantum mechanics. Each excited state is characterized by quantum numbers that describe its angular momentum, parity, and isospin. The angular momentum quantum number, J, is the integer or half-integer that is the measure of the total angular momentum of the energy state in units of $\hbar$,

$$\text{angular momentum} = J\hbar$$

The parity, P, of a nuclear energy level is a statement about what the nuclear structure of the state would look like if the spatial coordinates of all the nucleons were reversed. $P = +$ means the reversed state would look the same as the original; $P = -$ means the reversed state differs from the original. The isospin quantum number, I measures the property that results if neutron and proton coordinates were interchanged.

Nuclear scientists have developed several nuclear models that simplified the description of the nucleus and the mathematical calculations. These models still preserve the main features of nuclear structure.

5.4 Shell Model

The nuclear shell model is based on the analogous model for the orbital structure of atomic electrons in atoms, as refered to Martin & Graham, Nuclear & Partile Physics, pp. 222-227. [2]

5.4.1 Nuclear Magic Numbers

In nuclear physics, there exist a list of “magic numbers”, values of Z and N at which the nuclear binding is particularly strong. The nuclear magic numbers are found from experiment to be

$$N = 2, 8, 20, 28, 50, 82, 126 \quad Z = 2, 8, 20, 28, 50, 82 \tag{5.7}$$

and correspond to one or more closed shells, plus 8 nucleons filling the s and p subshells of a nuclei with a particular value of n. Nuclei with both N and Z having one of these values are called doubly magic, and have even greater stability.

A simple Coulomb potential is clearly not appropriate and some form that describes the effective potential of all the other nucleons is needed. Since the strong nuclear force is short-ranged the potential is expected to follow the form of the density distribution of nucleons in the nucleus. Hence

$$V_{central}(r) = \frac{-V_0}{1 + \exp[(r - R)/a]}, \tag{5.8}$$

where V_0, R and a are constants. This equation is best known as Woods-Saxon potential. However, although these potentials can be shown to offer an explanation for the lowest magic numbers, they do not work for the higher ones. This is true of all purely central potentials.

The crucial step in understanding the origin of the magic numbers was taken in 1949 by Mayer and Jensen who suggested that by analogy with atomic physics there should also be a spin-orbit term in the potential, so that the total potential is

$$V_{total} = V_{central}(r) + V_{ls}(r)(\mathbf{L} \cdot \mathbf{S}), \tag{5.9}$$

where $\mathbf{L}$ and $\mathbf{S}$ are the orbital and spin angular momentum operators for a single nucleon and $V_{ls}(r)$ is an arbitrary function of the radial coordinate. This form for the total potential is the same as used in atomic physics except for the presence of the function $V_{ls}(r)$. Once we have coupling between $\mathbf{L}$ and $\mathbf{S}$ then m_l and m_s are no longer good quantum numbers and we have to work with eigenstates of the total angular momentum vector $\mathbf{J}$, defined by $\mathbf{J} = \mathbf{L} + \mathbf{S}$. Squaring this, we have

$$\mathbf{J}^2 = \mathbf{L}^2 + \mathbf{S}^2 + 2\mathbf{L} \cdot \mathbf{S}, \tag{5.10}$$

$$\mathbf{L} \cdot \mathbf{S} = \frac{1}{2}(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2) \tag{5.11}$$

and hence the expectation value of $\mathbf{L} \cdot \mathbf{S}$, which we write as $\langle ls \rangle$, is

$$\langle ls \rangle = \frac{\hbar^2}{2}[j(j+1) - l(l+1) - s(s+1)] = \hbar^2 \begin{cases} l/2 & \text{for} j = l + \frac{1}{2} \\ -(l+1)/2 & \text{for} j = l - \frac{1}{2} \end{cases} \tag{5.12}$$

If spin, $s = \frac{1}{2}$ is used, the splitting between the two levels is thus

$$\Delta E_{ls} = \frac{2l+1}{2}\hbar^2 \langle V_{ls} \rangle . \tag{5.13}$$

Experimentally, it is found that $V_{ls}(r)$ is negative, which means that the state with $j = l + \frac{1}{2}$ has a lower energy than the state with $j = l - \frac{1}{2}$. This is opposite to the situation in atoms. Also, the splittings are substantial and increase linearly with l. Hence for higher l, crossings between levels can occur. Namely, for large l, the splitting of any two neighbouring degenerate levels can shift the $j = l - \frac{1}{2}$ state of the initial lower level to lie above the $j = l + \frac{1}{2}$ level of the previously higher level.

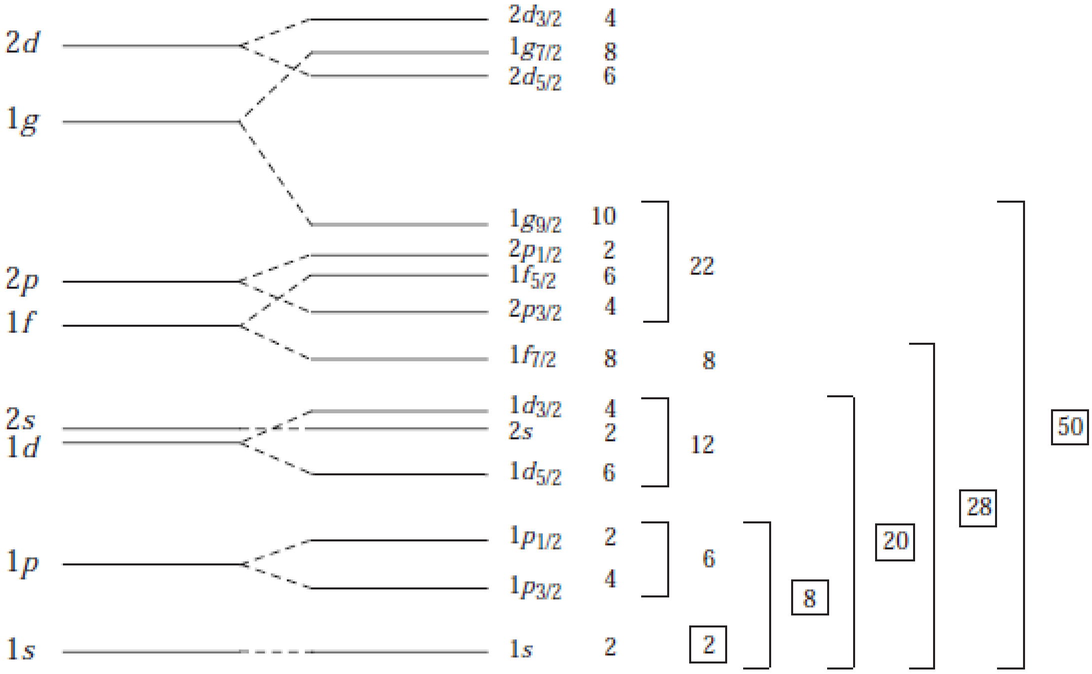

Figure 5.1: Low-lying energy levels in a single-particle shell model using a Woods-Saxon potential plus spin-orbit term. The intergers in boxes correspond to nuclear magic numbers. Martin, pp. 226 [2]

An example of resulting splittings up to the 2d state is shown in Figure 5.1, where the usual atomic spectroscopic notation has been used, i.e. levels are written nl_j with $s, p, d, f, g \ldots$ used for $l = 0, 1, 2, 3, 4, \ldots$. Magic numbers occur when there are particularly large gaps between groups of levels. Note that there is no restriction on the values of l for a given n, because unlike the atomis case, the strong nuclear potential is not

Coulombic.

The configuration of a real nuclide describes the filling of its energy levels (sub-shells), for protons and for neutrons, in order, with the notation $(nl_j)^k$ for each sub-shell, where k is the occupancy of the given sub-shell. Sometimes, for brevity, the complete filled sub-shells are not listed, and if the highest sub-shell is nearly filled, k can be given as a negative number, indicationg how far from being filled that sub-shell is. Using the ordering diagram above, and recall that the maximum occupancy of each sub-shell is $2j + 1$, the configuration for ^{17}O can be predicted:

$$(1s_{1/2})^2(1p_{3/2})^4(1p_{1/2})^2 \quad \text{for protons} \tag{5.14}$$

$$(1s_{1/2})^2(1p_{3/2})^4(1p_{1/2})^2(1d_{5/2})^1 \quad \text{for the neutrons} \tag{5.15}$$

Notice that all the proton sub-shells are filled, and that all the neutrons are in filled sub-shells except for the last one, which is in a sub-shell on its own. Most of the ground state properties of ^{17}O can therefore be found from just stating the neutron configuration as $(1d_{5/2})^1$.

5.5 The Single-Particle Shell Model

Hydrogen is the simplest atomis system because it consists of only one electron moving in the field of a heavy nucleus. [3] Next in simplicity are the alkali atoms which consist of a closed atomic shell plus one electron. In nuclear physics, the two-body system has only one bound state and does not provide much insight. In analogy to the atomic case, the next simplest cases then are nuclei with closed shells plus one valence nucleon or nuclides with closed shells minus one nucleon.

In the shell model, protons and neutrons are treated independently. For a subshell with a given value of the total angular momentum j, there are $2j + 1 = 2$ protons in this subshell. Since protons are fermions, the total wave function need to be antisymmetric. The spatial wave function of two protons in the same shell is symmetric, and consequently the spin function must be antisymmetric. Only one totally antisymmetric state can be formed from two protons, but a state described by one wave function only must have spin $J = 0$. The same argument holds for any closed subshell or shell of protons or neutrons: closed shells always have a total angular momentum of zero. The parity of a closed shell is even because there are an even number of nucleons filling it.

Ground-state spin and parity of nuclides with closed shells plus or minus a single particle are now straightforward to predict. Consider first a single proton outside a closed shell. Because the closed shell has zero angular momentum and even parity, angular momentum and parity of the nucleus are carried by the valence proton. A few examples are shown in Table 5.2. The agreement between predicted and observed values of spins and parities is complete.

Nuclide	Z	N	Shell-Model Assignment	Observed Spin and Parity
^{17}O	8	9	$d_{5/2}$	$\frac{5}{2}^+$
^{17}F	9	8	$d_{5/2}$	$\frac{5}{2}^+$
^{41}Sc	21	20	$f_{7/2}$	$\frac{7}{2}^-$
^{209}Pb	82	127	$g_{9/2}$	$\frac{9}{2}^+$
^{209}Bi	83	126	$h_{9/2}$	$\frac{9}{2}^-$

Figure 5.2: Ground-state spins and parities as predicted by the single-particle shell model and as observed. Henley, pp. 532 [3]

Next we turn to excited states. In the spirit of the extreme single-particle model, they are described as excitations of the valence nucleon alone; it moves into a higher orbit. The core is assumed to remain undisturbed. It is also known that the pairing energy is of the order about 2 MeV. At an excitation energy of a few MeV it is therefore possible that the valence nucleon remains in its ground state but that a pair from the the core is broken up and that one of the nucleons of the pair is promoted to the next higher shell. It is also possible that a pair is excited to the next higher shell. In either case, the resulting energy level is no longer describable by the single-particle approach. It is consequently not surprising to find "foregin" levels at a few MeV. Two examples are shown in Figure 5.3, both doubly magic nuclei plus one valence nucleon. In the case of ^{57}Ni, the single-particle shell-model assignments hold up to about 1 MeV, but above 2.5 MeV, foreign states appear. The foreign states are not really foreign. While they cannot be described in terms of the extreme single-particle shell model, they can be understood in terms of the general shell model, through excitations from the core. In the case of ^{209}Pb, the first such state appears at 2.15 MeV. The estimate of that core excitation will play a role at about 2 MeV is verified.

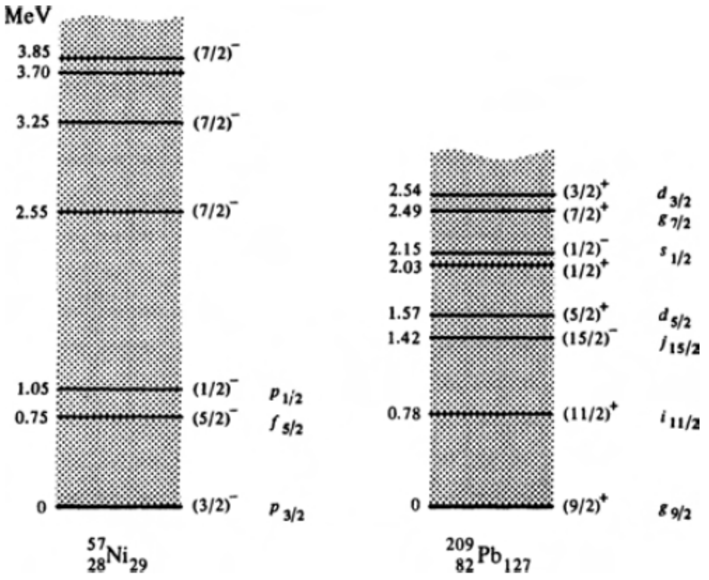

Figure 5.3: Excited states in ^{57}Ni and ^{209}Pb. The states that allow an unambiguos shell-model assignment are labeled witht he corresponding quantum numbers. Henley, pp. 533 [3]

5.6 Isospin

Charge independent of nuclear forces leads to the introduction of a new conserved quantum number, isospin. See Henley, Subatomic Physics, p. 225. [3] Isospin was introduced by Heisenberg in 1932 which he treated the neutron and the protoon as two states of one particle, the nucleon N. The two states presumably have the same mass, but the electromagnetic interaction makes the masses slightly different.

The difference between a proton and a neutron is analogous to the difference between spin-up and spin-down particles. The fundamental difference between ordinary spin and the isospin is that, unlike the spin, the isospin has nothing to do with rotations or spinning in the coordinate space, it hence cannot be coupled with the angular momenta of the nucleons.

To describe the two states of the nucleons, an isospin space is introduced, and the following analogy to the two spin states of a spin-$\frac{1}{2}$ particle is made, as from Zetttili. [16]:

Similar to the two states of an ordinary spin $\frac{1}{2}$ particle, the proton and the neutron are considered as the up and the down state of nucleon. Formally, the situation is described by introducing a new quantity, isospin I. The nucleon with isospin $\frac{1}{2}$ has $2I + 1 = 2$

	Spin-$\frac{1}{2}$	Nucleon in Isospin Space
Orientation	Up	Up, proton
	Down	Down, neutron

possible orientations in isospin space, while the three components of isospin vector I are denoted by I_1, I_2, and I_3. The value of I_3 behaves like z component vectors in atomic angular momentum which distinguishes, by definition, between the proton and the neutron. $I_3 = +\frac{1}{2}$ is the proton and $I_3 = -\frac{1}{2}$ is the neutron. The most convenient way to write the value of I and I_3 for a given state is by using a Dirac ket:

$$|I, I_3\rangle .$$

The proton is represented by $\left|\frac{1}{2}, \frac{1}{2}\right\rangle$ while neutron $\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$. The charge for the particle $|I, I_3\rangle$ is given by

$$q = e(I_3 + \frac{1}{2}). \tag{5.16}$$

With the values of the third component of I_3 given as before, the proton has charge e, and the neutron charge 0.

The states of the neutron and the proton are denoted by $|n\rangle$ and $|p\rangle$ respectively and then the operators for making the transition from one state to the other [17]:

$$\tau_+ |n\rangle = |p\rangle \quad \tau_- |p\rangle = |n\rangle . \tag{5.17}$$

Insisting that only these two states exist yields the conditions

$$\tau_+ |p\rangle = 0 \quad \text{and} \quad \tau_- |n\rangle = 0 \tag{5.18}$$

The mutually conjugate operators that satisfy the additional condition

$$\tau_- \ \text{and} \ (\tau_+)^+. \tag{5.19}$$

The simplest representation of the operators τ_+ and $\tau_-$is obtained with the 2×2 matrices

$$|p\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |n\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \tau_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \tau_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{5.20}$$

satisfying relations 5.17, 5.18, and 5.19.

The commutator of τ_+ and τ_- can be calculated easily by using 5.20 which denotes as τ_3. Thus

$$[\tau_+, \tau_-] = \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5.21}$$

By causing τ_3 to act on $|p\rangle$ and $|n\rangle$,

$$\tau_3 \, |p\rangle = |p\rangle \quad \text{and} \quad \tau_3 \, |n\rangle = - \, |n\rangle \, . \tag{5.22}$$

In other words, $|p\rangle$ and $|n\rangle$ are none than eigenstates of τ_3, with the corresponding eigenvalues being $+1$ and -1.
The linear combinations are introduced:

$$\begin{aligned} \tau_1 = (\tau_- + \tau_+) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \\ \tau_2 = \iota(\tau_- - \tau_+) = \iota \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \\ \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned} \tag{5.23}$$

Here the symbol ι works similarly to complex number i. Noticed that the matrices τ are Pauli matrices $\tau_1 = \tau_x, \tau_2 = \tau_y, \tau_3 = \tau_z$. Because spin S is defined by $\hat{S} = \frac{1}{2}\hat{\sigma}$, an isospin $\hat{I}$ can be written such that

$$\hat{I} = \frac{1}{2}\hat{\sigma} \;\text{ with }\; \hat{I} \wedge \hat{I} = \iota \hat{I} \;\text{ or better still }\; [I_k, I_l] = \iota \epsilon_{klm} I_m. \tag{5.24}$$

The isospin states $\pm\frac{1}{2}$ therefore represent the two states of the nucleon:

$$\begin{aligned} \text{proton state } \left|\frac{1}{2}\frac{1}{2}\right\rangle \, , \; I = \frac{1}{2} \text{ and } I_3 = \frac{1}{2} \\ \text{neutron state } \left|\frac{1}{2} - \frac{1}{2}\right\rangle \, , \; I = \frac{1}{2} \text{ and } I_3 = -\frac{1}{2}. \end{aligned}$$

On the other hand, a charge operator can be defined by using Equation 5.16 [16], i.e.

$$\hat{Q} = e(\hat{I}_3 + \frac{1}{2})$$

where e is the charge of the proton, with

$$\hat{Q} \left| p \right\rangle = e \left| p \right\rangle , \quad \hat{Q} \left| n \right\rangle = 0 \tag{5.25}$$

Due to strong interactions conserve isospin, for instance, a reaction like

$$d + d \rightarrow \alpha + \pi^0 \tag{5.26}$$

is forbidden since the isospin is not conserved, because the isospin of d and α are both zero and the isospin of the pion is equal to one; this leads to isospin zero for $(d + d)$ and isospin one for $(\alpha + \pi^0)$. The reaction was confirmed experiementally to be forbidden, since its cross-section is negligibly small. However, reactions such as

$$p + p \rightarrow d + \pi^+, \quad p + n \rightarrow d + \pi^0 \tag{5.27}$$

are allowed, since they conserve isospin.

5.6.1 Isospin in Nuclei

A nucleus with A nucleons, Z protons, and N neutrons, has a total charge Ze. The total charge can be written as a sum over all A nucleons with Equation 5.16:

$$Ze = \sum_{i=1}^{A} q_i = e(I_3 + \frac{1}{2}A), \tag{5.28}$$

where the third component of the total isospin is obtained by summing over all nucleons.

$$I_3 = \sum_{i=1}^{A} I_{3,i}. \tag{5.29}$$

The isospin $\hat{I}$ behaves algebraically like the ordinary spin, and the total isospin of the nucleus A is the sum over the isospins from all nucleons:

$$\hat{I} = \sum_{i=1}^{A} \hat{I}_i. \tag{5.30}$$

All states of a given nuclide are characterized by the same values of A and Z. According to Equation 5.28, all states of a nuclide have the same value of I_3, namely

$$I_3 = Z - \frac{1}{2}A = \frac{1}{2}(Z - N). \tag{5.31}$$

It is easy to assign the total isospin quantum number I. There are A isospin vectors with $I = \frac{1}{2}$, and since they add vectorially, they can add up to many different values of I. The maximum value of I is $\frac{1}{2}A$, and it occurs if the contributions from all nucleons are parallel. The minimum values is $|I_3|$, because a vector cannot be smaller than one of its components. I therefore satisfies

$$\frac{1}{2}|Z - N| \leq I \leq \frac{1}{2}A. \tag{5.32}$$

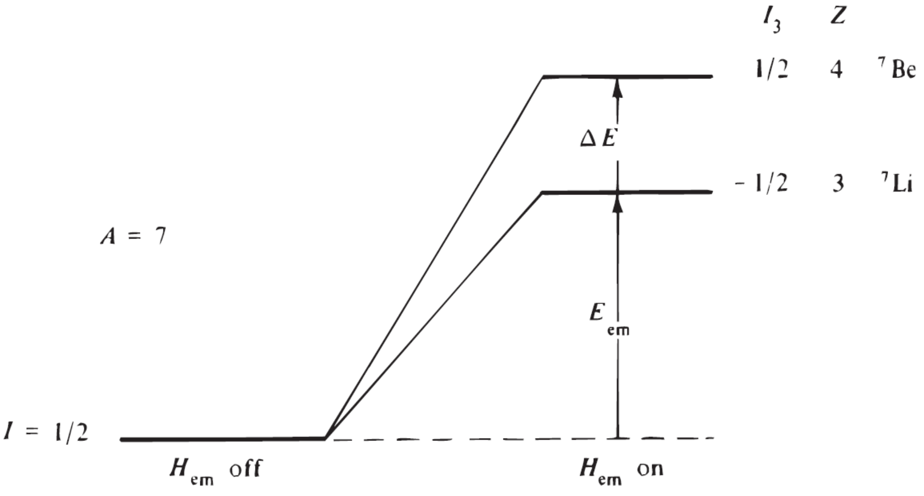

Figure 5.4: Isospin doublet. Without the electromagnectic interaction, the two substates are degenerate. With H_{em} switched on, the degeneracy is lifted, and each sublevel appears in a different isobar. The levels in the real nuclides are said to form an isospin multiplet, with reference to Henley, Subatomic Physics, p. 233. [3]

I is a good quantum number in a purely hadronic world, and each state of the nucleus can be characterized by a value of I. Equation 5.32 shows that I is integer if A is even and half-integer if A is odd. The state is $(2I + 1)$-fold degenerate. If the electromagnetic interaction is switched on, the degeneracy is broken, as indicated in Figure 5.4. Each of the substates is characterized by a unique value of I_3 and, as shown by Equation 5.28, appears in a different isobar. As long as the electromagnetic interaction is reasonably small $[(Ze^2/\hbar c) << 1]$ it is expected that real nuclear states will behave as described and consequently can be labeled by I.

It turns out that I can even be assigned to states in heavy nuclei where this condition is not fulfilled. Such states are called isobaric analog states which were discovered in 1961. Figure 5.4 are the isospin analogs of the Zeeman effect which shows that the degeneracy of the isospin result in a different isobar when H_{em} is swtiched on. In the magnetic spin case, the levels are labeled by J and J_z, and in the isospin case by I and I_3. In the magnetic case, the splitting is caused by the magnetic field, and in the isospin case by the Coulomb interaction.

The way to find the value of I is similar to the one used for particles: If all members of an isospin multiplet can be found, their number can be counted; it is $2I + 1$, and I is determined. All members of an isospin multiplet are expected to have the same quantum numbers, apart from I_3 and q. Properties other than discrete quantum numbers can be affected by the electromagnetic force but should still be approximately alike. The search is started in a given isobar, the levels with similar properties are looked for in neighboring isobars. In contrast to particle physics, the electromagnetic force produces two effects, a repulsion between the protons in the nucleus and a mass difference between neutron and proton. The Coulomb repulsion can be calculated, and the mass difference is taken from experiment. The energy difference between members of an isospin multiplet in isobars $(A, Z + 2)$ and (A, Z) is:

$$\Delta E = E(A, Z + 1) - E(A, Z) \approx \Delta E_{Coul} - (m_n - m_H)c^2. \tag{5.33}$$

The energies refer to the neutral atoms and include the electrons; $(m_n - m_H)c^2 = 0.782\mathrm{MeV}$ is the neutron-hydrogen atomic mass difference. The simplest estimate of the Coulomb energy is obtained by assuming that charge Ze is distributed uniformly through a sphere of radius R. The classical electrostatic energy is then given by

$$E_{Coul} = \frac{3}{5}\frac{(Ze)^2}{R}, \tag{5.34}$$

and it gives rise to the shift shown in Figure 5.4. The energy difference between isobars with charges $Z + 1$ and Z becomes approximately

$$\Delta E_{Coul} \approx \frac{6}{5}\frac{e^2}{R}Z \tag{5.35}$$

if both nuclides have equal radii. The values of nuclear spins vary from 0 to more than 10. This similar richness exist in the values of isospin as well. For instance, isospin singlets, $I = 0$, can appear only in nuclides with $N = Z$, as is evident from Equation 5.32. Such nuclides are called self-conjugate. The ground states of ^{2}H, ^{4}He, ^{6}Li, ^{8}Be, ^{12}C, ^{14}N, and ^{16}O have $I = 0$. ^{14}N is a good example, and the lowest levels of the $A = 14$ isobars are shown in Figure 5.5. Since A is even, only integer isospin values are allowed. If the ^{14}N ground state had a value of $I \neq 0$, similar levels would have to appear in ^{14}C and ^{14}O, with $I_3 = \pm 1$. These levels should have the same spin and parity as the ^{14}N ground state, namely 1^+.

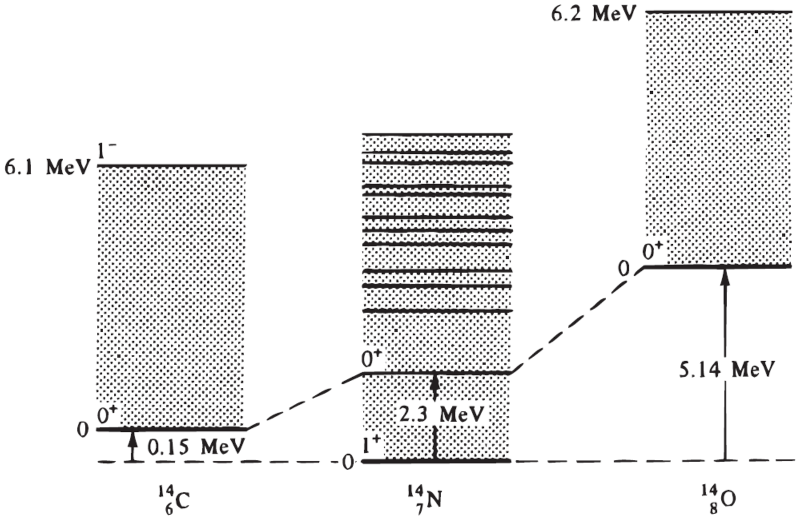

Figure 5.5: $A = 14$ isobars. The labels denote spin and parity, for instance, 0^+. The ground state of ^{14}N is an isospin singlet; the first excited state is a member of isospin triplet. Taken from Henley, Subatomic Physics, p. 234. [3]

Equation 5.33 permits a calculation of the approximate position: The level in ^{14}O should be about 3.0MeV higher, and the level in ^{14}C should be about 2.5MeV lower than the ^{14}N ground state. No such state exist. On the oxygen side, the first level appears at 5.14MeV and it has spin 1 and negative parity. On the ^{12}C side, the first level is higher and not lower, and it also has spin 1 and negative parity. All evidence indicates that the ^{14}N ground state has isospin 0.

Isospin doublets occur in mirror nuclides for which $Z = (A \pm 1)/2$. An example is shown in Figure 5.6. The ground state and the first five excited states have isospin $\frac{1}{2}$. Equation 5.33 predicts an energy shift of 1.3MeV, which is in reasonable agreement with the observed shift of 0.86MeV.

An example of an isospin triplet is shown in Figure 5.5. The ground states of ^{14}C and ^{14}O form an $I = 1$ triplet with the first excited state of ^{14}N. All three states have spin 0 and positive parity. The energies agree reasonably well with the prediction of Equation 5.33. Quartets and quintets have also been found, and the existence of isospin multiplets in isobars is well established.

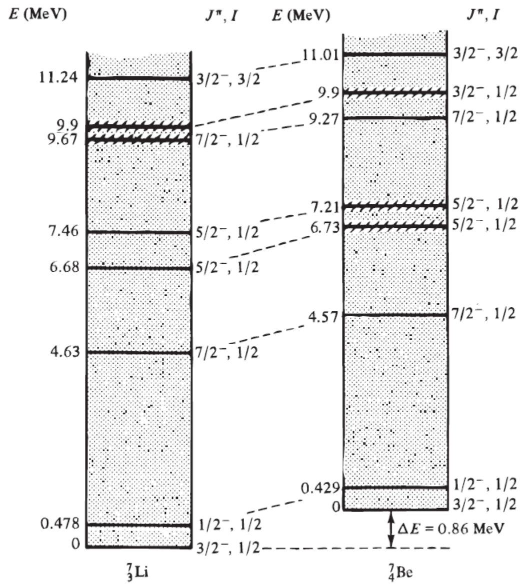

Figure 5.6: Level structure in the two isobars ^{7}Li and ^{7}Be. These two nuclides contain the same number of nucleons apart from electromagnetic effect, their level schemes should be identical. J^x denotes spin and parity of a level, I its isospin. Taken from Henley, Subatomic Physics, p. 235. [3]

5.7 Chapter Summary

This chapter discussed through all kind of nuclear characteristics account by angular momentum. No matter how advance and details one theory goes, today nuclear physics still traced down to Heisenberg model of nuclear iso-spin. It is worth saying that these are the fundamental when come to nuclear structure.

Chapter 6

Conclusion

First of all, physics of angular momentum is splitted into two major catagories, the orbital L and the spin S. Though in classical sense, they are not quite similar, as explained clearly by their name. However in quantum mechanics, the quantum numbers that play the roles hold the same meaning as related by:

l and s for magnitude component
m_l and m_s for directional component

The most important equations of the first two chapters are none other than as listed by equations 2.38, 2.39, 3.2, and 3.3.

Beyond the understanding of both sets in advance, mathematics are able to resolve themselves in addition of angular momentum. This approach in adding them up explained well some popular calculation and rules, some of them have been discussed in Chapter 4. As the discussion goes, different type of coupling schemes were introduced. The most well known will be referred directly to $L-S$ coupling and $j-j$ coupling, where they each represent extreme case. As mentioned before, in fact the real system is somewhere between the both.

To cope with the problem arise from technical difficulties in experiments involved particle and sub-particle state, physicist want a model to be as close to experimental datas as possible. Mathematical structure given by Clebsch-Gordan coefficient tidily relate uncoupled and coupled representation of angular momentum coupling. This link experiment data to a theoretical reference directly, provided by a full list of tables.

Despite the difficulties in finding a good nuclear model, physicist are never tired in searching for a better one to extract the nature of this tiny core. The quantum studies of nuclear structure involved more advance field theory such as Quantum Chromodynamics (QCD) whereby further studies are required. Even then, most of these high level theories traced back to simple visible model such as Heisenberg isospin.

Appendix A

Topics of Interest in Orbital Angular Momentum

A.1 Eigenfunction of Ladder Operator

This is an adaptation from Problem 4.18 of Introduction to Quantum Mechanics (2nd ed.) by Griffiths, page 166.
Based on hermitian the relation 2.28,

$$(L_\pm)^\dagger = (L_x \pm iL_y)^\dagger = (L_x \mp iL_y) = L_\mp \tag{A.1}$$

$$L_\pm L_\mp = L^2 - L_z^2 \pm \hbar L_z \tag{A.2}$$

and are given in the question:

$$L_\pm f_l^m = (A_l^m) f_l^{m\pm1} \tag{A.3}$$

by using a test function, say f_l^m itself,

$$\begin{aligned} L_\pm L_\mp f_l^m &= (L^2 - L_z^2 \pm \hbar L_z) f_l^m \\ &= L^2 f_l^m - L_z^2 f_l^m \pm \hbar L_z f_l^m \\ &= [\hbar^2 l(l+1) - \hbar^2 m(m \mp 1)] f_l^m \end{aligned} \tag{A.4}$$

but

$$\begin{aligned} L_\mp L_\pm f_l^m &= L_\mp (A_l^m) f_l^{m\pm1} \\ &= (A_l^m)(L_\pm)^\dagger f_l^{m\pm1} \\ &= |A_l^m|^2 f_l^m \\ &= \hbar^2 [l(l+1) - m(m \pm 1)] f_l^m \end{aligned} \tag{A.5}$$

So, $A_l^m = \hbar\sqrt{l(l+1) - m(m \pm 1)}$.

A.2 Spherical Harmonics

This is an adaptation from Section 4.1 of Introduction to Quantum Mechanics (2nd ed.) by Griffiths, page 131-139.
Time-independent Schrödinger equation speak:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi \tag{A.6}$$

In a spherical coordinates system (r, θ, ϕ), the Laplacian:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}(f^2\frac{\partial}{\partial r}) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}(\frac{\partial^2}{\partial\phi^2}) \tag{A.7}$$

where $r =$ radius, $\theta =$ zenith angle and $\phi =$ azimuthal angle, which leaves the Schrödinger equation in the form of:

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial\psi}{\partial r}) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial\psi}{\partial\theta}) + \frac{1}{r^2\sin^2\theta}(\frac{\partial^2\psi}{\partial\phi^2})\right] + V\psi = E\psi \tag{A.8}$$

Notice that there is a clear separation between the radial component r and angular part θ, ϕ, so, the separation of variables are:

$$\psi(r, \theta, \phi) = R(r)Y(\theta, \phi) \tag{A.9}$$

$$\frac{\partial\psi}{\partial r} = Y\frac{dR}{dr}\ ;\ \frac{\partial\psi}{\partial\theta} = R\frac{\partial Y}{\partial\theta} \text{ and } \frac{\partial^2\psi}{\partial\phi^2} = R\frac{\partial^2 Y}{\partial\phi^2} \tag{A.10}$$

By substituting these series of differential equation A.10 back into A.8 and further dividing it by $\psi = RY$ yields:

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2R}\frac{d}{dr}(r^2\frac{dR}{dr}) + \frac{1}{r^2Y\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial Y}{\partial\theta}) + \frac{1}{r^2Y\sin^2\theta\frac{\partial^2Y}{\partial\phi^2}}\right] + V = E \tag{A.11}$$

By multiplying the whole equation by $\frac{2m}{\hbar^2}r^2$, and rearranging it to obtain:

$$\frac{2mr^2}{\hbar^2}[E - V] + \frac{1}{R}\frac{d}{dr}(r^2\frac{dR}{dr}) = -\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2Y}{\partial\phi^2}\right] \tag{A.12}$$

With this clear separation, equation A.12 is equated to a separation constant λ_1, two differential equations are obtained:

$$\tfrac{1}{R}\tfrac{d}{dr}(r^2\tfrac{dR}{dr}) + \tfrac{2mr^2}{\hbar^2}(E-V) = \lambda_1 \quad \text{and} \tag{A.13}$$

$$\tfrac{1}{Y}\left[\tfrac{1}{\sin\theta}\tfrac{\partial}{\partial\theta}(\sin\theta\tfrac{\partial Y}{\partial\theta}) + \tfrac{1}{\sin^2\theta}\tfrac{\partial^2 Y}{\partial\phi^2}\right] = -\lambda_1 \tag{A.14}$$

Here, the interest is in the extraction of Y, the angular equation only. Multiply equation A.14 by $Y\sin^2\theta$ to get:

$$\sin\theta\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial Y}{\partial\theta}) + Y\sin^2\theta\lambda_1 = -\frac{\partial^2 Y}{\partial\phi^2} \tag{A.15}$$

By separation of variable again:

$$Y(\theta,\phi) = \Theta(\theta)\Phi(\phi) \tag{A.16}$$

$$\frac{\partial Y}{\partial\theta} = \Phi\frac{d\Theta}{d\theta} \quad \text{and} \quad \frac{\partial^2 Y}{\partial\phi^2} = \Theta\frac{d^2\Phi}{d\phi^2} \tag{A.17}$$

similarly, substitute them back to equation and dividing by $Y = \Theta\Phi$,

$$\frac{\sin\theta}{\Theta}\frac{d}{d\theta}(\sin\theta\frac{d\Theta}{d\theta}) + \lambda_1\sin^2\theta = -\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} \tag{A.18}$$

Meanwhile, a second separation constant, λ_2 is introduced such that:

$$\tfrac{\sin\theta}{\Theta}\tfrac{d}{d\theta}(\sin\theta\tfrac{d\Theta}{d\theta}) + \lambda_1\sin^2\theta = \lambda_2 \tag{A.19}$$

$$\tfrac{d^2\Phi}{d\phi^2} = -\Phi\lambda_2 \tag{A.20}$$

For $\Phi(\phi)$, 3 cases of λ_2 are considered:
case 1: $\lambda_2 = 0$, $\frac{d^2\Phi}{d\phi^2} = 0$ with general solution:

$$\Phi(\phi) = A\phi + B \tag{A.21}$$

and to look at the periodicity of ϕ, $\Phi(\phi) = \Phi(\phi + 2\pi)$,

$$A\phi + B = A(\phi + 2\pi) + B \;\Rightarrow\; A = 0 \tag{A.22}$$

which do not nullify that $B = 0$, and so

$$\Phi(\phi) = B \tag{A.23}$$

case 2: $\lambda_2 > 0$, say $\lambda_2 = m^2$, $\frac{d^2\Phi}{d\phi^2} + m^2\Phi = 0$;
let $\Phi(\phi) = e^{k\phi}$, $k^2e^{k\phi} + m^2e^{k\phi} = 0$, $k = \pm im$; which gives

$$\Phi(\phi) = Ae^{im\phi} + Be^{-im\phi} \tag{A.24}$$

or more compactly,

$$\Phi(\phi) = Ce^{im\phi} \tag{A.25}$$

by allowing $m \in \pm Z$. With $\Phi(\phi) = \Phi(\phi + 2\pi)$: $Ce^{im\phi} = Ce^{im(\phi+2\pi)}$

$$e^{im2\pi} = 1 \;\Rightarrow\; 2m\pi = 2n\pi \;\text{ where }\; m = n = \pm 1, \pm 2, \ldots \tag{A.26}$$

case 3: $\lambda_2 < 0$, say $\lambda_2 = -m^2$, $\frac{d^2\Phi}{d\phi^2} - m^2\Phi = 0$;
again let $\Phi(\phi) = e^{k\phi}$, $k^2e^{k\phi} - m^2e^{k\phi} = 0$, $k = \pm m$

$$\Phi(\phi) = De^{m\phi} + Ee^{-m\phi} = F\cosh(m\phi) + G\sinh(m\phi) \tag{A.27}$$

which totally disobey the condition $\Phi(\phi) = \Phi(\phi+2\pi)$. Thus, the general solution is given by:

$$\Phi_m(\phi) = C_m e^{im\phi} \;\text{ for }\; m = 0, \pm 1, \pm 2, \ldots \tag{A.28}$$

By $\lambda_2 = m^2$,

$$\frac{\sin\theta}{\Theta}\frac{d}{d\theta}(\sin\theta\frac{d\Theta}{d\theta}) + \lambda_1 \sin^2\theta = m^2 \tag{A.29}$$

To simplify the equation, use change of variable $x = \cos\theta$, then

$$\sin^2\theta = 1 - x^2 \tag{A.30}$$

$$\frac{dx}{d\theta} = -\sin\theta \tag{A.31}$$

$$\frac{d\Theta}{d\theta} = \frac{d\Theta}{dx}\frac{dx}{d\theta} = -\sin\theta\frac{d\Theta}{dx} \tag{A.32}$$

$$\begin{aligned}\frac{d}{d\theta}(-\sin^2\theta\frac{d\Theta}{dx}) &= -2\sin\theta\cos\theta\frac{d\Theta}{dx} - \sin^2\theta\frac{d}{d\theta}\frac{d\Theta}{dx} \\ &= -2x\sin\theta\frac{d\Theta}{dx} - \sin^2\theta\frac{d}{dx}(\frac{d\Theta}{dx})\frac{dx}{d\theta} \\ &= -2x\sin\theta\frac{d\Theta}{dx} + \sin^3\theta\frac{d^2\Theta}{dx^2} \end{aligned} \tag{A.33}$$

then,

$$-2x\sin^2\theta\frac{d\Theta}{dx} + \sin^4\theta\frac{d^2\Theta}{dx^2} + [\lambda_1\sin^2\theta - m^2]\Theta = 0 \tag{A.34}$$

divide by $\sin^2\theta = 1 - x^2$ to yield:

$$(1-x^2)\frac{d^2\Theta}{dx^2} - 2x\frac{d\Theta}{dx} + \left[\lambda_1 - \frac{m^2}{1-x^2}\right]\Theta = 0 \text{ with } |x| < 1 \tag{A.35}$$

This is associated Legendre equation whereby

$$\lambda_1 = l(l+1) \tag{A.36}$$

$$(1-x^2)\tfrac{d^2\Theta}{dx^2} - 2x\tfrac{d\Theta}{dx} + \left[l(l+1) - \tfrac{m^2}{1-x^2}\right]\Theta = 0 \tag{A.37}$$

The general solution take the form:

$$\Theta_{lm}(x) = d_1 P_l^m(x) + d_2 Q_l^m(x) \tag{A.38}$$

Since $Q_l^m(x)$ is not bounded at both end, the term vanishes by taking $d_2 = 0$, so

$$\Theta_{lm}(x) = d_1 P_l^m(x) \tag{A.39}$$

in terms of θ,

$$\Theta_{lm}(\theta) = d_1 P_l^m(\cos\theta) \tag{A.40}$$

Collectively,

$$Y(\theta,\phi) = a e^{im\phi} P_l^m(\cos\theta) \tag{A.41}$$

the coefficient a is to be determined by the initial normalization condition:

$$\begin{aligned} \textstyle\int |\psi|^2 d^3\mathbf{r} = 1 \quad &\text{with} \quad \psi(r,\theta,\phi) = R(r)Y(\theta,\phi) \\ &\text{and} \quad d^3\mathbf{r} = r^2 \sin\theta dr d\theta d\phi \end{aligned} \tag{A.42}$$

so that $\int |R|^2 r^2 dr \int\int |Y|^2 \sin\theta d\theta d\phi = 1$. Angular component, Y should fulfill:

$$\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi} |Y|^2 \sin\theta d\theta d\phi = 1 \tag{A.43}$$

with $|Y|^2 = Y^*Y = a^2 P_l^{m2}(\cos\theta)$,

$$a^2 \int_{\theta=0}^{\pi} P_l^{m2}(\cos\theta)\sin\theta d\theta \int_{\phi=0}^{2\pi} d\phi = 1 \tag{A.44}$$

The spherical harmonics can eventually be solved in this form:

$$Y_l^m(\theta,\phi) = \epsilon\sqrt{\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}} e^{im\phi} P_l^m(\cos\theta) \tag{A.45}$$

A.3 Eigenfunctions of L^2 and L_z

This is an adaptation from Section 4.3.2 of Introduction to Quantum Mechanics (2nd ed.) by Griffiths, page 167-169.
In spherical coordinates,

$$\begin{aligned}\mathbf{L} &= -i\hbar(\mathbf{r}\times\nabla)\\ &= -i\hbar[r(\hat{r}\times\hat{r})\frac{\partial}{\partial r}+(\hat{r}\times\hat{\theta})\frac{\partial}{\partial\theta}+(\hat{r}\times\hat{\phi})\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}]\\ &= -i\hbar(\hat{\phi}\frac{\partial}{\partial\theta}-\hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}) \qquad (A.46)\end{aligned}$$

where $\mathbf{r} = r\hat{r}$, $\hat{r}\times\hat{r} = 0$, $\hat{r}\times\hat{\theta} = \hat{\phi}$ and $\hat{r}\times\hat{\phi} = -\hat{\theta}$. The unit vectors $\hat{\theta}$ and $\hat{\phi}$ have their respective Cartesian form:

$$\hat{\theta} = (\cos\theta\cos\phi)\hat{\imath}+(\cos\theta\sin\phi)\hat{\jmath}-(\sin\theta)\hat{k} \qquad (A.47)$$

$$\hat{\phi} = -(\sin\phi)\hat{\imath}+(\cos\phi)\hat{\jmath} \qquad (A.48)$$

then

$$\mathbf{L} = -i\hbar[(-\sin\phi\hat{\imath}+\cos\phi\hat{\jmath})\frac{\partial}{\partial\theta}-(\cos\theta\cos\phi\hat{\imath}+\cos\theta\sin\phi\hat{\jmath}-\sin\theta\hat{k})\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}] \qquad (A.49)$$

gives the components L_x, L_y, L_z in spherical coordinates:

$$L_x = i\hbar(\sin\phi\frac{\partial}{\partial\theta}+\cos\phi\cot\theta\frac{\partial}{\partial\phi}) \qquad (A.50)$$

$$L_y = i\hbar(-\cos\phi\frac{\partial}{\partial\theta}+\sin\phi\cot\theta\frac{\partial}{\partial\phi}) \qquad (A.51)$$

$$\text{and} \qquad L_z = -i\hbar\frac{\partial}{\partial\phi} \qquad (A.52)$$

At this stage, with $L^2 = L_x^2 + L_y^2 + L_z^2$,

$$L_x^2 = -\hbar^2(\sin^2\phi\frac{\partial^2}{\partial\theta^2}+\cos^2\phi\cot^2\theta\frac{\partial^2}{\partial\phi^2}+2\sin\phi\cos\phi\cot\theta\frac{\partial}{\partial\phi}\frac{\partial}{\partial\theta}) \qquad (A.53)$$

$$L_y^2 = -\hbar^2(-\cos^2\phi\frac{\partial^2}{\partial\theta^2}+\sin^2\phi\cot^2\theta\frac{\partial^2}{\partial\phi^2}-2\sin\phi\cos\phi\cot\theta\frac{\partial}{\partial\phi}\frac{\partial}{\partial\theta}) \qquad (A.54)$$

$$L_z^2 = -\hbar^2\frac{\partial^2}{\partial\phi^2} \qquad (A.55)$$

thus,

$$\begin{aligned} L^2 &= -\hbar^2[\frac{\partial^2}{\partial\theta^2} + (\cot^2\theta + 1)\frac{\partial^2}{\partial\phi^2}] \\ &= -\hbar^2[\frac{\partial^2}{\partial\theta^2} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}] \end{aligned} \tag{A.56}$$

With this approach, some terms are dropped. Alternatively, recall equation 2.29, $L^2 = L_\pm L_\mp + L_z^2 \mp \hbar L_z$:

$$\begin{aligned} L_\pm &= L_x \pm iL_y \\ &= i\hbar[(\sin\phi \mp i\cos\phi)\frac{\partial}{\partial\theta} + (\cos\phi \pm i\sin\phi)\cot\theta\frac{\partial}{\partial\phi}] \\ &= \pm\hbar e^{\pm i\phi}(\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}) \end{aligned} \tag{A.57}$$

by using a test function ψ,

$$\begin{aligned} L_+L_-\psi &= \hbar e^{i\phi}(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi})[-\hbar e^{-i\phi}(\frac{\partial\psi}{\partial\theta} - i\cot\theta\frac{\partial\psi}{\partial\phi})] \\ &= -\hbar^2[\frac{\partial^2\psi}{\partial\theta^2} - i\frac{\partial}{\partial\theta}(\cot\theta\frac{\partial\psi}{\partial\phi}) + e^{i\phi}i\cot\theta\frac{\partial}{\partial\phi}(e^{-i\phi}\frac{\partial\psi}{\partial\theta}) \\ &\quad - e^{i\phi}i\cot\theta\frac{\partial}{\partial\phi}(e^{-i\phi}i\cot\theta\frac{\partial\psi}{\partial\phi})] \\ &= -\hbar^2[\frac{\partial^2\psi}{\partial\theta^2} + \frac{i}{\sin^2\theta}\frac{\partial\psi}{\partial\phi} - i\cot\theta\frac{\partial}{\partial\theta}\frac{\partial\psi}{\partial\phi} + ie^{i\phi}\cot\theta(-ie^{-i\phi})\frac{\partial\psi}{\partial\theta} \\ &\quad + i\cot\theta\frac{\partial}{\partial\phi}\frac{\partial\psi}{\partial\theta} - ie^{i\phi}\cot\theta(-i^2e^{-i\phi}\cot\theta\frac{\partial\psi}{\partial\phi}) + \cot^2\theta\frac{\partial^2\psi}{\partial\phi^2}] \\ &= -\hbar^2[\frac{\partial^2\psi}{\partial\theta^2} + \frac{i}{\sin^2\theta}\frac{\partial\psi}{\partial\phi} + \cot\theta\frac{\partial\psi}{\partial\theta} - i\cot^2\theta\frac{\partial\psi}{\partial\phi} + \cot^2\theta\frac{\partial^2\psi}{\partial\phi^2}] \\ &= -\hbar^2[\frac{\partial^2\psi}{\partial\theta^2} + \cot\theta\frac{\partial\psi}{\partial\theta} + \cot^2\theta\frac{\partial^2\psi}{\partial\phi^2} + i(\frac{1-\cos^2\theta}{\sin^2\theta})\frac{\partial\psi}{\partial\phi}] \end{aligned} \tag{A.58}$$

thus,

$$L_+L_- = -\hbar^2(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + cot^2\theta\frac{\partial^2}{\partial\phi^2} + i\frac{\partial}{\partial\phi}) \tag{A.59}$$

So that,

$$\begin{aligned} L^2 &= L_\pm L_\mp + L_z^2 \mp \hbar L_z \\ &\equiv L_+L_- + (-i\hbar^2\frac{\partial^2}{\partial\phi^2}) + i\hbar^2\frac{\partial}{\partial\phi} \\ &= -\hbar^2[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \cot^2\theta\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial\phi^2}] \\ &= -\hbar^2[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}] \end{aligned} \tag{A.60}$$

In comparison, previously the term $\cot\theta\frac{\partial}{\partial\theta}$ are lost.

Now, by knowing the eigenvalue of L^2 and L_z,

$$L^2 f_l^m = -\hbar^2[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}]f_l^m = \hbar^2 l(l+1) f_l^m \tag{A.61}$$

$$L_z f_l^m = -i\hbar\frac{\partial}{\partial\phi}f_l^m = \hbar m f_l^m \tag{A.62}$$

in comparison to:

$$\sin\theta\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial Y_l^m}{\partial\theta}) + \frac{\partial^2 Y_l^m}{\partial\phi^2} = -l(l+1)\sin^2\theta Y_l^m \tag{A.63}$$

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2 \tag{A.64}$$

indeed, $f_l^m \equiv Y_l^m$.

Appendix B

Topics of Interest in Atomic Physics

B.1 Non-degenerate Perturbation Theory

This is an adaptation from Section 6.1 of Introduction to Quantum Mechanics (2nd ed.) by Griffiths, page 249-254.

B.1.1 General Formulation

Schr$\ddot{o}$dinger Equation speak:

$$H\psi_n = E_n\psi_n \tag{B.1}$$

and unperturbed Schr$\ddot{o}$dinger Equation:

$$H^0\psi_n^0 = E_n^0\psi_n^0 \tag{B.2}$$

obtaining a complete set of orthonormal eigenfunction, ψ_n^0 as,

$$\left\langle \psi_n^0 | \psi_m^0 \right\rangle = \delta_{nm} \tag{B.3}$$

and the corresponding eigenvalues of E_n^0.

To begin with, the new Hamiltonian is written as the sum of two terms:

$$H = H^0 + \lambda H' \tag{B.4}$$

where H' is the perturbation and λ is a small number.

Next, ψ_n and E_n are expressed as power series in λ:

$$\begin{aligned} \psi_n &= \psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + \dots \quad &(B.5) \\ E_n &= E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots \quad &(B.6) \end{aligned}$$

Use equation B.4, B.5 and B.6 in equation B.1,

$$(H^0+\lambda H')(\psi_n^0+\lambda\psi_n^1+\lambda^2\psi_n^2+\dots) = (E_n^0+\lambda E_n^1+\lambda^2 E_n^2+\dots)(\psi_n^0+\lambda\psi_n^1+\lambda^2\psi_n^2+\dots) \quad (B.7)$$

collecting like power of λ:

$$\begin{aligned} H^0\psi_n^0 &+ \lambda(H^0\psi_n^1 + H'\psi_n^0) + \lambda^2(H^0\psi_n^0 + H'\psi_n^1) + \dots \\ &= E_n^0\psi_n^0 + \lambda(E_n^0\psi_n^1 + E_n^1\psi_n^0) + \lambda^2(E_n^0\psi_n^2 + E_n^1\psi_n^1 + E_n^2\psi_n^0) + \dots \quad (B.8) \end{aligned}$$

The lowest order λ^0;	$H^0\psi_n^0 = E_n^0\psi_n^0$
The first order λ^1;	$H^0\psi_n^1 + H'\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0$
The second order λ^2;	$H^0\psi_n^2 + H'\psi_n^1 = E_n^0\psi_n^2 + E_n^1\psi_n^1 + E_n^2\psi_n^0$

B.1.2 First-Order Theory

E_n^1 is the first-order correction to the nth eigenvalue and ψ_n^1 is the first-order correction to the nth eigenfunction. From

$$H^0\psi_n^1 + H'\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0 \quad (B.9)$$

Taking the inner product of the above equation with ψ_n^0

$$\langle \psi_n^0 | H^0\psi_n^1 \rangle + \langle \psi_n^0 | H'\psi_n^0 \rangle = E_n^0 \langle \psi_n^0 | \psi_n^1 \rangle + E_n^1 \langle \psi_n^0 | \psi_n^0 \rangle \quad (B.10)$$

but H^0 is Hermitian, $H^{0\dagger} = H^0$

$$\langle \psi_n^0 | H^0\psi_n^1 \rangle = \langle H^0\psi_n^0 | \psi_n^1 \rangle = E_n^0 \langle \psi_n^0 | \psi_n^1 \rangle \quad (B.11)$$

This cancel the first term of both sides of equation B.10. With $\langle \psi_n^0 | \psi_n^0 \rangle = 1$ the first-order correction to the energy is:

$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle \quad (B.12)$$

To find the first-order correction to the wave function, equation B.9 is rearranged to give

$$(H^0 - E_n^0)\psi_n^1 = -(H' - E_n^1)\psi_n^0 \quad (B.13)$$

ψ_n^1 can be expressed as a linear combination of ψ_m^0:

$$\psi_n^1 = \sum_{m \neq n} c_m^{(n)} \psi_m^0 \tag{B.14}$$

using the fact that ψ_m^0 satisfies the unperturbed Schrӧdinger equation B.2

$$\begin{aligned}(H^0 - E_n^0) \sum_{m \neq n} c_m^{(n)} \psi_m^0 &= -(H' - E_n^1)\psi_n^0 \\ &= \sum_{m \neq n} (c_m^{(n)} H^0 \psi_m^0 - E_n^0 c_m^{(n)} \psi_m^0) \\ &= \sum_{m \neq n} (E_m^0 - E_n^0) c_m^{(n)} \psi_m^0 \end{aligned} \tag{B.15}$$

Taking the inner product with ψ_l^0,

$$\sum_{m \neq n} (E_m^0 - E_n^0) c_m^{(n)} \left\langle \psi_l^0 | \psi_m^0 \right\rangle = - \left\langle \psi_l^0 | H' | \psi_n^0 \right\rangle + E_n^1 \left\langle \psi_l^0 | \psi_n^0 \right\rangle \tag{B.16}$$

If $l = n$, the left side is zero, equation B.12 is recovered, if $l \neq n$, instead

$$(E_m^0 - E_n^0) c_m^{(n)} = - \left\langle \psi_m^0 | H' | \psi_n^0 \right\rangle \tag{B.17}$$

$$c_m^{(n)} = \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \tag{B.18}$$

$$\psi_n^1 = \sum_{m \neq n} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \psi_m^0 \tag{B.19}$$

Notice that the coefficient is always true, since there is no $m = n$, as long as the unperturbed energy spectrum is non-degenerate.

B.2 Relativistic Correction for Hydrogen

This is an adaptation from Section 6.3.1 of Introduction to Quantum Mechanics (2nd ed.) by Griffiths, page 267-270.
With reference to equation 4.7, the first term in the Hamiltonian is supposed to represent kinetic energy,

$$T = \frac{1}{2} m v^2 = \frac{p^2}{2m} \tag{B.20}$$

and the canonical substitution $\mathbf{p} = -i\hbar\nabla$ yields the operators

$$T = -\frac{\hbar^2}{2m}\nabla^2 \tag{B.21}$$

The relativistic formula for kinetic energy is:

$$T = \frac{mc^2}{\sqrt{1-(v/c)^2}} - mc^2 \tag{B.22}$$

To express T in term of the (relativistic) momentum $p = \frac{mv}{\sqrt{1-(v/c)^2}}$ instead of velocity, notice that

$$\begin{aligned}
p^2c^2 + m^2c^4 &= \frac{m^2v^2c^2}{1-(v/c)^2} + m^2c^4 \\
&= \frac{m^2v^2c^2 + m^2c^4[1-(v/c)^2]}{1-(v/c)^2} \\
&= \frac{m^2v^2c^2 + m^2c^4 - m^2v^2c^2}{1-(v/c)^2} \\
&= \frac{m^2c^4}{1-(v/c)^2} \\
&= (T+mc^2)^2 \qquad (B.23)\\
T + mc^2 &= \sqrt{p^2c^2 + m^2c^4} \qquad (B.24)\\
T &= \sqrt{p^2c^2 + m^2c^4} - mc^2 \qquad (B.25)
\end{aligned}$$

This relativistic equation for kinetic energy reduced to the classical result, in the non-relativistic limit $p << mc$; expanding in powers of the small number p/mc, the kinetic is:

$$\begin{aligned}
T &= \sqrt{m^2c^4(1+\frac{p^2}{m^2c^2})} - mc^2 \\
&= mc^2[\sqrt{1+(\frac{p}{mc})^2} - 1] \\
&= mc^2[\sum_{k=0}^{\infty} \binom{\frac{1}{2}}{k} (\frac{p}{mc})^{2k} - 1] \\
&= mc^2[1 + \frac{1}{2}(\frac{p}{mc})^2 - \frac{1}{8}(\frac{p}{mc})^4 + \ldots - 1] \\
&= \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \ldots \qquad (B.26)
\end{aligned}$$

Hence, the lowest-order relativistic correction to the Hamiltonian is:

$$H'_r = -\frac{p^4}{8m^3c^2} \tag{B.27}$$

In the first-order perturbation theory, the correction to E_n is given by the expectation value of H' in the unperturbed state:

$$\begin{aligned} E_r^1 &= \langle H_r' \rangle = -\frac{1}{8m^3c^2} \langle \psi | p^4 | \psi \rangle \\ &= -\frac{1}{8m^3c^2} \langle p^2\psi | p^2\psi \rangle \end{aligned} \tag{B.28}$$

The Schrödinger equation (for the unperturbed states) obtained from time-independent form is:

$$[-\tfrac{\hbar^2}{2m}\nabla^2 + V(r)]\psi = E\psi \tag{B.29}$$

$$p^2\psi = 2m(E - V)\psi \tag{B.30}$$

and hence

$$\begin{aligned} E_r^1 &= -\frac{4m^2}{8m^3c^2} \langle (E - v)^2 \rangle \\ &= -\frac{1}{2mc^2}[E^2 - 2E\langle V \rangle + \langle V^2 \rangle] \end{aligned} \tag{B.31}$$

for hydrogen atom,

$$V(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} \tag{B.32}$$

$$E_r^1 = -\frac{1}{2mc^2}[E_n^2 + 2E_n(\frac{e^2}{4\pi\epsilon_0})\left\langle \frac{1}{r} \right\rangle + (\frac{e^2}{4\pi\epsilon_0})^2 \left\langle \frac{1}{r^2} \right\rangle] \tag{B.33}$$

where E_n is the Bohr energy of the state.
The expectation values of $\left\langle \frac{1}{r} \right\rangle$ and $\left\langle \frac{1}{r^2} \right\rangle$ in the (unperturbed) state ψ_{nlm} is explained in detail as following.

This is an adaptation from Problem 6.12 of Introduction to Quantum Mechanics (2nd ed.) by Griffiths, page 270.
Virial theorem for 3-dimensions,

$$2\langle T \rangle = \langle \mathbf{r} \cdot \nabla V \rangle \tag{B.34}$$

Again for hydrogen atom,

$$V = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$$

$$\nabla V = \frac{e^2}{4\pi\epsilon_0}\frac{1}{r^2}\hat{r} \tag{B.35}$$

$$\mathbf{r}\cdot\nabla V = r\hat{r}\cdot\frac{e^2}{4\pi\epsilon_0}\frac{\hat{r}}{r^2} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{r} = -V \tag{B.36}$$

hence $2\langle T\rangle = -\langle V\rangle$ Hamiltonian

$$\begin{aligned}
\langle H\rangle &= \langle T\rangle + \langle V\rangle = E_n && \text{(B.37)}\\
&= -\frac{1}{2}\langle V\rangle + \langle V\rangle && \text{(B.38)}\\
\frac{1}{2}\langle V\rangle &= E_n\\
\langle V\rangle &= 2E_n && \text{(B.39)}
\end{aligned}$$

for $E_n = -[\frac{m}{2\hbar^2}(\frac{e^2}{4\pi\epsilon_0})^2]\frac{1}{n^2}$ then

$$\langle V\rangle = -\tfrac{e^2}{4\pi\epsilon_0}\left\langle\tfrac{1}{r}\right\rangle = -\tfrac{m}{\hbar^2}(\tfrac{e^2}{4\pi\epsilon_0})^2\tfrac{1}{n^2} \tag{B.40}$$

$$\left\langle\tfrac{1}{r}\right\rangle = \tfrac{me^2}{4\pi\epsilon_0\hbar^2}\tfrac{1}{n^2} = \tfrac{1}{n^2a} \tag{B.41}$$

where $a = \frac{4\pi\epsilon_0\hbar^2}{me^2}$ the Bohr's radius.

This is an adaptation from Problem 6.33 of Introduction to Quantum Mechanics (2nd ed.) by Griffiths, page 288.
Feynman-Hellmann theorem:

$$\frac{\partial E_n}{\partial\lambda} = \left\langle\psi_n|\frac{\partial H}{\partial\lambda}|\psi_n\right\rangle \tag{B.42}$$

The effective Hamiltonian for the radial wave functions is:

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r} \tag{B.43}$$

and the eigenvalues are:

$$E_n = -\frac{me^4}{32\pi^2\epsilon_0^2\hbar^2(j_{max}+l+1)^2} \tag{B.44}$$

let $\lambda = l$,

$$\begin{aligned} \frac{\partial E_n}{\partial l} &= \frac{2me^4}{32\pi^2\epsilon_0^2\hbar^2(j_{max}+l+1)} = -\frac{2E_n}{n} && \text{(B.45)} \\ \frac{\partial H}{\partial l} &= \frac{\hbar^2}{2mr^2}(2l+1) && \text{(B.46)} \\ \text{so,} \quad -\frac{2E_n}{n} &= \frac{\hbar^2(2l+1)}{2m}\left\langle\frac{1}{r^2}\right\rangle && \text{(B.47)} \\ \text{or,} \quad \left\langle\frac{1}{r^2}\right\rangle &= -\frac{2mE_n}{n(2l+1)\hbar^2} = -\frac{4mE_1}{n^3(2l+1)\hbar^2} && \text{(B.48)} \end{aligned}$$

where $E_n = \frac{E_1}{n^2}$, but $-\frac{4mE_1}{\hbar^2} = \frac{2}{a^2}$, so that

$$\left\langle\frac{1}{r^2}\right\rangle = \frac{1}{n^3(l+1/2)a^2} \qquad \text{(B.49)}$$

Now, with equation B.41 and B.49, equation B.33 is rewritten as:

$$E_r^1 = -\frac{1}{2mc^2}[E_n^2 + 2E_n(\frac{e^2}{4\pi\epsilon_0})\frac{1}{n^2a} + (\frac{e^2}{4\pi\epsilon_0})^2\frac{1}{(l+1/2)n^3a^2}] \qquad \text{(B.50)}$$

from

$$\left.\begin{array}{lll} a = \frac{4\pi\epsilon_0\hbar^2}{me^2} & \rightarrow & \frac{e^2}{4\pi\epsilon_0} = \frac{\hbar^2}{ma} \\ E_n = -\frac{\hbar^2}{2ma^2n^2} & \rightarrow & -2n^2aE_n = \frac{\hbar^2}{ma} \end{array}\right\} \frac{e^2}{4\pi\epsilon_0} = -2n^2aE_n \qquad \text{(B.51)}$$

hence,

$$\begin{aligned} E_r^1 = -\frac{1}{2mc^2} &= -\frac{1}{2mc^2}[E_n^2 + 2E_n(-2m^2aE_n)\frac{1}{n^2a} + \frac{4n^4a^2E_n^2}{(l+1/2)n^3a^2}] \\ &= -\frac{1}{2mc^2}[E_n^2 - 4E_n^2 + \frac{4nE_n^2}{l+1/2}] \\ &= -\frac{1}{2mc^2}[\frac{4nE_n^2}{l+1/2} - 3E_n^2] \\ &= -\frac{E_n^2}{2mc^2}[\frac{4n}{l+1/2} - 3] && \text{(B.52)} \end{aligned}$$

Evidently the relativistic correction is smaller than E_n, by a factor of about $\frac{E_n}{mc^2} = 2\times10^{-5}$

B.3 Spin-Orbit Coupling

This is an adaptation from Section 6.3.2 of Introduction to Quantum Mechanics (2nd ed.) by Griffiths, page 271-274.

The Hamiltonian (electron in a magnetic field)

$$H = -\vec{\mu} \cdot \mathbf{B} \tag{B.53}$$

(i) The magnetic field of the proton, **B**.
If the proton is pictured as a continuous current loop, it's magnetic field can be calculated from the Biot-Savart law:

$$B = \frac{\mu_0 I}{2r} \tag{B.54}$$

with an effective current $I = \frac{e}{T}$, where e is the proton charge and T is the period of the orbit. The orbital angular momentum of the electron (in the rest frame of the nucleus) is:

$$L = mvr = \frac{2\pi mr^2}{T}, \text{where } v = \frac{2\pi r}{T} \tag{B.55}$$

$$\frac{1}{T} = \frac{L}{2\pi mr^2} \tag{B.56}$$

Moreover, **B** and **L** point in the same direction,

$$\mathbf{B} = \mu_0 \frac{e}{4\pi mr^3} \mathbf{L} \tag{B.57}$$

but $c^2 = \frac{1}{\epsilon_0 \mu_0}$, $\mu_0 = \frac{1}{\epsilon_0 c^2}$ thus,

$$\mathbf{B} = \frac{1}{4\pi\epsilon_0} \frac{e}{mc^2 r^3} \mathbf{L} \tag{B.58}$$

(ii) The magnetic dipole moment of the electron.
The magnetic dipole moment of a spinning charge is related to its (spin) angular momentum, the proportionality factor is the gyro magnetic ratio: $\vec{\mu} = \gamma \mathbf{S}$. Consider first a charge q smeared out around a ring of radius r, which rotates about the axis with period T. The magnetic dipole moment of the ring is defined as the current $\frac{q}{T}$ times the area πr^2:

$$\mu = IA = \frac{q\pi r^2}{T} \tag{B.59}$$

If the mass of the ring is m, its angular momentum is the moment of inertia mr^2 times the angular velocity $\frac{2\pi}{T}$:

$$S = I'\omega = \frac{2\pi mr^2}{T} \tag{B.60}$$

The gyro magnetic ratio for this configuration is

$$\gamma = \frac{\mu}{s} = (\frac{q\pi r^2}{T})(\frac{T}{2\pi mr^2}) = \frac{q}{2m} \tag{B.61}$$

Moreover, the direction of $\vec{\mu}$ and **S** are the same (or opposite if the charge is negative), so

$$\vec{\mu} = (\frac{q}{2m})\mathbf{S} \tag{B.62}$$

That was a purely classical calculation, however as it turns out the electron's magnetic moment is twice the classical value:

$$\vec{\mu}_e = -\frac{2}{m}\mathbf{S} \tag{B.63}$$

Plugging both results into equation B.53,

$$H = (\frac{e^2}{4\pi\epsilon_0})\frac{1}{m^2c^2r^3}\mathbf{S}\cdot\mathbf{L} \tag{B.64}$$

By an appropriate kinematic correction, known as Thomas precession (multiply 1/2):

$$H'_{SO} = (\frac{e^2}{8\pi\epsilon_0})\frac{1}{m^2c^2r^3}\mathbf{S}\cdot\mathbf{L} \tag{B.65}$$

the perturbed Hamiltonian for spin-orbit interaction. In the presence of spin-orbit coupling, the Hamiltonian no longer commutes with **L** and **S**, so the spin and orbital angular momentum are not separately conserved. However, H'_{SO} does commute with L^2, S^2 and the total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$ and hence these quantities are conserved

$$\begin{aligned} J^2 &= (\mathbf{L}+\mathbf{S})\cdot(\mathbf{L}+\mathbf{S}) \\ &= L^2 + S^2 + 2\mathbf{L}\cdot\mathbf{S} \qquad \text{(B.66)} \\ \text{so} \quad \mathbf{L}\cdot\mathbf{S} &= \frac{1}{2}(J^2 - L^2 - S^2) \qquad \text{(B.67)} \end{aligned}$$

and therefore the eigenvalues of $\mathbf{L}\cdot\mathbf{S}$ are

$$\frac{\hbar^2}{2}[j(j+1) - l(l+1) - s(s+1)] \tag{B.68}$$

The first order energy correction is:

$$\begin{aligned} E^1_{SO} &= \langle H'_{SO}\rangle = (\frac{e^2}{8\pi\epsilon_0})\frac{1}{m^2c^2}\left\langle\frac{\mathbf{L}\cdot\mathbf{S}}{r^3}\right\rangle \\ &= \frac{e^2}{8\pi\epsilon_0}\frac{1}{m^2c^2}\frac{\hbar^2}{2}[j(j+1) - l(l+1) - s(s+1)]\left\langle\frac{1}{r^3}\right\rangle \qquad \text{(B.69)} \end{aligned}$$

for electron, $s = \frac{1}{2}$; $s(s+1) = \frac{1}{2}(\frac{1}{2}+1) = \frac{3}{4}$

$$E^1_{SO} = \frac{e^2}{8\pi\epsilon_0}\frac{1}{m^2c^2}\frac{\hbar^2}{2}[j(j+1) - l(l+1) - \frac{3}{4}]\left\langle\frac{1}{r^3}\right\rangle \tag{B.70}$$

The expectation value of $\left\langle\frac{1}{r^3}\right\rangle$ is:

$$\left\langle\frac{1}{r^3}\right\rangle = \frac{1}{l(l+1)(l+1/2)n^3a^3} \tag{B.71}$$

This is an adaptation from Problem 6.35c of Introduction to Quantum Mechanics (2nd ed.) by Griffiths, page 289.
According to Kramer's relation

$$\frac{s+1}{n^2}\left\langle r^s\right\rangle - (2s+1)a\left\langle r^{s-1}\right\rangle + \frac{s}{4}[(el+1)^2 - s^2]a^2\left\langle r^{s-2}\right\rangle = 0 \tag{B.72}$$

if $s = -1$,

$$0 + a\left\langle\frac{1}{r^2}\right\rangle - \frac{1}{4}[(2l+1)^2 - 1]a^2\left\langle\frac{1}{r^3}\right\rangle = 0 \tag{B.73}$$

$$\frac{a^2}{4}[4l^2 + 4l + 1 - 1]\left\langle\frac{1}{r^3}\right\rangle = a\left\langle\frac{1}{r^2}\right\rangle \tag{B.74}$$

$$\frac{a}{4}[4l^2 + 4l]\left\langle\frac{1}{r^3}\right\rangle = \left\langle\frac{1}{r^2}\right\rangle \tag{B.75}$$

$$al(l+1)\left\langle\frac{1}{r^3}\right\rangle = \frac{1}{(l+1/2)n^3a^2} \tag{B.76}$$

$$\left\langle\frac{1}{r^3}\right\rangle = \frac{1}{l(l+1)(l+1/2)n^3a^3} \tag{B.77}$$

$$E^1_{SO} = \frac{e^2}{8\pi\epsilon_0}\frac{1}{m^2c^2}\{\frac{(\hbar^2/2)[j(j+1) - l(l+1) - 3/4]}{(l+1)(l+1/2)n^3a^3}\} \tag{B.78}$$

or, expressing it in term of E_n:

$$-2n^2aE_n = \frac{e^2}{4\pi\epsilon_0}\,,\ \frac{e^2}{8\pi\epsilon_0} = -n^2aE_n \tag{B.79}$$

$$\begin{aligned}
E^1_{SO} &= -\frac{n^2aE_n}{m^2c^2}\frac{\hbar^2}{2n^3a^3}\{\frac{j(j+1) - l(l+1) - 3/4}{l(l+1)(l+1/2)}\} && \text{(B.80)}\\
&= (-\frac{\hbar^2}{2ma^2n^2})\frac{E_n}{mc^2}\{\frac{n[j(j+1) - l(l+1) - 3/4]}{l(l+1)(l+1/2)}\} && \text{(B.81)}\\
&= \frac{E_n^2}{mc^2}\{\frac{n[j(j+1) - l(l+1) - 3/4]}{l(l+1)(l+1/2)}\} && \text{(B.82)}
\end{aligned}$$

It is remarkable that the relativistic correction and the spin-orbit coupling are of the same order, $\frac{E_n^2}{mc^2}$

B.4 Application of Hund's Rules in Spectroscopy Notation

The general ideas:

- The atomic number provides information on the electronic configuration.
- Fully filled orbitals fulfill $S = 0$ and $L = 0$, are thus be ignored when considering spectroscopy notation.
- Valence electrons or outermost non-fully filled orbit gives the occupancies of the orbit and orbitals. For a given l, $m_l = -l, -l+1, \ldots, l-1, l$.
- Hund's first rule implies that $E_{parallel} < E_{anti-parallel}$ since parallel spins add but anti-parallel spins minus, as highest S are obtain through addition instead of subtraction. However Pauli exclusion principle prohibit parallel pair in same orbital. Since n, l, m_l, s are all the same already, m_s cannot be the same anymore. So, basically, $\sum_i s_i \equiv \sum_i m_{si}$.
- Hund's second rule, together with $\sum_i l_i \equiv \sum_i m_{li}$ explains the sequence of adding electrons into an empty orbit with more than one orbitals. In a single spin direction, electrons are filled from high m_l to low m_l, then followed by pairing each one with opposite spin direction, from high m_l to low m_l as well.
- Hund's third rule is obvious. In fact, half-filled and fully-filled orbit always gives $L = 0$, that simply have $J = S$ for such cases.

For the special case as mentioned before, like Cr and Cu, the first point was skipped since their electronic configurations were affected by other factors. The rest can be obtained in a similar ways if their valance electronic configuration are known. Up to this steps, S, L and J are readily obtainable to be written as spectroscopy notation: ${}^{2S+1}\mathcal{L}_J$.

For C-12, the electronic configurations are: $1s^2 2s^2 2p^2$, valence electrons are $2p^2$, with $l = 1$, $m_l = -1, 0, 1$, there are total of 3 orbitals, with 6 occupancies.
-From Hund's first rule, both electrons should be in same spin, for example, $\uparrow\uparrow$; $S = \frac{1}{2} + \frac{1}{2} = 1$
-Based on Hund's second rule, first electron filled $m_l = 1$, while second electron filled

$m_l = 0$; $L = 1 + 0 = 1$.
-The valence orbit filled 2 out of 6, which is not more than half-filled, thus $J = |L - S| = 1 - 1 = 0$.
Hence, the spectroscopy notation of ground state C-12 is ${}^{2S+1}\mathcal{L}_J = {}^3 P_0$.

For Ni-28, the electronic configurations are: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^8 4s^2$, non-fully filled orbitals are from $3d^8$, with $l = 2$, $m_l = -2, -1, 0, 1, 2$, there are total of 5 orbitals, with 10 occupancies.
-From Hund's first rule, 2 unpaired and 3 paired electrons, namely: $\uparrow, \uparrow, \uparrow\downarrow, \uparrow\downarrow, \uparrow\downarrow$; $S = \frac{1}{2} + \frac{1}{2} + 0 + 0 + 0 = 1$
-Based on Hund's second rule, first 5 electron filled up the each orbitals with same spin, says $\uparrow$ (half-filled with $L_{half} = 0$), the sixth in $m_l = 2$, seventh in $m_l = 1$ and last one in $m_l = 0$; $L = L_{half} + 2 + 1 + 0 = 3$.
-Now that 8 out of 10 are in the orbit, which is already more than half-filled, thus $J = L + S = 3 + 1 = 4$.
Hence, the spectroscopy notation of ground state Ni-28 is ${}^{2S+1}\mathcal{L}_J = {}^3 F_4$.

B.5 The Clebsch-Gordan Coefficients Table for $\frac{1}{2} \times \frac{1}{2}$ and $1 \times \frac{1}{2}$ Systems

B.5.1 $\frac{1}{2} \times \frac{1}{2}$ Systems

This can be referred to electrons, protons or neutrons. Right now, the informations are:

$$j_1 = \frac{1}{2}\ ,\ m_1 = \pm\frac{1}{2}\ ;\ j_2 = \frac{1}{2}\ ,\ m_2 = \pm\frac{1}{2} \tag{B.83}$$

$$\left.\begin{array}{rcl} |j_1 - j_2| \leq & j & \leq j_1 + j_2 \\ \frac{1}{2} - \frac{1}{2} \leq & j & \leq \frac{1}{2} + \frac{1}{2} \\ 0 \leq & j & \leq 1 \end{array}\right\} \text{hence, } j = 0 \text{ or } j = 1 \tag{B.84}$$

$$\left.\begin{array}{l} m = m_1 + m_2 = \frac{1}{2} + \frac{1}{2} = 1 \\ m = -\frac{1}{2} - \frac{1}{2} = -1 \\ m = +\frac{1}{2} - \frac{1}{2} = -\frac{1}{2} + \frac{1}{2} = 0 \end{array}\right\} \text{hence, } m = 1, 0, -1 \tag{B.85}$$

There are four possible states as discussed before:
a.) $j = 1, m = 1 : \uparrow\uparrow$

$$|1, 1\rangle = 1 \left|\frac{1}{2}, \frac{1}{2}\right\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle \tag{B.86}$$

compared with,

$$|j, m\rangle = c\,|j_1, m_1\rangle \otimes |j_2, m_2\rangle \tag{B.87}$$

thus, $C^{\frac{1}{2}\frac{1}{2}1}_{\frac{1}{2}\frac{1}{2}1} = 1$.

b.) $j = 1, m = 0$: $\frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow)$

$$\begin{aligned} |1,0\rangle &= \frac{1}{\sqrt{2}}\left[\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle + \left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle\right] \\ &= \frac{1}{\sqrt{2}}\left(\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle\right) + \frac{1}{\sqrt{2}}\left(\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle\right) \end{aligned} \tag{B.88}$$

thus yield $C^{\frac{1}{2}\ \frac{1}{2}1}_{\frac{1}{2}-\frac{1}{2}0} = C^{\ \frac{1}{2}\frac{1}{2}1}_{-\frac{1}{2}\frac{1}{2}0} = \frac{1}{\sqrt{2}}$.

c.) $j = 1, m = -1$: $\downarrow\downarrow$

$$|1,-1\rangle = 1\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle \tag{B.89}$$

gives $C^{\ \frac{1}{2}\ \ \frac{1}{2}\ \ 1}_{-\frac{1}{2}-\frac{1}{2}-1} = 1$

d.) $j = 0, m = 0$: $\frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$

$$\begin{aligned} |0,0\rangle &= \frac{1}{\sqrt{2}}\left[\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle - \left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle\right] \\ &= \frac{1}{\sqrt{2}}\left|\frac{1}{2},\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},-\frac{1}{2}\right\rangle - \frac{1}{\sqrt{2}}\left|\frac{1}{2},-\frac{1}{2}\right\rangle \otimes \left|\frac{1}{2},\frac{1}{2}\right\rangle \end{aligned} \tag{B.90}$$

thus $C^{\frac{1}{2}\ \frac{1}{2}0}_{\frac{1}{2}-\frac{1}{2}0} = \frac{1}{\sqrt{2}}$ but $C^{\ \frac{1}{2}\frac{1}{2}0}_{-\frac{1}{2}\frac{1}{2}0} = -\frac{1}{\sqrt{2}}$. Hence, filling into table with notations:

$\frac{1}{2} \times \frac{1}{2}$		$j =$	1	1	0	1
$m_1 + m_2 = m =$			+1	0	0	-1
$+\frac{1}{2}$	$+\frac{1}{2}$		1			
$+\frac{1}{2}$	$-\frac{1}{2}$			$\sqrt{\frac{1}{2}}$	$\sqrt{\frac{1}{2}}$	
$-\frac{1}{2}$	$+\frac{1}{2}$			$\sqrt{\frac{1}{2}}$	$-\sqrt{\frac{1}{2}}$	
$-\frac{1}{2}$	$-\frac{1}{2}$					1

Table B.1: Clebsch-Gordan coefficients table of $\frac{1}{2} \times \frac{1}{2}$

B.5.2 $1 \times \frac{1}{2}$ Composite Systems

$$j_1 = 1\ ,\ m_1 = 0, \pm 1\ ;\ j_2 = \frac{1}{2}\ ,\ m_2 = \pm\frac{1}{2} \tag{B.91}$$

$$|j_1 - j_2| \leq \quad j \quad \leq j_1 + j_2 \tag{B.92}$$

$$\frac{1}{2} \leq \quad j \quad \leq \frac{3}{2} \tag{B.93}$$

By considering the ladder operators:

$$J_{\pm} |j, m\rangle = \sqrt{j(j+1) - m(m \pm 1)}\, |j, m \pm 1\rangle \tag{B.94}$$

$$J_{+} |j, m_{max}\rangle = J_{-} |j, m_{min}\rangle = 0 \tag{B.95}$$

which is used to obtain the following relations:

$$\begin{gathered}
J_{-} \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle = \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle \ , \ J_{-} \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle = 0 \\
J_{-} |1, 1\rangle = \sqrt{2}\, |1, 0\rangle \ , \ J_{-} |1, 0\rangle = \sqrt{2}\, |1, -1\rangle \ , \ J_{-} |1, -1\rangle = 0 \\
J_{+} \left|\tfrac{1}{2}, -\tfrac{1}{2}\right\rangle = \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle \ , \ J_{+} \left|\tfrac{1}{2}, \tfrac{1}{2}\right\rangle = 0 \\
J_{+} |1, -1\rangle = \sqrt{2}\, |1, 0\rangle \ , \ J_{+} |1, 0\rangle = \sqrt{2}\, |1, 1\rangle \ , \ J_{+} |1, 1\rangle = 0
\end{gathered} \tag{B.96}$$

(i.) For $j = j_1 + j_2 = \frac{3}{2}$, $m = \pm\frac{1}{2}, \pm\frac{3}{2}$, the four possible states $|j, m\rangle$ are:

$$\left|\frac{3}{2}, \frac{3}{2}\right\rangle \ , \ \left|\frac{3}{2}, \frac{1}{2}\right\rangle \ , \ \left|\frac{3}{2}, -\frac{1}{2}\right\rangle \quad \text{and} \quad \left|\frac{3}{2}, -\frac{3}{2}\right\rangle \tag{B.97}$$

a.)

$$\left|\frac{3}{2}, \frac{3}{2}\right\rangle = 1\, |1, 1\rangle \otimes \left|\frac{1}{2}\frac{1}{2}\right\rangle \tag{B.98}$$

gives $C^{1\,\frac{1}{2}\,\frac{3}{2}}_{1\,\frac{1}{2}\,\frac{3}{2}} = 1$.
b.)

$$\left|\frac{3}{2}, -\frac{3}{2}\right\rangle = 1\, |1, -1\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \tag{B.99}$$

gives $C^{\;1\;\;\frac{1}{2}\;\;\frac{3}{2}}_{-1\,-\frac{1}{2}\,-\frac{3}{2}} = 1$.
Before proceeding further the state $\left|\frac{3}{2}, \frac{1}{2}\right\rangle$ is first identified by:

$$J_{-} \left|\frac{3}{2}, \frac{3}{2}\right\rangle = J_{-} |1, 1\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle + |1, 1\rangle \otimes J_{-} \left|\frac{1}{2}, \frac{1}{2}\right\rangle \tag{B.100}$$

$$\sqrt{3} \left|\frac{3}{2}, \frac{1}{2}\right\rangle = \sqrt{2}\, |1, 0\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle + |1, 1\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \tag{B.101}$$

c.)

$$\left|\frac{3}{2}, \frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\, |1, 0\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle + \sqrt{\frac{1}{3}}\, |1, 1\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \tag{B.102}$$

thus, $C^{1\,\frac{1}{2}\,\frac{3}{2}}_{0\,\frac{1}{2}\,\frac{1}{2}} = \sqrt{\frac{2}{3}}$ and $C^{1\ \ \frac{1}{2}\,\frac{3}{2}}_{1\,-\frac{1}{2}\,\frac{1}{2}} = \sqrt{\frac{1}{3}}$.
The same goes to $\left|\frac{3}{2}, -\frac{1}{2}\right\rangle$, by using J_+:

$$J_+\left|\frac{3}{2}, -\frac{3}{2}\right\rangle = J_+\left|1,-1\right\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle + \left|1,-1\right\rangle \otimes J_+\left|\frac{1}{2}, -\frac{1}{2}\right\rangle \tag{B.103}$$

$$\sqrt{3}\left|\frac{3}{2}, -\frac{1}{2}\right\rangle = \sqrt{2}\left|1,0\right\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle + \left|1,-1\right\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle \tag{B.104}$$

d.)

$$\left|\frac{3}{2}, -\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left|1,0\right\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle + \sqrt{\frac{1}{3}}\left|1,-1\right\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle \tag{B.105}$$

thus $C^{1\ \ \frac{1}{2}\ \ \frac{3}{2}}_{0\,-\frac{1}{2}\,-\frac{1}{2}} = \sqrt{\frac{2}{3}}$ and $C^{\ \ 1\,\frac{1}{2}\ \ \frac{3}{2}}_{-1\,\frac{1}{2}\,-\frac{1}{2}} = \sqrt{\frac{1}{3}}$
(ii.) For $j = |j_1 - j_2| = \frac{1}{2}$, $m = \pm\frac{1}{2}$, there are two possible states of $|j,m\rangle$:

$$\left|\frac{1}{2}, \frac{1}{2}\right\rangle \quad \text{and} \quad \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \tag{B.106}$$

The trick here is by letting

$$\left|\frac{1}{2}, \frac{1}{2}\right\rangle = a\left|1,1\right\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle + b\left|1,0\right\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle \tag{B.107}$$

$$\left|\frac{1}{2}, -\frac{1}{2}\right\rangle = c\left|1,0\right\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle + d\left|1,-1\right\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle \tag{B.108}$$

where $a^2+b^2 = c^2+d^2 = 1$. To find the coefficients a, b, c and d, extra pieces of information are needed, as in:

$$\begin{aligned} J_+\left|\frac{1}{2}, \frac{1}{2}\right\rangle &= aJ_+\left|1,1\right\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle + a\left|1,1\right\rangle \otimes J_+\left|\frac{1}{2}, -\frac{1}{2}\right\rangle \\ &\quad + bJ_+\left|1,0\right\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle + b\left|1,0\right\rangle \otimes J_+\left|\frac{1}{2}, \frac{1}{2}\right\rangle \\ &= a\left|1,1\right\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle + \sqrt{2}b\left|1,1\right\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle \\ &= (a+\sqrt{2}b)\left|1,1\right\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle = 0 \end{aligned} \tag{B.109}$$

hence, $a + \sqrt{2}b = 0$, $a = -\sqrt{2}b$, $a^2 = 2b^2 = 1 - b^2$, so that $b^2 = \frac{1}{3}$, and $b = \pm\sqrt{\frac{1}{3}}$, while $a = \mp\sqrt{\frac{2}{3}}$.
The sign convention is such a way that the filling of the table is regular, $a = \sqrt{\frac{2}{3}}$ and $b = -\sqrt{\frac{1}{3}}$.

Similarly, for the case of $\left|\frac{1}{2}, -\frac{1}{2}\right\rangle$,

$$\begin{aligned} J_- \left|\frac{1}{2}, -\frac{1}{2}\right\rangle &= cJ_- \left|1,0\right\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle + c\left|1,0\right\rangle \otimes J_- \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \\ &\quad + dJ_- \left|1,-1\right\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle + d\left|1,-1\right\rangle \otimes J_- \left|\frac{1}{2}, \frac{1}{2}\right\rangle \\ &= \sqrt{2}c\left|1,-1\right\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle + d\left|1,-1\right\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \\ &= (\sqrt{2}c + d)\left|1,-1\right\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle = 0 \end{aligned} \tag{B.110}$$

hence, $\sqrt{2}c + d = 0$, $d = -\sqrt{2}c$, $d^2 = 2c^2 = 1 - c^2$, then $c^2 = \frac{1}{3}$, $c = \pm\sqrt{\frac{1}{3}}$, $d = \mp\sqrt{\frac{2}{3}}$. with the sign being $c = \sqrt{\frac{1}{3}}$ and $d = -\sqrt{\frac{2}{3}}$.

e.)

$$\left|\frac{1}{2}, \frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left|1,1\right\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle - \sqrt{\frac{1}{3}}\left|1,0\right\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle \tag{B.111}$$

$C^{1\ \ \frac{1}{2}\ \frac{1}{2}}_{1\ -\frac{1}{2}\ \frac{1}{2}} = \sqrt{\frac{2}{3}}$, $C^{1\ \frac{1}{2}\ \ \frac{1}{2}}_{0\ \frac{1}{2}\ -\frac{1}{2}} = -\sqrt{\frac{1}{3}}$.

f.)

$$\left|\frac{1}{2}, -\frac{1}{2}\right\rangle = \sqrt{\frac{1}{3}}\left|1,0\right\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle - \sqrt{\frac{2}{3}}\left|1,-1\right\rangle \otimes \left|\frac{1}{2}, \frac{1}{2}\right\rangle \tag{B.112}$$

$C^{1\ \ \frac{1}{2}\ \ \frac{1}{2}}_{1\ -\frac{1}{2}\ -\frac{1}{2}} = \sqrt{\frac{1}{3}}$, $C^{\ \ 1\ \frac{1}{2}\ \ \frac{1}{2}}_{-1\ \frac{1}{2}\ -\frac{1}{2}} = -\sqrt{\frac{2}{3}}$.

These fill the table accordingly:

$1 \times \frac{1}{2}$		$j =$	$\frac{3}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{3}{2}$
$m_1 + m_2 = m =$			$+\frac{3}{2}$	$+\frac{1}{2}$	$+\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{3}{2}$
$+1$	$+\frac{1}{2}$		1					
$+1$	$-\frac{1}{2}$			$\sqrt{\frac{1}{3}}$	$\sqrt{\frac{2}{3}}$			
0	$+\frac{1}{2}$			$\sqrt{\frac{2}{3}}$	$-\sqrt{\frac{1}{3}}$			
0	$-\frac{1}{2}$					$\sqrt{\frac{2}{3}}$	$\sqrt{\frac{1}{3}}$	
-1	$+\frac{1}{2}$					$\sqrt{\frac{1}{3}}$	$-\sqrt{\frac{2}{3}}$	
-1	$-\frac{1}{2}$							1

Table B.2: Clebsch-Gordan coefficients table of $1 \times \frac{1}{2}$

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