Applications of Group Theory to Few-Body Physics

by

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Abstract

Over the past fifteen years, there have been persistent claims of anomalous nuclear reactions in condensed matter environments. A Unified Model [38] has been proposed to systematically account for most of these anomalies. However, all the work done so far has used simple scalar nuclear Hamiltonians. In this thesis, we develop the tools necessary to use a realistic nuclear Hamiltonian in the Unified Model.

A natural way to include a realistic nuclear potential in the Unified Model is via the method of coupled-channel equations. The phenomenological nuclear interaction chosen is the Hamada-Johnston potential [40]. The major portion of the thesis is devoted to deriving the coupled-channel equations with explicit symmetry constraints for the Hamada-Johnston potential. A critical input in this derivation is the calculation of the matrix elements of the various channels. We develop a systematic method, based on group theory, for calculating matrix elements of few-body correlated spatial wavefunctions. This method can, in some sense, be considered a generalization of Racah's viewpoint [17] of calculating shell-model matrix elements.

Towards the end, two related, but somewhat different topics are explored. Firstly, a simple phonon-coupled nuclear reaction, the photodisintegration of the deuteron, is investigated. While no observable results are computed, this work should be considered a first step in calculating the effects of the lattice on nuclear reactions. Secondly, Lie algebra theory is used to understand the coherent decay, from the highest symmetry state in N-level systems, in terms of the usual Dicke [21] algebra.

Thesis Supervisor: Peter L. Hagelstein
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Chapter 1

Introduction

Over the last fifteen years, various experimental claims have been made with regard to anomalous nuclear reactions in the condensed matter state [12, 55]. Based on these experimental results, Peter Hagelstein has proposed a "Unified Phonon-Coupled $SU(N)$"model which seems to explain almost all the anomalies systematically [38]. Hagelstein, using simple scalar nuclear Hamiltonians, has made a preliminary analysis of his model. The initial results have been very promising. Recognizing the fact that the nuclear Hamiltonian is far from being a scalar potential, the next logical step is to use a realistic nuclear Hamiltonian with all its angular, spin and isospin[1] terms. However, phonon operators will modify the spatial part of the wavefunction. Thus the natural way to couple the lattice and nuclear degrees of freedom is to try and "scalarize" each spatial channel. In this thesis, group theory is used to derive the coupled-channel equations for the Hamada-Johnston potential [40]. These equations can now be used to calculate the first realistic consequences of phonon-coupled nuclear reaction theory.

We recognize that the subject of anomalous nuclear reactions in metal deuterides is extremely controversial and many in the scientific community consider it akin to alchemy. However, we feel that this question of "cold fusion" is far too important and the experimental claims (while lacking complete reproducibility) are far too numerous and persistent

[1] Isospin is formally completely analogous to spin. We will briefly discuss it in section 4.2. For now it can be considered a "nuclear degree of freedom."

to be ignored completely. This thesis can be regarded as a step to help resolve this controversy.

In the remainder of this chapter, we give some background on the phonon-coupled unified model, which is the motivation for undertaking the present work. We then explain how our research fits within this approach to condensed matter nuclear reactions, provide a brief outline of our method and state the reasons for our choice of the nuclear Hamiltonian. We end the chapter with a brief summary of the important features of the thesis.

1.1 Unified Phonon-Coupled $SU(N)$ Model

The commonly held view in the physics community is that fusion reactions in the condensed matter state can very well be described by vacuum nuclear physics. Their basic argument is that the nuclear interaction takes place far too quickly for the reaction to influence neighboring atoms[2]. Similarly, while nuclear energies are on the order of MeV's, the maximum phonon energy is only $50\,meV$; hence exchanging a few phonons cannot modify a nuclear reaction. However, as stated above, over the past fifteen years, there have been persistent experimental claims of anomalies by respected laboratories and serious researchers [39]. Based on such evidence, it has been conjectured [38] in the Phonon-Coupled Unified Model that vacuum nuclear physics cannot adequately explain all nuclear reactions in a lattice.

The fundamental theoretical issue is the coupling of phonons to the nuclei. The first thing to realize is that the nuclear force (even for that matter the Coulombic interaction) can be considered a highly non-linear phonon operator. As such, when we try to couple the lattice to nuclear degrees of freedom, perturbation theory on vacuum nuclear physics is bound to fail. Thus, we need a completely new way of approaching condensed matter nuclear physics.

In the Unified Model, the condensed matter environment is formally included through the

[2]Atoms are separated on the angstrom scale where as the nuclear force has a range of 10 fermis and nuclear reactions take place on the order of 10^{-21} seconds.

Lattice Resonating Group Method [38]. This is a generalization of the Resonating Group Method [101] of vacuum nuclear physics. In this model the basic *ansatz* is to write out a trial variational wavefunction Ψ_t in the form

$$\Psi_t = \sum_j \Phi_j F_j$$

where the Φ_j keep track of the nuclear structure of the reactants and the channel separation factors, F_j, describe the relative coordinates of the reactants. The optimization of channel separation factors leads to

$$EF_j = \langle \Phi_j | H | \Phi_j \rangle F_j + \sum_{k \neq j} \langle \Phi_j | H - E | \Phi_k F_k \rangle$$

In the generalization to include phonons, Hagelstein starts by a different trial wavefunction

$$\Psi_t = \sum_j \Phi_j \Psi_j$$

where the Φ_j keep track of the nuclear structure of the reactants as before, but the Ψ_j are the lattice channel separation factors which describe the relative coordinates of the reactants as well as the particles in the lattice. The optimization of channel separation factors leads to

$$E\Psi_j = \langle \Phi_j | H | \Phi_j \rangle \Psi_j + \sum_{k \neq j} \langle \Phi_j | H - E | \Phi_k \Psi_k \rangle$$

Now, at least, the phonons have formally been accounted for. Hagelstein's conjecture is that [38]:

> All the anomalies in metal deuterides can be accounted for theoretically within this formulation that generalizes the vacuum models to include the local solid state environment. No other new basic physics is required beyond what is needed in textbooks, at least in principle.

1.2 The Motivation for this Research

Hagelstein has assumed simple scalar nuclear Hamiltonians in his Lattice Resonating Group Method and analyzed the coupled-channel equations. As discussed above, a more realistic nuclear potential, such as the Hamada-Johnston (H-J), should be used to make this analysis more rigorous[3]. In the Unified Model, the nuclear interaction takes place between two, three or four nucleons[4]. Over the past decades, the few-nucleon problem has received a great deal of attention from the nuclear physics community and there are a number of techniques available to solve the few-body nuclear problem [34, 57]. However, within the framework of the Unified Model the most natural way to include the nuclear potential was through the coupled-channel equations for the H-J potential (with each channel being specified by the spatial symmetry, spin and isospin). This could be achieved for each channel by algebraically removing the spin and isospin parts of the nuclear potential. While there were some useful results for the three-body case [4, 18, 45], for the four-body case we found no comparable work which explicitly dealt with the specification of the spatial channels [11, 53] . Even the three-body work was not clear, comprehensive or systematic.

The main goal of this thesis is to derive the coupled-channel three and four-body equations for the H-J interaction so that the Unified Model could be used to make realistic predictions. Hence, this thesis should be viewed as a step towards generating the tools necessary to calculate the effects of the lattice on nuclear reactions.

1.3 Outline of Our Method

In order to derive the coupled-channel equations, we first need to construct the nuclear wavefunctions. These can most naturally be built by using the following facts

- Nucleons are fermions and hence they obey the *Generalized Pauli Exclusion Principle* of being antisymmetric under the exchange of space, spin and isospin.

[3] We will discuss the reason for choosing H-J in section 1.4.

[4] A nucleon is a proton or a neutron.

- *Schur-Weyl duality* connects angular momenta (space, spin or isospin) and symmetry under permutations.

Generalized Clebsch-Gordan coefficients can then be used to construct appropriate wavefunctions for the various channels.

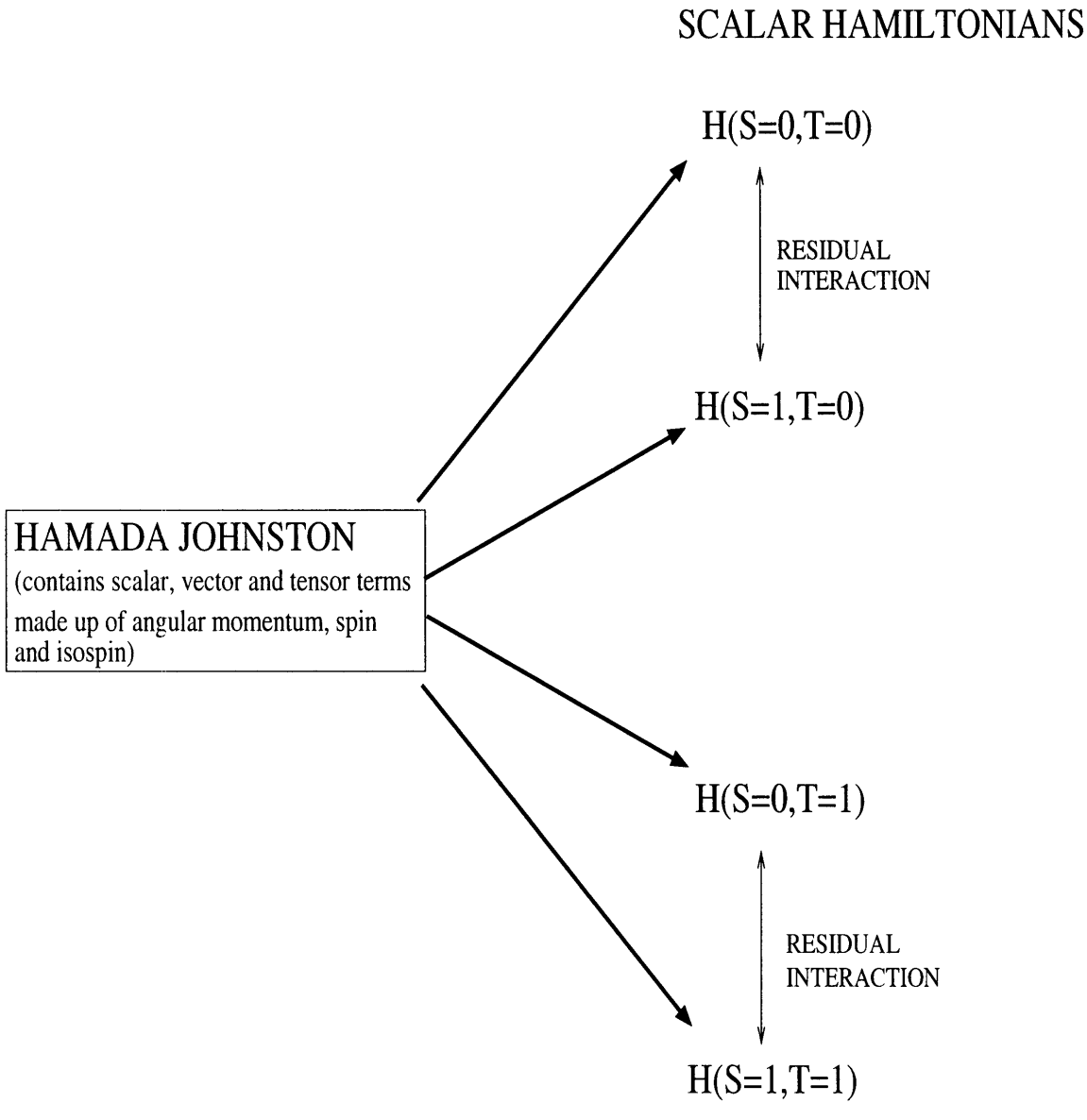
After construction of the wavefunctions, we need to evaluate the matrix elements so that we can derive the coupled-channel equations. Methods for calculating matrix elements of one-body and two-body operators with multi-particle wavefunctions were developed due to the pioneering work of Racah [70, 71, 72, 73]. These techniques were extended for the nuclear problem by Jahn [25, 48, 49] (for LS coupling) and by Flowers [23, 29] (for j-j coupling). It should be noted that all these calculations were done for the *nuclear shell model* [17]. In its simplest manifestation, the shell model is an independent particle approximation. Associated with it is the picture of nucleons having well-defined orbitals in some potential well.

However, in the applications we have in mind, we will mostly be dealing with variational correlated spatial wavefunctions. Historically, for correlated functions, the Hamiltonians were confined to purely scalar radial interactions [10]. Later on, tensor forces were introduced [7]. Around the same time Laskar [60], assuming symmetric spatial wavefunctions, worked out the few-nucleon case with central forces. However, we did not find any reference in the literature which systematically deals with the H-J potential. Thus, our approach to matrix element calculation, should be considered a generalization of the methods initiated by Racah to variational correlated spatial wavefunctions.

This calculation then leads us to the scalar few-body multi-channel equations for the H-J potential, which could be solved numerically. It should be mentioned here that, with trivial modifications, this analysis could also be applied to some of the more modern nuclear potentials [58] as well.

As a corollary, this thesis also opens up the field of low/medium energy nuclear physics to non-experts. This happens because now the few-body nuclear problem is reduced to a concrete set of coupled partial differential equations. Hence, with sufficient numerical

expertise, these equations can be solved for any few-body nuclear problem.



1.4 The Nuclear Hamiltonian

Despite the fact that the nuclear interaction is not well-understood, starting in the 1930's, physicists began to model various nuclear phenomena. The natural place to start was with

the simplest scalar nuclear potential e.g.

$$\sum_j -\frac{\hbar^2}{2m_j}\vec{\nabla}_j^2 + \sum_{j,k} V_0 e^{-\alpha(|\vec{r}_j - \vec{r}_k|^2)}$$

Unfortunately such a potential does not even bind deuterium, triton and helium with approximately the right nuclear sizes [37].

There were also early signs [91] of the so-called "exchange forces" e.g. during a proton-neutron collision, it seems as if a proton is exchanging its charge, instead of its momentum, with a neutron. Given such experimental evidence and the hopelessness of the simple nuclear Hamiltonians, physicists quickly moved onto more complicated scalar potentials; a typical example [76] (ignoring the Coulombic part) was

$$H = \sum_i -\frac{1}{2}\vec{\nabla}_i^{\,2} + \sum_{i<j}\{(1-g)P_{ij} + gP_{ij}Q_{ij}\}J(r_{ij})$$

where the P_{ij} and Q_{ij} are operators which exchange the space and spin variables, respectively. While such potentials began to at least bind all the light nuclei with approximately the right sizes, the deviation from experimental values was still significant. Such scalar models were also unable to account for the quadrupole moment of the deuteron [77]. Hence it was realized that to make sensible nuclear models, vector and tensor terms had to be added to the Hamiltonian.

In the 1950's, a major experimental program was undertaken to understand nucleon-nucleon interaction and build empirical potentials fitted to scattering and bound-state deuteron data. This eventually resulted in a new class of realistic potentials in the early 1960's [40, 61, 78]. These potentials were significantly more complicated as compared to the earlier models and contained all sorts of scalar, vector and tensor terms. A typical example is the H-J [40] potential.

The H-J potential between nucleon 1 and nucleon 2 can be written in the form

$$V = V_C + V_T S_{12} + V_{LS}\vec{L}.\vec{S} + V_{LL}L_{12}$$

where

$$
\begin{aligned}
V_C &= \vec{\tau}_1.\vec{\tau}_2\ \vec{\sigma}_1.\vec{\sigma}_2\ y_C(r_{12}) \\
V_T &= \vec{\tau}_1.\vec{\tau}_2\ y_T(r_{12}) \\
S_{12} &= 3\frac{(\vec{\sigma}_1.\vec{r})(\vec{\sigma}_2.\vec{r})}{r^2} - \vec{\sigma}_1.\vec{\sigma}_2 \\
V_{LS} &= y_{LS}(r_{12}) \\
V_{LL} &= y_{LL}(r_{12}) \\
L_{12} &= \vec{\sigma}_1.\vec{\sigma}_2\vec{L}^2 - \frac{1}{2}(\vec{\sigma}_1.\vec{L})(\vec{\sigma}_2.\vec{L}) - \frac{1}{2}(\vec{\sigma}_2.\vec{L})(\vec{\sigma}_1.\vec{L}) \\
\vec{L} &= \vec{L}_1 + \vec{L}_2 \\
\vec{S} &= \frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)
\end{aligned}
$$

The y's are defined to be

$$
\begin{aligned}
y_C^\alpha(x) &= 0.08\frac{\mu}{3}Y(x)\{1 + a_C Y(x) + b_C Y^2(x)\} \\
y_T^\alpha(x) &= 0.08\frac{\mu}{3}Z(x)\{1 + a_T Y(x) + b_T Y^2(x)\} \\
y_{LS}^\alpha(x) &= \mu G_{LS} Y^2(x)\{1 + b_{LS} Y(x)\} \\
y_{LL}^\alpha(x) &= \mu G_{LL} x^{-2} Z(x)\{1 + a_{LL} Y(x) + b_{LL} Y^2(x)\}
\end{aligned}
$$

where the α stands for singlet-odd, singlet-even, triplet-odd or triplet-even (singlet/triplet stands for the spin wavefunction and even/odd for the parity of the spatial wavefunction) and μ is the pion mass.

As explained above, our interest in nuclear phenomena is a by-product of our desire to better understand phonon-coupled nuclear reactions. To do this, we need realistic solutions of the few-body nuclear Hamiltonian. As we have discussed, the pre-1960 nuclear models are too primitive to give us reliable answers. H-J is one of the first realistic nuclear potentials. Since the H-J, many new potentials have been introduced e.g. the Paris[58], Bonn [44], Urbana[59] and Argonne[102]. However, decades of experience with H-J has shown that it

gives reasonable results for the few-nucleon problem [45, 51, 99] and it is still being used by the nuclear physics community [1, 67, 69]. Hence we can conclude that using the H-J potential is a reasonable starting point for understanding nuclear reactions in a lattice. If the calculations of the unified model with H-J point to some new nuclear phenomenon, then it would be worthwhile to use one of the modern day potentials to refine the calculations.

1.5 Organization of the Thesis

Chapter 2 and 3 give a brief overview of the necessary portions of group representation theory. The mathematically inclined reader may also want to read Appendix A, which discusses the role of symmetric polynomials.

Chapter 4 explains the method of construction of the wavefunctions. The results of the calculation for the three-body and four-body cases are given in chapters 5 and 6. The results of chapter 6 are new. We have not seen a systematic enumeration of the completely antisymmetric four-body nuclear wavefunctions in the literature.

Beginning with chapter 7, the focus shifts to calculation of the matrix elements of the H-J potential. We generalize Racah's method to correlated, variational spatial wavefunctions. In this process we find two facts which are of some fundamental importance:

- Racah's method for the shell-model works by choosing the *last* two particles to have special symmetry properties. We find that for correlated functions, it is best to expand the wavefunction with the *first* two particles having distinguished symmetry.
- Clebsch-Gordan coefficients of $SU(2)$ can be naturally used to construct the spin or isospin Yamanouchi basis of the group of permutations.

In chapters 8 and 9, we give the results for the 3-body and 4-body matrix elements. Then in chapter 10, we bring together the results of chapters 8 and 9 to derive the coupled-channel equations for the 2, 3 and 4-body cases. These coupled-channel equations have a clear and simple channel-specification. We have not seen such a result in the literature i.e. complete separation of the spatial part with explicit symmetry requirements.

Chapter 11 begins to explore the possibility of phonon-coupled nuclear reactions. In this chapter, we look at threshold photodisintegration of the deuteron in the presence of a highly excited phonon mode. Since we are considering low energy photons, the precise form of the nuclear interaction is insignificant [65, 82, 86] and the use of multi-channel equations is not required. However, had we been interested in nuclear reactions at higher energies, we would then have to use the full H-J potential to do the computations. Hence, this chapter establishes the basic framework for phonon-coupled nuclear reactions. For higher energies or other nuclear reactions, we would have to use the wavefunctions obtained by solving the coupled-channel H-J equations.

Chapter 12 deals with a somewhat different but related problem. It has been known that coherence between atoms that radiatively decay can lead to an enhancement in the decay rate. This is called Dicke superradiance [21]. A similar kind of enhancement has been proposed by Hagelstein to be involved in his cold fusion model. The question of whether Dicke coherence can be obtained in the case of models more complicated than two-level systems has become of interest. The chapter is an attempt to simply understand such effects using Schur-Weyl duality and Lie algebra theory. In this respect it is more abstract as compared to the rest of the thesis. However the conclusions are very simple and straightforward, and can be used by anybody familiar with angular momentum algebra.

Chapter 13 summarizes the contributions of the thesis and discusses possible future research.

Chapter 2

Theory Of Group Representations

In this chapter we build up some of the tools necessary for the construction of the nuclear wavefunctions. One of the most natural ways to construct wavefunctions is to use group representation theory. While such an approach leads to a very elegant and simple construction, it requires the use of somewhat formidable machinery from mathematics [24, 31, 41].

The purpose of this chapter is to make the use of representation theory accessible to the reader who is familiar with angular momentum algebra. Thus, this chapter is an attempt to build a "representation theory to quantum mechanics dictionary". We will repeatedly appeal to facts from angular momentum algebra to "prove" general results for arbitrary groups [1]. For the construction of the wavefunctions, we need to understand the representations of the group of permutations, $S(n)$, and their interaction with the representations of $SU(2)$. These groups are defined to be

$$\begin{aligned} S(n) &= \{\text{Group of permutations of } n \text{ objects}\} \\ SU(2) &= \{\text{Group of } 2 \times 2 \text{ unitary matrices of determinant } 1\} \end{aligned}$$

This connection will be explored in chapter 3. However, for now, we focus on general representation theory. The two most important concepts in this chapter are:

[1] By arbitrary, we mean either a finite or a compact Lie group.

1. The generalization of Clebsch-Gordan(CG) coefficients to arbitrary groups.

2. Construction of projection operators.

Both of these will be critical in the construction of the wavefunctions.

2.1 Two Applications of Representation Theory

Group representation theory is tremendously useful to physicists. Here we will only consider two applications. The first one, spherical harmonics, is familiar to us from quantum mechanics. However, in this thesis, we will mainly be interested in the second application, namely in the construction of the wavefunctions.

2.1.1 Breaking up the Hilbert space

Consider a closed physical system. We expect such a system to be invariant under the group of rotations, $SO(3)$, where

$$SO(3) \quad = \quad \{\text{Group of } 3 \times 3 \text{ real orthogonal matrices of determinant } 1\}$$

This means that given an eigenstate of our system, all the rotated states should have the same energy eigenvalue. Hence if $\psi_n(r)$ is an eigenfunction of the Hamiltonian with energy E_n, then all the functions[2], $\rho(R)\psi_n(r)$, where $\rho(R)$ is an arbitrary rotation operator, have energy E_n. Now if we consider the vector space spanned by all these functions, this vector space (by construction) is *invariant* under the action of the operators $\rho(R)$. All the wavefunctions in this subspace can be characterized by an eigenvalue, l, of angular momentum. In this way we naturally get a *representation* of $SO(3)$[3].

[2]All the functions may not be linearly independent.

[3]We have tacitly assumed that we are dealing with bosons. If we were dealing with fermions, the theory would be a bit more complicated. In quantum mechanics we deal with rays and not vectors. This means that representations are defined only up to a phase. So what we get in this case are not representations of $SO(3)$, but *projective representations*, which are essentially a way of saying that we do not care about phases. Now it turns out that projective representations of groups like $SO(3)$ are just ordinary representations of the

Hence, we have managed to break up our Hilbert space into smaller noninteracting pieces. This means that we can write a general wavefunction as[4]

$$\psi(\theta, \phi, r) = \sum_{l=0}^{\infty} \left[\sum_{m=-l}^{l} c_{lm} Y_m^{(l)} \right] f_l(r) \tag{2.1}$$

This way of decomposing the wavefunction is useful because under rotations, the $Y_m^{(l)}$ only transform into other $Y_{m'}^{(l)}$'s [5]. Even if the Hamiltonian is not invariant under rotations, calculation of matrix elements of irreducible tensor operators becomes much easier due to the Wigner-Eckart theorem [81]. It can be shown that the above results i.e. labeling of the eigenfunctions and tensor methods can be generalized to arbitrary groups.

2.1.2 Construction of the wavefunctions

Representation theory is also very helpful in building up wavefunctions. The construction of the two-body electronic wavefunction is a textbook example in quantum mechanics. It is based on the *Pauli Exclusion Principle*. Provided spin is a good quantum number, the total wavefunction is either a product of space-symmetric and spin-antisymmetric or a product of space-antisymmetric and spin-symmetric eigenfunctions where

$$\begin{aligned} \text{space symmetric} &= \frac{1}{2}\left[f(\vec{r}_1, \vec{r}_2) + f(\vec{r}_2, \vec{r}_1)\right] \\ \text{space antisymmetric} &= \frac{1}{2}\left[f(\vec{r}_1, \vec{r}_2) - f(\vec{r}_2, \vec{r}_1)\right] \end{aligned}$$

universal covering groups [2]. For $SO(3)$ the universal covering group is $SU(2)$. So we should actually be considering the representations of $SU(2)$. Please note that group theory and quantum mechanics only tell us the group whose representations we should consider. The realization of group representations is a *physical* input (derived from experiment) into the theory i.e. group theory does not imply that any of the representations are actually realized in nature.

[4]We have not discussed how we get the label m. Since $SO(2) \subset SO(3)$, any irreducible representation of $SO(3)$ is also a (in general reducible) representation of $SO(2)$. $SO(2)$ representations are labeled by m. This is a standard way of uniquely labeling vectors in our Hilbert space. We will see examples of such a procedure in the next chapter when we talk about the Yamanouchi labels for the symmetric group.

[5]Or in the language that we will learn, for any l the $Y_m^{(l)}$ form a *representation* of the rotation group.

$$\text{spin symmetric} = \begin{cases} \uparrow\uparrow \\ \frac{\uparrow\downarrow+\downarrow\uparrow}{\sqrt{2}} \\ \downarrow\downarrow \end{cases}$$

$$\text{spin antisymmetric} = \frac{\uparrow\downarrow - \downarrow\uparrow}{\sqrt{2}}$$

However, when we get to the three-electron case, our intuition does not work as well. Of course, we still have the obvious case i.e. the product of space-antisymmetric with spin-symmetric where (now denoting 1,2,3 to represent $\vec{r}_1, \vec{r}_2, \vec{r}_3$ and $\alpha(i)$ for $\uparrow$ (i) and $\beta(i)$ for $\downarrow$ (i))[6]

$$\begin{aligned}\text{space antisymmetric} = \frac{1}{6}[&f(123) + f(312) + f(231) - f(132) \\ &- f(213) - f(321)]\end{aligned}$$

$$\text{spin symmetric} = \begin{cases} \alpha(1)\alpha(2)\alpha(3) \\ \frac{1}{\sqrt{3}}\{\alpha(1)\alpha(2)\beta(3) + \alpha(1)\beta(2)\alpha(3) \\ +\beta(1)\alpha(2)\alpha(3)\} \\ \frac{1}{\sqrt{3}}\{\alpha(1)\beta(2)\beta(3) + \beta(1)\alpha(2)\beta(3) \\ +\beta(1)\beta(2)\alpha(3)\} \\ \beta(1)\beta(2)\beta(3) \end{cases}$$

We do not have the product of space-symmetric with spin-antisymmetric because there is no completely antisymmetric three-particle spin-wavefunction (since we only have two possible z-directed spins). But do these wavefunctions exhaust the Hilbert space?

The answer to this question lies in the observation that there seems to be a link between

[6]This change in notation is adopted for convenience in later chapters.

the symmetry of the spin wavefunction under permutations of particles and the total spin e.g. for both the two and the three-particle case, symmetric spin wavefunctions are associated with the maximum possible total spin. In fact our observation is a consequence of a deep and beautiful relation called the Schur-Weyl duality. This duality exists between the representations of the symmetric and unitary groups. In our case, this duality implies that there exist two copies of a "mixed symmetry" representation of the symmetric group[7]. CG coefficients of the symmetric group then allow us to construct the few-body wavefunctions.

However, our interest is in the nuclear and not in the few-electron case. For nucleons the *Generalized Pauli Exclusion Principle* states that the total wavefunction of a nucleon, made up of spatial, spin and isospin parts, must be antisymmetric under the exchange of any two particles. Once the Schur-Weyl duality and CG techniques are understood, the extension to the nuclear case is completely obvious. The results of this calculation are given in chapters 4 and 5.

Before we can outline some important ideas in representation theory, we need to understand what a *group* is.

2.2 Basic Group Theory

Let us consider three different groups

- The integers under addition.
- The non-zero real numbers under multiplication.
- 3×3 real orthogonal matrices of determinant 1, under multiplication. This is usually denoted by $SO(3)$.

In the first example, if we add two integers, we get another integer. Also given an integer a, if we add $-a$ to it, we get the integer 0. 0 is the unique integer such that $a + 0 = 0 + a = a$.

[7]These will turn out to be nothing more than the familiar fact that when we add three spin $\frac{1}{2}$ particles, we get two orthogonal total $S = \frac{1}{2}$ states.

$-a$ is called the inverse of a and 0 the identity element. The second example has the same properties as the first one i.e. given two real numbers, we can multiply them to get another real number. Given a real number b if we multiply it by $1/b$ we get 1. 1 is the unique real number such that $b.1 = 1.b = b$.

Formally, we get the same structure in the third case, with matrix multiplication replacing multiplication of real numbers, matrix inversion taking the place of reciprocals and the identity matrix replacing 1. However, we know that such matrices represent rotations in ordinary three-dimensional space[8]. Irrespective of the physical content, there are obvious similarities in the structure of all of these objects.

Hence we define a *group* to be a set $G = \{a, b, c...\}$ with an associative law of composition, denoted by $a \circ b$, which satisfies the following axioms.

1. There exists a unique element $e \in G$ such that for any element $a \in G$, $a \circ e = a$ and $e \circ a = a$. The element e is called the *identity*.

2. For every element $a \in G$ there exists a unique $b \in G$ such that $a \circ b = e$ and $b \circ a = e$. The element b is called the *inverse* of a.

So, depending on the group, the $\circ$ here can stand for "integer addition", "real number multiplication", "matrix multiplication", "composition of permutations", "composition of rotations" etc.

The simplest example of a group is $G = \{e\}$. Clearly it satisfies all the axioms of a group. Next, we can consider the group G of *order*[9] 2 i.e. $G = \{e, a\}$ with $a \circ a = e$. As the order of the group increases, the number of possible groups quickly multiplies. However, we move on to the rotation group, which is the main example of this chapter. This will naturally lead us to representation theory.

[8]Please note that all these groups have an infinite number elements in them. We will mostly be dealing with finite groups or compact Lie groups (like $SO(3)$ or $SU(2)$). Such Lie groups are very well understood in the mathematics literature. We will adopt the typical physicists view that going from the discrete to the continuum just involves changing "a sum to an integral".

[9]Order of a group G is the number of elements in the set G and is denoted by $|G|$.

2.2.1 The rotation group

Let us consider

$$G = \{\text{Group of all rotations in three dimensions}\}$$

This group acts to rotate our apparatus in physical 3-D space. Any $R \in G$ is going to correspond to a rotation operator $\rho(R)$ on the Hilbert space (i.e. the physically rotated apparatus will correspond to a rotated ket). Please note that we are dealing with two *distinct* groups i.e. the group of rotations in real physical space, and its corresponding group on the Hilbert space. These two groups will have distinct laws of composition. In physical space we can consider the effect on our apparatus of one rotation R_1 followed by another rotation R_2 to get a rotation $R_2 \circ R_1$. We would like the rotation operators, $\rho(R_i)$, to obey

$$\rho(R_2 \circ R_1) = \rho(R_2) \bullet \rho(R_1) \tag{2.2}$$

where, on the L.H.S. we are composing group elements in G and on the R.H.S. we are composing the operators $\rho(R_i)$ on the Hilbert Space. In fact Equation 2.2 captures the essence of what it means to be a *representation*.

Equation 2.2 is also an example of something called a *homomorphism*. A homomorphism between two groups G and H, with group composition laws $\circ$ and $\bullet$ respectively, is defined to be a map $\rho : G \to H$ such that $\rho(a \circ b) = \rho(a) \bullet \rho(b)$.

Another simple example of a homomorphism is given by the exponential map, where G is the real numbers under addition, and H is the positive real numbers under multiplication. Then the property that exponential map is group homomorphism reads

$$e^{a+b} = e^a e^b$$

An *isomorphism* is a homomorphism which is one-to-one and onto. We will frequently write $a \circ b$ as just ab.

2.3 Basic Definitions in Representation Theory

We intuitively already know what a representation is, i.e. $Y_m^{(l)}$ form a representation of $SO(3)$. However, in order to give a precise definition, let us revisit the example in section 2.2.1 of the rotation group. Recall that we required our operators to satisfy

$$\rho(R_1 \circ R_2) = \rho(R_1) \bullet \rho(R_2) \tag{2.3}$$

Abstractly, this is a homomorphism from the group G to the group of invertible linear operators on the Hilbert space [10] i.e. a map

$$\rho : G \to GL(V) \tag{2.4}$$

which maps a rotation R to the linear operator $\rho(R)$ [11]. Since ρ is a homomorphism, Equation 2.3 is satisfied.

Hence a *representation* of a group G on a finite-dimensional complex vector space V is defined to be a homomorphism $\rho : G \to GL(V)$. The dimension of V is called the *dimension of the representation.* It is also common to blur the distinction between representations and vector spaces.

Two representations (ρ_i, V_i) $i = 1, 2$ of G are considered *equivalent* if there is a linear isomorphism T such that for every $g \in G$, $\rho_2(g) \circ T = T \circ \rho_1(g)$. A representation (ρ, V) is *unitary* if there is an inner product $\langle \cdot, \cdot \rangle$ on V s.t. for every $g \in G$ and $u, v \in V$, $\langle \rho(g)v, \rho(g)u \rangle = \langle u, v \rangle$. It is a fact that every representation is equivalent to a unitary representation.

[10] Let V be the Hilbert space. Then by $GL(V)$ we mean the *automorphisms* of V. If $V = C^n$, then $GL(V)$ is nothing more than the group of complex invertible $n \times n$ matrices.

[11] $\rho(R)$ represents R on the Hilbert space.

2.3.1 Matrix representations

From linear algebra we know that given a linear operator, $\rho(a)$, on a n-dimensional complex (or real) vector space V, by choosing a basis of V, this problem can be reduced to an $n \times n$ matrix acting on C^n. The recipe is that if $\{v_1, \ldots, v_n\}$ is a basis of V and $\rho_a v_i = \sum_{j=1}^{n} \Gamma_{ji} v_j$, then Γ_{ji} is the matrix of ρ_a in the basis $\{v_1, v_2 \ldots, v_n\}$. So after choosing a basis, the entire theory of finite representations reduces to dealing with matrices, e.g. equivalent representations are nothing more than matrices equivalent under a similarity transformation.

2.3.2 Spherical harmonics

Consider the simplest possible case of $l = 0$. Then V is the space spanned by $Y_0^{(0)}$. This is a one dimensional complex vector space. There is a homomorphism

$$\rho : G \to GL(V) \tag{2.5}$$

which maps R to $\rho(R)$. But as it stands, the equation does not tell us much; we need to specify more explicitly the linear operator $\rho(R)$, i.e. how does it act on the vector space V? We define it to be

$$\begin{aligned} \rho(R) &: V \to V \\ \rho(R) Y_0^{(0)}(\hat{\vec{n}}) &= Y_0^{(0)}(\hat{\vec{n}}) \end{aligned} \tag{2.6}$$

The linear operator $\rho(R)$ does not seem to be doing much. In fact this representation is called the *trivial* representation, which means that all the rotation operators, $\rho(R)$, act as the identity on $Y_0^{(0)}$ [12].

Next, we can consider the vector space V, spanned by $Y_m^{(l)}$ for fixed l. Again we want to

[12] It is obvious that the trivial representation is a representation since it satisfies the homomorphism property.

explicitly know the action of the linear operator $\rho'(R)$ on V. This is defined by

$$\begin{aligned} \rho'(R) : V &\to V \\ \rho'(R)Y_m^{(l)}(\hat{\vec{n}}) &= Y_m^{(l)}(R^{-1}\hat{\vec{n}}) \\ &= \sum_{m'} Y_{m'}^{(l)}(\hat{\vec{n}})D_{m'm}^{(l)}(R) \end{aligned} \tag{2.7}$$

where the $D_{m'm}^{(l)}(R)$ are some matrix coefficients. The reader is presumed to be familiar with this equation from quantum mechanics. Now this is to be understood as the action of a linear operator on a vector space. The reader can verify[13] that $\rho'(R_1)\rho'(R_2) = \rho'(R_1R_2)$ does indeed hold.

2.3.3 Irreducible representations

When considering representations of $SO(3)$ for a rotationally invariant Hamiltonian, it is almost frivolous to consider the $Y_m^{(l)}$ for different l. The reason being that the various l do not get transformed into each other under rotations. However for a given l, consider the vector space V, spanned by all the $Y_m^{(l)}$ for $-l \leq m \leq l$. We need to include all the m's since arbitrary rotations do inevitably mix the various spherical harmonics. In this sense V is the smallest vector space that can form a representation of the rotation group: it is irreducible. A representation $\rho : G \to GL(V)$ is called *irreducible* if V has no *proper invariant subspace* W [14]. The example with spherical harmonics correctly suggests that it should always be possible to break up a space into a direct sum of irreducible ones.

Hence, if we take for G the group $SO(3)$ and for V the invariant vector space generated by the rotation operators, $\rho(R)$, applied to $Y_m^{(l)}$, then the homomorphism $\rho : R \to \rho(R)$ is an irreducible $2l + 1$ dimensional representation of the group of rotations[15]. Now consider the group $SO(2) \subset SO(3)$, where $SO(2) = \{$Group of 2×2 orthogonal matrices of determinant

[13]Using the well-known properties of the $D_{m'm}^{(l)}(R)$.

[14]A vector subspace $W \subset V$ is a proper invariant subspace if $\rho(R)W \subset W$ for every element $\rho(R) \in G$ where G is a group of operators on the Hilbert Space (e.g. rotations), and $W \neq V$ and $W \neq 0$.

[15]Frequently the representations are labeled by the vector space V.

1}. We can consider $SO(2)$ to be rotations around the z-axis. While V is irreducible with respect to $SO(3)$, there is no reason for it to be irreducible with respect to $SO(2)$. In fact we know that it is reducible. It is a well-known fact that representations of $SO(2)$ are labeled by m [24]. So for each m, $Y_m^{(l)}$ forms a 1-dimensional irreducible representation of $SO(2)$ i.e. as a representation of $SO(2)$

$$V = Y_l^{(l)} \oplus Y_{l-1}^{(l)} \oplus \cdots Y_{-l+1}^{(l)} \oplus Y_{-l}^{(l)}$$

In this way we get unique labels for all our basis vectors[16].

In terms of matrices, consider the set of matrices of all the operators of our group. If, by a change of basis, they cannot *all be simultaneously block diagonalized*, the representation is irreducible.

With this section we wrap up our basic introduction to representation theory. Now we come to an extremely important part of the chapter: the generalization of the concept of CG coefficients to an arbitrary group.

2.4 Clebsch-Gordan Theory

The canonical example in this section is angular momentum algebra from quantum mechanics. The purpose of this section is to look at this familiar example from a somewhat different perspective, so that we can easily generalize the concepts to other groups. We already know that the concepts of angular momentum addition and CG coefficients are very useful in quantum mechanics. We will similarly find that the generalization of these concepts to arbitrary groups, especially $S(n)$, is essential to our construction of the few-body wavefunctions.

[16] Admittedly the reasoning is a bit circular since we started with $Y_m^{(l)}$s. We could have started with polynomials and *derived* the Cartesian expansion of the $Y_m^{(l)}$s [97].

2.4.1 Direct product of representations

We first have to understand the meaning of direct products of vector spaces[17]. Given a spinless particle of angular momentum l_1, the various $|l_1, m_1\rangle$ form a representation of the rotation group. Similarly for a spinless particle of angular momentum l_2, the $|l_2, m_2\rangle$ form another representation of the rotation group. Then a direct product of the two representations is $|l_1, l_2, m_1, m_2\rangle = |l_1, m_1\rangle \otimes |l_2, m_2\rangle$. We can generalize this to arbitrary vector spaces. Suppose we have two vector spaces V and W. If V has basis $\{v_1, \ldots, v_n\}$ and W has basis $\{w_1, \ldots, w_m\}$ then $V \otimes W$ is nm dimensional and has basis $\{v_i \otimes w_j\}$. If $v = \sum \alpha_i v_i$ and $w = \sum \beta_j w_j$ then

$$v \otimes w = \sum_{i,j} \alpha_i \beta_j v_i \otimes w_j \tag{2.8}$$

From the above equation it is easy to verify that the product is bilinear (i.e. linear in each variable) and distributive (relations like $v \otimes (w + x) = v \otimes w + v \otimes x$ hold).

We know from quantum mechanics that given $|l, m_l\rangle \otimes |s, m_s\rangle = |l, s, m_l, m_s\rangle$ the rotation operators $\rho(R)$ can act on the tensor product space in the obvious way i.e.

$$\left[\rho^{(l)} \otimes \rho^{(s)}\right](R)|l, m_l\rangle \otimes |s, m_s\rangle = \rho^{(l)}(R)|l, m_l\rangle \otimes \rho^{(s)}(R)|s, m_s\rangle \tag{2.9}$$

The different superscripts "l" and "s" on $\rho(R)$ are simply meant to distinguish that R has two different representations on the two different vector spaces, spanned respectively by spherical harmonics and spin eigenfunctions. This construction is completely general. Suppose we are given two representations ρ and σ i.e.

$$\begin{aligned} \rho &: G \to GL(V) \\ \sigma &: G \to GL(W) \end{aligned} \tag{2.10}$$

Then we can define the *tensor product* or *direct product* of representations [18]. It is denoted

[17] These are also known in the mathematics literature as *tensor products*.

[18] Please note that although we have given a basis dependent definition of the tensor product, it is in fact

by $\rho \otimes \sigma$ where

$$\rho \otimes \sigma : G \to GL(V \otimes W) \tag{2.11}$$

We still have to concretely define the action of the linear operator $[\rho \otimes \sigma](g)$ (for any $g \in G$), on the vector space $V \otimes W$. This is done by using the representations ρ and σ as

$$[\rho \otimes \sigma](g)v \otimes w = \rho(g)v \otimes \sigma(g)w \tag{2.12}$$

Sometimes we will not use the words "vector space" or "representation" before "tensor product". This convention is quite standard in the literature and sometimes even $\otimes$ is not written.

In terms of matrices, let C be the matrix representation of $\rho(g)$ and D be the matrix representation of $\sigma(g)$ w.r.t. to the above bases. Then the matrix of $(\rho \otimes \sigma)(g)$ w.r.t $v_i \otimes w_j$ is

$$[\rho \otimes \sigma](g)v_i \otimes w_j = \sum_{kl} C_{li} D_{kj} v_l \otimes w_k \tag{2.13}$$

Or in other words $([\rho \otimes \sigma](g))_{lk,ij} = C_{li} D_{kj}$. In terms of matrices, if C is the matrix of $\rho(a)$ and D is the matrix of $\rho'(a)$ then $(C \times D)_{ij,kl} = C_{ik} D_{jl}$, where each row and column has a double index.

2.4.2 Angular momentum addition

Consider a two-electron spinless atom. There is no reason for individual angular momenta to be conserved. However we know that due to rotational invariance, the total angular momentum must be conserved. Hence we need to add the individual orbital angular momenta to get a total angular momentum. The basic idea is that we can add two momenta, $\vec{L}_1$ and $\vec{L}_2$, to give a new angular momentum $\vec{L}$ i.e.

$$|l_1 l_2; lm\rangle = \sum_{m_1, m_2} C^{l,m}_{l_1,m_1;l_2,m_2} |l_1 m_1 l_2 m_2\rangle \tag{2.14}$$

intrinsically defined.

where the $C^{l,m}_{l_1,m_1;l_2,m_2}$ are some coefficients. This equation should be viewed as a change of basis in the space of $W = V^{(l_1)} \otimes V^{(l_2)}$, where $V^{(l_1)}$ is spanned by $|l_1, m_1\rangle$ and $V^{(l_2)}$ is spanned by $|l_2, m_2\rangle$. W has dimension $(2l_1 + 1)(2l_2 + 1)$. We take this space and break it up into subspaces labeled by total angular momentum l and total z-directed angular momentum m. Consider two $l_1 = l_2 = 1$ electrons. The angular momentum eigenkets form a $3 \times 3 =$ 9-dimensional space. This space can be broken up into a 5-dimensional subspace labeled by $l = 2$, a 3-dimensional subspace labeled by $l = 1$ and a 1-dimensional subspace labeled by $l = 0$. If we choose a basis of each of these subspaces, then the rotation operator will itself be block-diagonalized. This is an obvious consequence of the fact that the various (total) angular momenta do not mix under a rotation i.e. thinking of rotation operators as matrices, we are choosing a basis such that $D^{(l_1)} \otimes D^{(l_2)}$ is block-diagonalized.

$$\begin{pmatrix} D^{(2)} & & \\ & D^{(1)} & \\ & & D^{(0)} \end{pmatrix}$$

In our new terminology, we are decomposing the representation on $V^{(l_1)} \otimes V^{(l_2)}$ into irreducible representations of the rotation group. So we can write the same thing in more abstract (basis independent) notation as

$$D^{(l_1)} \otimes D^{(l_2)} = D^{(l_1+l_2)} \oplus D^{(l_1+l_2-1)} \oplus \ldots D^{(|l_1-l_2|)} \tag{2.15}$$

The process of decomposing a tensor product of representations into irreducible ones and the expansion of the bases of the new irreducible representations in terms of the old basis elements is completely general. The advantage of a basis-independent approach is that a basis need not be chosen until we start doing explicit calculations. Sometimes basis-dependent arguments can mystify simple results. So it is useful to spend some time trying to understand the more abstract version. But we first need to explain the symbol $\oplus$ for vector spaces and for representations.

2.4.3 Direct sum of representations

Before we define what we mean by direct sum of representations, we should define what a direct sum of vector spaces is. The canonical example to bear in mind is how we can take $\mathbb{R}^n$ (n-dimensional real space) and break it up into $\mathbb{R}^m$ and $\mathbb{R}^{n-m}$. We can say that

$$\mathbb{R}^n = \mathbb{R}^m \oplus \mathbb{R}^{n-m}$$

Mathematically speaking if W_1 and W_2 are vector subspaces of V, then V is called the *direct sum* of W_1 and W_2 if every vector $v \in V$ can be written uniquely as $w_1 + w_2$ where $w_i \in W_i$ and $W_1 \cap W_2 = 0$. Then $V = W_1 \oplus W_2$.

Given two representations (ρ_i, V_i) $i = 1, 2$ of G, we can form a new representation of the group, called the *direct sum* of the two representations on the vector space $V_1 \oplus V_2$. This is denoted by $\rho_1 \oplus \rho_2$ and is defined by

$$(\rho_1 \oplus \rho_2)(g)(v_1 \oplus v_2) = \rho_1(g)v_1 \oplus \rho_2(g)v_2 \quad v_i \in V_i \tag{2.16}$$

We know that any given representation can be broken up into a finite number of irreducible representations [19]. Hence we have the important statement that every representation is equivalent to a direct sum of irreducible representations i.e. (with the usual abuse of notation by blurring the distinction between representations and vector spaces)

$$V = W_1 \oplus W_2 \ldots \oplus W_n \tag{2.17}$$

Choosing a basis of each of the W_i, and putting them together to get a basis of V, shows that $\rho(g)$, for *all* $g \in G$, can be *simultaneously block diagonalized.* Hence we come to the conclusion that in order to understand representations of any group, we only need to learn about its irreducible representations.

[19] If (ρ, V) is a representation, and W_1 is an invariant subspace, the orthogonal complement is also an invariant subspace. Now use induction on dimension of V.

2.4.4 Clebsch-Gordan series

[20]As we know from Equation 2.15, the tensor product of two irreducible representations $\rho^{(\alpha)}$ and $\rho^{(\beta)}$ is in general reducible.

$$\rho^{(\alpha)} \otimes \rho^{(\beta)} = \sum_{\gamma=1}^{\zeta} \oplus n_\gamma \rho^{(\gamma)} \tag{2.18}$$

where the sum is over all the irreducible representations $\rho^{(\gamma)}$ of the group G (total ζ in number), and n_γ is the multiplicity of the irreducible representation (γ) in the tensor product. This is called the *Clebsch-Gordan series*. So Equation 2.15 is the Clebsch-Gordan series of $D^{(l_1)} \otimes D^{(l_2)}$ (where each representation has multiplicity $n_\gamma = 1$).

2.4.5 Clebsch-Gordan coefficients

Continuing the example of angular momentum addition, we know that

$$|l_1 l_2; lm\rangle = \sum_{m_1,m_2} C^{l,m}_{l_1,m1;l_2,m_2} |l_1, m_1\rangle \otimes |l_2, m_2\rangle \tag{2.19}$$

where the $C^{l,m}_{l_1,m1;l_2,m_2}$ are called the Clebsch-Gordan coefficients. These are simply the coefficients of the matrix of the change of basis from $|l_1 m_1 l_2 m_2\rangle$ to $|l_1 l_2; lm\rangle$. This again applies to all groups in general.

Consider two vector representations $(\rho^{(\alpha)}, V)$ and $(\rho^{(\beta)}, W)$. V has basis $\{v_1^{(\alpha)}, \ldots, v_n^{(\alpha)}\}$ and W has basis $\{w_1^{(\beta)}, \ldots, w_m^{(\beta)}\}$. Then $V \otimes W$ is nm dimensional and has $\{v_i^{(\alpha)} \otimes w_j^{(\beta)}\}$ as a basis. However by Equation 2.18 we know that there exists another basis $\{u_k^{(\gamma),t}\}$, $1 \le \gamma \le \zeta$, $1 \le t \le n_\gamma$ for $V \otimes W$, such that for fixed γ and t, the vectors $\{u_k^{(\gamma),t}\}$, $1 \le k \le d_\gamma$ form a basis for an irreducible representation $\rho^{(\gamma)}$, where d_γ is the dimension of γ. Hence it must

[20]The following sections are essentially taken from [24].

be possible to choose linear combinations of basis elements $v_i^{(\alpha)} \otimes w_j^{(\beta)}$ such that

$$u_k^{(\gamma),t} = \sum_{ij} C(\alpha\beta\gamma t, ijk) v_i^{(\alpha)} \otimes w_j^{(\beta)} \tag{2.20}$$

which transform irreducibly according to the representation γ (provided $n_\gamma \neq 0$). The C's are called the *Clebsch-Gordan coefficients*. Hence the CG coefficients should be considered as forming a change of basis matrix. The new basis has the property that it brings out the underlying group structure most explicitly. While Equation 2.18 makes it obvious that CG coefficients exist, we know from quantum mechanics, the explicit calculation of these coefficients is a hard and laborious job. This is true for an arbitrary group as well.

2.4.6 Wigner-Eckart theorem

Let (ρ, V) be a representation of a group G. If S is any other linear operator on V then

$$\rho(g_a)'S = S' = \rho(g_a)S\rho(g_a^{-1})$$

is a representation of G on $End(V)$, where $End(V)$ is the vector space of all linear operators on V (e.g. if $V = R^n$, then $End(V)$ is just the vector space of $n \times n$ matrices). If we can find operators such that

$$\rho(g_a)'S_i^{(\alpha)} = \rho(g_a)S_i(\alpha)\rho(g_a^{-1}) = \sum_{j=1}^{d_\alpha} \rho_{ji}^{(\alpha)}(g_a)S_j^{(\alpha)} \tag{2.21}$$

where d_α is the dimension of the irreducible representation (α) of G, then clearly the operators $S_i^{(\alpha)}$ form an irreducible representation equivalent to (α).

Now for functions like

$$\psi_{ij} = S_i^{(\alpha)} \phi_j^{(\beta)}$$

where (α) and (β) label irreducible representations of G, it is easy to see that ϕ_{ij} transforms according to the direct product representation $(\alpha) \otimes (\beta)$. Using Equation 2.18 or Equation 2.20, we can see that there exists a $C(\alpha\beta\gamma' t, ijk')$ such that

$$\psi_{ij} = \sum_{\gamma',t,k'} C(\alpha\beta\gamma' t, ijk')\psi_{k'}^{(\gamma')t} \tag{2.22}$$

Hence

$$(\phi_k^{(\gamma)}, S_i^{(\alpha)}\phi_j(\beta)) = \sum_t C(\alpha\beta\gamma t, ijk)(\phi_k(\gamma), \psi_k^{(\gamma)t}) \tag{2.23}$$

This equation has far reaching consequences.

1. If (γ) does not appear in Clebsch-Gordan series of $(\alpha) \otimes (\beta)$, the matrix element in Equation 2.23 vanishes.

2. If the group is simply reducible (i.e. there is no summation over t, which means that in the Equation 2.18 of Clebsch-Gordan series $n_\gamma = 1$ for all γ), then

$$(\phi_k^{(\gamma)}, S_i^{(\alpha)}\phi_j^{(\beta)}) = C(\alpha\beta\gamma, ijk)\langle\phi^{(\gamma)}||S^{(\alpha)}||\phi^{(\beta)}\rangle$$

where $\langle\phi^{(\gamma)}||S^{(\alpha)}||\phi^{(\beta)}\rangle = (\phi_k^{(\gamma)}, \psi_k^{(\gamma)})$ (it can be shown that this reduced matrix element is independent of k). The importance of this separation is that the i, j, k dependence is all in the Clebsch-Gordan coefficient.

2.5 Projection Operators

We are interested in representation theory so that we can construct wavefunctions which transform according to particular representations of the symmetric group[21]. For construc-

[21]While projection operators can be constructed for Lie groups like $SU(2)$, it is not common to do so in a course in quantum mechanics [98]. Hence in this section we will not try and make the connection to angular momentum algebra.

tion of these wavefunctions, projections operators are very useful e.g. given any function of f of x, y, using $P = \frac{(e)+(12)}{2}$ or $P = \frac{(e)-(12)}{2}$, we can symmetrize it by considering $g(x, y) = \frac{f(x,y)+f(y,x)}{2}$ and antisymmetrize it by considering $h(x, y) = \frac{f(x,y)-f(y,x)}{2}$.

We first define the generalization of these operators to an arbitrary group and then show that the definition is consistent, for $S(2)$, with the naive idea of symmetrization and antisymmetrization.

The projection operators are very simple to construct provided we have representations given in matrix form. Suppose the representation label is κ and $\Gamma^{\kappa}(A_j)$ is the matrix of the group element A_j, the group has n elements and the representation is unitary of dimension d_{κ}. Then the projection operators are defined by

$$\rho^{\kappa}_{kl} = \frac{d_{\kappa}}{n} \sum_{j=1}^{n} (\Gamma^{\kappa}(A_j)_{kl})^* A_j \tag{2.24}$$

These d_{κ}^2 operators are called projection operators. Take any arbitrary function f and define (for fixed l)

$$f^{\kappa}_{kl} = \rho^{\kappa}_{kl} f \tag{2.25}$$

These form a set of partner functions in the irreducible representation Γ^{κ}. By applying all projection operators we get a $d_{\kappa} \times d_{\kappa}$ square array of functions

$$\begin{matrix} f^{\kappa}_{11} & f^{\kappa}_{12} & \cdots & f^{\kappa}_{1d_{\kappa}} \\ f^{\kappa}_{21} & f^{\kappa}_{22} & \cdots & f^{\kappa}_{2d_{\kappa}} \\ \vdots & \vdots & \vdots & \vdots \\ f^{\kappa}_{d_{\kappa}1} & f^{\kappa}_{d_{\kappa}2} & \cdots & f^{\kappa}_{d_{\kappa}d_{\kappa}} \end{matrix}$$

The functions in any one single column form a set of partners in Γ^{κ}. However different columns may not be independent nor do they need to be non-vanishing. In fact for certain functions the entire array can vanish, signifying that the particular function has no "component" corresponding to the particular irreducible representation.

2.5.1 Projection operators for $S(2)$

$S(2) = \{e, (12)\}$ is a very simple group. A moment's reflection shows that it can have only two irreducible representations and they are both 1-dimensional i.e the "symmetric" and "sign". In the "symmetric" representation both elements get mapped to 1, and for the "sign" representation e gets mapped to 1 and (12) gets mapped to -1. The matrix of the symmetric representation (it is merely a number since it is a 1-dimensional representation) is

- (1) for e (identity permutation)
- (1) for (12) (exchange permutation)

The matrix of the sign representation is

- (1) for e
- (-1) for (12)

So from the definition of projection operators we conclude that

$$\rho_{sym} = \frac{e + (12)}{2}$$
$$\rho_{sign} = \frac{e - (12)}{2}$$

Hence $\frac{f(x,y)+f(y,x)}{2}$ and $\frac{f(x,y)-f(y,x)}{2}$ are the components that transform according to the symmetric and sign representations of $S(2)$. So we can see that when we were naively constructing our two-particle wavefunctions, we were actually using projection operators.

Chapter 3

Representation Theory Of $S(n)$ and $SU(2)$

The previous chapter was mainly devoted to learning a language to describe representations. In this chapter, we will specifically learn about the *symmetric group*, $S(n)$, and the *special unitary group*, $SU(2)$. These groups play a crucial role in the construction of the wavefunctions. Our goal is not to try and prove the well-known facts about representations of $S(n)$[1] and $SU(2)$, but to get some understanding of the important theorems by looking at a few simple examples.

Before we begin our discussion, let us summarize some relevant facts about the irreducible representations of $SU(2)$. We already know from quantum mechanics that

1. j (integer and half-integer) labels all the irreducible representations of SU(2).
2. Each basis vector has two labels, namely j and m, to identify it[2].
3. The combined label (j, m), uniquely identifies each basis vector in the irreducible representation.

[1]For applications to Hagelstein's models we only need results for the three-body and four-body cases. So wherever convenient, we will limit our discussion to $S(3)$ and $S(4)$.

[2]This is possible because $U(1) \subset SU(2)$ ($U(1)$ in this context means matrices of the form $e^{i\theta}I$ where I is the identity), and every irreducible representation of $SU(2)$, decomposes into a reducible representation of $U(1)$. The $U(1)$ representations are labeled by m.

4. The angular momenta can be coupled using the "vector model" for angular momentum addition. In group theory language, it means that we know the CG series for $SU(2)$.

5. The CG coefficients can be easily calculated using standard formulas.

6. For two particles there is a curious link between symmetry under permutations and total spin, i.e. the symmetric spin wavefunction corresponds to $S = 1$ and the anti-symmetric wavefunction corresponds to $S = 0$.

From our experience with quantum mechanics, we also know that all these properties prove to be extremely useful in various calculations. Since, for the construction of the wavefunctions, we have to deal with $S(n)$, we would hope that its irreducible representations also satisfy similar properties. Luckily it does indeed turn out to be true, and we will find that

1. There is a pictorial way to label all the irreducible representations of $S(n)$. These are called *Young diagrams*.

2. Using $S(1) \subset S(2) \subset \ldots S(n-1) \subset S(n)$, we can get labels for our basis vectors. These are called the *Yamanouchi symbols*.

3. The Young diagrams and the Yamanouchi symbols together uniquely identify each basis vector in the irreducible representation[3].

4. There are general formulas for the CG series of $S(n)$. Since these results are not relevant to us, we merely quote the formulas for the CG series of $S(3)$ and $S(4)$.

5. The values of the CG coefficients are known. Since we merely want to use these coefficients in our calculations, we refer the reader to various tables of CG coefficients in the literature.

6. There is a deep connection between representations of $S(n)$ and $SU(2)$ called the Schur-Weyl duality[4].

[3]In fact it will turn out that we do not need the Young diagram explicitly, since the Yamanouchi symbols contain within them the information required to reconstruct the Young diagram.

[4]This relationship between the representations of $S(n)$ and $SU(m)$ is a rich and beautiful subject involving symmetric functions, combinatorics and Lie theory. The interested reader should consult [30, 31].

This chapter is intended to give the reader some understanding of these properties, so that in the next chapter we can use them to construct our nuclear wavefunctions.

Finally, the notation used to denote permutations should be mentioned. Permutations in $S(n)$ will be denoted in cycle notation where e.g. $(1, 3, 5)(2, 4)$ means that under a permutation particle 1 goes to particle 3, particle 3 to particle 5, particle 5 to particle 1, particle 2 to particle 4 and particle 4 to particle 2. Similarly $(1, 2, 3)$ means that particle 1 goes to particle 2, particle 2 to particle 3 and particle 3 to particle 1.

3.1 The Symmetric Group and Construction of Wavefunctions

Our interest is in few-body nuclear systems. According to standard nuclear physics, the proton and neutron are considered to be the "same" particle, but with a different z-directed isospin. Hence, all the few-body nuclear systems will consist of identical fermions. This means that $S(n)$ commutes with the Hamiltonian H. From our general discussion of irreducible representations of $SO(3)$, we know that

- The eigenfunctions can be labeled by the irreducible representations of $S(n)$.
- The degeneracy is at least equal to the dimension of the representation.

So in principle, eigenfunctions could be labeled by any representation of the symmetric group. However, by the Pauli exclusion principle, for fermions, only the "sign", and for bosons, only the "trivial" representation is allowed. Thus in this case, representation theory does not seem to give us particularly useful information.

However, representation theory does become interesting, once we start to think about constructing wavefunctions. There is no Pauli exclusion principle operating on the individual space, spin or isospin pieces. So long as the overall wavefunction is antisymmetric, the space, spin and isospin parts are free to belong to any representation of $S(n)$. We can then use CG coefficients to construct an overall antisymmetric wavefunction.

But first we need to state some important properties of the representations of the symmetric group.

3.2 Representation Theory of the Symmetric Group

Given any function $f(1, 2)$, it can be broken up into a symmetric part and an antisymmetric part i.e.

$$f(1,2) = \frac{f(1,2) + f(2,1)}{2} + \frac{f(1,2) - f(2,1)}{2}$$

Hence we can conclude that the symmetric group only has the *trivial* and the *sign* representations. However, when we are dealing with more than two particles, the results are not obvious. To proceed further, we need to know certain facts about the symmetric group.

Representation theory of the symmetric group has a venerable history [41, 80, 100] and is still actively pursued in the mathematics literature [96]. The amazing property of the symmetric group is that all the representations can be enumerated in a very simple way. This enumeration is important for us, since we want to write down a complete set of wavefunctions in our Hilbert space. It can most easily be done via the graphical method of *Young diagrams*. Even after the enumeration, we will need some convenient labels for our basis vectors of the vector space (which carries the irreducible representation). These will be the *Yamanouchi symbols*.

3.2.1 Young diagrams

Consider a *partition* of n i.e. $\lambda_1 \geq \lambda_2 \geq \ldots \lambda_n \geq 0$ such that $\lambda_1 + \lambda_2 + \ldots \lambda_n = n$. These can be denoted by *Young diagrams*. These diagrams are just a graphical way of representing partitions, e.g. for $n = 8$, if $\lambda_1 = 3, \lambda_2 = 2, \lambda_3 = 2, \lambda_4 = 1$, we can picturize it as  .

The amazing fact is that the Young diagrams, which partition n, label all the inequivalent irreducible representations of $S(n)$ e.g. for $S(2)$ the two irreducible representations are (trivial representation) and (sign representation).

We will need the enumeration for $S(3)$ and $S(4)$.

- For $S(3)$ we have  ,  and  .
- For $S(4)$ we have , , , and .

3.2.2 Yamanouchi symbols

There is a simple way to calculate the dimension d_η of the representation $\Gamma^{(\eta)}$ labeled by a Young diagram η. First a *tableau* is simply a Young diagram with entries (allowing repeats in general) in $1, 2, \ldots, n$. A *standard tableau* is a tableau in which the numbers increase from left to right in a row and from top to bottom in a column. A *normal tableau* is a standard tableau in which the numbers increase as one goes from left to right, starting out at the top of the diagram and going towards the bottom[5]. Then d_η is simply the number of standard tableau corresponding to the Young diagram η.

The labeling of the d_η basis vectors of an irreducible representation of $S(n)$ is obtained by looking at the chain of groups $S(1) \subset S(2) \ldots \subset S(n-1) \subset S(n)$ i.e. given an irreducible representation of $S(n)$, we break it up (in general) into a linear combination of irreducible representations of $S(n-1)$ and so on till we get to $S(1)$. This way we get a *unique* label for each of our basis vectors of the irreducible representation of $S(n)$. This label is called the *Yamanouchi symbol.* It is simply the symbol $[r_n r_{n-1} \ldots r_1]$ where r_i is the row of i in the standard tableau corresponding to the basis vector[6]. The vectors labeled by the Yamanouchi symbol have the property that they are always symmetric or antisymmetric under the exchange of the first two particles. This will later on turn out to be very useful in the calculation of the matrix elements.

3.2.3 Enumeration of Yamanouchi symbols

For $n = 3$, we have three representations.

[5]Hence for each Young diagram there is only one unique normal tableau.

[6]Sometimes we will ignore the brackets around the Yamanouchi symbol and write it as $r_n r_{n-1} \ldots r_1$.

-  . It is 1-dimensional with basis vector [111]. This is the trivial or symmetric representation.

-  . It is 2-dimensional with basis vectors [211] and [121][7]. This is the mixed representation.

-  . It is 1-dimensional with basis vector [321]. This is the antisymmetric or sign representation.

For $n = 4$, there are five representations.

-  . It is 1-dimensional with basis vector [1111]. This is the trivial representation.

-  . It is 3-dimensional with basis vectors [2111], [1211], [1121].

-  . It is 2-dimensional with basis vectors [2211] and [2121].

-  . It is 3-dimensional with basis vectors [3211], [3121] and [1321].

-  . It is 1-dimensional with basis vector [4321]. This is the antisymmetric or sign representation.

To construct our wavefunctions, we will be considering linear combinations of direct product of wavefunctions which transform according to particular representations of $S(n)$. For this we need to know the CG series of $S(n)$.

3.2.4 Clebsch-Gordan series of $S(n)$

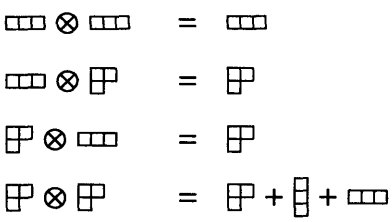
The CG series of $S(n)$ are known. However, we only need some [8] of the CG series for $S(3)$ and $S(4)$.

The required results for $S(3)$ are

[7]Here [211] is a normal tableau, whereas [121] is a standard tableau.

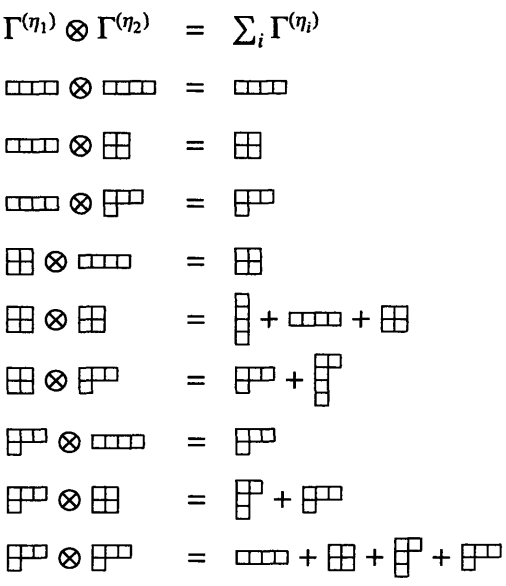
[8]Since we will also be dealing with representations of $SU(2)$, we will see that this interaction restricts the Young diagrams to two rows only.

$$\Gamma^{(\eta_1)} \otimes \Gamma^{(\eta_2)} = \sum_i \Gamma^{(\eta_i)}$$



And for $S(4)$ the useful results are

$$\Gamma^{(\eta_1)} \otimes \Gamma^{(\eta_2)} = \sum_i \Gamma^{(\eta_i)}$$



3.2.5 Clebsch-Gordan coefficients of $S(n)$

As we know from experience with quantum mechanics, the CG coefficient problem is always much harder than the CG series problem. The main reason for this is that while the series is independent of a basis, for the calculation of the CG coefficients, we have to choose a basis[9], and basis-dependent calculations are always tedious. As is true for the CG coefficients of any group, we also have to deal with the annoying but important question of phases.

Hamermesh [41] did important and fundamental work on the CG coefficients. Schindler and Mirman [87, 88, 89] explicitly worked out the CG coefficients for general $S(n)$. How-

[9]By definition it is the matrix for a change of basis.

	[211].[211]′	[211].[121]′	[121].[211]′	[121].[121]′
[321]	0	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$	0
[211]	$\frac{1}{\sqrt{2}}$	0	0	$-\frac{1}{\sqrt{2}}$
[121]	0	$-\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$	0
[111]	$\frac{1}{\sqrt{2}}$	0	0	$\frac{1}{\sqrt{2}}$

Table 3.1: CG coefficients of $S(3)$

ever, their results are numerical and do not implement phase conventions rigorously. Later on the subject was extensively studied by Jin-Quan Chen and others [13, 14, 32]. Unlike Schindler and Mirman, they were much more careful about the phase conventions. Another improvement over the previous work was, that instead of numerical tables, their results were given in terms of square roots of simple rational numbers. However as pointed out by Stancu and Pepin [95], there are some phase-related discrepancies in these tables as well . We will be using the tables from [94, 95]. The tables are too large to be reproduced here and the reader can easily find these in the references cited. However, to give a feel for how to use these CG coefficients we reproduce Table 3.1 from Hamermesh [41] for $S(3)$. And now we go through an example to illustrate how to use Table 3.1.

An example on the use of CG coefficients

Suppose we are given two functions which transform according to the $\ydiagram{2,1}$ representation of $S(3)$ and we want to construct a function which transforms according to the $\ydiagram{1,1,1}$ representation. Table 3.1 shows that we can construct such a vector. It is obtained by taking the linear combination

$$[321] = \frac{1}{\sqrt{2}}\left([211] \otimes [121]' - [121] \otimes [211]'\right) \tag{3.1}$$

Similarly if we want to construct a totally symmetric function from mixed symmetry functions, Table 3.1 tells us that[10]

$$[111] = \frac{1}{\sqrt{2}}\left([211].[211]' + [121].[121]'\right)$$

[10]As mentioned before, sometimes we will not write the $\otimes$ symbol.

transforms according to the ⊡⊡ representation.

This example will be the canonical way that we will construct our antisymmetric wavefunctions. In the construction of the wavefunctions we will particularly be interested in the sign representation, since our wavefunctions have to be completely antisymmetric. We would like to know when does the tensor product of two irreducible representations contain the sign representation. The answer is given by the following lemma

Lemma. $\rho^{(\alpha)} \otimes \rho^{(\beta)}$ contains the sign (antisymmetric) representation if and only if (β) is conjugate to (α) (Conjugate representation is constructed by flipping the Young diagram about its diagonal e.g. is conjugate to). In fact we can say that

$$|(1^n)[n, n-1, \ldots, 1]\rangle = \sqrt{\frac{1}{d_\alpha}} \sum_{[Y]} (-1)^{(n_Y^\alpha)} |(\alpha)[Y]\rangle \otimes |(\tilde{\alpha})[\tilde{Y}]\rangle$$

where (1^n) is the completely antisymmetric Young diagram with the Yamanouchi symbol $[n, n-1, \ldots, 1]$, n_Y^α is the number of transpositions necessary to bring the standard tableau, $[Y]$, to a normal tableau and d_α is the dimension of the irreducible representation, (α). $(\tilde{\alpha})$ and $\left[\tilde{Y}\right]$ are the conjugate Young diagram and Yamanouchi symbol to (α) and $[Y]$ respectively.

This lemma gives us another way to verify Equation 3.1 because we know that

- () is a two-dimensional representation.
- is conjugate to itself.
- [211] is a normal tableau conjugate to [121].
- [121] requires one transposition to become the normal tableau [211].

3.3 Representations of $SU(2)$

We already know all the representations of $SU(2)$ from quantum mechanics[11]. These are labeled by one quantum number, i.e. the angular momentum (integer and half-integer). For our multi-particle states, we will construct wavefunctions in which each particle has spin (or isospin) = $\frac{1}{2}$. Such states can easily be constructed using the standard techniques of CG coefficients of $SU(2)$. However, this would hide the symmetry properties of the wavefunctions. Hence we should look at this problem from the purely group-theoretical point of view of chapter 2.

We will use the spin space as the carrier space for the representations (isospin is completely equivalent). Let $\phi_1 = \uparrow$, and $\phi_2 = \downarrow$, be the basis of the 2-dimensional representation of $SU(2)$ (corresponding to $S = \frac{1}{2}$).

Since an n-particle system is under consideration, we are interested in the vector space T_2^n spanned by all tensors of the form $\Phi = \phi_i(1)...\phi_p(n)$, when the subscripts are all 1 or 2. This vector space has dimension 2^n. From chapter 2, we know that since the space spanned by ϕ_1 and ϕ_2 forms a representation of $SU(2)$, T_2^n also forms a representation of $SU(2)$. But this is in general reducible. The entire space T_2^n can be decomposed into independent subspaces of type $((\eta), m)$ where η is a Young diagram labeling an irreducible representation of $S(n)$ and $1 \leq m \leq d_\eta$ [12] i.e.

$$T_2^n = \sum_\eta \sum_{m=1}^{d_\eta} T_2^{(\eta),m} \tag{3.2}$$

where each subspace $T_2^{(\eta),m}$ is an irreducible representation of $SU(2)$.

3.4 Schur-Weyl Duality

Equation 3.2 is extremely important for the following reasons

- Each subspace $T_2^{(\eta),m}$ is an irreducible representation of $SU(2)$.

[11] The notation and discussion in this and the following section closely follow [24].

[12] In fact in this way we get all the irreducible representations of $SU(2)$.

- Given any basis function of the $T_2^{(\eta),m}$, say $T_2^{(\eta),1}$, it partners with basis functions in $T_2^{(\eta),2}, \ldots, T_2^{(\eta),d_\eta}$ to form a d_η-dimensional representation of $S(n)$.

- The subspace

$$T_2^{\eta} = \sum_{m=1}^{d_\eta} T_2^{(\eta),m} \tag{3.3}$$

  is invariant under $S(n) \times SU(2)$. We can find basis vectors $\phi_{tx}^{(\eta)}$ of $T^{(\eta)}$ s.t. if $\mu(\eta)$ is the dimension of $T_2^{(\eta),m}$, then we can think of these as forming a matrix

$$\begin{matrix} \Phi_{11}^{\eta} & \Phi_{12}^{\eta} & \ldots & \Phi_{1\mu(\eta)}^{\eta} \\ \Phi_{21}^{\eta} & \Phi_{22}^{\eta} & \ldots & \Phi_{2\mu(\eta)}^{\eta} \\ \vdots & \vdots & \vdots & \vdots \\ \Phi_{d_\eta 1}^{\eta} & \Phi_{d_\eta 2}^{\eta} & \ldots & \Phi_{d_\eta \mu(\eta)}^{\eta} \end{matrix}$$

  where each row forms an irreducible representation of $SU(2)$ and each column an irreducible representation of $S(n)$.

This is the beautiful duality between $SU(2)$[13] and $S(n)$. The following facts will be useful for us:

1. The dimension $\mu(\eta)$ of the irreducible representation corresponding to the Young diagram (η) is equal to the number of different *permissible* ways of placing n integers from the set $\{1, 2\}$ in the diagram (η). By a permissible way we mean that integers are in non-decreasing order in a row (from left to right) and strictly increasing as we go down a column.

2. One immediate corollary of the above fact is that for $SU(2)$ we do not need to consider any Young diagram with more than two rows.

All this may seem a bit abstract, so we now go through a few simple examples to make these results concrete.

[13] In general it is between $SU(m)$ and $S(n)$.

3.4.1 Examples of Schur-Weyl duality

Let us consider some simple examples to clarify the concepts. For $n = 2$, T_2^n is 4-dimensional. The product wavefunctions are $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$. The irreducible representations of $S(2)$ are labeled by $\eta_1 = \square\square$ and $\eta_2 = \begin{smallmatrix}\square\\\square\end{smallmatrix}$. They are both 1-dimensional. Then

$$T_2^{\eta_1} : \quad |\uparrow\uparrow\rangle \quad \frac{|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle}{\sqrt{2}} \quad |\downarrow\downarrow\rangle$$

and

$$T_2^{\eta_2} : \quad \frac{|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle}{\sqrt{2}}$$

For $n = 3$, T_2^n is 8-dimensional. We know that there are 3 irreducible representations denoted by $\begin{smallmatrix}\square\\\square\\\square\end{smallmatrix}$, $\begin{smallmatrix}\square\square\\\square\end{smallmatrix}$ and $\square\square\square$. The last one is ruled out by fact 2 of the last subsection. $\eta_1 = \square\square\square$ is 1-dimensional as a representation of $S(3)$ (the trivial representation). However, from fact 1 of last subsection we know that as a representation of $SU(2)$ it is 4-dimensional. This is the $S = \frac{3}{2}$ representation with

$$T_2^{\eta_1} : \quad |\uparrow\uparrow\uparrow\rangle \quad \frac{1}{\sqrt{3}}(|\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\uparrow\rangle + \downarrow\uparrow\uparrow\rangle) \quad \frac{1}{\sqrt{3}}(|\uparrow\downarrow\downarrow\rangle \downarrow\uparrow\uparrow\rangle + \downarrow\downarrow\uparrow\rangle) \quad |\downarrow\downarrow\downarrow\rangle$$

Let $\eta_2 = \begin{smallmatrix}\square\square\\\square\end{smallmatrix}$. As a representation of $S(3)$, it is 2-dimensional. From fact 1 of the last subsection we know that as a representation of $SU(2)$, it is also 2-dimensional and $T_2^{\eta_2}$ is given by

$$\begin{array}{cc} \frac{2|\uparrow\uparrow\downarrow\rangle-|\uparrow\downarrow\uparrow\rangle-|\downarrow\uparrow\uparrow\rangle}{\sqrt{6}} & \frac{2|\downarrow\downarrow\uparrow\rangle-|\downarrow\uparrow\downarrow\rangle-|\uparrow\downarrow\downarrow\rangle}{\sqrt{6}} \\ \frac{|\uparrow\downarrow\uparrow\rangle-|\downarrow\uparrow\uparrow\rangle}{\sqrt{2}} & \frac{|\downarrow\uparrow\downarrow\rangle-|\uparrow\downarrow\downarrow\rangle}{\sqrt{2}} \end{array}$$

Each column forms a $\begin{smallmatrix}\square\square\\\square\end{smallmatrix}$ representation of $S(3)$ and each row forms a $\begin{smallmatrix}\square\square\\\square\end{smallmatrix}$ representation of $SU(2)$. Schur-Weyl duality for two and three-particle spin wavefunctions, is also illustrated in Figure 3-1.

Before we end this chapter, we want to discuss how the symmetric group operates on multi-particle wavefunctions. This will become important when we construct wavefunctions in the next chapter. There, the symmetric group will be acting on wavefunctions, for which

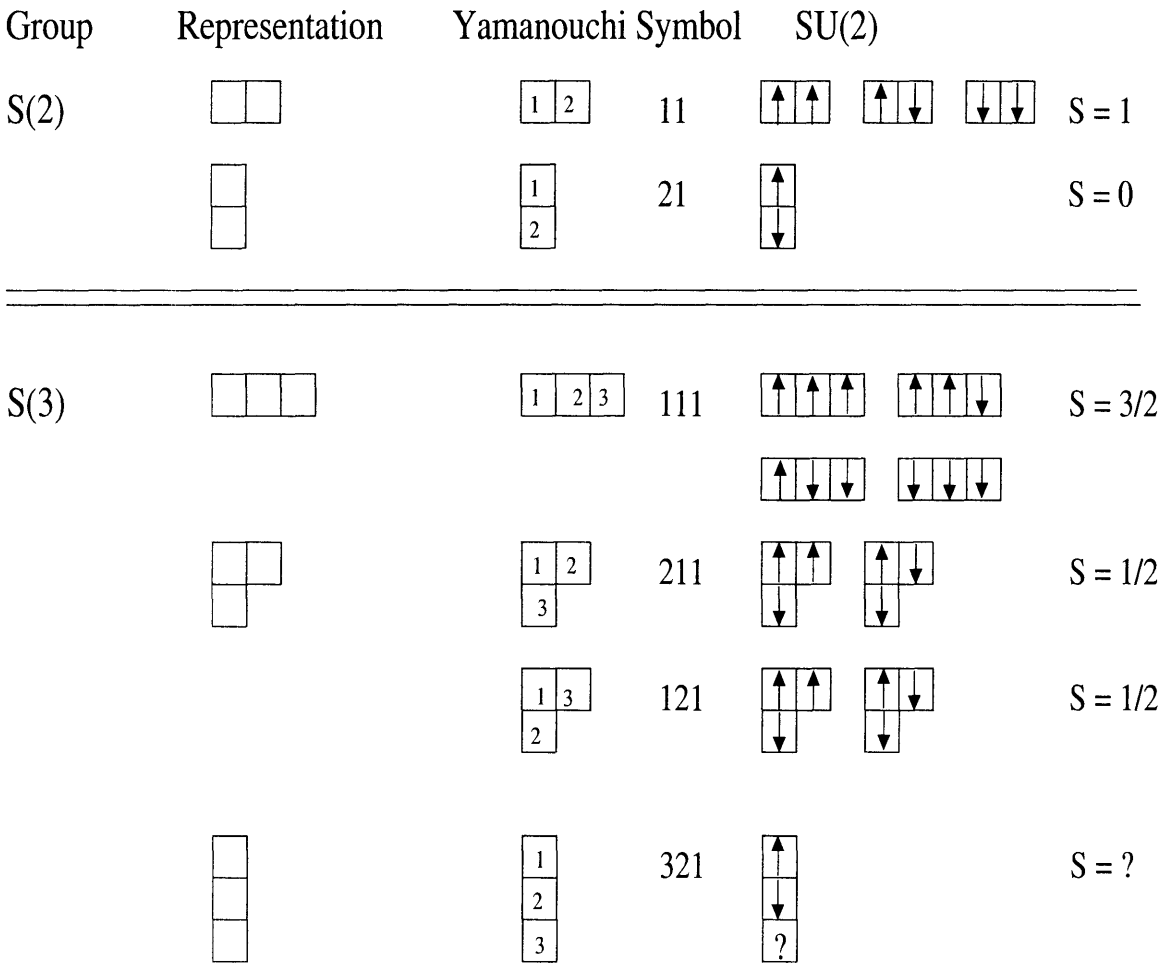


Figure 3-1: Schur-Weyl Duality

we need to fix a convention.

3.5 Action of the Symmetric Group on Many-Particle Functions

There are two standard ways that one can make the symmetric group act on a function, i.e. it can be a left action or a right action. We assume that it is a left action and the group acts directly on the particle labels e.g. $(12)f(132) = f(231)$. That this is a group homomorphism (it has to be, since that is how elements in the group algebra act) can be explicitly checked, e.g. since $(123) = (12) \circ (23)$ then

$$\begin{aligned} (23)f(213) &= f(312) \\ (12)f(312) &= f(321) \\ (123)f(213) &= f(321) \end{aligned}$$

When considering spin or isospin, we want to follow the same conventions as for the spatial wavefunctions. Consider $f(123) = \alpha(1)\beta(2)\gamma(3)$. Then according to our convention

$$\begin{aligned} (123)\alpha(1)\beta(2)\gamma(3) &= \alpha(2)\beta(3)\gamma(1) \\ (123)\alpha(2)\beta(3)\gamma(1) &= \alpha(3)\beta(1)\gamma(2) \end{aligned}$$

Now consider spin up and spin down as functions of particle labels. Say

$$\alpha(1) = \uparrow_1 \quad \beta(2) = \downarrow_2 \quad \gamma(3) = \uparrow_3$$

with $f(123) = \alpha(1)\beta(2)\gamma(3)$. Then

$$\begin{aligned}(123)f(123) &= \alpha(2)\beta(3)\gamma(1)\\ (123)f(231) &= \alpha(3)\beta(1)\gamma(2)\\ (132)f(123) &= \alpha(3)\beta(1)\gamma(2)\end{aligned}$$

Since $(123) \circ (123) = (132)$, we can see that everything is consistent.

Note that this convention is in accord with the usual left action of the symmetric group on the tensor space by inverse of the group element, i.e. usually we say that

$$\sigma(v_1 \otimes v_2 \otimes v_3) = v_{\sigma^{-1}(1)} \otimes v_{\sigma^{-1}(2)} \otimes v_{\sigma^{-1}(3)}$$

Using $\sigma = (123)$ and $v_1 = \uparrow$, $v_2 = \downarrow$ and $v_3 = \uparrow$, we can see that

$$(123)(v_1 \otimes v_2 \otimes v_3) = v_3 \otimes v_1 \otimes v_2 = \uparrow\uparrow\downarrow$$

exactly as before.

Chapter 4

Construction Of The Wavefunctions

The previous two chapters discussed aspects of group theory most relevant for us. Now, we can begin to apply representation theory for the construction of wavefunctions. Before we outline our method, we would like to discuss why is it completely natural to use group theory to construct few-body wavefunctions. The reason is based on the following facts:

- The overall nuclear wavefunction has to belong to the antisymmetric representation of $S(n)$.
- The various channels in a nuclear reaction are specified by spin, isospin and other relevant quantum numbers. Specifying spin and isospin implies constraining the $SU(2)$ representation that the spin/isospin wavefunction can belong to.
- Schur-Weyl duality links the representations of $S(n)$ and $SU(2)$.

This argument is schematically presented in Figure 4-1.

Our method will be to use [1]

1. Projection operators to construct space, spin and isospin wavefunctions which transform according to particular representations of $S(n)$.

[1] Similar ideas are used in the literature for multi-quark calculations [42, 93].

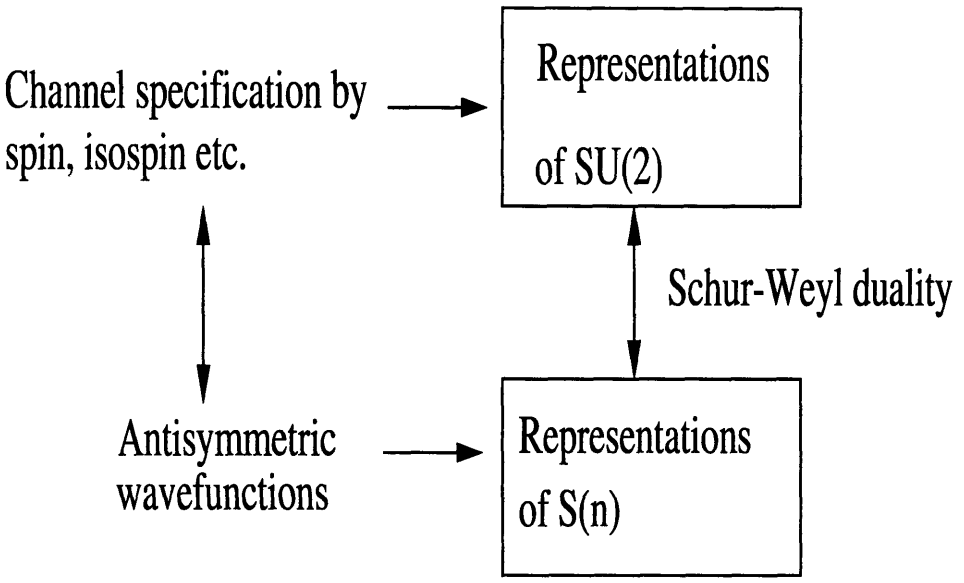


Figure 4-1: Reasons for using group theory for the construction of wavefunctions

2. CG coefficients of $S(n)$ to construct the appropriate linear combinations of space, spin and isospin to form a completely antisymmetric wavefunction.

In this chapter, we also describe a new method, of constructing spin or isospin wavefunctions of the appropriate symmetry. This method, which is based on angular momentum addition, is far simpler as compared to earlier techniques [85].

In order to elucidate the principles involved, we will exclusively deal with the three-body nuclear case [20]. While a completely similar calculation can be carried out for the four-body problem, this is computationally much more complicated, and does not involve any significant new concepts. However, to establish the form of the wavefunctions and our notation, we will begin by looking at the familiar two-body example. After that we will explicitly construct the projection operators for $S(3)$ and use them to build the wavefunctions of the appropriate symmetry. At the end of this chapter, with the help of CG coefficients, we will construct the completely antisymmetric wavefunctions.

Spin	⇒	*Space*
Symmetric	⇒	Antisymmetric
Antisymmetric	⇒	Symmetric

Table 4.1: Symmetry constraints on two-body atomic wavefunctions

4.1 Two-electron System

This is the simplest example in which we see the CG coefficients at work. The coefficients are 1, so the calculation is trivial[2].

The construction of product wavefunctions for two-electron systems is a standard topic in quantum mechanics textbooks. It is based on the *Pauli exclusion principle*, which as shown in Table 4.1, imposes stringent constraints on the wavefunction.

If we denote $m_S = \frac{1}{2}$ by α, $m_S = -\frac{1}{2}$ by β then the actual wavefunctions are

$$\text{spin symmetric} = \begin{cases} \alpha(1)\alpha(2) \\ \frac{1}{\sqrt{2}}\{\alpha(1)\beta(2) + \beta(1)\alpha(2)\} \\ \beta(1)\beta(2) \end{cases}$$

$$\text{spin antisymmetric} = \frac{1}{\sqrt{2}}\{\alpha(1)\beta(2) - \beta(1)\alpha(2)\}$$

$$\text{space symmetric} = \frac{f(r_1, r_2) + f(r_2, r_1)}{2}$$

$$\text{space antisymmetric} = \frac{f(r_1, r_2) - f(r_2, r_1)}{2}$$

The complete wavefunction is constructed by taking appropriate products e.g.

[2]Please note that we are talking about the CG coefficients of the $S(2)$ and not the usual CG coefficients of angular momentum addition.

$$\alpha(1)\alpha(2)\frac{f(r_1, r_2) - f(r_2, r_1)}{2}$$

Please note that this is not normalized since $\frac{f(r_1,r_2)-f(r_2,r_1)}{2}$ cannot be normalized until we know the form of the $f(\cdot)$. This inability to normalize will be a constant feature of this construction. However, this is not a serious drawback, since any given spatial wavefunction can be normalized. The next simple system we consider is the two-nucleon system. However, before deriving its wavefunction, we need to summarize some properties of isospin.

4.2 Isospin

The concept of isospin was introduced by Heisenberg [43]. The Coulombic interaction between protons is much weaker than the strong force between two nucleons. Hence we can ignore the Coulombic part of the interaction. This is also reflected in the fact that many of the properties of *mirror nuclei* are very similar . Mirror nuclei are nuclei which have the same total number of protons and neutrons e.g. ^3He and ^3H. Thus we can postulate that the strong nuclear force does not distinguish between protons and neutrons[3]. Nucleons are then assigned an extra degree of freedom called *isospin* and the protons and neutrons are considered the same particle, but with different z-directed isospin. We will only be interested in some formal properties of isospin, which we summarize here.

- Formally isospin is the same as spin. So all the usual spin algebra works in the case of isospin as well.
- The proton is represented by $\uparrow$ with $M_T = \frac{1}{2}$
- The neutron is represented by $\downarrow$ with $M_T = -\frac{1}{2}$.
- Nuclear reactions mediated by the strong force conserve T and M_T[4].

[3] Actually there is a difference between *charge symmetry* and *charge independence* [16].
[4] Isospin is not conserved by electromagnetic or weak interactions [91].

Spin	*Isospin*	⇒	*Space*
Symmetric	Symmetric	⇒	Antisymmetric
Symmetric	Antisymmetric	⇒	Symmetric
Antisymmetric	Symmetric	⇒	Symmetric
Antisymmetric	Antisymmetric	⇒	Antisymmetric

Table 4.2: Symmetry constraints on two-body nuclear wavefunctions

While we will only be using these properties, the concept of isospin is very useful in particle and nuclear physics and allows important predictions to be made in scattering/decay experiments [33].

4.3 Two-nucleon System

The construction of the two-particle nuclear wavefunctions takes places in a completely analogous manner to the two-electron case except that we include isospin. The Generalized Pauli Exclusion Principle states that the total wavefunction (including isospin) has to be antisymmetric under the exchange of any two particles. Hence the wavefunctions have the symmetry requirements as given in Table 4.2.

If we denote $m_S = \frac{1}{2}$ by α, $m_S = -\frac{1}{2}$ by β, $m_T = \frac{1}{2}$ by μ, $m_T = -\frac{1}{2}$ by ν, then the explicit wavefunctions are

$$\text{spin symmetric} = \begin{cases} \alpha(1)\alpha(2) \\ \frac{1}{\sqrt{2}}\{\alpha(1)\beta(2)+\beta(1)\alpha(2)\} \\ \beta(1)\beta(2) \end{cases}$$

$$\text{spin antisymmetric} = \frac{1}{\sqrt{2}}\{\alpha(1)\beta(2)-\beta(1)\alpha(2)\}$$

$$\text{isospin symmetric} = \begin{cases} \mu(1)\mu(2) \\ \frac{1}{\sqrt{2}}\{\mu(1)\nu(2)+\mu(2)\nu(1)\} \\ \nu(1)\nu(2) \end{cases}$$

$$\text{isospin antisymmetric} = \frac{1}{\sqrt{2}}\{\mu(1)\nu(2)-\mu(2)\nu(1)\}$$

$$\text{space symmetric} = \frac{f(r_1, r_2)+f(r_2, r_1)}{2}$$

$$\text{space antisymmetric} = \frac{f(r_1, r_2)-f(r_2, r_1)}{2}$$

The complete (unnormalized) wavefunction is constructed by taking appropriate products e.g.

$$\alpha(1)\alpha(2)\frac{1}{\sqrt{2}}\{\mu(1)\nu(2)-\nu(1)\mu(2)\}\frac{f(r_1, r_2)+f(r_2, r_1)}{2}$$

Again, the wavefunction cannot be normalized until we know the explicit form of f. These examples seem completely straight forward, and use no knowledge of group theory. However, as we saw in chapter 2, when we tried to deal with the three-body problem, we encountered some serious difficulties. Now that we have enough theoretical background, we can proceed (with the method outlined at the beginning of the chapter) to write down the wavefunctions. We first need the projection operators for $S(3)$.

4.4 Explicit Three-body Projection Operators

There are three irreducible representations of $S(3)$. Obviously we have the 1-dimensional trivial and sign representations. The trivial representation matrices are all 1 and the sign representation matrices are 1 or -1 depending on the sign of the permutation. We only have to worry about the 2-dimensional mixed representation $\boxplus$.

The matrices in the *Standard Young-Yamanouchi* representation are well known [41, 94]. These are

$$e = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad (12) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad (23) = \begin{pmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$$
$$(13) = \begin{pmatrix} \frac{-1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \quad (123) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \quad (132) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \tag{4.1}$$

The rows and columns are labeled by the Yamanouchi symbols in descending order i.e. they are labeled by [211] and [121]. Now that we have these matrices, we can use them to construct the projection operators easily. For the mixed representation, we get

$$\begin{aligned}
\rho_{11} &= \frac{2}{6}\left[e + (12) - \frac{1}{2}(23) - \frac{1}{2}(13) - \frac{1}{2}(123) - \frac{1}{2}(132)\right] \\
\rho_{21} &= \frac{2}{6}\left[\frac{\sqrt{3}}{2}(23) - \frac{\sqrt{3}}{2}(13) - \frac{\sqrt{3}}{2} + \frac{\sqrt{3}}{2}(132)\right] \\
\rho_{12} &= \frac{2}{6}\left[\frac{\sqrt{3}}{2}(23) - \frac{\sqrt{3}}{2}(13) + \frac{\sqrt{3}}{2}(123) - \frac{\sqrt{3}}{2}(132)\right] \\
\rho_{22} &= \frac{2}{6}\left[e - (12) + \frac{1}{2}(23) + \frac{1}{2}(13) - \frac{1}{2}(123) - \frac{1}{2}(132)\right]
\end{aligned} \tag{4.2}$$

For the trivial representation, we have

$$\rho = \frac{1}{6}\left[e + (12) + (23) + (13) + (123) + (132)\right] \tag{4.3}$$

and for the sign representation

$$\rho = \frac{1}{6}[e + (123) + (132) - (23) - (12) - (13)] \tag{4.4}$$

In the next two sections we will apply these projection operators to space and spin/isospin wavefunctions. It is important to note that since the rows and columns of the matrices in Equation 4.1 are labeled by the Yamanouchi symbol, the projected functions[5] can also be labeled by the Yamanouchi symbol. This can be shown by an explicit computation. The upshot is that by using the projection operators, we directly get the projected functions which can be labeled by [211] or [121] and which transform according to the $\boxplus$ representation of $S(3)$. The labeling depends on the row of the matrix and not on the column.

4.5 Construction of Space Wavefunctions

We know that given any functions f, $\rho_{11}f$ and $\rho_{21}f$ form partners in an irreducible representation (provided it is non-zero). Similarly $\rho_{12}f$ and $\rho_{22}f$ form partners in an irreducible representation (provided it is non-zero). Given an arbitrary function $f(123)$ i.e. a function which depends on the coordinates of the three particles, we can apply the projection operators to get

$$\begin{aligned}
\rho_{11}f(123) &= \frac{2}{6}\left[f(123) + f(213) - \frac{1}{2}f(132) - \frac{1}{2}f(321) - \frac{1}{2}f(231) - \frac{1}{2}f(312)\right] \\
\rho_{21}f(123) &= \frac{2}{6}\left[\frac{\sqrt{3}}{2}\{f(132) - f(321) - f(231) + f(312)\}\right] \\
\rho_{12}f(123) &= \frac{2}{6}\left[\frac{\sqrt{3}}{2}\{f(132) - f(321) + f(231) - f(312)\}\right] \\
\rho_{22}f(123) &= \frac{2}{6}\left[f(123) - f(213) + \frac{1}{2}f(132) + \frac{1}{2}f(321) - \frac{1}{2}f(231) - \frac{1}{2}f(312)\right]
\end{aligned}$$

[5]By projected functions we mean the functions that we get by applying projection operators of Equation 4.2 to a given function.

Using the statement at the end of the last section we can label $\rho_{11}f$ and $\rho_{12}f$ by [211][6]. Similarly $\rho_{21}f$ and $\rho_{22}f$ can be labeled by [121][7]. In this way we see that the projection operators give us the required basis vectors directly.

4.6 Construction of Spin/Isospin Wavefunctions

The construction of spin or isospin wavefunctions is exactly similar because formally the spin and isospin algebra is the same. We will explicitly treat spin, but all the arguments go through in exactly the same way for isospin by replacing "spin up" by "isospin up" and "spin down" by "isospin down" respectively.

Given the $\square\square$ representation of spin, we know from chapter 3, that its total spin is $S = \frac{3}{2}$. We can get all the four wavefunctions by considering the following four spin wavefunctions and applying projection operator of $\square\square$ to them. These are

$$\alpha(1)\alpha(2)\alpha(3),\ \alpha(1)\alpha(2)\beta(3),\ \alpha(1)\beta(2)\beta(3),\ \beta(1)\beta(2)\beta(3)$$

After symmetrization and normalization we get,

$$\begin{aligned}
&\alpha(1)\alpha(2)\alpha(3)\\
&\tfrac{1}{\sqrt{3}}\{\alpha(1)\alpha(2)\beta(3)+\alpha(1)\beta(2)\alpha(3)+\beta(1)\alpha(2)\alpha(3)\}\\
&\tfrac{1}{\sqrt{3}}\{\alpha(1)\beta(2)\beta(3)+\beta(1)\alpha(2)\beta(3)+\beta(1)\beta(2)\alpha(3)\}\\
&\beta(1)\beta(2)\beta(3)
\end{aligned} \tag{4.5}$$

Note that as mentioned in chapter 3, each one of these functions individually forms a 1-dimensional irreducible representation of $S(3)$ and collectively form a 4-dimensional irreducible representation of $SU(2)$; both of these are labeled by $\square\square$.

Similarly we know that the $\begin{smallmatrix}\square\\\square\end{smallmatrix}$ representation has total spin $S = \frac{1}{2}$. To construct the spin

[6]Since both belong to the first row.

[7]Since these belong to the second column.

wavefunctions we use the appropriate projection operators on

$$\alpha(1)\alpha(2)\beta(3),\ \alpha(1)\beta(2)\beta(3)$$

If we apply ρ_{ij} to these functions we get

$$\begin{aligned}
&\tfrac{1}{\sqrt{6}}\{\beta(1)\alpha(2)+\alpha(1)\beta(2)\}\alpha(3)-\sqrt{\tfrac{2}{3}}\alpha(1)\alpha(2)\beta(3)\\
&\tfrac{1}{\sqrt{2}}\{\beta(1)\alpha(2)-\alpha(1)\beta(2)\}\alpha(3)\\
&\tfrac{1}{\sqrt{6}}\{\beta(1)\alpha(2)+\alpha(1)\beta(2)\}\beta(3)-\sqrt{\tfrac{2}{3}}\beta(1)\beta(2)\alpha(3)\\
&\tfrac{1}{\sqrt{2}}\{\beta(1)\alpha(2)-\alpha(1)\beta(2)\}\beta(3)
\end{aligned} \tag{4.6}$$

Again, as mentioned in chapter 3, the first two wavefunctions form a 2-dimensional irreducible representation of $S(3)$ and the last two form another copy of the same 2-dimensional irreducible representation. However wavefunctions 1 and 3 form a 2-dimensional irreducible representation of $SU(2)$ as do wavefunctions 2 and 4. This is the beautiful Schur-Weyl duality at work! As for the spatial case, the Yamanouchi label of a symmetry-adapted basis vector depends on the projection operator that was applied to obtain it i.e. wavefunctions 1 and 3 are labeled by [211] and wavefunctions 2 and 4 are labeled by [121].

However, we have found an easier way, based on angular momentum algebra, to do the same construction for multi-particle spin/isospin wavefunctions.

4.7 Clebsch-Gordan Approach

Note that in this section we are using the CG coefficients of $SU(2)$ i.e. the ones that are routinely taught in a quantum mechanics course. Projection operators are generally useful because they can be applied to any function. However if we are only interested in spin or isospin, we can use a simpler method based on addition of angular momentum.

The Yamanouchi symbol gives us a clue as to the construction of appropriate wavefunctions without the use of the projection operators. The construction of the completely symmetric

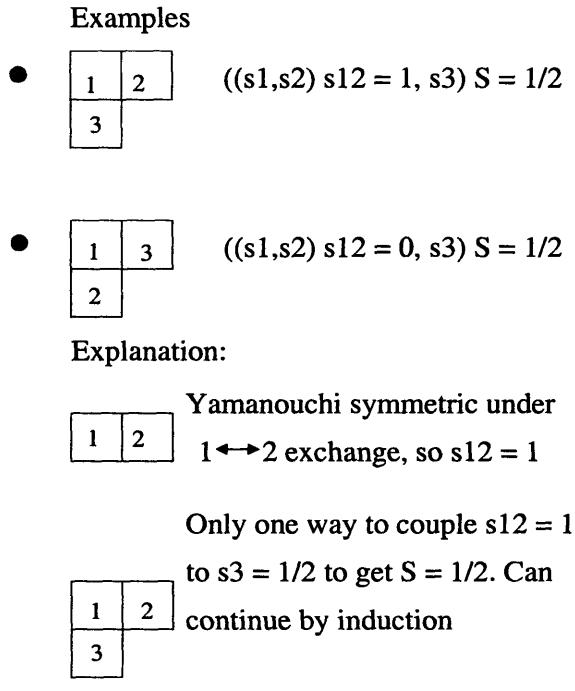


Figure 4-2: Clebsch-Gordan approach to constructing spin/isospin wavefunctions

wavefunction is straightforward via the Clebsch-Gordan approach. One simply couples $j_1 = \frac{1}{2}$ to $j_2 = \frac{1}{2}$ to get $J_{12} = 1$ which in turn is coupled to $j_3 = \frac{1}{2}$ to get a total $J = \frac{3}{2}$.

The mixed symmetry representation is a bit more interesting. Consider the spin wavefunction [211]. Particle labels 1 and 2 are in the top row and particle label 3 is in the second row. So it suggests that we should first couple particle 1 to 2 to build a state of $J_{12} = 1$ and then couple $J_{12} = 1$ to $j_3 = \frac{1}{2}$ to get a total $J = \frac{1}{2}$. However in order to construct [121], we couple $j_1 = \frac{1}{2}$ to $j_2 = \frac{1}{2}$ to get a total state of $J_{12} = 0$ which in turn couples to the $j_3 = \frac{1}{2}$ state to get the $J = \frac{1}{2}$ state.

This construction depends on the fact that given a fixed number of particles, there is a one-one correspondence between the Young diagrams and spin of the wavefunctions. This can be generalized to any number of particles e.g. in order to construct the spin wavefunction corresponding to [1211], we couple $j_1 = \frac{1}{2}$ to $j_2 = \frac{1}{2}$ to get $J_{12} = 1$, then couple $J_{12} = 1$ to $j_3 = \frac{1}{2}$ to get $J_{123} = \frac{1}{2}$ and then couple $J_{123} = \frac{1}{2}$ to $j_4 = \frac{1}{2}$ to get a final $J = 1$.

This method is illustrated in Figure 4-2. Now at this point it is still possible that the wavefunctions we get from the projection operators and the ones that we get from the CG ap-

proach may differ by a phase factor. However, in all our calculations, we have found that there is no phase difference between the two approaches. It is also important to point out that this approach will break down for any other special unitary group other than $SU(2)$, because no one-one correspondence exists between Young diagrams and total angular momentum for the higher dimensional unitary groups.

By using either projection operators or the $SU(2)$ (only for spin/isospin) CG coefficients, we can now construct space, spin and isospin wavefunctions with the prescribed symmetry. However, we still need to mix appropriate combinations of these wavefunctions in order to construct a totally antisymmetric wavefunction. This is done via the CG coefficients of the symmetric group.

4.8 Explicit Construction of Wavefunctions

In this section we will use the wavefunction with $S = \frac{1}{2}$ and $T = \frac{1}{2}$ as an example of our method of constructing wavefunctions. We already know that:

1. Both the spin and isospin wavefunctions belong to the $\ydiagram{2,1}$ representation[8]. This is a consequence of Schur-Weyl duality.

2. The relevant CG series is

$$\ydiagram{2,1} \otimes \ydiagram{2,1} = \ydiagram{2} \oplus \ydiagram{2,1} \oplus \ydiagram{1,1}$$

3. From each of $\ydiagram{2}$, $\ydiagram{2,1}$, $\ydiagram{1,1}$, using the conjugate tableau for space, (i.e. $\ydiagram{1,1}$, $\ydiagram{2,1}$, $\ydiagram{2}$ respectively) we can construct three different antisymmetric wavefunctions. This is a consequence of using the lemma in section 3.2.5.

From Table 3.1[9]

[8]We have intentionally not mentioned whether it is a representation of $S(3)$ or $SU(2)$, since from Schur-Weyl duality we know that these functions form a representation under both the groups.

[9]The subscripts of R, S or T on the Yamanouchi symbols tell us which part of the wavefunction we are considering e.g. $[211]_S$ is a spin wavefunction with Yamanouchi symbol [211] where as $[211]_{ST}$ is a spin-isospin wavefunction with Yamanouchi symbol [211].

$$[211]_{ST} = \frac{1}{\sqrt{2}}\{[211]_S[211]_T - [121]_S[121]_T\}$$

$$[121]_{ST} = -\frac{1}{\sqrt{2}}\{[211]_S[121]_T + [121]_S[211]_T\}$$

$$[321]_{ST} = \frac{1}{\sqrt{2}}\{[211]_S[121]_T - [121]_S[211]_T\}$$

$$[111]_{ST} = \frac{1}{\sqrt{2}}\{[211]_S[211]_T + [121]_S[121]_T\}$$

Using Table 3.1 again[10], the antisymmetric wavefunction corresponding to $\square\!\square_{ST}$ is

$$[321]_{RST} = \frac{1}{\sqrt{2}}\{[211]_R[121]_{ST} - [121]_R[211]_{ST}\}$$

The antisymmetric wavefunction corresponding to $\square\square\square_{ST}$ is

$$[321]_{RST} = [321]_R[111]_{ST}$$

And the antisymmetric wavefunction corresponding to $\begin{smallmatrix}\square\\\square\end{smallmatrix}_{ST}$ is

$$[321]_{RST} = [111]_R[321]_{ST}$$

Since in the previous sections we have already constructed basis functions for space, spin and isospin corresponding to [321], [211], [121] and [111] representations, we have now completed our objective of constructing few-body wavefunctions.

For the $S = T = \frac{1}{2}$ case we were considering, the three wavefunctions are (without taking into account the different m_S and m_T values)

[10]Or the lemma in section 3.2.5.

$$\psi = \frac{1}{\sqrt{2}}\{f^1(-\frac{1}{\sqrt{2}})(q^1v^2 + q^2v^1) - f^2(\frac{1}{\sqrt{2}})(q^1v^1 - q^2v^2)\}$$

$$\psi' = f^4(\frac{1}{\sqrt{2}})(q^1v^1 + q^2v^2)$$

$$\psi'' = f^3(\frac{1}{\sqrt{2}})(q^1v^2 - q^2v^1)$$

where

- q is used for spin
- v for isospin
- f for space
- The superscripts on the q's, v's and f's represent the particular Yamanouchi basis vector with

[2 1 1] = 1	mixed symmetry
[1 2 1] = 2	mixed symmetry
[1 1 1] = 3	symmetric part
[3 2 1] = 4	antisymmetric part

Chapter 5

Summary Of Three-body Wavefunctions

This chapter summarizes our results for the construction of the three-body wavefunctions. In some ways, our approach resembles the method initiated by Jahn and others [29, 48, 49] for the shell model. Later on, group theory was applied to various three-body calculations [4, 5, 9, 18, 19, 20, 45, 46, 64, 84, 103]. However, we have not found a completely systematic treatment of the three-body problem in the literature that explicitly treats the symmetry properties of the spatial parts of general wavefunctions. We will first enumerate the possible symmetries of a three-body wavefunction. The CG series of $S(3)$ restricts the wavefunction to the form give in Table 5.1. For example, the last line of Table 5.1 implies that when we tensor a $S = \frac{1}{2}$ representation with $T = \frac{1}{2}$, we get a $2 \times 2 = 4$ dimensional representation of $S(3)$. This breaks up into a 2-dimensional representation  , a 1-dimensional representation  and another 1-dimensional representation  . As we saw in chapter 4, in order to get a totally antisymmetric wavefunction, we need to combine the part with the spatial part (of conjugate symmetry) . This gives us one antisymmetric

spin	*isospin*	=	⇒	*space*
 $S = \frac{3}{2}$	$T = \frac{3}{2}$		⇒	
 $S = \frac{3}{2}$	$T = \frac{1}{2}$		⇒	
$S = \frac{1}{2}$	$T = \frac{3}{2}$		⇒	
$S = \frac{1}{2}$	$T = \frac{1}{2}$		⇒	

Table 5.1: Symmetry constraints on three-body nuclear wavefunctions

wavefunction. We can also combine the $\begin{smallmatrix}\square\\\square\end{smallmatrix}$ with the spatial symmetry $\square\square$ to get another antisymmetric wavefunction. And finally we can combine the $\square\square$ with the spatial symmetry $\begin{smallmatrix}\square\\\square\end{smallmatrix}$ to get the third antisymmetric wavefunction. This exhausts the possibility of constructing antisymmetric wavefunctions from $S = \frac{1}{2}$ and $T = \frac{1}{2}$.

We are also going to label $m_S = \frac{1}{2}$ as α, $m_S = -\frac{1}{2}$ as β, $m_T = \frac{1}{2}$ as μ and $m_T = -\frac{1}{2}$ as ν. Now we explicitly write out the wavefunctions for each of the 4 possible cases (corresponding to each row of the table above). The labeling of the wavefunctions is done according to the standard Yamanouchi method.

5.1 Spin = $\frac{3}{2}$, Isospin = $\frac{3}{2}$

Since spin and isospin are completely symmetric, the spatial part is completely anti-symmetric and it is trivial to write down the wavefunction [1].

5.2 Spin = $\frac{3}{2}$, Isospin = $\frac{1}{2}$

Spin is $\square\square$ and Isospin is $\begin{smallmatrix}\square\square\\\square\end{smallmatrix}$.

$$[321]_{RST} = \frac{1}{\sqrt{2}}\{[211]_R[121]_{ST} - [121]_R[211]_{ST}\}$$

where

$$[121]_{ST} = [111]_S[121]_T$$

$$[211]_{ST} = [111]_S[211]_T$$

[1] It is just a simple product of the usual $S = \frac{3}{2}$ and $T = \frac{3}{2}$ wavefunctions.

5.3 Spin = $\frac{1}{2}$, Isospin = $\frac{3}{2}$

It is clear that, as before

$$[211]_{ST} = [211]_S[111]_T$$

$$[121]_{ST} = [121]_S[111]_T$$

Then we can write down the total wavefunction as

$$[321]_{RST} = \frac{1}{\sqrt{2}}\{[211]_R[121]_{ST} - [121]_R[211]_{ST}\}$$

5.4 Spin = $\frac{1}{2}$, Isospin = $\frac{1}{2}$

$$[321]_{RST} = \frac{1}{\sqrt{2}}\{[211]_R[121]_{ST} - [121]_R[211]_{ST}\}$$

The other two antisymmetric wavefunctions are constructed by

$$[321]_{RST} = [321]_R[111]_{ST}$$

$$[321]_{RST} = [111]_R[321]_{ST}$$

where

$$[211]_{ST} = \frac{1}{\sqrt{2}}\{[211]_S[211]_T - [121]_S[121]_T\}$$

$$[121]_{ST} = -\frac{1}{\sqrt{2}}\{[211]_S[121]_T + [121]_S[211]_T\}$$

[2 1 1] = 1	mixed symmetry
[1 2 1] = 2	mixed symmetry
[1 1 1] = 3	symmetric part
[3 2 1] = 4	antisymmetric part

Table 5.2: Shorthand for three-Particle Yamanouchi symbol

$$[321]_{ST} = \frac{1}{\sqrt{2}}\{[211]_S[121]_T - [121]_S[211]_T\}$$

$$[111]_{ST} = \frac{1}{\sqrt{2}}\{[211]_S[211]_T + [121]_S[121]_T\}$$

5.5 Notation

To simplify the notation, we use q for spin, v for isospin and f for the space part of the wavefunction. The superscripts on the q's, v's and f's represent the particular Yamanouchi basis vector. The shorthand for Yamanouchi symbols is given in Table 5.2.

5.6 Spin Wavefunctions

Let us define spin wavefunctions corresponding to various m_S values and permutation symmetries. We will denote them by $q^a_{m_S}$, where the subscript refers to the value of m_S and the superscript labels the various Yamanouchi basis vectors defined in Table 5.2.

5.6.1 $m_S = \frac{3}{2}$

□□□

$$[111]_{\frac{3}{2}} = q^3_{\frac{3}{2}} = \alpha(1)\alpha(2)\alpha(3)$$

5.6.2 $m_S = \frac{1}{2}$

$$[211]_{\frac{1}{2}} = q^1_{\frac{1}{2}} = \frac{1}{\sqrt{6}}\{\beta(1)\alpha(2) + \alpha(1)\beta(2)\}\alpha(3) - \sqrt{\frac{2}{3}}\alpha(1)\alpha(2)\beta(3)$$

$$[121]_{\frac{1}{2}} = q^2_{\frac{1}{2}} = \frac{1}{\sqrt{2}}\{\beta(1)\alpha(2) - \alpha(1)\beta(2)\}\alpha(3)$$

$$[111]_{\frac{1}{2}} = q^3_{\frac{1}{2}} = \frac{1}{\sqrt{3}}\{\alpha(1)\alpha(2)\beta(3) + \alpha(1)\beta(2)\alpha(3) + \beta(1)\alpha(2)\alpha(3)\}$$

5.6.3 $m_S = -\frac{1}{2}$

$$[211]_{-\frac{1}{2}} = q^1_{-\frac{1}{2}} = \frac{1}{\sqrt{6}}\{\beta(1)\alpha(2) + \alpha(1)\beta(2)\}\beta(3) - \sqrt{\frac{2}{3}}\beta(1)\beta(2)\alpha(3)$$

$$[121]_{-\frac{1}{2}} = q^2_{-\frac{1}{2}} = \frac{1}{\sqrt{2}}\{\beta(1)\alpha(2) - \alpha(1)\beta(2)\}\beta(3)$$

$$[111]_{-\frac{1}{2}} = q^3_{\frac{1}{2}} = \frac{1}{\sqrt{3}}\{\alpha(1)\beta(2)\beta(3) + \beta(1)\alpha(2)\beta(3) + \beta(1)\beta(2)\alpha(3)\}$$

5.6.4 $m_S = -\frac{3}{2}$

$$[111]_{-\frac{3}{2}} = q^{3}_{-\frac{3}{2}} = \beta(1)\beta(2)\beta(3)$$

5.7 Isospin Wavefunctions

In a completely analogous way to the spin wavefunctions, we can define isospin wavefunctions with the q's replaced by the v's.

5.8 Space Wavefunctions

Please note that the superscript is the Yamanouchi symbol from Table 5.2 and the subscript refers to the row in the matrix representation.

$$[111]_R = f^3_1 = \frac{1}{6}[f(123) + f(132) + f(213) + f(321) + f(231) + f(312)]$$

$$[211]_R = f^1_1 = \frac{2}{6}\left[f(123) + f(213) - \frac{1}{2}f(132) - \frac{1}{2}f(321) - \frac{1}{2}f(231) - \frac{1}{2}f(312)\right]$$

$$[121]_R = f^2_1 = \frac{2}{6}\left[\frac{\sqrt{3}}{2}\{f(132) - f(321) - f(231) + f(312)\}\right]$$

Or we can use the other pair

$$[211]_R = f^1_2 = \frac{2}{6}\left[\frac{\sqrt{3}}{2}\{f(132) - f(321) + f(231) - f(312)\}\right]$$

$S=\frac{3}{2}$	$T=\frac{3}{2}$	$\psi = f^4q^3v^3$
$S=\frac{3}{2}$	$T=\frac{1}{2}$	$\psi = \frac{1}{\sqrt{2}}\{f^1q^3v^2 - f^2q^3v^1\}$
$S=\frac{1}{2}$	$T=\frac{3}{2}$	$\psi = \frac{1}{\sqrt{2}}\{f^1q^2v^3 - f^2q^1v^3\}$
$S=\frac{1}{2}$	$T=\frac{1}{2}$	$\psi = \frac{1}{\sqrt{2}}\{f^1(-\frac{1}{\sqrt{2}})(q^1v^2 + q^2v^1) - f^2(\frac{1}{\sqrt{2}})(q^1v^1 - q^2v^2)\}$
		$\psi = f^4(\frac{1}{\sqrt{2}})(q^1v^1 + q^2v^2)$
		$\psi = f^3(\frac{1}{\sqrt{2}})(q^1v^2 - q^2v^1)$

Table 5.3: Complete three-body nuclear wavefunctions

$$[121]_R = f_2^2 = \frac{2}{6}\left[f(123) - f(213) + \frac{1}{2}f(132) + \frac{1}{2}f(321) - \frac{1}{2}f(231) - \frac{1}{2}f(312)\right]$$

$$[321]_R = f^4 = \frac{1}{6}\left[f(123) + f(231) + f(312) - f(132) - f(321) - f(213)\right]$$

As we observed in chapter 2, these pairs can turn out to be linearly dependent if the functions have certain symmetries.

5.9 Summary

In Table 5.3, we give the complete three-body nuclear wavefunctions. In that table q is used for spin, v for isospin and f for the space part of the wavefunction. The superscripts on the q's, v's and f's represent the particular Yamanouchi basis vector as defined in Table 5.2.

5.10 Atomic Wavefunctions

$S=\frac{3}{2}$	$\psi = q^3f^4$
$S=\frac{1}{2}$	$\psi = \frac{1}{\sqrt{2}}\{f^1q^2 - f^2q^1\}$

Table 5.4: Complete three-body atomic wavefunctions

In a completely analogous way (it is much simpler, since we do not need to combine isospin), in Table 5.4 we write down the atomic wavefunctions (with the same definitions of space and spin as for nuclear wavefunctions).

Chapter 6

Summary Of Four-body Wavefunctions

In this chapter we summarize the results for the construction of the four-body wavefunctions. These results are new. Unlike the three-body case, where we found some work with a similar approach, we have not been able to find any paper explicitly dealing with the spatial symmetries of the four-body wavefunctions. The literature on the variational approach to the four-body problem is *ad hoc* and not systematic [11, 52, 53, 68]. However, in our approach to few-body nuclear physics, the four-body case naturally follows from the method that is adopted for three nucleons. We will first enumerate the possible symmetries of a four-body wavefunction. The CG series of $S(4)$ restricts the wavefunction to the form give in Table 6.1.

We are again going to label $m_S = \frac{1}{2}$ as α, $m_S = -\frac{1}{2}$ as β, $m_T = \frac{1}{2}$ as μ and $m_T = -\frac{1}{2}$ as ν. Now we explicitly write out the wavefunctions for each of the 9 possible cases (corresponding to each row of the table above).

6.1 Spin = 2, Isospin = 2

Since spin and isospin are completely symmetric, the spatial part is completely anti-symmetric and it is trivial to write down the wavefunction.

spin	*isospin*	=	⇒ *space*
$S=2$	$T=2$		
$S=2$	$T=0$		
$S=2$	$T=1$		
$S=0$	$T=2$		
$S=0$	$T=0$	+ +	+ +
$S=0$	$T=1$	+	+
$S=1$	$T=2$		
$S=1$	$T=0$	+	+
$S=1$	$T=1$	+ + +	+ + +

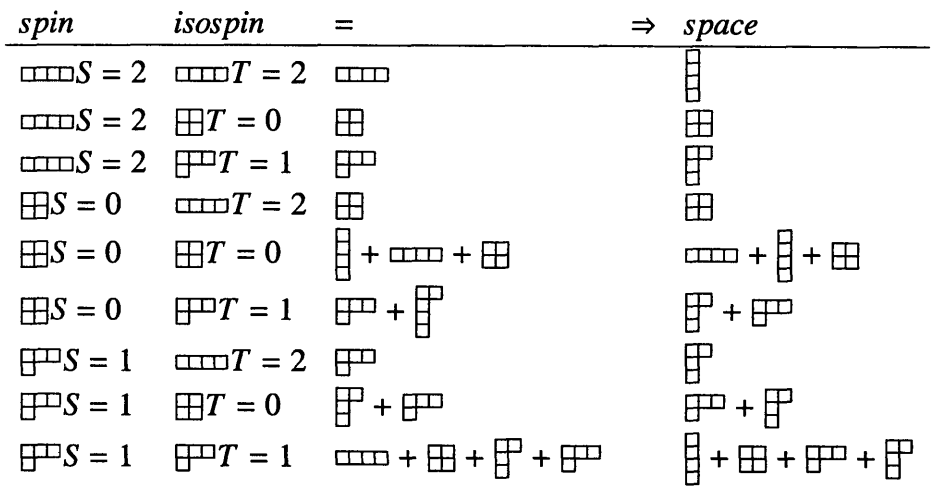


Table 6.1: Symmetry constraints on four-body nuclear wavefunctions

6.2 Spin = 2, Isospin = 0

$$[4321]_{RST} = \frac{1}{\sqrt{2}}\{[2211]_R[2121]_{ST} - [2121]_R[2211]_{ST}\}$$

where

$$[2121]_{ST} = [1111]_S[2121]_T$$

$$[2211]_{ST} = [1111]_S[2211]_T$$

6.3 Spin = 2, Isospin = 1

$$[4321]_{RST} = \frac{1}{\sqrt{3}}\{[3211]_R[1121]_{ST} - [3121]_R[1211]_{ST} + [1321]_R[2111]_{ST}\}$$

where

$$[2111]_{ST} = [1111]_S[2111]_T$$

$$[1211]_{ST} = [1111]_S[1211]_T$$

$$[1121]_{ST} = [1111]_S[1121]_T$$

6.4 Spin = 0, Isospin = 2

$$[4321]_{RST} = \frac{1}{\sqrt{2}}\{[2211]_R[2121]_{ST} - [2121]_R[2211]_{ST}\}$$

where

$$[2121]_{ST} = [2121]_S[1111]_T$$

$$[2211]_{ST} = [2211]_S[1111]_T$$

6.5 Spin = 0, Isospin = 0

$$[4321]_{RST} = [4321]_R[1111]_{ST}$$

$$[4321]_{RST} = \frac{1}{\sqrt{2}}\{[2211]_R[2121]_{ST} - [2121]_R[2211]_{ST}\}$$

$$[4321]_{RST} = [1111]_R[4321]_{ST}$$

where

$$[1111]_{ST} = \frac{1}{\sqrt{2}}\{[2211]_S[2211]_T + [2121]_S[2121]_T\}$$

$$[2211]_{ST} = \frac{1}{\sqrt{2}}\{[2211]_S[2211]_T - [2121]_S[2121]_T\}$$

$$[2121]_{ST} = \frac{-1}{\sqrt{2}}\{[2211]_S[2121]_T + [2121]_S[2211]_T\}$$

$$[4321]_{ST} = \frac{1}{\sqrt{2}}\{[2211]_S[2121]_T - [2121]_S[2211]_T\}$$

6.6 Spin = 0, Isospin = 1

$$[4321]_{RST} = \frac{1}{\sqrt{3}}\{[3211]_R[1121]_{ST} - [3121]_R[1211]_{ST} + [1321]_R[2111]_{ST}\}$$

$$[4321]_{RST} = \frac{1}{\sqrt{3}}\{[2111]_R[1321]_{ST} - [1211]_R[3121]_{ST} + [1121]_R[3211]_{ST}\}$$

where

$$[2111]_{ST} = \frac{1}{\sqrt{2}}\{[2211]_S[1211]_T + [2121]_S[1121]_T\}$$

$$[1211]_{ST} = \frac{1}{2}\{2[2211]_S[2111]_T + [2211]_S[1211]_T - [2121]_S[1121]_T\}$$

$$[1121]_{ST} = \frac{1}{2}\{2[2121]_S[2111]_T - [2121]_S[1211]_T - [2211]_S[1121]_T\}$$

$$[3211]_{ST} = \frac{1}{2}\{2[2211]_S[2111]_T - [2211]_S[1211]_T + [2121]_S[1121]_T\}$$

$$[3121]_{ST} = \frac{1}{2}\{2[2121]_S[2111]_T + [2121]_S[1211]_T + [2211]_S[1121]_T\}$$

$$[1321]_{ST} = \frac{1}{\sqrt{2}}\{-[2121]_S[1211]_T + [2211]_S[1121]_T\}$$

6.7 Spin = 1, Isospin = 2

$$[4321]_{RST} = \frac{1}{\sqrt{3}}\{[3211]_R[1121]_{ST} - [3121]_R[1211]_{ST} + [1321]_R[2111]_{ST}\}$$

where

$$[1121]_{ST} = [1121]_S[1111]_T$$

$$[1211]_{ST} = [1211]_S[1111]_T$$

$$[2111]_{ST} = [2111]_S[1111]_T$$

6.8 Spin = 1, Isospin = 0

$$[4321]_{RST} = \frac{1}{\sqrt{3}}\{[3211]_R[1121]_{ST} - [3121]_R[1211]_{ST} + [1321]_R[2111]_{ST}\}$$

$$[4321]_{RST} = \frac{1}{\sqrt{3}}\{[2111]_R[1321]_{ST} - [1211]_R[3121]_{ST} + [1121]_R[3211]_{ST}\}$$

where

$$[2111]_{ST} = \frac{1}{\sqrt{2}}\{[1211]_S[2211]_T + [1121]_S[2121]_T\}$$

$$[1211]_{ST} = \frac{1}{2}\{2[2111]_S[2211]_T + [1211]_S[2211]_T - [1121]_S[2121]_T\}$$

$$[1121]_{ST} = \frac{1}{2}\{2[2111]_S[2121]_T - [1211]_S[2121]_T - [1121]_S[2211]_T\}$$

$$[3211]_{ST} = \frac{1}{2}\{2[2111]_S[2211]_T - [1211]_S[2211]_T + [1121]_S[2121]_T\}$$

$$[3121]_{ST} = \frac{1}{2}\{2[2111]_S[2121]_T + [1211]_S[2121]_T + [1121]_S[2211]_T\}$$

$$[1321]_{ST} = \frac{1}{\sqrt{2}}\{-[1211]_S[2121]_T + [1121]_S[2211]_T\}$$

6.9 Spin = 1, Isospin = 1

$$[4321]_{RST} = [4321]_R[1111]_{ST}$$

$$[4321]_{RST} = \frac{1}{\sqrt{2}}\{[2211]_R[2121]_{ST} - [2121]_R[2211]_{ST}\}$$

$$[4321]_{RST} = \frac{1}{\sqrt{3}}\{[2111]_R[1321]_{ST} - [1211]_R[3121]_{ST} + [1121]_R[3211]_{ST}\}$$

$$[4321]_{RST} = \frac{1}{\sqrt{3}}\{[3211]_R[1121]_{ST} - [3121]_R[1211]_{ST} + [1321]_R[2111]_{ST}\}$$

where

$$[1111]_{ST} = \frac{1}{\sqrt{3}}\{[2111]_S[2111]_T + [1211]_S[1211]_T + [1121]_S[1121]_T\}$$

$$[2111]_{ST} = \frac{1}{\sqrt{6}}\{4[2111]_S[2111]_T - [1211]_S[1211]_T - [1121]_S[1121]_T\}$$

$$[1211]_{ST} = \frac{1}{\sqrt{6}}\{-[2111]_S[1211]_T - [1211]_S[2111]_T + 2[1211]_S[1211]_T - 2[1121]_S[1211]_T\}$$

$$[1121]_{ST} = \frac{-1}{\sqrt{6}}\{[2111]_S[1121]_T + 2[1211]_S[1121]_T + [1121]_S[2111]_T + 2[1121]_S[1211]_T\}$$

$$[2211]_{ST} = \frac{1}{\sqrt{6}}\{2[2111]_S[1211]_T + 2[1211]_S[2111]_T + [1211]_S[1211]_T - [1121]_S[1121]_T\}$$

$$[2121]_{ST} = \frac{1}{\sqrt{6}}\{2[2111]_S[1121]_T - [1211]_S[1121]_T + 2[1121]_S[2211]_T - [1121]_S[1211]_T\}$$

$$[3211]_{ST} = \frac{1}{\sqrt{2}}\{[2111]_S[1211]_T - [1211]_S[2111]_T\}$$

$$[3121]_{ST} = \frac{1}{\sqrt{2}}\{[2111]_S[1121]_T - [1121]_S[2111]_T\}$$

$$[1321]_{ST} = \frac{1}{\sqrt{2}}\{[1211]_S[1121]_T - [1121]_S[1211]_T\}$$

6.10 Notation

As in the previous chapter, in order to simplify the notation, we use q for spin, v for isospin and f for the space part of the wavefunction. The superscripts on the q's, v's and f's represent the particular Young-Yamanouchi basis vector. The short-hand for the Yamanouchi symbol is given in Table 6.2

[1 1 1 1] = 1	[2 1 2 1] = 6
[2 1 1 1] = 2	[3 2 1 1] = 7
[1 2 1 1] = 3	[3 1 2 1] = 8
[1 1 2 1] = 4	[1 3 2 1] = 9
[2 2 1 1] = 5	[4 3 2 1] = 10

Table 6.2: Shorthand for four-particle Yamanouchi symbol

6.11 Spin Wavefunctions

As in the three-body case, let us define spin wavefunctions corresponding to various m_S values and permutation symmetries. We will denote them by $q^a_{m_S}$, where the subscript refers to the value of m_S and the superscript labels the various Yamanouchi basis vectors defined in Table 6.2.

6.11.1 $m_S = 2$

$$[1111]_2 = q^1_2 = \alpha(1)\alpha(2)\alpha(3)\alpha(4)$$

6.11.2 $m_S = 1$

$$[1111]_1 = q^1_1 = \frac{1}{2}\{\alpha(1)\alpha(2)\alpha(3)\beta(4) + \alpha(1)\alpha(2)\beta(3)\alpha(4) + \alpha(1)\beta(2)\alpha(3)\alpha(4) + \beta(1)\alpha(2)\alpha(3)\alpha(4)\}$$

$$[2111]_1 = q_1^2 = \frac{1}{\sqrt{12}}\{3\alpha(1)\alpha(2)\alpha(3)\beta(4) - \alpha(1)\beta(2)\alpha(3)\alpha(4) - \alpha(1)\alpha(2)\beta(3)\alpha(4) - \beta(1)\alpha(2)\alpha(3)\alpha(4)\}$$

$$[1211]_1 = q_1^3 = \frac{1}{\sqrt{6}}\{2\alpha(1)\alpha(2)\beta(3)\alpha(4) - \alpha(1)\beta(2)\alpha(3)\alpha(4) - \beta(1)\alpha(2)\alpha(3)\alpha(4)\}$$

$$[1121]_1 = q_1^4 = \frac{1}{\sqrt{2}}\{\alpha(1)\beta(2)\alpha(3)\alpha(4) - \beta(1)\alpha(2)\alpha(3)\alpha(4)\}$$

6.11.3 $m_S = 0$

$$[1111]_0 = q_0^1 = \frac{1}{\sqrt{6}}\{\alpha(1)\alpha(2)\beta(3)\beta(4) + \alpha(1)\beta(2)\alpha(3)\beta(4) + \alpha(1)\beta(2)\beta(3)\alpha(4) + \beta(1)\alpha(2)\alpha(3)\beta(4) + \beta(1)\alpha(2)\beta(3)\alpha(4) + \beta(1)\beta(2)\alpha(3)\alpha(4)\}$$

$$[2111]_0 = q_0^2 = \frac{-1}{\sqrt{6}}\{\alpha(1)\alpha(2)\beta(3)\beta(4) + \alpha(1)\beta(2)\alpha(3)\beta(4) + \beta(1)\alpha(2)\alpha(3)\beta(4) - \beta(1)\beta(2)\alpha(3)\alpha(4) - \beta(1)\alpha(2)\beta(3)\alpha(4) - \alpha(1)\beta(2)\beta(3)\alpha(4)\}$$

$$[1211]_0 = q_0^3 = \frac{-1}{\sqrt{6}}\{2\alpha(1)\alpha(2)\beta(3)\beta(4) - 2\beta(1)\beta(2)\alpha(3)\alpha(4) - \alpha(1)\beta(2)\alpha(3)\beta(4) - \beta(1)\alpha(2)\alpha(3)\beta(4) + \alpha(1)\beta(2)\beta(3)\alpha(4) + \beta(1)\alpha(2)\beta(3)\alpha(4)\}$$

$$[1121]_0 = q_0^4 = \frac{-1}{2}\{\alpha(1)\beta(2)\alpha(3)\beta(4) - \beta(1)\alpha(2)\alpha(3)\beta(4) + \alpha(1)\beta(2)\beta(3)\alpha(4) - \beta(1)\alpha(2)\beta(3)\alpha(4)\}$$

$$[2211]_0 = q_0^5 = \frac{1}{\sqrt{12}}\{2\alpha(1)\alpha(2)\beta(3)\beta(4) + 2\beta(1)\beta(2)\alpha(3)\alpha(4) - \alpha(1)\beta(2)\alpha(3)\beta(4) - \beta(1)\alpha(2)\alpha(3)\beta(4) - \alpha(1)\beta(2)\beta(3)\alpha(4) - \beta(1)\alpha(2)\beta(3)\alpha(4)\}$$

$$[2121]_0 = q_0^6 = \frac{1}{2}\{\alpha(1)\beta(2)\alpha(3)\beta(4) - \beta(1)\alpha(2)\alpha(3)\beta(4) + \beta(1)\alpha(2)\beta(3)\alpha(4) - \alpha(1)\beta(2)\beta(3)\alpha(4)\}$$

6.11.4 m_S = -1

$$[1111]_{-1} = q_{-1}^1 = \frac{1}{2}\{\alpha(1)\beta(2)\beta(3)\beta(4) + \beta(1)\alpha(2)\beta(3)\beta(4) + \beta(1)\beta(2)\alpha(3)\beta(4) + \beta(1)\beta(2)\beta(3)\alpha(4)\}$$

$$[2111]_{-1} = q_{-1}^2 = \frac{1}{\sqrt{12}}\{3\beta(1)\beta(2)\beta(3)\alpha(4) - \alpha(1)\beta(2)\beta(3)\beta(4) - \beta(1)\alpha(2)\beta(3)\beta(4) - \beta(1)\beta(2)\alpha(3)\beta(4)\}$$

$$[1211]_{-1} = q^3_{-1} = \frac{1}{\sqrt{6}}\{2\beta(1)\beta(2)\alpha(3)\beta(4) - \alpha(1)\beta(2)\beta(3)\beta(4) - \beta(1)\alpha(2)\beta(3)\beta(4)\}$$

$$[1121]_{-1} = q^4_{-1} = \frac{-1}{\sqrt{2}}\{\alpha(1)\beta(2)\beta(3)\beta(4) - \beta(1)\alpha(2)\beta(3)\beta(4)\}$$

6.11.5 m_S = -2

□□□□

$$[1111]_{-2} = q^1_{-2} = \beta(1)\beta(2)\beta(3)\beta(4)$$

6.12 Isospin Wavefunctions

In a completely analogous way to the spin wavefunctions, we can define isospin wavefunctions with the q's replaced by the v's.

6.13 Space Wavefunctions

Please note that the superscript is the Yamanouchi symbol from Table 6.2 and the subscript refers to the row in the matrix representation.

□□□□

$$\begin{aligned}[1111]_R = f^1_1 \;=\; & \frac{1}{24}[f(1234) + f(1243) + f(1324) + f(1432) + f(1423) \\ & + f(1342) + f(3214) + f(4231) + f(4213) + f(3241) \\ & + f(2134) + f(4132) + f(2431) + f(3124) + f(2314) \\ & + f(2143) + f(4123) + f(3412) + f(2341) + f(4321) \\ & + f(2413) + f(3142) + f(3421) + f(4312)]\end{aligned}$$

$$
\begin{aligned}
[2111]_R = f_1^2 \;=\; & \frac{3}{24}\Big[f(1234) - \frac{1}{3}f(1243) + f(1324) - \frac{1}{3}f(1432) - \frac{1}{3}f(1423) \\
& - \frac{1}{3}f(1342) + f(3214) - \frac{1}{3}f(4231) - \frac{1}{3}f(4213) - \frac{1}{3}f(3241) \\
& + f(2134) - \frac{1}{3}f(4132) - \frac{1}{3}f(2431) + f(3124) + f(2314) \\
& - \frac{1}{3}f(2143) - \frac{1}{3}f(4123) - \frac{1}{3}f(3412) - \frac{1}{3}f(2341) - \frac{1}{3}f(4321) \\
& - \frac{1}{3}f(2413) - \frac{1}{3}f(3142) - \frac{1}{3}f(3421) - \frac{1}{3}f(4312)\Big]
\end{aligned}
$$

$$
\begin{aligned}
[1211]_R = f_1^3 \;=\; & \frac{3}{24}\Big[\frac{\sqrt{8}}{3}f(1243) - \frac{\sqrt{2}}{3}f(1432) + \frac{\sqrt{8}}{3}f(1423) - \frac{\sqrt{2}}{3}f(1342) \\
& - \frac{\sqrt{2}}{3}f(4231) + \frac{\sqrt{8}}{3}f(4213) - \frac{\sqrt{2}}{3}f(3241) - \frac{\sqrt{2}}{3}f(4132) \\
& - \frac{\sqrt{2}}{3}f(2431) + \frac{\sqrt{8}}{3}f(2143) + \frac{\sqrt{8}}{3}f(4123) - \frac{\sqrt{2}}{3}f(3412) \\
& - \frac{\sqrt{2}}{3}f(2341) - \frac{\sqrt{2}}{3}f(4321) + \frac{\sqrt{8}}{3}f(2413) - \frac{\sqrt{2}}{3}f(3142) \\
& - \frac{\sqrt{2}}{3}f(3421) - \frac{\sqrt{2}}{3}f(4312)\Big]
\end{aligned}
$$

$$
\begin{aligned}
[1121]_R = f_1^4 \;=\; & \frac{3}{24}\sqrt{\frac{2}{3}}\,[f(1432) + f(1342) - f(4231) - f(3241) + f(4132) \\
& - f(2431) + f(3412) - f(2341) - f(4321) + f(3142) \\
& - f(3421) + f(4312)]
\end{aligned}
$$

$$
\begin{aligned}
[2111]_R = f_2^2 \;=\; & \frac{3}{24}\Big[\frac{\sqrt{8}}{3}f(1243) - \frac{\sqrt{2}}{3}f(1432) - \frac{\sqrt{2}}{3}f(1423) + \frac{\sqrt{8}}{3}f(1342) \\
& - \frac{\sqrt{2}}{3}f(4231) - \frac{\sqrt{2}}{3}f(4213) + \frac{\sqrt{8}}{3}f(3241) - \frac{\sqrt{2}}{3}f(4132) \\
& - \frac{\sqrt{2}}{3}f(2431) + \frac{\sqrt{8}}{3}f(2143) - \frac{\sqrt{2}}{3}f(4123) - \frac{\sqrt{2}}{3}f(3412) \\
& + \frac{\sqrt{8}}{3}f(2341) - \frac{\sqrt{2}}{3}f(4321) - \frac{\sqrt{2}}{3}f(2413) + \frac{\sqrt{8}}{3}f(3142) \\
& - \frac{\sqrt{2}}{3}f(3421) - \frac{\sqrt{2}}{3}f(4312)\Big]
\end{aligned}
$$

$$
\begin{aligned}
[1211]_R = f_2^3 \;=\; & \frac{3}{24}\Big[f(1234) + \frac{1}{3}f(1243) - \frac{1}{2}f(1324) + \frac{5}{6}f(1432) - \frac{1}{6}f(1423) \\
& - \frac{1}{6}f(1342) - \frac{1}{2}f(3214) + \frac{5}{6}f(4231) - \frac{1}{6}f(4213) - \frac{1}{6}f(3241) \\
& + f(2134) + \frac{5}{6}f(4132) + \frac{5}{6}f(2431) - \frac{1}{2}f(3124) - \frac{1}{2}f(2314) \\
& + \frac{1}{3}f(2143) - \frac{1}{6}f(4123) - \frac{2}{3}f(3412) - \frac{1}{6}f(2341) - \frac{2}{3}f(4321) \\
& - \frac{1}{6}f(2413) - \frac{1}{6}f(3142) - \frac{2}{3}f(3421) - \frac{2}{3}f(4312)\Big]
\end{aligned}
$$

$$
\begin{aligned}
[1121]_R = f_2^4 \;=\; & \frac{3}{24}\left[\frac{\sqrt{3}}{2}f(1324) + \frac{1}{2\sqrt{3}}f(1432) + \frac{\sqrt{3}}{2}f(1423) + \frac{1}{2\sqrt{3}}f(1342)\right. \\
& - \frac{\sqrt{3}}{2}f(3214) - \frac{1}{2\sqrt{3}}f(4231) - \frac{\sqrt{3}}{2}f(4213) - \frac{1}{2\sqrt{3}}f(3241) \\
& + \frac{1}{2\sqrt{3}}f(4132) - \frac{1}{2\sqrt{3}}f(2431) + \frac{\sqrt{3}}{2}f(3124) - \frac{\sqrt{3}}{2}f(2314) \\
& + \frac{\sqrt{3}}{2}f(4123) - \frac{1}{\sqrt{3}}f(3412) - \frac{1}{2\sqrt{3}}f(2341) + \frac{1}{\sqrt{3}}f(4321) \\
& - \frac{\sqrt{3}}{2}f(2413) + \frac{1}{2\sqrt{3}}f(3142) + \frac{1}{\sqrt{3}}f(3421) \\
& \left. - \frac{1}{\sqrt{3}}f(4312)\right]
\end{aligned}
$$

$$
\begin{aligned}
[2111]_R = f_3^2 \;=\; & \frac{3}{24}\sqrt{\frac{2}{3}}\,[f(1432) + f(1423) - f(4231) - f(4213) - f(4132) + f(2431) \\
& - f(4123) + f(3412) - f(4321) + f(2413) + f(3421) - f(4312)]
\end{aligned}
$$

$$
\begin{aligned}
[1211]_R = f_3^3 \;=\; & \frac{3}{24}\left[\frac{\sqrt{3}}{2}f(1324) + \frac{1}{2\sqrt{3}}f(1432) + \frac{1}{2\sqrt{3}}f(1423) + \frac{\sqrt{3}}{2}f(1342)\right. \\
& - \frac{\sqrt{3}}{2}f(3214) - \frac{1}{2\sqrt{3}}f(4231) - \frac{1}{2\sqrt{3}}f(4213) - \frac{\sqrt{3}}{2}f(3241) \\
& - \frac{1}{2\sqrt{3}}f(4132) + \frac{1}{2\sqrt{3}}f(2431) - \frac{\sqrt{3}}{2}f(3124) + \frac{\sqrt{3}}{2}f(2314) \\
& - \frac{1}{2\sqrt{3}}f(4123) - \frac{1}{\sqrt{3}}f(3412) + \frac{\sqrt{3}}{2}f(2341) \\
& + \frac{1}{\sqrt{3}}f(4321) + \frac{1}{2\sqrt{3}}f(2413) - \frac{\sqrt{3}}{2}f(3142) - \frac{1}{\sqrt{3}}f(3421) \\
& \left. + \frac{1}{\sqrt{3}}f(4312)\right]
\end{aligned}
$$

$$[1121]_R = f_3^4 = \frac{3}{24}\Big[f(1234) + \frac{1}{2}f(1324) + \frac{1}{2}f(1432) + \frac{1}{2}f(1423) + \frac{1}{2}f(1342) + \frac{1}{2}f(3214) + \frac{1}{2}f(4231) + \frac{1}{2}f(4213) + \frac{1}{2}f(3241) - f(2134) - \frac{1}{2}f(4132) - \frac{1}{2}f(2431) - \frac{1}{2}f(3124) - \frac{1}{2}f(2314) - f(2143) - \frac{1}{2}f(4123) - \frac{1}{2}f(2341) - \frac{1}{2}f(2413) - \frac{1}{2}f(3142)\Big]$$

$$[3211]_R = f_1^7 = \frac{3}{24}\Big[f(1234) - f(1243) - \frac{1}{2}f(1324) - \frac{1}{2}f(1432) + \frac{1}{2}f(1423) + \frac{1}{2}f(1342) - \frac{1}{2}f(3214) - \frac{1}{2}f(4231) + \frac{1}{2}f(4213) + \frac{1}{2}f(3241) + f(2134) - \frac{1}{2}f(4132) - \frac{1}{2}f(2431) - \frac{1}{2}f(3124) - \frac{1}{2}f(2314) - f(2143) + \frac{1}{2}f(4123) + \frac{1}{2}f(2341) + \frac{1}{2}f(2413) + \frac{1}{2}f(3142)\Big]$$

$$[3121]_R = f_1^8 = \frac{3}{24}\Big[\frac{\sqrt{3}}{2}f(1324) + \frac{1}{2\sqrt{3}}f(1432) - \frac{1}{2\sqrt{3}}f(1423) - \frac{\sqrt{3}}{2}f(1342) - \frac{\sqrt{3}}{2}f(3214) - \frac{1}{2\sqrt{3}}f(4231) + \frac{1}{2\sqrt{3}}f(4213) + \frac{\sqrt{3}}{2}f(3241) + \frac{1}{2\sqrt{3}}f(4132) - \frac{1}{2\sqrt{3}}f(2431) + \frac{\sqrt{3}}{2}f(3124) - \frac{\sqrt{3}}{2}f(2314) - \frac{1}{2\sqrt{3}}f(4123) + \frac{1}{\sqrt{3}}f(3412) + \frac{\sqrt{3}}{2}f(2341) - \frac{1}{\sqrt{3}}f(4321) + \frac{1}{2\sqrt{3}}f(2413) - \frac{\sqrt{3}}{2}f(3142) - \frac{1}{\sqrt{3}}f(3421) + \frac{1}{\sqrt{3}}f(4312)\Big]$$

$$[1321]_R = f_1^9 = \frac{3}{24}\frac{\sqrt{2}}{3}[-f(1432) + f(1423) + f(4231) - f(4213) - f(4132) + f(2431) + f(4123) + f(3412) - f(4321) - f(2413) - f(3421) + f(4312)]$$

$$[3211]_R = f_2^7 = \frac{3}{24}\left[\frac{\sqrt{3}}{2}f(1324) + \frac{1}{2\sqrt{3}}f(1432) - \frac{\sqrt{3}}{2}f(1423) - \frac{1}{2\sqrt{3}}f(1342) - \frac{\sqrt{3}}{2}f(3214) - \frac{1}{2\sqrt{3}}f(4231) + \frac{\sqrt{3}}{2}f(4213) + \frac{1}{2\sqrt{3}}f(3241) - \frac{1}{2\sqrt{3}}f(4132) + \frac{1}{2\sqrt{3}}f(2431) - \frac{\sqrt{3}}{2}f(3124) + \frac{\sqrt{3}}{2}f(2314) + \frac{\sqrt{3}}{2}f(4123) + \frac{1}{\sqrt{3}}f(3412) - \frac{1}{2\sqrt{3}}f(2341) - \frac{1}{\sqrt{3}}f(4321) - \frac{\sqrt{3}}{2}f(2413) + \frac{1}{2\sqrt{3}}f(3142) + \frac{1}{\sqrt{3}}f(3421) - \frac{1}{\sqrt{3}}f(4312)\right]$$

$$[3121]_R = f_2^8 = \frac{3}{24}\left[f(1234) - \frac{1}{3}f(1243) + \frac{1}{2}f(1324) - \frac{5}{6}f(1432) - \frac{1}{6}f(1423) - \frac{1}{6}f(1342) + \frac{1}{2}f(3214) - \frac{5}{6}f(4231) - \frac{1}{6}f(4213) - \frac{1}{6}f(3241) - f(2134) + \frac{5}{6}f(4132) + \frac{5}{6}f(2431) - \frac{1}{2}f(3124) - \frac{1}{2}f(2314) + \frac{1}{3}f(2143) + \frac{1}{6}f(4123) - \frac{2}{3}f(3412) + \frac{1}{6}f(2341) - \frac{2}{3}f(4321) + \frac{1}{6}f(2413) + \frac{1}{6}f(3142) + \frac{2}{3}f(3421) + \frac{2}{3}f(4312)\right]$$

$$[1321]_R = f_2^9 = \frac{3}{24}\left[\frac{\sqrt{8}}{3}f(1243) - \frac{\sqrt{2}}{3}f(1432) + \frac{\sqrt{2}}{3}f(1423) - \frac{\sqrt{8}}{3}f(1342)\right.$$
$$- \frac{\sqrt{2}}{3}f(4231) + \frac{\sqrt{2}}{3}f(4213) - \frac{\sqrt{8}}{3}f(3241) + \frac{\sqrt{2}}{3}f(4132)$$
$$+ \frac{\sqrt{2}}{3}f(2431) - \frac{\sqrt{8}}{3}f(2143) - \frac{\sqrt{2}}{3}f(4123) + \frac{\sqrt{2}}{3}f(3412)$$
$$+ \frac{\sqrt{8}}{3}f(2341) + \frac{\sqrt{2}}{3}f(4321) - \frac{\sqrt{2}}{3}f(2413) + \frac{\sqrt{8}}{3}f(3142)$$
$$\left. - \frac{\sqrt{2}}{3}f(3421) - \frac{\sqrt{2}}{3}f(4312)\right]$$

$$[3211]_R = f_3^7 = \frac{3}{24}\sqrt{\frac{2}{3}}[-f(1432) + f(1342) + f(4231) - f(3241) + f(4132) - f(2431)$$
$$+ f(3412) + f(2341) - f(4321) - f(3142) + f(3421) - f(4312)]$$

$$[3121]_R = f_3^8 = \frac{3}{24}\left[\frac{\sqrt{8}}{3}f(1243) - \frac{\sqrt{2}}{3}f(1432) - \frac{\sqrt{8}}{3}f(1423) + \frac{\sqrt{2}}{3}f(1342)\right.$$
$$- \frac{\sqrt{2}}{3}f(4231) - \frac{\sqrt{8}}{3}f(4213) + \frac{\sqrt{2}}{3}f(3241) + \frac{\sqrt{2}}{3}f(4132)$$
$$+ \frac{\sqrt{2}}{3}f(2431) - \frac{\sqrt{8}}{3}f(2143) + \frac{\sqrt{8}}{3}f(4123) + \frac{\sqrt{2}}{3}f(3412)$$
$$- \frac{\sqrt{2}}{3}f(2341) + \frac{\sqrt{2}}{3}f(4321) + \frac{\sqrt{8}}{3}f(2413) - \frac{\sqrt{2}}{3}f(3142)$$
$$\left. - \frac{\sqrt{2}}{3}f(3421) - \frac{\sqrt{2}}{3}f(4312)\right]$$

$$[1321]_R = f_3^9 = \frac{3}{24}\Big[f(1234) + \frac{1}{3}f(1243) - f(1324) + \frac{1}{3}f(1432) - \frac{1}{3}f(1423) - \frac{1}{3}f(1342) - f(3214) + \frac{1}{3}f(4231) - \frac{1}{3}f(4213) - \frac{1}{3}f(3241) - f(2134) - \frac{1}{3}f(4132) - \frac{1}{3}f(2431) + f(3124) + f(2314) - \frac{1}{3}f(2143) + \frac{1}{3}f(4123) - \frac{1}{3}f(3412) + \frac{1}{3}f(2341) - \frac{1}{3}f(4321) + \frac{1}{3}f(2413) + \frac{1}{3}f(3142) + \frac{1}{3}f(3421) + \frac{1}{3}f(4312)\Big]$$

⊞

$$[2211]_R = f_1^5 = \frac{2}{24}\Big[f(1234) + f(1243) - \frac{1}{2}f(1324) - \frac{1}{2}f(1432) - \frac{1}{2}f(1423) - \frac{1}{2}f(1342) - \frac{1}{2}f(3214) - \frac{1}{2}f(4231) - \frac{1}{2}f(4213) - \frac{1}{2}f(3241) + f(2134) - \frac{1}{2}f(4132) - \frac{1}{2}f(2431) - \frac{1}{2}f(3124) - \frac{1}{2}f(2314) + f(2143) - \frac{1}{2}f(4123) + f(3412) - \frac{1}{2}f(2341) + f(4321) - \frac{1}{2}f(2413) - \frac{1}{2}f(3142) + f(3421) + f(4312)\Big]$$

$$[2121]_R = f_1^6 = \frac{2}{24}\frac{\sqrt{3}}{2}[f(1324) - f(1432) - f(1423) + f(1342) - f(3214) + f(4231) + f(4213) - f(3241) - f(4132) + f(2431) + f(3124) - f(2314) - f(4123) - f(2341) + f(2413) + f(3142)]$$

$$[2211]_R = f_2^5 = \frac{2}{24}\frac{\sqrt{3}}{2}[f(1324) - f(1432) + f(1423) - f(1342) - f(3214) + f(4231) - f(4213) + f(3241) + f(4132) - f(2431) - f(3124) + f(2314) - f(4123) - f(2341) + f(2413) + f(3142)]$$

$$[2121]_R = f_2^6 = \frac{2}{24}\Big[f(1234) - f(1243) + \frac{1}{2}f(1324) + \frac{1}{2}f(1432) - \frac{1}{2}f(1423) - \frac{1}{2}f(1342) + \frac{1}{2}f(3214) + \frac{1}{2}f(4231) - \frac{1}{2}f(4213) - \frac{1}{2}f(3241) - f(2134) - \frac{1}{2}f(4132) - \frac{1}{2}f(2431) - \frac{1}{2}f(3124) - \frac{1}{2}f(2314) + f(2143) + \frac{1}{2}f(4123) + f(3412) + \frac{1}{2}f(2341) + f(4321) + \frac{1}{2}f(2413) + \frac{1}{2}f(3142) - f(3421) - f(4312)\Big]$$

$$[4321]_R = f_1^{10} = \frac{1}{24}[f(1234) - f(1243) - f(1324) - f(1432) + f(1423) + f(1342) - f(3214) - f(4231) + f(4213) + f(3241) - f(2134) + f(4132) + f(2431) + f(3124) + f(2314) + f(2143) - f(4123) + f(3412) - f(2341) + f(4321) - f(2413) - f(3142) - f(3421) - f(4312)]$$

6.14 Summary

In Table 6.3, the complete four-body nuclear wavefunctions are given. As in the three-body case, q is used for spin, v for isospin and f for the space part of the wavefunction.

$S=2$	$T=2$	$\psi = f^{10}q^1v^1$
$S=2$	$T=0$	$\psi = \frac{1}{\sqrt{2}}\{f^5q^1v^6 - f^6q^1v^5\}$
$S=2$	$T=1$	$\psi = \frac{1}{\sqrt{3}}\{f^7q^1v^4 - f^8q^1v^3 + f^9q^1v^2\}$
$S=0$	$T=2$	$\psi = \frac{1}{\sqrt{2}}\{f^5q^6v^1 - f^6q^5v^1\}$
$S=0$	$T=0$	$\psi = f^{10}\frac{1}{\sqrt{2}}\{q^5v^5 + q^6v^6\}$
		$\psi = \frac{1}{\sqrt{2}}\{f^5(\frac{-1}{\sqrt{2}})(q^5v^6 + q^6v^5) - f^6(\frac{1}{\sqrt{2}})(q^5v^5 - q^6v^6)\}$
		$\psi = f^1(\frac{1}{\sqrt{2}})\{q^5v^6 - q^6v^5\}$
$S=0$	$T=1$	$\psi = \frac{1}{\sqrt{3}}\{f^7\frac{1}{2}(2q^6v^2 - q^6v^3 - q^5v^4) - f^8\frac{1}{2}(2q^5v^2 + q^5v^3 - q^6v^4)$ $+f^9\frac{1}{\sqrt{2}}(q^5v^3 + q^6v^4)\}$
		$\psi = \frac{1}{\sqrt{3}}\{f^2\frac{1}{\sqrt{2}}(-q^6v^3 + q^5v^4) - f^3\frac{1}{2}(2q^6v^2 + q^6v^3 + q^5v^4) +$ $f^4\frac{1}{2}(2q^5v^2 - q^5v^3 + q^6v^4)\}$
$S=1$	$T=2$	$\psi = \frac{1}{\sqrt{3}}\{f^7(q^4v^1) - f^8(q^3v^1) + f^9(q^2v^1)\}$
$S=1$	$T=0$	$\psi = \frac{1}{\sqrt{3}}\{f^7\frac{1}{2}(2q^2v^6 - q^3v^6 - q^4v^5) - f^8\frac{1}{2}(2q^2v^5 + q^3v^5 - q^4v^6)$ $+f^9\frac{1}{\sqrt{2}}(q^3v^5 + q^4v^6)\}$
		$\psi = \frac{1}{\sqrt{3}}\{f^2\frac{1}{\sqrt{2}}(-q^3v^6 + q^4v^5) - f^3\frac{1}{2}(2q^2v^6 + q^3v^6 + q^4v^5) +$ $f^4\frac{1}{2}(2q^2v^5 - q^3v^5 + q^4v^6)\}$
$S=1$	$T=1$	$\psi = f^{10}\frac{1}{\sqrt{3}}(q^2v^2 + q^3v^3 + q^4v^4)$
		$\psi = \frac{1}{\sqrt{2}}\{f^5\frac{1}{\sqrt{6}}(2q^2v^4 - q^3v^4 + 2q^4v^5 - q^4v^3)$ $-f^6\frac{1}{\sqrt{6}}(2q^2v^3 + 2q^3v^2 + q^3v^3 - q^4v^4)\}$
		$\psi = \frac{1}{\sqrt{3}}\{f^2\frac{1}{\sqrt{2}}(q^3v^4 - q^4v^3) - f^3\frac{1}{\sqrt{2}}(q^2v^4 - q^4v^2)$ $+f^4\frac{1}{\sqrt{2}}(q^2v^3 - q^3v^2)\}$
		$\frac{1}{\sqrt{3}}\{f^7\frac{-1}{\sqrt{6}}(q^2v^4 + 2q^3v^4 + q^4v^2 + 2q^4v^3)$ $-f^8\frac{1}{\sqrt{6}}(-q^2v^3 - q^3v^2 + 2q^3v^3 - 2q^4v^3)$ $+f^9\frac{1}{\sqrt{6}}(4q^2v^2 - q^3v^3 - q^4v^4)\}$

Table 6.3: Complete four-body nuclear wavefunctions

The superscripts on the q's, v's and f's represent the particular Young-Yamanouchi basis vector as defined in Table 6.2.

6.15 Atomic Wavefunctions

In a completely analogous way (it is much simpler, since we do not need to combine Isospin), in Table 6.4, we write down the atomic wavefunctions (with the same definitions of space and spin as for nuclear wavefunctions). It should be noted that this notation

$S = 2$	$\psi = f^{10}q^1$
$S = 1$	$\psi = \frac{1}{\sqrt{3}}\{f^7q^4 - f^8q^3 + f^9q^2\}$
$S = 0$	$\psi = \frac{1}{\sqrt{2}}\{f^5q^6 - f^6q^5\}$

Table 6.4: Complete four-body atomic wavefunctions

does not differentiate between the various M_S values.

Chapter 7

Matrix Elements: First Attempt

In the first few chapters, we have used group theory for the systematic construction of few-body nuclear wavefunctions. In this chapter we will use those wavefunctions to calculate the matrix elements for the H-J potential. These matrix elements will eventually, in chapter 10, lead us to the coupled-channel equations.

As discussed in the introduction, systematic methods for calculating matrix elements of one-body and two-body operators in the nuclear shell model were developed due to the pioneering work of Racah, Jahn and others. Racah's approach, by giving special status to the *last* two particles, achieves tremendous simplification for these matrix element calculations. However, in the phonon-coupled model, we will use correlated wavefunctions. Hence we wanted to explore whether it is possible to generalize Racah's method to arbitrary wavefunctions. The answer, as we will demonstrate, is unfortunately negative, and retrospectively completely obvious: Racah's method is based on treating two nucleons as special and there is no natural way for correlated wavefunctions to do so.

However, in order to see how far Racah's method can help us, we want to emulate it as much as possible. So the natural scheme for us turns out to be

1. Use Racah's method on spin and isospin (since these are angular momentum eigenstates). For this we need to expand our wavefunction in terms of a basis which has explicit symmetry under the exchange of the last two particles.

2. Leave our spatial functions in their original form.

3. Evaluate our matrix element, with the result given in terms of multidimensional spatial integrals.

However, going through these calculations it will become obvious that such a method fails completely for the H-J potential i.e. *it cannot in principle be applied to H-J*. However, even if we were not dealing with H-J, we observe that

1. Since we cannot utilize the full power of Racah's method, there is no particular advantage in working with the last two particles.

2. In fact for variational correlated wavefunctions, it is much better to give special status to the *first* two particles. This is a radical departure from Racah's established approach of more than fifty years.

We will first write out the H-J potential in terms of Racah's irreducible tensor operators. This simplifies the calculation of the two-body, two-particle matrix elements. These matrix elements will also be utilized in the next two chapters.

7.1 H-J Potential

The Hamada-Johnston potential between nucleon 1 and nucleon 2 can be written in the form

$$V = V_C + V_T S_{12} + V_{LS} \vec{L}.\vec{S} + V_{LL} L_{12} \tag{7.1}$$

where

$$
\begin{aligned}
V_C &= \vec{\tau}_1.\vec{\tau}_2\ \vec{\sigma}_1.\vec{\sigma}_2\ y_C(r_{12}) \\
V_T &= \vec{\tau}_1.\vec{\tau}_2 y_T(r_{12}) \\
S_{12} &= \frac{3(\vec{\sigma}_1.\vec{r})(\vec{\sigma}_2.\vec{r})}{r^2} - \vec{\sigma}_1.\vec{\sigma}_2 \\
V_{LS} &= y_{LS}(r_{12}) \\
V_{LL} &= y_{LL}(r_{12}) \\
L_{12} &= \vec{\sigma}_1.\vec{\sigma}_2\vec{L}^2 - \frac{1}{2}(\vec{\sigma}_1.\vec{L})(\vec{\sigma}_2.\vec{L}) - \frac{1}{2}(\vec{\sigma}_2.\vec{L})(\vec{\sigma}_1.\vec{L}) \\
\vec{L} &= \vec{L}_1 + \vec{L}_2 \\
\vec{S} &= \frac{\vec{\sigma}_1 + \vec{\sigma}_2}{2}
\end{aligned}
$$

The definitions of the y's are

$$
\begin{aligned}
y_C(x) &= 0.08\frac{\mu}{3}Y(x)\{1 + a_C Y(x) + b_C Y^2(x)\} \\
y_T(x) &= 0.08\frac{\mu}{3}Z(x)\{1 + a_T Y(x) + b_T Y^2(x)\} \\
y_{LS}(x) &= \mu G_{LS} Y^2(x)\{1 + b_{LS} Y(x)\} \\
y_{LL}(x) &= \mu G_{LL} x^{-2} Z(x)\{1 + a_{LL} Y(x) + b_{LL} Y^2(x)\}
\end{aligned}
$$

where the pion mass $\mu = 139.4 = (1.415fm)^{-1}$ and the nucleon mass $M = 6.73\mu$. The inter-nucleon distance, x, is measured in μ^{-1} and

$$
\begin{aligned}
Y(x) &= \frac{e^{-x}}{x} \\
Z(x) &= (1 + \frac{3}{x} + \frac{3}{x^2})Y(x)
\end{aligned}
$$

The numerical values of the parameters are given in (using a hard core radius of $x_0 = 0.343$ in all the states) Table 7.1.

state	a_C	b_C	a_T	b_T	G_{LS}	b_{LS}	G_{LL}	a_{LL}	b_{LL}
singlet even	+8.7	+10.6					−0.000891	+0.2	−0.2
triplet odd	−9.07	+3.48	−1.29	+0.55	+0.1961	−7.12	−0.000891	−7.26	+6.92
triplet even	+6.0	−1.0	−0.5	+0.2	+0.0743	−0.1	+0.00267	+1.8	−0.4
singlet odd	−8.0	+12.0					−0.00267	+2.0	+6.0

Table 7.1: Parameter values for H-J potential

7.2 H-J and Irreducible Tensor Operators

The form given above is not suitable for matrix element calculations since most of these two-body potentials are not written as irreducible tensor operators. However this transformation to tensor operators can easily be made. This form was first published by Boersma [6], who gives the nuclear force in terms of

$$\sum_K [S^{[K]} \times V^{[K]}]^{[0]}$$

This notation is standard in the angular momentum literature [17] and is a succinct way of using Clebsch-Gordan coefficients[1] to couple two tensor operators of rank K to give an operator of rank 0.

We reproduce Table 1[2] from [6] as Table 7.2.

Interaction	K	$S^{[K]}$	$V^{[K]}$
V_C	0	$(\vec{\sigma}(1).\vec{\sigma}(2))(\vec{\tau}(1).\vec{\tau}(2))$	1
V_{LS}	1	$\frac{i}{2}\sqrt{3}(\sigma_\kappa^{[1]}(1) + \sigma_\kappa^{[1]}(2))$	$L_\kappa^{[1]}$
V_T	1	$2\sqrt{6\pi}(\vec{\tau}(1).\vec{\tau}(2)[\vec{\sigma}(1) \times \vec{\sigma}(2)]_\kappa^{[2]}$	$Y_\kappa^{[2]}$
$V_{L_{12}}$	0	$\frac{2}{3}\vec{\sigma}(1).\vec{\sigma}(2)$	$\vec{L}.\vec{L}$
$V_{L_{12}}$	2	$-\sqrt{5}[\vec{\sigma}(1) \times \vec{\sigma}(2)]_\kappa^{[2]}$	$[\vec{L} \times \vec{L}]_\kappa^{[2]}$

Table 7.2: H-J as irreducible tensor operators

In the next few subsections we verify that the Boersma definitions are consistent with Hamada-Johnston.

[1]The usual $SU(2)$ ones of angular momentum addition.

[2]Boersma uses $\vec{\sigma}(1)$ instead of $\vec{\sigma}_1$ etc.

7.2.1 V_C

There is no need to modify this part, since it is given in the form of an irreducible tensor operator.

7.2.2 V_T

The definitions of $S_k^{[2]}$ and $V_k^{[2]}$ from Table 7.2 are

$$\begin{aligned} S_k^{[2]} &= [\vec{\sigma}_1 \times \vec{\sigma}_2]_k^{[2]} \\ V_k^{[2]} &= Y_k^{[2]} 2\sqrt{6\pi} \end{aligned}$$

In order to figure out what $S_k^{[2]}$ is, we need to use Clebsch-Gordan coefficients (in the usual way we add angular momentum). Explicitly,

$$\begin{aligned} [S^{[2]} \times V^{[2]}]^{[0]} &= C^{0,0}_{2,-2;2,2} S_{-2}^{[2]} V_2^{[2]} + C^{0,0}_{1,-1;1,1} S_{-1}^{[2]} V_1^{[2]} + C^{0,0}_{1,0;1,0} S_0^{[2]} V_0^{[2]} \\ &\quad + C^{0,0}_{1,1;1,-1} S_1^{[1]} V_{-1}^{[1]} + C^{0,0}_{2,2;2,-2} S_2^{[2]} V_{-2}^{[2]} \\ &= 3\frac{(\vec{\sigma}_1.\vec{r})(\vec{\sigma}_2.\vec{r})}{r^2} - \vec{\sigma}_1.\vec{\sigma}_2 \end{aligned}$$

where the $C^{l,m}_{l_1,m_1;l_2,m_2}$ are the Clebsch-Gordan coefficients. This is exactly the form as written out in the H-J Hamiltonian.

7.2.3 V_{LS}

Using

$$\begin{aligned} S_k^{[1]} &= \frac{i}{2}\sqrt{3}(\sigma_k^{[1]} + \sigma_k^{[2]}) \\ V_k^{[1]} &= L_k^{[1]} \end{aligned}$$

we can see that

$$\begin{aligned}[S^{[1]} \times V^{[1]}]^{[0]} &= C^{0,0}_{1,-1;1,1} S^{[1]}_{-1} V^{[1]}_{1} + C^{0,0}_{1,0;1,0} S^{[1]}_{0} V^{[1]}_{0} \\ &\quad + C^{0,0}_{1,1;1,-1} S^{[1]}_{1} V^{[1]}_{-1} \\ &= -i\vec{\sigma}.\vec{L}\end{aligned}$$

There seems to be a discrepancy of $-i$ between the Hamada-Johnston result and Boersma's tensor operators: we have not found a way to resolve it, and believe that Boersma probably included this factor in his definition of y_{LS}. For our calculations, we will be using the H-J definition, since it is well-established and widely used.

7.2.4 V_{LL}

There are two components of V_{LL}. One is the $K = 0$ and the other is the $K = 2$ component. The 0 component is very simple and the 2 component is analogous to the tensor force, V_T. The $K = 0$ component is

$$\begin{aligned}S^{[0]}_{0} &= \frac{2}{3}\vec{\sigma}_1.\vec{\sigma}_2 \\ V^{[0]}_{0} &= \vec{L}.\vec{L}\end{aligned}$$

Hence $[S^{[0]} \times V^{[0]}]^{[0]} = \frac{2}{3}\vec{\sigma}_1.\vec{\sigma}_2\vec{L}.\vec{L}$.

For the $K = 2$ component, using

$$\begin{aligned}S^{[2]}_{k} &= -\sqrt{5}[\vec{\sigma}_1 \times \vec{\sigma}_2]^{[2]}_{k} \\ V^{[2]}_{k} &= [\vec{L} \times \vec{L}]^{[2]}\end{aligned}$$

after a brief calculation we get

$$[S^{[2]} \times V^{[2]}]^{[0]} = \frac{1}{3}(\vec{\sigma}_1).(\vec{\sigma}_2)\vec{L}^2 - \frac{1}{2}\left\{(\vec{\sigma}_1.\vec{L})(\vec{\sigma}_2.\vec{L}) + (\vec{\sigma}_2.\vec{L})(\vec{\sigma}_1.\vec{L})\right\}$$

Adding the 0 and the 2 components we get

$$\vec{\sigma}_1.\vec{\sigma}_2\vec{L}^2 - \frac{1}{2}((\vec{\sigma}_1.\vec{L})(\vec{\sigma}_2.\vec{L}) + (\vec{\sigma}_2.\vec{L})(\vec{\sigma}_1.\vec{L}))$$

exactly as in the H-J Hamiltonian.

7.3 Two-body Matrix Elements

Since we have expressed our potential as a linear combination of irreducible tensor operators, two-body matrix elements can easily be calculated. We only calculate the spin matrix elements since, as the calculation in subsection 7.3.1 will show, that the $\vec{\tau}_1 \cdot \vec{\tau}_2$ is a diagonal operator with values -1 or 3. The results of these subsections are important and will also be utilized in the next two chapters.

7.3.1 V_C

We want to evaluate

$$\langle s_1 = \frac{1}{2}, s_2 = \frac{1}{2}, S, M_S|\vec{\sigma}_1.\vec{\sigma}_2|s_1' = \frac{1}{2}, s_2' = \frac{1}{2}, S', M_{S'}\rangle = (-1)^{s_1'+s_2+S}\begin{Bmatrix} s_1 & s_2 & S \\ s_2' & s_1' & 1 \end{Bmatrix}(s_1\|\vec{\sigma}_1\|s_1')(s_2\|\vec{\sigma}_2\|s_2)\delta_{S,S'}\delta_{M_S,M_{S'}} \tag{7.2}$$

Using Wigner-Eckart, we can easily see that

$$(s_1 = \frac{1}{2}\|\vec{\sigma}_1\|s_1 = \frac{1}{2}) = \sqrt{6}$$

Plugging this value into Equation 7.2, we get the result that for $S = 0$ (hence $S' = 0$),

$$\langle s_1 = \frac{1}{2}, s_2 = \frac{1}{2}, S, M_S | \vec{\sigma}_1 . \vec{\sigma}_2 | s_1' = \frac{1}{2}, s_2' = \frac{1}{2}, S', M_{S'} \rangle = -3$$

And for $S = 1$ (hence $S' = 1$)

$$\langle s_1 = \frac{1}{2}, s_2 = \frac{1}{2}, S, M_S | \vec{\sigma}_1 . \vec{\sigma}_2 | s_1' = \frac{1}{2}, s_2' = \frac{1}{2}, S', M_{S'} \rangle = \delta_{M_S, M_{S'}}$$

7.3.2 V_T

We want to evaluate

$$\langle s_1 = \frac{1}{2}, s_2 = \frac{1}{2}, S, M_S | 3 \frac{[\vec{\sigma}_1 \times \vec{\sigma}_2]^{(2)} . [\vec{r}_{12} \times \vec{r}_{12}]^{(2)}}{r_{12}^2} | s_1' = \frac{1}{2}, s_2' = \frac{1}{2}, S', M_{S'} \rangle \tag{7.3}$$

In order to calculate this matrix element, we need to know

$$\langle s_1 = \frac{1}{2}, s_2 = \frac{1}{2}, S, M_S | [\vec{\sigma}_1 \times \vec{\sigma}_2]^{(2)}_m | s_1' = \frac{1}{2}, s_2' = \frac{1}{2}, S', M_{S'} \rangle =$$
$$\frac{C^{S,M_S}_{S',M_{S'};2,m}}{\sqrt{2S'+1}} (s_1 = \frac{1}{2}, s_2 = \frac{1}{2}, S || [\vec{\sigma}_1 \times \vec{\sigma}_2]^{(2)} || s_1' = \frac{1}{2}, s_2' = \frac{1}{2} S_2') \tag{7.4}$$

One can easily evaluate

$$(s_1 = \frac{1}{2}, s_2 = \frac{1}{2}, S || [\vec{\sigma}_1 \times \vec{\sigma}_2]^{(2)} || s_1' = \frac{1}{2}, s_2' = \frac{1}{2} S_2') =$$
$$\sqrt{(2S+1)(2 \times 2 + 1)(2S'+1)} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & S \\ \frac{1}{2} & \frac{1}{2} & S' \\ 1 & 1 & 2 \end{Bmatrix} (\frac{1}{2} || \vec{\sigma} || \frac{1}{2})^2$$

Putting everything together, we find that the Equation 7.3 is non-zero only for $S = S' = 1$. The matrix elements are given in Table 7.3.

M_S	M'_S	$\langle S=1, M_S \lvert S_{12} \rvert S'=1, M_{S'} \rangle$
-1	-1	$\frac{2z^2-x^2-y^2}{r^2}$
-1	0	$-3\sqrt{2}\frac{(x+iy)z}{r^2}$
-1	1	$3\frac{(x+iy)^2}{r^2}$
0	0	$\frac{2x^2+2y^2-4z^2}{r^2}$
0	1	$3\sqrt{2}\frac{(x+iy)z}{r^2}$
1	1	$\frac{2z^2-x^2-y^2}{r^2}$

Table 7.3: S_{12} Matrix Elements

M_S	M'_S	$\langle S=1, M_S \lvert \vec{L}.\vec{S} \rvert S'=1, M_{S'} \rangle$
-1	-1	$-L_z$
-1	0	$\frac{L_+}{\sqrt{2}}$
-1	1	0
0	0	0
0	1	$\frac{L_+}{\sqrt{2}}$
1	1	L_z

Table 7.4: $\vec{L}.\vec{S}$ Matrix Elements

7.3.3 V_{LS}

Taking $\vec{S} = \frac{\vec{\sigma}_1+\vec{\sigma}_2}{2}$, we want to get the matrix elements of $\vec{L}.\vec{S}$. Again the non-zero coupling is only between $S = S' = 1$. The matrix elements are given in Table 7.4.

7.3.4 V_{LL}

The operator is

$$\theta = \frac{2}{3}\vec{\sigma}_1.\vec{\sigma}_2\vec{L}^2 + \left[-\sqrt{5}[\sigma(1)\times\sigma(2)]^{(2)}\times[\vec{L}\times\vec{L}]^{(2)}\right]^{(0)}$$

Since the first part resembles V_C and the second V_T, the details of the matrix element calculation are very similar to the V_C and V_T matrix elements which we have already calculated.

M_S	M'_S	$\langle S=1, M_S \vert\theta\vert S'=1, M_{S'}\rangle$
-1	-1	$L_x^2 + L_y^2$
-1	0	$\frac{1}{\sqrt{2}}[L_+L_z + L_zL_+]$
-1	1	$-L_+^2$
0	0	$2L_z^2$
0	1	$-\frac{1}{\sqrt{2}}[L_+L_z + L_zL_+]$
1	1	$L_x^2 + L_y^2$

Table 7.5: L_{12} Matrix Elements

The only non-zero coupling is for $S = S' = 1$ or for $S = S' = 0$. For $S = 0$,

$$\langle S=0, M_S=0\vert\theta\vert S'=0, M_{S'}=0\rangle = -2\vec{L}^2 \tag{7.5}$$

The results are given in Table 7.5 for S = 1.

7.4 Standard Approach of Matrix Element Evaluation

In this section we describe the standard way of evaluating two-body matrix elements. This method was developed for shell-model calculations and is most effective when it is used on angular momentum eigenstates.

The first observation that we make is that the potential is completely symmetric, and the wavefunctions are completely antisymmetric under the exchange of any two particles. This allows us to prove the following lemma:

Lemma. *If ψ and ϕ are completely antisymmetric, then*

$$\langle\psi\vert \sum_{1<i<j\leq n} V_{ij}\vert\phi\rangle = \frac{n(n-1)}{2}\langle\psi\vert V_{pq}\vert\phi\rangle$$

where $1 \leq p < q \leq n$.

Proof. It will be sufficient to show that all the terms in the sum $\sum_{1<i<j\leq n}\langle\psi\vert V_{ij}\vert\phi\rangle$ are equal.

Suppose P is the operator which permutes particle labels 2 and 3, leaving 1 fixed. Then

$$\begin{aligned}\langle\psi|V_{12}|\phi\rangle &= \langle\psi|P^{-1}PV_{12}P^{-1}P|\phi\rangle \\ &= \langle -\psi|V_{13}|-\phi\rangle \\ &= \langle\psi|V_{13}|\phi\rangle\end{aligned}$$

Because of this lemma, our work reduces by a factor of 3 for the three-body calculation and a factor of 6 for the four-body one. Note that this argument depends only on the symmetry properties of the operators and wavefunctions and has nothing to do with the shell model. Hence this lemma will hold in our case as well. While this is a significant simplification, the task ahead is still quite daunting.

Let us suppose that we can expand our completely antisymmetric n-particle wavefunction as a linear superposition of products of $n-2$ particle wavefunctions, Ψ_{n-2}, and two-particle functions, Ψ_2, i.e.

$$\begin{aligned}\Psi_n &= \sum_{\alpha,\beta} \xi_{\alpha\beta}\Psi_{n-2}(\alpha)\Psi_2(\beta) \\ \Psi'_n &= \sum_{\mu,\nu} \xi_{\mu\nu}\Psi'_{n-2}(\mu)\Psi'_2(\nu)\end{aligned} \tag{7.6}$$

where Ψ_{n-2} is completely antisymmetric under the exchange of the coordinates of the first $n-2$ particles, and Ψ_2 is antisymmetric under the exchange of the coordinates of the last 2 particles. This dramatically simplifies the matrix element calculation because $V_{n-1,n}$ only acts on the last two coordinates i.e.

$$\langle\Psi_n|V_{n-1,n}|\Psi'_n\rangle = \sum_{\alpha\beta\mu\nu} \xi_{\alpha\beta}\xi_{\mu\nu}\langle\Psi_{n-2}(\alpha)|\Psi'_{n-2}(\mu)\rangle\ \langle\Psi_2(\beta)|V|\Psi'_2(\nu)\rangle$$

This is the basic idea of Racah's method. It reduces the matrix element of a two-body operator with antisymmetric n-particle wavefunctions to calculating simple dot products and two-body matrix elements with two-body wavefunctions. In this approach, all the

work is done in calculating the coefficients $\xi_{\alpha\beta}$ and $\xi_{\mu\nu}$ in Equation 7.6. These are called the *coefficients of fractional parentage*. Instead of showing how to calculate these coefficients, we refer the reader to Appendix B, chapter 7 of [54] and the rather detailed papers by Jahn and others [25, 48, 49]. Briefly, however, the basic method is to write each space, spin and isospin wavefunction as a linear combination of products of functions of $n-2$ particles and 2 particles e.g. using ψ for space, we would write,

$$\psi_n = \sum_j c_j \psi^j_{n-2} \psi^j_2$$

where c_j are some coefficients, ψ^j_{n-2} is an $n-2$ particle wavefunction which transforms according to the jth irreducible representation of $S(n-2)$ and ψ^j_2 is symmetric or anti-symmetric under the exchange of the last two particles. Even without going into details of how these coefficients are calculated, we can see that for arbitrary correlated spatial wavefunctions, there cannot be any meaningful expansion in terms of wavefunctions that are antisymmetric in the first $n-2$ and last 2 particles. Hence we conclude that Racah's method cannot be generalized to arbitrary wavefunctions.

7.5 New Wavefunctions

We know from the previous section that Racah's method will not be completely applicable in our case. However, for our first attempt, we still try to follow the classical method as much as possible. As explained above, this means that only for spin and isospin wavefunctions, we will assign special symmetry properties to the last two particles.

Note that we are not defining new wavefunctions, but merely expanding them in a basis of functions that have explicit symmetry under permutations of the last two particles. For the three-body problem only the $T = \frac{1}{2}$ state corresponds to physically observed particles. While the notation used in chapters 4 and 5 was convenient for the purposes of enumeration, it is not convenient for the purposes of calculation of matrix elements. Using ψ for space, ϕ for spin and Γ for isospin, and denoting the Yamanouchi symbol in parentheses, we can

see from chapter 4 that the relevant wavefunctions are

$$\begin{aligned}
\Psi_1 &= \psi(111)\frac{1}{\sqrt{2}}[\phi(211)\Gamma(121) - \phi(121)\Gamma(211)] \\
\Psi_2 &= \psi(321)\frac{1}{\sqrt{2}}[\phi(211)\Gamma(211) + \phi(121)\Gamma(121)] \\
\Psi_3 &= -\frac{1}{2}\psi(211)[\phi(211)\Gamma(121) + \phi(121)\Gamma(211)] \\
&\quad -\frac{1}{2}\psi(121)[\phi(211)\Gamma(211) - \phi(121)\Gamma(121)] \\
\Psi_4 &= \frac{1}{\sqrt{2}}[\psi(211)\phi(111)\Gamma(121) - \psi(121)\phi(111)\Gamma(211)]
\end{aligned}$$

These spin and isospin wavefunctions have no particular symmetry under the exchange of particles 2 and 3. However we can define two new wavefunctions i.e.

$$\begin{aligned}
\phi(\overline{12}1) &= \phi(s_a = \frac{1}{2}, s_b = \frac{1}{2}, s_c = \frac{1}{2}(S_{bc} = 1), S = \frac{1}{2}, M_S) \\
\phi(\tilde{12}1) &= \phi(s_a = \frac{1}{2}, s_b = \frac{1}{2}, s_c = \frac{1}{2}(S_{bc} = 0), S = \frac{1}{2}, M_S)
\end{aligned}$$

where the ϕ's are constructed by vector coupling s_a to S_{bc}[3]. By an explicit calculation we can see that $\phi(\overline{12}1)$ is symmetric and $\phi(\tilde{12}1)$ is antisymmetric under the exchange of the last two particles. Now we need to expand our spin/isospin functions with the Yamanouchi symbol 211 or 121 in terms of the $\phi(\overline{12}1)$ and $\phi(\tilde{12}1)$. The details of this computation are given in Appendix B. The results are

$$\begin{aligned}
\phi(121) &= \frac{\sqrt{3}}{2}\phi(\overline{12}1) - \frac{1}{2}\phi(\tilde{12}1) \\
\phi(211) &= \frac{1}{2}\phi(\overline{12}1) + \frac{\sqrt{3}}{2}\phi(\tilde{12}1)
\end{aligned}$$

Using this expansion we can rewrite our wavefunctions as

[3] S_{bc} is the spin obtained by coupling s_b to s_c.

$$
\begin{aligned}
\Psi_1 &= \psi(111)\frac{1}{\sqrt{2}}\left[\phi(\tilde{1}\bar{2}1)\Gamma(\bar{1}\bar{2}1) - \phi(\bar{1}\bar{2}1)\Gamma(\tilde{1}\bar{2}1)\right] \\
\Psi_2 &= \psi(321)\frac{1}{\sqrt{2}}\left[\phi(\bar{1}\bar{2}1)\Gamma(\bar{1}\bar{2}1) + \phi(\tilde{1}\bar{2}1)\Gamma(\tilde{1}\bar{2}1)\right] \\
\Psi_3 &= \frac{1}{2}\psi(211)\left[\frac{\sqrt{3}}{2}\phi(\tilde{1}\bar{2}1)\Gamma(\tilde{1}\bar{2}1) - \frac{1}{2}\phi(\tilde{1}\bar{2}1)\Gamma(\bar{1}\bar{2}1) - \frac{1}{2}\phi(\bar{1}\bar{2}1)\Gamma(\tilde{1}\bar{2}1) - \frac{\sqrt{3}}{2}\phi(\bar{1}\bar{2}1)\Gamma(\bar{1}\bar{2}1)\right] \\
&\quad -\frac{1}{2}\psi(121)\left[\frac{1}{2}\phi(\tilde{1}\bar{2}1)\Gamma(\tilde{1}\bar{2}1) + \frac{\sqrt{3}}{2}\phi(\tilde{1}\bar{2}1)\Gamma(\bar{1}\bar{2}1) + \frac{\sqrt{3}}{2}\phi(\bar{1}\bar{2}1)\Gamma(\tilde{1}\bar{2}1) - \frac{1}{2}\phi(\bar{1}\bar{2}1)\Gamma(\bar{1}\bar{2}1)\right] \\
\Psi_4 &= \frac{1}{\sqrt{2}}\left[\psi(211)\phi(111)\Gamma(121) - \psi(121)\phi(111)\Gamma(211)\right]
\end{aligned}
$$

7.6 An Example

We can calculate matrix elements in both the old basis and the new basis. Because of the Lemma in section 7.4, we know that

$$\langle\Psi_i|\theta_{12}|\Psi_j\rangle = \langle\Psi_i|\theta_{23}|\Psi_j\rangle$$

To see this explicitly let us concretely work out a particular case e.g. $\langle\Psi_1|\vec{\tau}_1.\vec{\tau}_2 S_{12}|\Psi_4\rangle$ and compare it to $\langle\Psi_1|\vec{\tau}_2.\vec{\tau}_3 S_{23}|\Psi_4\rangle$. Using our wavefunctions and Appendix B, we easily see that

$$
\begin{aligned}
\langle\Psi_1|\vec{\tau}_1.\vec{\tau}_2 S_{12} y_T|\Psi_4\rangle &= -\frac{3}{2}\int \psi(111)\langle\phi(211)|S_{12} y_T|\phi(111)\rangle\psi(121) \\
\langle\Psi_1|\vec{\tau}_2.\vec{\tau}_3 S_{23} y_T|\Psi_4\rangle &= -\frac{3}{4}\int \psi(111)\langle\phi(\bar{1}\bar{2}1)|S_{23} y_T|\phi(111)\rangle\psi(211) - \\
&\quad \frac{3\sqrt{3}}{4}\int \psi(111)\langle\phi(\bar{1}\bar{2}1)|S_{23} y_T|\phi(111)\rangle\psi(121)
\end{aligned}
$$

Ostensibly they do not seem equal. However, let us look at a concrete case. Say $M_S = \frac{1}{2}$

and $M'_S = \frac{3}{2}$. Then[4]

$$\begin{aligned}
\langle\Psi_1(M_S)|\vec{\tau}_1.\vec{\tau}_2 S_{12}|\Psi_4(M'_S\rangle &= \frac{3\sqrt{6}}{2}\int \psi(111)\frac{x_{12}+iy_{12}}{r_{12}^2} z_{12} y_T(r_{12})\psi(211) \\
\langle\Psi_1(M_S)|\vec{\tau}_2.\vec{\tau}_3 S_{23}|\Psi_4(M'_S)\rangle &= -\frac{3}{4}\int \psi(111)\sqrt{6}\frac{x_{23}+iy_{23}}{r_{23}^2} z_{23} y_T(r_{23})\psi(211) - \\
&\quad \frac{3\sqrt{3}}{4}\int \psi(111)\sqrt{6}\frac{x_{23}+iy_{23}}{r_{23}^2} z_{23} y_T(r_{23})\psi(121) \qquad (7.7)
\end{aligned}$$

However we can expand $\psi(211)$ and $\psi(121)$ as

$$\begin{aligned}
\psi(211) &= \frac{1}{2}\psi^s + \frac{\sqrt{3}}{2}\psi^a \\
\psi(121) &= \frac{\sqrt{3}}{2}\psi^s - \frac{1}{2}\psi^a
\end{aligned}$$

where s = symmetric and a = antisymmetric refer to the symmetry under the $2 \leftrightarrows 3$ transposition. Using the fact that due to symmetry only ψ^s will couple to $\overline{\psi}$, we come to the conclusion that

$$\langle\Psi_1(M_S)|\vec{\tau}_2.\vec{\tau}_3 S_{23}|\Psi_4(M'_S)\rangle = -\frac{3\sqrt{6}}{2}\int \psi(111)\frac{x_{23}+iy_{23}}{r_{23}} z_{23} y_T(r_{23}^2)\psi^s$$

We now see that apart from an insignificant overall phase factor the two matrix elements are the same.

This example was very illustrative. We have learnt that, for correlated functions, it is immaterial which two particles we choose to make special. However it is critical that we choose the *same* two particles for the space, spin and isospin parts of the wavefunction. If we do not, then we get a spurious coupling between $\psi(111)$ and ψ^a, which in general,

[4]Equation 7.7 clearly shows, why this method does not make sense for the H-J. The problem is that the y_T in the H-J has hidden superscripts which tell us whether the matrix element is to be calculated with respect to even-triplet, even-singlet, odd-triplet or odd-singlet states. However, for the $\vec{\tau}_2.\vec{\tau}_3 S_{23}$ case, we can see that there is non-zero coupling between odd and even states. Hence practically speaking, we would not know which value of y_T to use.

complicates the computation. However, for H-J, this coupling leads to an even more serious problem: it leads to ambiguities because of the form (even-singlet etc.) of the H-J and we cannot calculate the matrix element.

7.7 An Observation

Historically, in this field, the expansion has always been done in the last two particles. This was probably been done for two reasons, one of which is fundamental and the other, probably conventional.

- Physically it was natural to think about the many-electron (or many-nucleon) problem as building up the shells by putting in one electron (or nucleon) at a time. This naturally leads to the particle numbering in which the last particles were in the outer shells. This we believe to be a conventional reason.
- However, there is a deeper reason why it makes sense to use this numbering. In Appendix B and the references cited there, we can see that for uncorrelated spatial wavefunctions (e.g. shell model wavefunctions), to utilize the full power of Racah's method, we need Racah's factorization Lemma. This lemma only makes sense if we treat the last two nucleons as special.

However, in our case, since we cannot use Racah's Lemma, it is better for us to expand in the first two coordinates. The reason for choosing the first two particles is that given a function f corresponding to any Yamanouchi symbol Y, f is always either symmetric or antisymmetric under the exchange of the first two particles (because 1 always has to appear in the left-most top-most box and 2 has to be adjacent to it. And in a Yamanouchi symbol, when two consecutive integers appear in consecutive rows (and the same column) they are antisymmetric and when they appear in consecutive columns (and the same row) they are symmetric). This approach has the advantage that we do not have to do any work on our original wavefunctions.

We have learnt four important lessons from this chapter:

1. We should keep our symmetries consistent.

2. If we do nothing to our spatial wavefunctions, because of the way they were constructed, they will be symmetric or antisymmetric under the exchange of the first two particles.

3. Since we are not using the classical method, it is not advisable to transform all the wavefunctions into being symmetric or antisymmetric under the exchange of last two particles. We are better off using our original wavefunctions.

4. Because we will be taking our matrix element with the V_{12} operators, expressing our wavefunctions in terms of singlets or triplets, made up by coupling particles 1 and 2, will make our computations easier.

We will apply these ideas in the next two chapters to calculate our matrix elements.

Chapter 8

Three-body Matrix Elements

From the last chapter, we know that since our wavefunctions are arbitrary, we will not be able to utilize the full power of Racah's method. However, we will get some simplifications due to our approach: symmetry will prevent the coupling of symmetric and antisymmetric states. As noted in the last chapter, we should rewrite our wavefunctions so that the coupling is between particles 1 and 2. This will make the computation much easier. We will then calculate the three-body matrix element in two steps:

1. First, we only calculate the isospin part of the matrix element. In this step we can use the fact that V_{12} is symmetric under the exchange of 1 and 2, so there can be no coupling between symmetric and antisymmetric states[1].

2. We then tabulate the results for the spin matrix elements.

The results of Step 1 are multi-dimensional spatial integrals of spin matrix elements. We can use the spin matrix elements from Step 2, to reduce the results of Step 1 to multi-dimensional spatial integrals. This approach was followed because there are two classes of operators in the H-J potential: those with $\vec{\tau}_1.\vec{\tau}_2$. dependence and those with no isospin dependence. From section 7.3 we know that $\vec{\tau}_1.\vec{\tau}_2$ is a diagonal operator with a value -3 for a singlet and +1 for a triplet. Hence, it is convenient to remove the isospin dependence

[1]This is a direct consequence of the Wigner-Eckart theorem applied to the symmetric group. It can also be seen directly since there are only two representations of $S(2)$.

from the matrix elements first. The spin matrix elements are also not difficult to evaluate since we have expanded our spin wavefunctions in terms of singlets and triplets made from particles 1 and 2. Hence, we can use our two-body results from section 7.3 to compute the matrix elements. These calculations can be done by hand but get to be somewhat tedious. We checked these calculations by using Mathematica.

8.1 Three-body Wavefunctions

For our applications, we are only interested in the $T = \frac{1}{2}$ state. Using

$$\begin{aligned}
\phi(211) &= \alpha^s \\
\phi(121) &= \alpha^a \\
\phi(111) &= \overline{\phi} \\
\Gamma(211) &= \beta^s \\
\Gamma(121) &= \beta^a \\
\psi(111) &= \overline{\psi} \\
\psi(321) &= \tilde{\psi} \\
\psi(211) &= \psi^s \\
\psi(121) &= \psi^a
\end{aligned}$$

as our new shorthand, we can rewrite our wavefunctions as

S = $\frac{1}{2}$

$$\begin{aligned}
\Psi_1 &= \overline{\psi}\frac{1}{\sqrt{2}}[\alpha^s\beta^a - \alpha^a\beta^s] \\
\Psi_2 &= \tilde{\psi}\frac{1}{\sqrt{2}}[\alpha^s\beta^s + \alpha^a\beta^a] \\
\Psi_3 &= -\frac{1}{2}\psi^s[\alpha^s\beta^a + \alpha^a\beta^s] - \frac{1}{2}\psi^a[\alpha^s\beta^s - \alpha^a\beta^a]
\end{aligned}$$

$\mathbf{S} = \frac{3}{2}$

$$\Psi_4 = \frac{1}{\sqrt{2}}\left[\psi^s\overline{\phi}\beta^a - \psi^a\overline{\phi}\beta^s\right]$$

8.2 Matrix Elements

In the Hamada-Johnston potential the operators are either of the form $\vec{\tau}_1.\vec{\tau}_2\theta$ or just θ, where θ has no dependence on the isospin variables.

8.2.1 Isospin dependent matrix elements

$$\langle\Psi_1(M_S, M_T)|\vec{\tau}_1.\vec{\tau}_2\theta|\Psi_1(M'_S, M'_I)\rangle = \frac{1}{2}\int\overline{\psi}^*\left[-3y^{et}\langle\alpha^s|\theta|\alpha^s\rangle + y^{es}\langle\alpha^a|\theta|\alpha^a\rangle\right]\overline{\psi}\delta_{M_T,M'_T}$$

$$\langle\Psi_1(M_S, M_T)|\vec{\tau}_1.\vec{\tau}_2\theta|\Psi_2(M'_S, M'_I)\rangle = 0$$

$$\langle\Psi_1(M_S, M_T)|\vec{\tau}_1.\vec{\tau}_2\theta|\Psi_3(M'_S, M'_I)\rangle = \frac{1}{2\sqrt{2}}\int\overline{\psi}^*\left[3y^{et}\langle\alpha^s|\theta|\alpha^s\rangle + y^{es}\langle\alpha^a|\theta|\alpha^a\rangle\right]\psi^s\delta_{M_T,M'_T}$$

$$\langle\Psi_1(M_S, M_T)|\vec{\tau}_1.\vec{\tau}_2\theta|\Psi_4(M'_S, M'_I)\rangle = -\frac{3}{2}\int\overline{\psi}^* y^{et}\langle\alpha^s|\theta|\overline{\phi}\rangle\psi^s\delta_{M_T,M'_T}$$

$$\langle \Psi_2(M_S, M_T)|\vec{\tau}_1.\vec{\tau}_2\theta|\Psi_2(M'_S, M'_I)\rangle =$$
$$\frac{1}{2}\int \tilde{\psi}^* \left[y^{ot}\langle\alpha^s|\theta|\alpha^s\rangle - 3y^{os}\langle\alpha^a|\theta|\alpha^a\rangle\right]\tilde{\psi}\delta_{M_T,M'_T}$$

$$\langle \Psi_2(M_S, M_T)|\vec{\tau}_1.\vec{\tau}_2\theta|\Psi_3(M'_S, M'_I)\rangle =$$
$$-\frac{1}{2\sqrt{2}}\int \tilde{\psi}^* \left[y^{ot}\langle\alpha^s|\theta|\alpha^s\rangle + 3y^{os}\langle\alpha^a|\theta|\alpha^a\rangle\right]\psi^a\delta_{M_T,M'_T}$$

$$\langle \Psi_2(M_S, M_T)|\vec{\tau}_1.\vec{\tau}_2\theta|\Psi_4(M'_S, M'_I)\rangle =$$
$$-\frac{1}{2}\int \tilde{\psi}^* y^{ot}\langle\alpha^s|\theta|\bar{\phi}\rangle\psi^a\delta_{M_T,M'_T}$$

$$\langle \Psi_3(M_S, M_T)|\vec{\tau}_1.\vec{\tau}_2\theta|\Psi_3(M'_S, M'_I)\rangle =$$
$$\frac{1}{4}\int \psi^{s*} \left[-3y^{et}\langle\alpha^s|\theta|\alpha^s\rangle + y^{es}\langle\alpha^a|\theta|\alpha^a\rangle\right]\psi^s\delta_{M_T,M'_T} +$$
$$\frac{1}{4}\int \psi^{a*} \left[y^{ot}\langle\alpha^s|\theta|\alpha^s\rangle - 3y^{os}\langle\alpha^a|\theta|\alpha^a\rangle\right]\psi^a\delta_{M_T,M'_T}$$

$$\langle \Psi_3(M_S, M_T)|\vec{\tau}_1.\vec{\tau}_2\theta|\Psi_4(M'_S, M'_I)\rangle =$$
$$\frac{3}{2\sqrt{2}}\int \psi^{s*} y^{et}\langle\alpha^s|\theta|\bar{\phi}\rangle\psi^s\delta_{M_T,M'_T} + \frac{1}{2\sqrt{2}}\int \psi^{a*} y^{ot}\langle\alpha^s|\theta|\bar{\phi}\rangle\psi^a\delta_{M_T,M'_T}$$

$$\langle \Psi_4(M_S, M_T)|\vec{\tau}_1.\vec{\tau}_2\theta|\Psi_4(M'_S, M'_I)\rangle =$$
$$-\frac{3}{2}\int \psi^{s*}\langle y^{et}\overline{\phi}|\theta|\overline{\phi}\rangle\psi^s\delta_{M_T,M'_T} + \frac{1}{2}\int \psi^{a*}y^{ot}\langle\overline{\phi}|\theta|\overline{\phi}\rangle\psi^a\delta_{M_T,M'_T}$$

8.2.2 Isospin independent matrix elements

$$\langle \Psi_1(M_S, M_T)|\theta|\Psi_1(M'_S, M'_I)\rangle =$$
$$\frac{1}{2}\int \overline{\psi}^*\left[y^{et}\langle\alpha^s|\theta|\alpha^s\rangle + y^{es}\langle\alpha^a|\theta|\alpha^a\rangle\right]\overline{\psi}\delta_{M_T,M'_T}$$

$$\langle \Psi_1(M_S, M_T)|\theta|\Psi_2(M'_S, M'_I)\rangle = 0$$

$$\langle \Psi_1(M_S, M_T)|\theta|\Psi_3(M'_S, M'_I)\rangle =$$
$$-\frac{1}{2\sqrt{2}}\int \overline{\psi}^*\left[y^{et}\langle\alpha^s|\theta|\alpha^s\rangle - y^{es}\langle\alpha^a|\theta|\alpha^a\rangle\right]\psi^s\delta_{M_T,M'_T}$$

$$\langle \Psi_1(M_S, M_T)|\theta|\Psi_4(M'_S, M'_I)\rangle =$$
$$\frac{1}{2}\int \overline{\psi}^* y^{et}\langle\alpha^s|\theta|\overline{\phi}\rangle\psi^s\delta_{M_T,M'_T}$$

$$\langle \Psi_2(M_S, M_T)|\theta|\Psi_2(M'_S, M'_I)\rangle =$$
$$\frac{1}{2}\int \tilde{\psi}^*\left[y^{ot}\langle\alpha^s|\theta|\alpha^s\rangle + y^{os}\langle\alpha^a|\theta|\alpha^a\rangle\right]\tilde{\psi}\delta_{M_T,M'_T}$$

$$\langle \Psi_2(M_S, M_T)|\theta|\Psi_3(M'_S, M'_I)\rangle =$$
$$-\frac{1}{2\sqrt{2}} \int \tilde{\psi}^* \left[y^{ot} \langle \alpha^s|\theta|\alpha^s\rangle - y^{os} \langle \alpha^a|\theta|\alpha^a\rangle \right] \psi^a \delta_{M_T, M'_T}$$

$$\langle \Psi_2(M_S, M_T)|\theta|\Psi_4(M'_S, M'_I)\rangle =$$
$$-\frac{1}{2} \int \tilde{\psi}^* y^{ot} \langle \alpha^s|\theta|\overline{\phi}\rangle \psi^a \delta_{M_T, M'_T}$$

$$\langle \Psi_3(M_S, M_T)|\theta|\Psi_3(M'_S, M'_I)\rangle =$$
$$\frac{1}{4} \int \psi^{s*} \left[y^{et} \langle \alpha^s|\theta|\alpha^s\rangle + y^{es} \langle \alpha^a|\theta|\alpha^a\rangle \right] \psi^s \delta_{M_T, M'_T} +$$
$$\frac{1}{4} \int \psi^{a*} \left[y^{ot} \langle \alpha^s|\theta|\alpha^s\rangle + y^{os} \langle \alpha^a|\theta|\alpha^a\rangle \right] \psi^a \delta_{M_T, M'_T}$$

$$\langle \Psi_3(M_S, M_T)|\theta|\Psi_4(M'_S, M'_I)\rangle =$$
$$-\frac{1}{2\sqrt{2}} \int \psi^{s*} y^{et} \langle \alpha^s|\theta|\overline{\phi}\rangle \psi^s \delta_{M_T, M'_T} + \frac{1}{2\sqrt{2}} \int \psi^{a*} y^{ot} \langle \alpha^s|\theta|\overline{\phi}\rangle \psi^a \delta_{M_T, M'_T}$$

$$\langle \Psi_4(M_S, M_T)|\theta|\Psi_4(M'_S, M'_I)\rangle =$$
$$\frac{1}{2} \int \psi^{s*} y^{et} \langle \overline{\phi}|\theta|\overline{\phi}\rangle \psi^s \delta_{M_T, M'_T} + \frac{1}{2} \int \psi^{a*} y^{ot} \langle \overline{\phi}|\theta|\overline{\phi}\rangle \psi^a \delta_{M_T, M'_T}$$

Thus, in order to evaluate these matrix elements, we need to know the various spin matrix elements, which are tabulated in the next section.

8.3 Spin Matrix Elements

We know that the first two particles can couple to form a singlet or a triplet. Hence, we can rewrite our wavefunctions of chapter 5 as [2]

$$
\begin{aligned}
\alpha^s(\frac{1}{2}) &= \sqrt{\frac{2}{3}}|S=1,M_S=1\rangle\downarrow -\frac{1}{\sqrt{3}}|S=1,M_S=0\rangle\uparrow \\
\alpha^s(-\frac{1}{2}) &= \frac{1}{\sqrt{3}}|S=1,M_S=0\rangle\downarrow -\sqrt{\frac{2}{3}}|S=1,M_S=-1\rangle\uparrow \\
\alpha^a(\frac{1}{2}) &= |S=0\rangle\uparrow \\
\alpha^a(-\frac{1}{2}) &= |S=0\rangle\downarrow \\
\overline{\phi}(\frac{3}{2}) &= |S=1,M_S=1\rangle\uparrow \\
\overline{\phi}(\frac{1}{2}) &= \sqrt{\frac{2}{3}}|S=1,M_S=0\rangle\uparrow +\frac{1}{\sqrt{3}}|S=1,M_S=1\rangle\downarrow \\
\overline{\phi}(-\frac{1}{2}) &= \sqrt{\frac{2}{3}}|S=1,M_S=0\rangle\downarrow +\frac{1}{\sqrt{3}}|S=1,M_S=-1\rangle\uparrow \\
\overline{\phi}(-\frac{3}{2}) &= |S=1,M_S=-1\rangle\downarrow
\end{aligned}
$$

Now we can simply evaluate these three-body matrix elements[3] in terms of the two-body matrix elements of the last chapter. The results are

[2] Since isospin is completely analogous to spin, we do not explicitly rewrite the isospin part.

[3] In the following formulas we skip the S label in the triplet state i.e. $|S=1,M_S\rangle = |M_S\rangle$ but write down all the quantum numbers for the singlet case.

$$
\begin{aligned}
\langle \alpha^s(\frac{1}{2})|\theta_{12}|\alpha^s(\frac{1}{2})\rangle &= \frac{2}{3}\langle 1|\theta_{12}|1\rangle + \frac{1}{3}\langle 0|\theta_{12}|0\rangle \\
\langle \alpha^s(\frac{1}{2})|\theta_{12}|\alpha^s(-\frac{1}{2})\rangle &= \frac{\sqrt{2}}{3}\langle 1|\theta_{12}|0\rangle + \frac{\sqrt{2}}{3}\langle 0|\theta_{12}|-1\rangle \\
\langle \alpha^s(\frac{1}{2})|\theta_{12}|\overline{\phi}(\frac{3}{2})\rangle &= -\frac{1}{\sqrt{3}}\langle 0|\theta_{12}|1\rangle \\
\langle \alpha^s(\frac{1}{2})|\theta_{12}|\overline{\phi}(\frac{1}{2})\rangle &= \frac{\sqrt{2}}{3}\langle 1|\theta_{12}|1\rangle - \frac{\sqrt{2}}{3}\langle 0|\theta_{12}|0\rangle \\
\langle \alpha^s(\frac{1}{2})|\theta_{12}|\overline{\phi}(-\frac{1}{2})\rangle &= \frac{2}{3}\langle 1|\theta_{12}|0\rangle - \frac{1}{3}\langle 0|\theta_{12}|-1\rangle \\
\langle \alpha^s(\frac{1}{2})|\theta_{12}|\overline{\phi}(-\frac{3}{2})\rangle &= \sqrt{\frac{2}{3}}\langle 1|\theta_{12}|-1\rangle
\end{aligned}
$$

$$
\begin{aligned}
\langle \alpha^s(-\frac{1}{2})|\theta_{12}|\alpha^s(-\frac{1}{2})\rangle &= \frac{1}{3}\langle 0|\theta_{12}|0\rangle + \frac{2}{3}\langle -1|\theta_{12}|-1\rangle \\
\langle \alpha^s(-\frac{1}{2})|\theta_{12}|\overline{\phi}(\frac{3}{2})\rangle &= -\sqrt{\frac{2}{3}}\langle -1|\theta_{12}|1\rangle \\
\langle \alpha^s(-\frac{1}{2})|\theta_{12}|\overline{phi}(\frac{1}{2})\rangle &= -\frac{2}{3}\langle -1|\theta_{12}|0\rangle + \frac{1}{3}\langle 0|\theta_{12}|1\rangle \\
\langle \alpha^s(-\frac{1}{2})|\theta_{12}|\overline{\phi}(-\frac{1}{2})\rangle &= \frac{\sqrt{2}}{3}\langle 0|\theta_{12}|0\rangle - \frac{\sqrt{2}}{3}\langle -1|\theta_{12}|-1\rangle \\
\langle \alpha^s(-\frac{1}{2})|\theta_{12}|\overline{\phi}(-\frac{3}{2})\rangle &= \frac{1}{\sqrt{3}}\langle 0|\theta_{12}|-1\rangle \\
\langle \alpha^a(\frac{1}{2})|\theta_{12}|\alpha^a(\frac{1}{2})\rangle &= \langle S=0, M_S=0|\theta_{12}|S=0, M_S=0\rangle
\end{aligned}
$$

$$
\begin{aligned}
\langle \alpha^a(\frac{1}{2})|\theta_{12}|\alpha^a(-\frac{1}{2})\rangle &= 0 \\
\langle \alpha^a(-\frac{1}{2})|\theta_{12}|\alpha^a(-\frac{1}{2})\rangle &= \langle S=0, M_S=0|\theta_{12}|S=0, M_S=0\rangle \\
\langle \bar{\phi}(\frac{3}{2})|\theta_{12}|\bar{\phi}(\frac{3}{2})\rangle &= \langle 1|\theta_{12}|1\rangle \\
\langle \bar{\phi}(\frac{3}{2})|\theta_{12}|\bar{\phi}(\frac{1}{2})\rangle &= \sqrt{\frac{2}{3}}\langle 1|\theta_{12}|0\rangle \\
\langle \bar{\phi}(\frac{3}{2})|\theta_{12}|\bar{\phi}(-\frac{1}{2})\rangle &= \frac{1}{\sqrt{3}}\langle 1|\theta_{12}|-1\rangle \\
\langle \bar{\phi}(\frac{3}{2})|\theta_{12}|\bar{\phi}(-\frac{3}{2})\rangle &= 0
\end{aligned}
$$

$$
\begin{aligned}
\langle \bar{\phi}(\frac{1}{2})|\theta_{12}|\bar{\phi}(\frac{1}{2})\rangle &= \frac{2}{3}\langle 0|\theta_{12}|0\rangle + \frac{1}{3}\langle 1|\theta_{12}|1\rangle \\
\langle \bar{\phi}(\frac{1}{2})|\theta_{12}|\bar{\phi}(-\frac{1}{2})\rangle &= \frac{\sqrt{2}}{3}\langle 0|\theta_{12}|-1\rangle + \frac{\sqrt{2}}{3}\langle 1|\theta_{12}|0\rangle \\
\langle \bar{\phi}(\frac{1}{2})|\theta_{12}|\bar{\phi}(-\frac{3}{2})\rangle &= \frac{1}{\sqrt{3}}\langle 1|\theta_{12}|-1\rangle
\end{aligned}
$$

$$
\begin{aligned}
\langle \bar{\phi}(-\frac{1}{2})|\theta_{12}|\bar{\phi}(-\frac{1}{2})\rangle &= \frac{2}{3}\langle 0|\theta_{12}|0\rangle + \frac{1}{3}\langle -1|\theta_{12}|-1\rangle \\
\langle \bar{\phi}(-\frac{1}{2})|\theta_{12}|\bar{\phi}(-\frac{3}{2})\rangle &= \sqrt{\frac{2}{3}}\langle 0|\theta_{12}|-1\rangle \\
\langle \bar{\phi}(-\frac{3}{2})|\theta_{12}|\bar{\phi}(-\frac{3}{2})\rangle &= \langle -1|\theta_{12}|-1\rangle
\end{aligned}
$$

Chapter 9

Four-body Matrix Elements

In this chapter we will summarize our results for the four-body matrix elements. These are completely new results. The wavefunctions used will be from chapter 6, since these functions naturally have appropriate symmetry properties under the exchange of particles 1 and 2.

^4He has T = 0. This is the case that we will be dealing with here. For the evaluation of the matrix elements, we repeat the techniques of chapter 8. Namely, we will first expand our spin/isospin wavefunctions (which have special properties under $1 \leftrightarrows 2$), in terms of a basis in which the first two particles are coupled to form singlets and triplets. We then calculate the four-body matrix element in two steps

1. Evaluate the isospin dependent matrix element first.

2. Tabulate the results for the spin matrix elements.

9.1 Four-body Wavefunctions

Using the shorthand that

$$\phi(2211, M_S = 0) \quad = \quad \phi^s$$

$$
\begin{aligned}
\phi(2121, M_S = 0) &= \phi^a \\
\phi(2111, M_S) &= \alpha^s(M_S) \\
\phi(1211, M_S) &= \beta^s(M_S) \\
\phi(1121, M_S) &= \gamma^a(M_S) \\
\phi(1111, M_S) &= \overline{\phi}(M_S) \\
\Gamma(2211, M_T = 0) &= \Gamma^s \\
\Gamma(2121, M_T = 0) &= \Gamma^a \\
\Gamma(1111, M_T) &= \overline{\Gamma}
\end{aligned}
$$

we see that the $T = 0$ wavefunctions are

S = 0

$$
\begin{aligned}
\Psi_1 &= \psi(1111)\frac{1}{\sqrt{2}}[\phi^s\Gamma^a - \phi^a\Gamma^s] \\
\Psi_2 &= \psi(4321)\frac{1}{\sqrt{2}}[\phi^s\Gamma^s + \phi^a\Gamma^a] \\
\Psi_3 &= -\frac{1}{2}\psi(2211)[\phi^s\Gamma^a + \phi^a\Gamma^s] - \frac{1}{2}\psi(2121)[\phi^s\Gamma^s - \phi^a\Gamma^a]
\end{aligned}
$$

S = 1

$$
\begin{aligned}
\Psi_4 &= \frac{1}{\sqrt{6}}\psi(2111)[\beta^s\Gamma^a - \gamma^a\Gamma^s] + \\
&\quad \frac{1}{2\sqrt{3}}\psi(1211)\left[\sqrt{2}\alpha^s\Gamma^a + \beta^s\Gamma^a + \gamma^a\Gamma^s\right] + \\
&\quad \frac{1}{2\sqrt{3}}\psi(1121)\left[-\sqrt{2}\alpha^s\Gamma^s + \beta^s\Gamma^s - \gamma^a\Gamma^a\right] \\
\Psi_5 &= \frac{1}{2\sqrt{3}}\psi(3211)\left[\sqrt{2}\alpha^s\Gamma^a - \beta^s\Gamma^a - \gamma^a\Gamma^s\right] - \\
&\quad \frac{1}{2\sqrt{3}}\psi(3121)\left[\sqrt{2}\alpha^s\Gamma^s + \beta^s\Gamma^s - \gamma^a\Gamma^a\right] + \\
&\quad \frac{1}{\sqrt{6}}\psi(1321)[\beta^s\Gamma^s + \gamma^a\Gamma^a]
\end{aligned}
$$

S = 2

$$\Psi_6 = \frac{1}{\sqrt{2}}\left[\psi(2211)\bar{\phi}\Gamma^a - \psi(2121)\bar{\phi}\Gamma^s\right]$$

9.2 Matrix Elements

As with the three-body case, we use the observation that the nuclear force operators are of two types i.e. they are either of the form $\vec{\tau}_1.\vec{\tau}_2\theta_{12}$ or θ_{12} where θ_{12} depends on the spatial and spin parts only.

9.2.1 Isospin dependent matrix elements

Using $V = \vec{\tau}_1.\vec{\tau}_2\theta_{12}$, we can write down the matrix elements (dropping the subscripts on θ.

$$\langle\Psi_1|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_1\rangle = \frac{1}{2}\int\bar{\psi}^*\left[-3y^{et}\langle\phi^s|\theta|\phi^s\rangle + y^{es}\langle\phi^a|\theta|\phi^a\rangle\right]\bar{\psi}$$

$$\langle\Psi_1|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_2\rangle = 0$$

$$\langle\Psi_1|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_3\rangle = -\frac{1}{2\sqrt{2}}\int\bar{\psi}^*\left[-3y^{et}\langle\phi^s|\theta|\phi^s\rangle - y^{es}\langle\phi^a|\theta|\phi^a\rangle\right]\psi^s$$

$$\begin{aligned}\langle\Psi_1|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_4\rangle = {} & \frac{1}{2\sqrt{3}}\int\bar{\psi}^*\left[-3y^{et}\langle\phi^s|\theta|\beta^s\rangle + y^{es}\langle\phi^a|\theta|\gamma^a\rangle\right]\psi(2111) \\ & + \frac{1}{2\sqrt{6}}\int\bar{\psi}^*\left[-3\sqrt{2}y^{et}\langle\phi^s|\theta|\alpha^s\rangle - 3y^{et}\langle\phi^s|\theta|\beta^s\rangle - y^{es}\langle\phi^a|\theta|\gamma^a\rangle\right]\psi(1211)\end{aligned}$$

$$\langle\Psi_1|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_5\rangle = \frac{1}{2\sqrt{6}}\int\overline{\psi}^*\left[-3\sqrt{2}y^{et}\langle\phi^s|\theta|\alpha^s\rangle + 3y^{et}\langle\phi^s|\theta|\beta^s\rangle\right]\psi(3211) + \frac{1}{2\sqrt{6}}\int\overline{\psi}^* y^{es}\langle\phi^a|\theta|\gamma^a\rangle\psi(3211)$$

$$\langle\Psi_1|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_6\rangle = \frac{1}{2}\int\overline{\psi}^* y^{et}\left[-3\langle\phi^s|\theta|\overline{\phi}\rangle\right]\psi(2211)$$

$$\langle\Psi_2|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_2\rangle = \frac{1}{2}\int\psi(4321)^*\left[y^{ot}\langle\phi^s|\theta|\phi^s\rangle - 3y^{os}\langle\phi^a|\theta|\phi^a\rangle\right]\psi(4321)$$

$$\langle\Psi_2|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_3\rangle = -\frac{1}{2\sqrt{2}}\int\psi(4321)^*\left[y^{ot}\langle\phi^s|\theta|\phi^s\rangle + 3y^{os}\langle\phi^a|\theta|\phi^a\rangle\right]\psi(2121)$$

$$\langle\Psi_2|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_4\rangle = \frac{1}{2\sqrt{6}}\int\psi(4321)^*\left[-\sqrt{2}y^{ot}\langle\phi^s|\theta|\alpha^s\rangle + y^{ot}\langle\phi^s|\theta|\beta^s\rangle + 3y^{os}\langle\phi^a|\theta|\gamma^a\rangle\right]\psi(1121)$$

$$\langle\Psi_2|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_5\rangle = -\frac{1}{2\sqrt{6}}\int\psi(4321)^*\left[\sqrt{2}y^{ot}\langle\phi^s|\theta|\alpha^s\rangle + y^{ot}\langle\phi^s|\theta|\beta^s\rangle + 3y^{os}\langle\phi^a|\theta|\gamma^a\rangle\right]\psi(3121) + \frac{1}{2\sqrt{3}}\int\psi(4321)^*\left[y^{ot}\langle\phi^s|\theta|\beta^s\rangle - 3y^{os}\langle\phi^a|\theta|\gamma^a\rangle\right]\psi(1321)$$

$$\langle\Psi_2|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_6\rangle = \frac{1}{2}\int\psi(4321)^*\left[-y^{os}\langle\phi^s|\theta|\overline{\phi}\rangle\right]\psi(2121)$$

$$\langle\Psi_3|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_3\rangle = \frac{1}{4}\int\psi(2211)^*\left[-3y^{et}\langle\phi^s|\theta|\phi^s\rangle + y^{es}\langle\phi^a|\theta|\phi^a\rangle\right]\psi(2211)$$
$$+\frac{1}{4}\int\psi(2121)^*\left[y^{ot}\langle\phi^s|\theta|\phi^s\rangle - 3y^{os}\langle\phi^a|\theta|\phi^a\rangle\right]\psi(2121)$$

$$\langle\Psi_3|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_4\rangle = -\frac{1}{2\sqrt{6}}\int\psi(2211)^*\left[-3y^{et}\langle\phi^s|\theta|\beta^s\rangle - y^{es}\langle\phi^a|\theta|\gamma^a\rangle\right]\psi(2111) -$$
$$\frac{1}{4\sqrt{3}}\int\psi(2211)^*\left[-3\sqrt{2}y^{et}\langle\phi^s|\theta|\alpha^s\rangle - 3y^{et}\langle\phi^s|\theta|\beta^s\rangle + y^{es}\langle\phi^a|\theta|\gamma^a\rangle\right]\psi(1211) -$$
$$\frac{1}{4\sqrt{3}}\int\psi(2121)^*\left[-\sqrt{2}y^{ot}\langle\phi^s|\theta|\alpha^s\rangle + y^{ot}\langle\phi^s|\theta|\beta^s\rangle - 3y^{os}\langle\phi^a|\theta|\gamma^a\rangle\right]\psi(1121)$$

$$\langle\Psi_3|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_5\rangle = \frac{-1}{4\sqrt{3}}\int\psi(2211)^*\left[-3y^{et}\sqrt{2}\langle\phi^s|\theta|\alpha^s\rangle + 3y^{et}\langle\phi^s|\theta_{12}|\beta\rangle - y^{es}\langle\phi^a|\theta|\gamma^a\rangle\right]\psi(3211)$$
$$+\frac{1}{4\sqrt{3}}\int\psi(2121)^*\left[\sqrt{2}y^{et}\langle\phi^s|\theta|\alpha^s\rangle + y^{et}\langle\phi^s|\theta|\beta^s\rangle - 3y^{es}\langle\phi^a|\theta|\gamma^a\rangle\right]\psi(3121)$$
$$-\frac{1}{2\sqrt{6}}\int\psi(2121)^*\left[y^{ot}\langle\phi^s|\theta|\beta^s\rangle + 3y^{os}\langle\phi^a|\theta|\gamma^a\rangle\right]\psi(1321)$$

$$\langle\Psi_3|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_6\rangle = -\frac{1}{2\sqrt{2}}\int\psi(2211)^*\left[-3y^{et}\langle\phi^s|\theta|\bar{\phi}\rangle\right]\psi(2211) +$$
$$\frac{1}{2\sqrt{2}}\int\psi(2121)^*\left[y^{ot}\langle\phi^s|\theta|\bar{\phi}\rangle\right]\psi(2121)$$

$$\begin{aligned}
\langle\Psi_4|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_4\rangle &= \frac{1}{6}\int \psi(2111)^*\left[-3y^{et}\langle\beta^s|\theta|\beta^s\rangle + y^{es}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(2111) + \\
&\frac{1}{6\sqrt{2}}\int \psi(2111)^*\left[-3\sqrt{2}y^{et}\langle\beta^s|\theta|\alpha^s\rangle - 3y^{et}\langle\beta^s|\theta|\beta^s\rangle - y^{es}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(1211) + \\
&\frac{1}{6\sqrt{2}}\int \psi(1211)^*\left[-3\sqrt{2}y^{et}\langle\alpha^s|\theta|\beta^s\rangle - 3y^{et}\langle\beta^s|\theta|\beta^s\rangle - y^{es}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(2111) \\
&+\frac{1}{12}\int \psi(1211)^*\left[-6y^{et}\langle\alpha^s|\theta|\alpha^s\rangle - 3y^{et}\langle\beta^s|\theta|\beta^s\rangle - 3\sqrt{2}y^{et}\langle\alpha^s|\theta|\beta^s\rangle\right. \\
&\left. - 3\sqrt{2}y^{et}\langle\beta^s|\theta|\alpha^s\rangle + y^{es}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(1211) + \frac{1}{12}\int \psi(1121)^*\left[2y^{ot}\langle\alpha^s|\theta|\alpha^s\rangle+\right. \\
&\left. y^{ot}\langle\beta^s|\theta|\beta^s\rangle - \sqrt{2}y^{ot}\langle\alpha^s|\theta|\beta^s - \sqrt{2}y^{ot}\langle\beta^s|\theta|\alpha^s\rangle - 3y^{os}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(1121)
\end{aligned}$$

$$\begin{aligned}
\langle\Psi_4|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_5\rangle &= \frac{1}{6\sqrt{2}}\int \psi(2111)^*\left[-3\sqrt{2}y^{et}\langle\beta^s|\theta|\alpha^s\rangle + 3y^{et}\langle\beta^s|\theta|\beta^s\rangle + y^{es}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(3211) + \\
&\frac{1}{12}\int \psi(1211)^*\left[-6y^{et}\langle\alpha^s|\theta|\alpha^s\rangle + 3y^{et}\langle\beta^s|\theta|\beta^s\rangle + 3\sqrt{2}y^{et}\langle\alpha^s|\theta|\beta^s\rangle-\right. \\
&\left. 3\sqrt{2}y^{et}\langle\beta^s|\theta|\alpha^s\rangle - y^{es}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(3211) - \frac{1}{12}\int \psi(1121)^*\left[-2y^{ot}\langle\alpha^s|\theta|\alpha^s\rangle+\right. \\
&\left. y^{ot}\langle\beta^s|\theta|\beta^s\rangle - \sqrt{2}y^{ot}\langle\alpha^s|\theta|\beta^s\rangle + \sqrt{2}y^{ot}\langle\beta^s|\theta|\alpha^s\rangle - 3y^{os}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(3121) + \\
&\frac{1}{6\sqrt{2}}\int \psi(1121)^*\left[-\sqrt{2}y^{ot}\langle\alpha^s|\theta|\beta^s\rangle + y^{ot}\langle\beta^s|\theta|\beta^s\rangle + 3y^{os}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(1321)
\end{aligned}$$

$$\begin{aligned}
\langle\Psi_4|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_6\rangle &= \frac{1}{2\sqrt{3}}\int \psi(2111)^*\left[-3y^{et}\langle\beta^s|\theta|\bar{\phi}\rangle\right]\psi(2211) + \\
&\frac{1}{2\sqrt{6}}\int \psi(1211)^*\left[-3\sqrt{2}y^{et}\langle\alpha^s|\theta|\bar{\phi}\rangle - 3y^{et}\langle\beta^s|\theta|\bar{\phi}\rangle\right]\psi(2211) + \\
&\frac{1}{2\sqrt{6}}\int \psi(1121)^*\left[y^{ot}\sqrt{2}\langle\alpha^s|\theta|\bar{\phi}\rangle - y^{ot}\langle\beta^s|\theta|\bar{\phi}\rangle\right]\psi(2121)
\end{aligned}$$

$$\begin{aligned}\langle\Psi_5|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_5\rangle &= \frac{1}{12}\int\psi(3211)^*\Big[-6y^{et}\langle\alpha^s|\theta|\alpha^s\rangle - 3y^{et}\langle\beta^s|\theta|\beta^s\rangle + 3\sqrt{2}y^{et}\langle\alpha^s|\theta|\beta^s\rangle + \\ &3\sqrt{2}y^{et}\langle\beta^s|\theta|\alpha^s\rangle + y^{es}\langle\gamma^a|\theta|\gamma^a\rangle\Big]\psi(3211) + \frac{1}{12}\int\psi(3121)^*\Big[2y^{ot}\langle\alpha^s|\theta|\alpha^s\rangle + \\ &y^{ot}\langle\beta^s|\theta|\beta^s\rangle + \sqrt{2}y^{ot}\langle\alpha^s|\theta|\beta^s\rangle + y^{ot}\sqrt{2}\langle\beta^s|\theta|\alpha^s\rangle - 3y^{os}\langle\gamma^a|\theta|\theta^a\rangle\Big]\psi(3121) - \\ &\frac{1}{6\sqrt{2}}\int\psi(3121)^*\Big[\sqrt{2}y^{ot}\langle\alpha^s|\theta|\beta^s\rangle + y^{ot}\langle\beta^s|\theta|\beta^s\rangle + 3y^{os}\langle\gamma^a|\theta|\gamma^a\rangle\Big]\psi(1321) - \\ &\frac{1}{6\sqrt{2}}\int\psi(1321)^*\Big[\sqrt{2}y^{ot}\langle\beta^s|\theta|\alpha^s\rangle + y^{ot}\langle\beta^s|\theta|\beta^s\rangle + 3y^{os}\langle\gamma^a|\theta|\gamma^a\rangle\Big]\psi(3121) + \\ &\frac{1}{6}\int\psi(1321)^*\Big[y^{ot}\langle\beta^s|\theta|\beta^s\rangle - 3y^{os}\langle\gamma^a|\theta|\gamma^a\rangle\Big]\psi(1321)\end{aligned}$$

$$\begin{aligned}\langle\Psi_5|\vec{\tau}_1.\vec{\tau}_2\theta_{12}|\Psi_6\rangle &= \frac{1}{2\sqrt{6}}\int\psi(3211)^*\Big[-3\sqrt{2}y^{et}\langle\alpha^s|\theta|\overline{\phi}+3y^{et}\langle\beta^s|\theta|\overline{\phi}\rangle\Big]\psi(2211) - \\ &\frac{1}{2\sqrt{6}}\int\psi(3121)^*\Big[-\sqrt{2}y^{ot}\langle\alpha^s|\theta|\overline{\phi}\rangle - y^{ot}\langle\beta^s|\theta|\overline{\phi}\rangle\Big]\psi(2121) + \\ &\frac{1}{2\sqrt{3}}\int\psi(1321)^*\Big[-y^{ot}\langle\beta^s|\theta|\overline{\phi}\rangle\Big]\psi(2121)\end{aligned}$$

$$\begin{aligned}\langle\Psi_6|\theta|\Psi_6\rangle &= \frac{1}{2}\int\psi(2211)^*\Big[-3y^{et}\langle\overline{\phi}|\theta|\overline{\phi}\rangle\Big]\psi(2211) + \\ &\frac{1}{2}\int\psi(2121)^*\Big[y^{ot}\langle\overline{\phi}|\theta|\overline{\phi}\rangle\Big]\psi(2121)\end{aligned}$$

9.2.2 Isospin independent matrix elements

$$\langle\Psi_1|\theta_{12}|\Psi_1\rangle = \frac{1}{2}\int\overline{\psi}^*\Big[y^{et}\langle\phi^s|\theta|\phi^s\rangle + y^{es}\langle\phi^a|\theta|\phi^a\rangle\Big]\overline{\psi}$$

$$\langle \Psi_1 | \theta_{12} | \Psi_2 \rangle = 0$$

$$\langle \Psi_1 | \theta_{12} | \Psi_3 \rangle = -\frac{1}{2\sqrt{2}} \int \overline{\psi}^* \left[y^{et} \langle \phi^s | \theta | \phi^s \rangle - y^{es} \langle \phi^a | \theta | \phi^a \rangle \right] \psi^s$$

$$\begin{aligned} \langle \Psi_1 | \theta_{12} | \Psi_4 \rangle = & \frac{1}{2\sqrt{3}} \int \overline{\psi}^* \left[y^{et} \langle \phi^s | \theta | \beta^s \rangle + y^{es} \langle \phi^a | \theta | \gamma^a \rangle \right] \psi(2111) \\ & + \frac{1}{2\sqrt{6}} \int \overline{\psi}^* \left[y^{et} \sqrt{2} \langle \phi^s | \theta | \alpha^s \rangle + y^{et} \langle \phi^s | \theta | \beta^s \rangle - y^{es} \langle \phi^a | \theta | \gamma^a \rangle \right] \psi(1211) \end{aligned}$$

$$\begin{aligned} \langle \Psi_1 | \theta_{12} | \Psi_5 \rangle = & \frac{1}{2\sqrt{6}} \int \overline{\psi}^* \left[\sqrt{2} y^{et} \langle \phi^s | \theta | \alpha^s \rangle - y^{et} \langle \phi^s | \theta | \beta^s \rangle \right] \psi(3211) \\ & + \frac{1}{2\sqrt{6}} \int \overline{\psi}^* \left[y^{es} \langle \phi^a | \theta | \gamma^a \rangle \right] \psi(3211) \end{aligned}$$

$$\langle \Psi_1 | \theta_{12} | \Psi_6 \rangle = \frac{1}{2} \int \overline{\psi}^* \left[y^{et} \langle \phi^s | \theta | \overline{\phi} \rangle \right] \psi(2211)$$

$$\langle \Psi_2 | \theta_{12} | \Psi_2 \rangle = \frac{1}{2} \int \psi(4321)^* \left[y^{ot} \langle \phi^s | \theta | \phi^s \rangle + y^{os} \langle \phi^a | \theta | \phi^a \rangle \right] \psi(4321)$$

$$\langle \Psi_2 | \theta_{12} | \Psi_3 \rangle = -\frac{1}{2\sqrt{2}} \int \psi(4321)^* \left[y^{ot} \langle \phi^s | \theta | \phi^s \rangle - y^{os} \langle \phi^a | \theta | \phi^a \rangle \right] \psi(2121)$$

$$\langle \Psi_2 | \theta_{12} | \Psi_4 \rangle = \frac{1}{2\sqrt{6}} \int \psi(4321)^* \left[-\sqrt{2} y^{ot} \langle \phi^s | \theta | \alpha^s \rangle + y^{ot} \langle \phi^s | \theta | \beta^s \rangle - y^{os} \langle \phi^a | \theta | \gamma^a \rangle \right] \psi(1121)$$

$$\langle \Psi_2 | \theta_{12} | \Psi_5 \rangle = -\frac{1}{2\sqrt{6}} \int \psi(4321)^* \left[\sqrt{2} y^{ot} \langle \phi^s | \theta | \alpha^s \rangle + y^{ot} \langle \phi^s | \theta | \beta^s \rangle - y^{os} \langle \phi^a | \theta | \gamma^a \rangle \right] \psi(3121) +$$
$$\frac{1}{2\sqrt{3}} \int \psi(4321)^* \left[y^{ot} \langle \phi^s | \theta | \beta^s \rangle + y^{os} \langle \phi^a | \theta | \gamma^a \rangle \right] \psi(1321)$$

$$\langle \Psi_2 | \theta_{12} | \Psi_6 \rangle = -\frac{1}{2} \int \psi(4321)^* \left[y^{ot} \langle \phi^s | \theta | \bar{\phi} \rangle \right] \psi(2121)$$

$$\langle \Psi_3 | \theta_{12} | \Psi_3 \rangle = \frac{1}{4} \int \psi(2211)^* \left[y^{et} \langle \phi^s | \theta | \phi^s \rangle + y^{es} \langle \phi^a | \theta | \phi^a \rangle \right] \psi(2211)$$
$$+\frac{1}{4} \int \psi(2121)^* \left[y^{ot} \langle \phi^s | \theta | \phi^s \rangle + y^{os} \langle \phi^a | \theta | \phi^a \rangle \right] \psi(2121)$$

$$\langle \Psi_3 | \theta_{12} | \Psi_4 \rangle = -\frac{1}{2\sqrt{6}} \int \psi(2211)^* \left[y^{et} \langle \phi^s | \theta | \beta^s \rangle - y^{es} \langle \phi^s | \theta | \gamma^a \rangle \right] \psi(2111) -$$
$$\frac{1}{4\sqrt{3}} \int \psi(2211)^* \left[\sqrt{2} y^{et} \langle \phi^s | \theta | \alpha^s \rangle + y^{et} \langle \phi^s | \theta | \beta^s \rangle + y^{es} \langle \phi^a | \theta | \gamma^a \rangle \right] \psi(1211) -$$
$$\frac{1}{4\sqrt{3}} \int \psi(2121)^* \left[-\sqrt{2} y^{ot} \langle \phi^s | \theta | \alpha^s \rangle + y^{ot} \langle \phi^s | \theta | \beta^s \rangle + y^{os} \langle \phi^a | \theta | \gamma^a \rangle \right] \psi(1121)$$

$$\langle\Psi_3|\theta_{12}|\Psi_5\rangle = -\frac{1}{4\sqrt{3}}\int\psi(2211)^*\left[\sqrt{2}y^{et}\langle\phi^s|\theta|\alpha^s\rangle - y^{et}\langle\phi^s|\theta|\beta\rangle - y^{es}\langle\phi^a|\theta|\gamma^a\rangle\right]\psi(3211)$$
$$+\frac{1}{4\sqrt{3}}\int\psi(2121)^*\left[\sqrt{2}y^{ot}\langle\phi^s|\theta|\alpha^s\rangle + y^{ot}\langle\phi^s|\theta|\beta^s\rangle + y^{os}\langle\phi^a|\theta|\gamma^a\rangle\right]\psi(3121)$$
$$-\frac{1}{2\sqrt{6}}\int\psi(2121)^*\left[y^{ot}\langle\phi^s|\theta|\beta^s\rangle - y^{os}\langle\phi^a|\theta|\gamma^a\rangle\right]\psi(1321)$$

$$\langle\Psi_3|\theta_{12}|\Psi_6\rangle = -\frac{1}{2\sqrt{2}}\int\psi(2211)^*\left[y^{et}\langle\phi^s|\theta|\bar{\phi}\rangle\right]\psi(2211) +$$
$$\frac{1}{2\sqrt{2}}\int\psi(2121)^*\left[y^{ot}\langle\phi^s|\theta|\bar{\phi}\rangle\right]\psi(2121)$$

$$\langle\Psi_4|\theta_{12}|\Psi_4\rangle = \frac{1}{6}\int\psi(2111)^*\left[y^{et}\langle\beta^s|\theta|\beta^s\rangle + y^{es}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(2111) +$$
$$\frac{1}{6\sqrt{2}}\int\psi(2111)^*\left[\sqrt{2}y^{et}\langle\beta^s|\theta|\alpha^s\rangle + y^{et}\langle\beta^s|\theta|\beta^s\rangle - y^{es}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(1211) +$$
$$\frac{1}{6\sqrt{2}}\int\psi(1211)^*\left[\sqrt{2}y^{et}\langle\alpha^s|\theta|\beta^s\rangle + y^{et}\langle\beta^s|\theta|\beta^s\rangle - y^{es}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(2111) +$$
$$\frac{1}{12}\int\psi(1211)^*\left[2y^{et}\langle\alpha^s|\theta|\alpha^s\rangle + y^{et}\langle\beta^s|\theta|\beta^s\rangle + \sqrt{2}y^{et}\langle\alpha^s|\theta|\beta^s\rangle + \sqrt{2}y^{et}\langle\beta^s|\theta|\alpha^s\rangle +\right.$$
$$y^{es}\langle\gamma^a|\theta|\gamma^a\rangle]\psi(1211) + \frac{1}{12}\int\psi(1121)^*\left[2y^{ot}\langle\alpha^s|\theta|\alpha^s\rangle + y^{ot}\langle\beta^s|\theta|\beta^s\rangle -\right.$$
$$\left.\sqrt{2}y^{ot}\langle\alpha^s|\theta|\beta^s - \sqrt{2}y^{ot}\langle\beta^s|\theta|\alpha^s\rangle + y^{os}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(1121)$$

$$\langle\Psi_4|\theta_{12}|\Psi_5\rangle = \frac{1}{6\sqrt{2}}\int\psi(2111)^*\left[\sqrt{2}y^{et}\langle\beta^s|\theta|\alpha^s\rangle - y^{et}\langle\beta^s|\theta|\beta^s\rangle + y^{es}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(3211) +$$
$$\frac{1}{12}\int\psi(1211)^*\left[2y^{et}\langle\alpha^s|\theta|\alpha^s\rangle - y^{et}\langle\beta^s|\theta|\beta^s\rangle - \sqrt{2}y^{et}\langle\alpha^s|\theta|\beta^s\rangle + \sqrt{2}y^{et}\langle\beta^s|\theta|\alpha^s\rangle -\right.$$
$$\left.y^{es}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(3211) - \frac{1}{12}\int\psi(1121)^*\left[-2y^{ot}\langle\alpha^s|\theta|\alpha^s\rangle + y^{ot}\langle\beta^s|\theta|\beta^s\rangle -\right.$$
$$\left.\sqrt{2}y^{ot}\langle\alpha^s|\theta|\beta^s\rangle + \sqrt{2}y^{ot}\langle\beta^s|\theta|\alpha^s\rangle + y^{os}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(3121) +$$
$$\frac{1}{6\sqrt{2}}\int\psi(1121)^*\left[-\sqrt{2}y^{ot}\alpha^s|\theta|\beta^s\rangle + y^{ot}\langle\beta^s|\theta|\beta^s\rangle - y^{os}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(1321)$$

$$\langle\Psi_4|\theta_{12}|\Psi_6\rangle = \frac{1}{2\sqrt{3}}\int\psi(2111)^*\left[y^{et}\langle\beta^s|\theta|\bar{\phi}\rangle\right]\psi(2211) +$$
$$\frac{1}{2\sqrt{6}}\int\psi(1211)^*\left[\sqrt{2}y^{et}\langle\alpha^s|\theta|\bar{\phi}\rangle + y^{et}\langle\beta^s|\theta|\bar{\phi}\rangle\right]\psi(2211) +$$
$$\frac{1}{2\sqrt{6}}\int\psi(1121)^*\left[\sqrt{2}y^{ot}\langle\alpha^s|\theta|\bar{\phi}\rangle - y^{ot}\langle\beta^s|\theta|\bar{\phi}\rangle\right]\psi(2121)$$

$$\langle\Psi_5|\theta_{12}|\Psi_5\rangle = \frac{1}{12}\int\psi(3211)^*\left[2y^{et}\langle\alpha^s|\theta|\alpha^s\rangle + y^{et}\langle\beta^s|\theta|\beta^s\rangle - \sqrt{2}y^{et}\langle\alpha^s|\theta|\beta^s\rangle - \sqrt{2}y^{et}\langle\beta^s|\theta|\alpha^s\rangle +\right.$$
$$\left.y^{es}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(3211) + \frac{1}{12}\int\psi(3121)^*\left[2y^{ot}\langle\alpha^s|\theta|\alpha^s\rangle + y^{ot}\langle\beta^s|\theta|\beta^s\rangle +\right.$$
$$\left.\sqrt{2}y^{ot}\langle\alpha^s|\theta|\beta^s\rangle + \sqrt{2}y^{ot}\langle\beta^s|\theta|\alpha^s\rangle + y^{os}\langle\gamma^a|\theta|\theta^a\rangle\right]\psi(3121) +$$
$$\frac{1}{6\sqrt{2}}\int\psi(3121)^*\left[\sqrt{2}y^{ot}\langle\alpha^s|\theta|\beta^s\rangle + y^{ot}\langle\beta^s|\theta|\beta^s\rangle - y^{os}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(1321) -$$
$$\frac{1}{6\sqrt{2}}\int\psi(1321)^*\left[\sqrt{2}y^{ot}\langle\beta^s|\theta|\alpha^s\rangle + y^{ot}\langle\beta^s|\theta|\beta^s\rangle - y^{os}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(3121) +$$
$$\frac{1}{6}\int\psi(1321)^*\left[y^{ot}\langle\beta^s|\theta|\beta^s\rangle + y^{os}\langle\gamma^a|\theta|\gamma^a\rangle\right]\psi(1321)$$

$$\langle \Psi_5 | \theta_{12} | \Psi_6 \rangle = \frac{1}{2\sqrt{6}} \int \psi(3211)^* \left[\sqrt{2} y^{et} \langle \alpha^s | \theta | \bar{\phi} \rangle - y^{et} \langle \beta^s | \theta | \bar{\phi} \rangle \right] \psi(2211) -$$
$$\frac{1}{2\sqrt{6}} \int \psi(3121)^* \left[-\sqrt{2} y^{ot} \langle \alpha^s | \theta | \bar{\phi} \rangle - y^{ot} \langle \beta^s | \theta | \bar{\phi} \rangle \right] \psi(2121) +$$
$$\frac{1}{2\sqrt{3}} \int \psi(1321)^* \left[-y^{ot} \langle \beta^s | \theta | \bar{\phi} \rangle \right] \psi(2121)$$

$$\langle \Psi_6 | \theta | \Psi_6 \rangle = \frac{1}{2} \int \psi(2211)^* \left[y^{et} \langle \bar{\phi} | \theta | \bar{\phi} \rangle \right] \psi(2211) +$$
$$\frac{1}{2} \int \psi(2121)^* \left[y^{ot} \langle \bar{\phi} | \theta | \bar{\phi} \rangle \right] \psi(2121)$$

9.3 Spin Matrix Elements

We can express our spin/isospin wavefunctions in terms of a basis which has explicit coupling between particles 1 and 2. The results are[1]

$$\begin{aligned}
\phi(2211, M_S = 0) &= -\frac{1}{\sqrt{6}}|S = 1, M_S = 0\rangle \uparrow\downarrow + \frac{1}{\sqrt{3}}|S = 1, M_S = 1\rangle \downarrow\downarrow - \\
&\quad \frac{1}{\sqrt{6}}|S = 1, M_S = 0\rangle \downarrow\uparrow + \frac{1}{\sqrt{3}}|S = 1, M_S = -1\rangle \uparrow\uparrow \\
\phi(2121, M_S = 0) &= \frac{1}{\sqrt{2}}\left[|S = 0, M_S = 0\rangle \uparrow\downarrow - |S = 0, M_S = 0\rangle \downarrow\uparrow\right] \\
\phi(2111, M_S = 1) &= \frac{\sqrt{3}}{2}|S = 1, M_S = 1\rangle \uparrow\downarrow - \frac{1}{2\sqrt{3}}|S = 1, M_S = 1\rangle \downarrow\uparrow - \\
&\quad \frac{1}{\sqrt{6}}|S = 1, M_S = 0\rangle \uparrow\uparrow \\
\phi(2111, M_S = 0) &= \frac{1}{\sqrt{6}}|S = 1, M_S = 1\rangle \downarrow\downarrow + \frac{1}{\sqrt{3}}|S = 1, M_S = 0\rangle \uparrow\downarrow - \\
&\quad \frac{1}{\sqrt{3}}|S = 1, M_S = 0\rangle \downarrow\uparrow - \frac{1}{\sqrt{6}}|S = 1, M_S = -1\rangle \uparrow\uparrow \\
\phi(2111, M_S = -1) &= \frac{1}{\sqrt{6}}|S = 1, M_S = 0\rangle \downarrow\downarrow + \frac{1}{2\sqrt{3}}|S = 1, M_S = -1\rangle \uparrow\downarrow - \\
&\quad \frac{\sqrt{3}}{2}|S = 1, M_S = -1\rangle \downarrow\uparrow
\end{aligned}$$

$$\begin{aligned}
\phi(1211, M_S = 1) &= \sqrt{\frac{2}{3}}|S = 1, M_S = 1\rangle \downarrow\uparrow - \frac{1}{\sqrt{3}}|S = 1, M_S = 0\rangle \uparrow\uparrow \\
\phi(1211, M_S = 0) &= \frac{1}{\sqrt{3}}|S = 1, M_S = 1\rangle \downarrow\downarrow - \frac{1}{\sqrt{6}}|S = 1, M_S = 0\rangle \uparrow\downarrow + \\
&\quad \frac{1}{\sqrt{6}}|S = 1, M_S = 0\rangle \downarrow\uparrow - \frac{1}{\sqrt{3}}|S = 1, M_S = -1\rangle \uparrow\uparrow \\
\phi(1211, M_S = -1) &= \frac{1}{\sqrt{3}}|S = 1, M_S = 0\rangle \downarrow\downarrow - \sqrt{\frac{2}{3}}|S = 1, M_S = -1\rangle \uparrow\downarrow
\end{aligned}$$

[1] Isospin is completely analogous to spin, so we only give the spin wavefunctions.

$$
\begin{aligned}
\phi(1121, M_S = 1) &= |S = 0, M_S = 0\rangle \uparrow\uparrow \\
\phi(1121, M_S = 0) &= \frac{1}{\sqrt{2}}\left[|S = 0, M_S = 0\rangle \uparrow\downarrow + |S = 0, M_S = 0\rangle \downarrow\uparrow\right] \\
\phi(1121, M_S = -1) &= |S = 0, M_S = 0\rangle \downarrow\downarrow \\
\phi(1111, M_S = 2) &= |S = 1, M_S = 1\rangle \uparrow\uparrow \\
\phi(1111, M_S = 1) &= \frac{1}{2}|S = 1, M_S = 1\rangle [\uparrow\downarrow + \downarrow\uparrow] + \frac{1}{\sqrt{2}}|S = 1, M_S = 0\rangle \uparrow\uparrow
\end{aligned}
$$

$$
\begin{aligned}
\phi(1111, M_S = 0) &= \frac{1}{\sqrt{6}}|S = 1, M_S = 1\rangle \downarrow\downarrow + \frac{1}{\sqrt{3}}|S = 1, M_S = 0\rangle [\uparrow\downarrow + \downarrow\uparrow] + \\
&\quad \frac{1}{\sqrt{6}}|S = 1, M_S = -1\rangle \uparrow\uparrow \\
\phi(1111, M_S = -1) &= \frac{1}{2}|S = 1, M_S = -1\rangle [\uparrow\downarrow + \downarrow\uparrow] + \frac{1}{\sqrt{2}}|S = 1, M_S = 0\rangle \downarrow\downarrow \\
\phi(1111, M_S = -2) &= |S = 1, M_S = -1\rangle \downarrow\downarrow
\end{aligned}
$$

Now we can simply evaluate these four-body matrix elements[2] in terms of the two-body matrix elements of chapter 7. The results are

$$
\begin{aligned}
\langle \phi^s|\theta|\phi^s\rangle &= \frac{1}{3}\langle -1|\theta|-1\rangle + \frac{1}{3}\langle 0|\theta|0\rangle + \frac{1}{3}\langle 1|\theta|1\rangle \\
\langle \phi^s|\theta|\alpha^s(1)\rangle &= -\frac{1}{3\sqrt{2}}\langle -1|\theta|0\rangle - \frac{1}{3\sqrt{2}}\langle 0|\theta|1\rangle \\
\langle \phi^s|\theta|\alpha^s(0)\rangle &= \frac{1}{3\sqrt{2}}\langle 1|\theta|1\rangle - \frac{1}{3\sqrt{2}}\langle -1|\theta|-1\rangle \\
\langle \phi^s|\theta|\alpha^s(-1)\rangle &= \frac{1}{3\sqrt{2}}\langle 0|\theta|-1\rangle + \frac{1}{3\sqrt{2}}\langle 1|\theta|0\rangle \\
\langle \phi^s|\theta|\beta^s(1)\rangle &= -\frac{1}{3}\langle -1|\theta|0\rangle - \frac{1}{3}\langle 0|\theta|1\rangle
\end{aligned}
$$

[2]In the following formulas we skip the S label in the triplet state i.e. $|S = 1, M_S\rangle = |M_S\rangle$ but write down all the quantum numbers for the singlet case.

$$\langle \phi^s|\theta|\beta^s(0)\rangle = \frac{1}{3}\langle 1|\theta|1\rangle - \frac{1}{3}\langle -1|\theta|-1\rangle$$
$$\langle \phi^s|\theta|\beta^s(-1)\rangle = \frac{1}{3}\langle 0|\theta|-1\rangle + \frac{1}{3}\langle 1|\theta|0\rangle$$
$$\langle \phi^s|\theta|\bar{\phi}(2)\rangle = \frac{1}{\sqrt{3}}\langle -1|\theta|1\rangle$$

$$\langle \phi^s|\theta|\bar{\phi}(1)\rangle = \frac{1}{\sqrt{6}} - \langle 1|\theta|0\rangle - \frac{1}{\sqrt{6}}\langle 0|\theta|1\rangle$$
$$\langle \phi^s|\theta|\bar{\phi}(0)\rangle = \frac{1}{3\sqrt{2}}\langle -1|\theta|-1\rangle - \frac{\sqrt{2}}{3}\langle 0|\theta|0\rangle + \frac{1}{3\sqrt{2}}\langle 1|\theta|1\rangle$$

$$\langle \phi^s|\theta|\bar{\phi}(-1)\rangle = \frac{1}{\sqrt{6}}\langle 1|\theta|0\rangle - \frac{1}{\sqrt{6}}\langle 0|\theta|-1\rangle$$
$$\langle \phi^s|\theta|\bar{\phi}(-2)\rangle = \frac{1}{\sqrt{3}}\langle 1|\theta|-1\rangle$$
$$\langle \phi^a|\theta|\phi^a\rangle = \langle S=0, M_S 0|\theta|S=0, M_S=0\rangle$$

$$\langle \phi^a|\theta|\gamma^a(1)\rangle = 0$$
$$\langle \phi^a|\theta|\gamma^a(0)\rangle = 0$$
$$\langle \phi^a|\theta|\gamma^a(-1)\rangle = 0$$
$$\langle \alpha^s(1)|\theta|\alpha^s(1)\rangle = \frac{1}{6}\langle 0|\theta|0\rangle + \frac{5}{6}\langle 1|\theta|1\rangle$$
$$\langle \alpha^s(1)|\theta|\alpha^s(0)\rangle = \frac{1}{6}\langle 0|\theta|-1\rangle + \frac{2}{3}\langle 1|\theta|0\rangle$$

$$\langle\alpha^s(1)|\theta|\alpha^s(-1)\rangle = \frac{1}{2}\langle 1|\theta|-1\rangle$$

$$\langle\alpha^s(1)|\theta|\beta^s(1)\rangle = \frac{1}{3\sqrt{2}}\langle 0|\theta|0\rangle - \frac{1}{3\sqrt{2}}\langle 1|\theta|1\rangle$$

$$\langle\alpha^s(1)|\theta|\beta^s(0)\rangle = \frac{1}{3\sqrt{2}}\langle 0|\theta|-1\rangle - \frac{\sqrt{2}}{3}\langle 1|\theta|0\rangle$$

$$\langle\alpha^s(1)|\theta|\beta^s(-1)\rangle = -\frac{1}{\sqrt{2}}\langle 1|\theta|-1\rangle$$

$$\langle\alpha^s(1)|\theta|\bar{\phi}(2)\rangle = -\frac{1}{\sqrt{6}}\langle 0|\theta|1\rangle$$

$$\langle\alpha^s(1)|\theta|\bar{\phi}(1)\rangle = -\frac{1}{2\sqrt{3}}\langle 0|\theta|0\rangle + \frac{1}{2\sqrt{3}}\langle 1|\theta|1\rangle$$

$$\langle\alpha^s(1)|\theta|\bar{\phi}(0)\rangle = -\frac{1}{6}\langle 0|\theta|-1\rangle + \frac{1}{3}\langle 1|\theta|0\rangle$$

$$\langle\alpha^s(1)|\theta|\bar{\phi}(-1)\rangle = \frac{1}{2\sqrt{3}}\langle 1|\theta|-1\rangle$$

$$\langle\alpha^s(1)|\theta|\bar{\phi}(-2)\rangle = 0$$

$$\langle\alpha^s(0)|\theta|\alpha^s(0)\rangle = \frac{1}{6}\langle -1|\theta|-1\rangle + \frac{2}{3}\langle 0|\theta|0\rangle + \frac{1}{6}\langle 1|\theta|1\rangle$$

$$\langle\alpha^s(0)|\theta|\alpha^s(-1)\rangle = \frac{2}{3}\langle 0|\theta|-1\rangle + \frac{1}{6}\langle 1|\theta|0\rangle$$

$$\langle\alpha^s(0)|\theta|\beta^s(1)\rangle = \frac{1}{3\sqrt{2}}\langle -1|\theta|0\rangle - \frac{\sqrt{2}}{3}\langle 0|\theta|1\rangle$$

$$\langle\alpha^s(0)|\theta|\beta^s(0)\rangle = \frac{1}{3\sqrt{2}}\langle -1|\theta|-1\rangle - \frac{2}{3\sqrt{2}}\langle 0|\theta|0\rangle + \frac{1}{3\sqrt{2}}\langle 1|\theta|1\rangle$$

$$\langle\alpha^s(0)|\theta|\beta^s(-1)\rangle = -\frac{\sqrt{2}}{3}\langle 0|\theta|-1\rangle + \frac{1}{3\sqrt{2}}\langle 1|\theta|0\rangle$$

$$\langle\alpha^s(0)|\theta|\bar{\phi}(2)\rangle = -\frac{1}{\sqrt{6}}\langle -1|\theta|1\rangle$$

$$\langle\alpha^s(0)|\theta|\bar{\phi}(1)\rangle = -\frac{1}{2\sqrt{3}}\langle -1|\theta|0\rangle$$

$$
\begin{aligned}
\langle \alpha^s(0)|\theta|\overline{\phi}(0)\rangle &= -\frac{1}{6}\langle -1|\theta|-1\rangle + \frac{1}{6}\langle 1|\theta|1\rangle \\
\langle \alpha^s(0)|\theta|\overline{\phi}(-1)\rangle &= \frac{1}{2\sqrt{3}}\langle 1|\theta|0\rangle \\
\langle \alpha^s(0)|\theta|\overline{\phi}(-2)\rangle &= \frac{1}{\sqrt{6}}\langle 1|\theta|-1\rangle
\end{aligned}
$$

$$
\begin{aligned}
\langle \alpha^s(-1)|\theta|\alpha^s(-1)\rangle &= \frac{5}{6}\langle -1|\theta|-1\rangle + \frac{1}{6}\langle 0|\theta|0\rangle \\
\langle \alpha^s(-1)|\theta|\beta^s(1)\rangle &= -\frac{1}{\sqrt{2}}\langle -1|\theta|1\rangle \\
\langle \alpha^s(-1)|\theta|\beta^s(0)\rangle &= -\frac{\sqrt{2}}{3}\langle -1|\theta|0\rangle + \frac{1}{3\sqrt{2}}\langle 0|\theta|1\rangle
\end{aligned}
$$

$$
\begin{aligned}
\langle \alpha^s(-1)|\theta|\beta^s(-1)\rangle &= -\frac{1}{3\sqrt{2}}\langle -1|\theta|-1\rangle + \frac{1}{3\sqrt{2}}\langle 0|\theta|0\rangle \\
\langle \alpha^s(-1)|\theta|\overline{\phi}(2)\rangle &= 0 \\
\langle \alpha^s(-1)|\theta|\overline{\phi}(1)\rangle &= -\frac{1}{2\sqrt{3}}\langle -1|\theta|1\rangle \\
\langle \alpha^s(-1)|\theta|\overline{\phi}(0)\rangle &= -\frac{1}{3}\langle -1|\theta|0\rangle + \frac{1}{6}\langle 0|\theta|1\rangle \\
\langle \alpha^s(-1)|\theta|\overline{\phi}(-1)\rangle &= -\frac{1}{2\sqrt{3}}\langle -1|\theta|-1\rangle + \frac{1}{2\sqrt{3}}\langle 0|\theta|0\rangle \\
\langle \alpha^s(-1)|\theta|\overline{\phi}(-2)\rangle &= \frac{1}{\sqrt{6}}\langle 0|\theta|-1\rangle
\end{aligned}
$$

$$
\begin{aligned}
\langle \beta^s(1)|\theta|\beta^s(1)\rangle &= \frac{1}{3}\langle 0|\theta|0\rangle + \frac{2}{3}\langle 1|\theta|1\rangle \\
\langle \beta^s(1)|\theta|\beta^s(0)\rangle &= \frac{1}{3}\langle 0|\theta|-1\rangle + \frac{1}{3}\langle 1|\theta|0\rangle \\
\langle \beta^s(1)|\theta|\beta^s(-1)\rangle &= 0 \\
\langle \beta^s(1)|\theta|\overline{\phi}(2)\rangle &= -\frac{1}{\sqrt{3}}\langle 0|\theta|1\rangle \\
\langle \beta^s(1)|\theta|\overline{\phi}(1)\rangle &= -\frac{1}{\sqrt{6}}\langle 0|\theta|0\rangle + \frac{1}{\sqrt{6}}\langle 1|\theta|1\rangle
\end{aligned}
$$

$$
\begin{aligned}
\langle \beta^s(1)|\theta|\bar{\phi}(0)\rangle &= -\frac{1}{3\sqrt{2}}\langle 0|\theta|-1\rangle + \frac{\sqrt{2}}{3}\langle 1|\theta|0\rangle \\
\langle \beta^s(1)|\theta|\bar{\phi}(-1)\rangle &= \frac{1}{\sqrt{6}}\langle 1|\theta|-1\rangle \\
\langle \beta^s(1)|\theta|\bar{\phi}(-2)\rangle &= 0 \\
\langle \beta^s(0)|\theta|\beta^s(0)\rangle &= \frac{1}{3}\langle -1|\theta|-1\rangle + \frac{1}{3}\langle 0|\theta|0\rangle + \frac{1}{3}\langle 1|\theta|1\rangle \\
\langle \beta^s(0)|\theta|\beta^s(-1)\rangle &= \frac{1}{3}\langle 0|\theta|-1\rangle + \frac{1}{3}\langle 1|\theta|0\rangle
\end{aligned}
$$

$$
\begin{aligned}
\langle \beta^s(0)|\theta|\bar{\phi}(2)\rangle &= -\frac{1}{\sqrt{3}}\langle -1|\theta|1\rangle \\
\langle \beta^s(0)|\theta|\bar{\phi}(1)\rangle &= -\frac{1}{\sqrt{6}}\langle -1|\theta|0\rangle \\
\langle \beta^s(0)|\theta|\bar{\phi}(0)\rangle &= -\frac{1}{3\sqrt{2}}\langle -1|\theta|-1\rangle + \frac{1}{3\sqrt{2}}\langle 1|\theta|1\rangle \\
\langle \beta^s(0)|\theta|\bar{\phi}(-1)\rangle &= \frac{1}{\sqrt{6}}\langle 1|\theta|0\rangle \\
\langle \beta^s(0)|\theta|\bar{\phi}(-2)\rangle &= \frac{1}{\sqrt{3}}\langle 1|\theta|-1\rangle
\end{aligned}
$$

$$
\begin{aligned}
\langle \beta^s(-1)|\theta|\beta^s(-1)\rangle &= \frac{2}{3}\langle -1|\theta|-1\rangle + \frac{1}{3}\langle 0|\theta|0\rangle \\
\langle \beta^s(-1)|\theta|\bar{\phi}(2)\rangle &= 0 \\
\langle \beta^s(-1)|\theta|\bar{\phi}(1)\rangle &= -\frac{1}{\sqrt{6}}\langle -1|\theta|1\rangle \\
\langle \beta^s(-1)|\theta|\bar{\phi}(0)\rangle &= -\frac{\sqrt{2}}{3}\langle -1|\theta|0\rangle + \frac{1}{3\sqrt{2}}\langle 0|\theta|1\rangle \\
\langle \beta^s(-1)|\theta|\bar{\phi}(-1)\rangle &= -\frac{1}{\sqrt{6}}\langle -1|\theta|-1\rangle + \frac{1}{\sqrt{6}}\langle 0|\theta|0\rangle \\
\langle \beta^s(-1)|\theta|\bar{\phi}(-2)\rangle &= \frac{1}{\sqrt{3}}\langle 0|\theta|-1\rangle \\
\langle \gamma^a(1)|\theta|\gamma^a(1)\rangle &= \langle S=0, M_S 0|\theta|S=0, M_S=0\rangle
\end{aligned}
$$

$$
\begin{aligned}
\langle \gamma^a(1)|\theta|\gamma^a(0)\rangle &= 0 \\
\langle \gamma^a(1)|\theta|\gamma^a(-1)\rangle &= 0 \\
\langle \gamma^a(0)|\theta|\gamma^a(0)\rangle &= \langle S=0, M_S 0|\theta|S=0, M_S=0\rangle \\
\langle \gamma^a(0)|\theta|\gamma^a(-1)\rangle &= 0 \\
\langle \gamma^a(-1)|\theta|\gamma^a(-1)\rangle &= \langle S=0, M_S 0|\theta|S=0, M_S=0\rangle \\
\langle \bar{\phi}(2)|\theta|\bar{\phi}(2)\rangle &= \langle 1|\theta|1\rangle \\
\langle \bar{\phi}(2)|\theta|\bar{\phi}(1)\rangle &= \frac{1}{\sqrt{2}}\langle 1|\theta|0\rangle \\
\langle \bar{\phi}(2)|\theta|\bar{\phi}(0)\rangle &= \frac{1}{\sqrt{6}}\langle 1|\theta|-1\rangle \\
\langle \bar{\phi}(2)|\theta|\bar{\phi}(-1)\rangle &= 0
\end{aligned}
$$

$$
\begin{aligned}
\langle \bar{\phi}(2)|\theta|\bar{\phi}(-2)\rangle &= 0 \\
\langle \bar{\phi}(1)|\theta|\bar{\phi}(1)\rangle &= \frac{1}{2}\langle 0|\theta|0\rangle + \frac{1}{2}\langle 1|\theta|1\rangle \\
\langle \bar{\phi}(1)|\theta|\bar{\phi}(0)\rangle &= \frac{1}{2\sqrt{3}}\langle 0|\theta|-1\rangle + \frac{1}{\sqrt{3}}\langle 1|\theta|0\rangle \\
\langle \bar{\phi}(1)|\theta|\bar{\phi}(-1)\rangle &= \frac{1}{2}\langle 1|\theta|-1\rangle \\
\langle \bar{\phi}(1)|\theta|\bar{\phi}(-2)\rangle &= 0
\end{aligned}
$$

$$
\begin{aligned}
\langle \bar{\phi}(0)|\theta|\bar{\phi}(0)\rangle &= \frac{1}{6}\langle -1|\theta|-1\rangle + \frac{2}{3}\langle 0|\theta|0\rangle + \frac{1}{6}\langle 1|\theta|1\rangle \\
\langle \bar{\phi}(0)|\theta|\bar{\phi}(-1)\rangle &= \frac{1}{\sqrt{3}}\langle 0|\theta|-1\rangle + \frac{1}{2\sqrt{3}}\langle 1|\theta|0\rangle \\
\langle \bar{\phi}(0)|\theta|\bar{\phi}(-2)\rangle &= \frac{1}{\sqrt{6}}\langle 1|\theta|-1\rangle \\
\langle \bar{\phi}(-1)|\theta|\bar{\phi}(-1)\rangle &= \frac{1}{2}\langle -1|\theta|-1\rangle + \frac{1}{2}\langle 0|\theta|0\rangle \\
\langle \bar{\phi}(-1)|\theta|\bar{\phi}(-2)\rangle &= \frac{1}{\sqrt{2}}\langle 0|\theta|-1\rangle \\
\langle \bar{\phi}(-2)|\theta|\bar{\phi}(-2)\rangle &= \langle -1|\theta|-1\rangle
\end{aligned}
$$

Chapter 10

Coupled-Channel Equations

In this chapter we will complete our task of scalarizing the H-J, the fundamental goal of this research project. We shall explicitly write down the coupled channel equations for the H-J potential. We are not aware of such a result in the literature i.e. coupled-channel equations for the H-J potential with explicit symmetry requirements on the spatial wavefunctions. For applications, these coupled-channel equations need to be solved numerically. These are very complicated coupled partial differential equations. We presume that in order to solve them, certain approximations will have to be made e.g. in certain cases *LS* terms are known to be small. For such problems, *LS* terms could be ignored. Since these differential equations are exact, the user of these differential equations, depending on the application, can make the relevant approximations to get physical results.

In this chapter, first by employing projection operators, we give a formal derivation of the coupled-channel equations. In the same section, we then show that such operators can indeed be constructed in our case. However, it is well-known, that while projection operator formalism is conceptually very simple, in practice it is not easy to compute with; the technique to use is the variational method. So we re-derive the formal coupled-channel equations via the variational method. This shows how the matrix elements of the previous chapters lead us to the coupled-channel equations directly. At the end, we tabulate some of the results for the 2-body, 3-body and 4-body cases. We do not derive all the coupled-channel equations because these can easily be written down using the matrix elements of

the previous two chapters. These results are only presented to give the reader a feel for the form of these equations.

A note of warning to the reader: the coupled-channel equations that we derive are not democratized i.e. the Hamiltonian only contains interactions between particles 1 and 2. The reason for this peculiarity is, that when we calculate the matrix elements, we give special status to particles 1 and 2. Hence, the results of the coupled-channel equations are given, with the interaction between particles 1 and 2 only. Not only is this physically unnatural, it also makes numerical computations somewhat difficult. At the end of the chapter, we show why, in the case of H-J potential, even the brute force method of matrix element calculation does not easily yield the democratized coupled-channel equations. However, the ground-state case is easy, so at the end of the chapter, we give the democratized versions of the two, three and four-body ground-state coupled-channel equations. More work is required to find a general method to yield democratized coupled-channel equations.

10.1 Projection Operators

Coupled-channel equations are formally based on Feshbach's projection operators [27, 28].

For simplicity we assume that we can expand our wavefunction as

$$\Psi = \Psi_1 + \Psi_2$$

Then

$$E(\Psi_1 + \Psi_2) = H(\Psi_1 + \Psi_2)$$

Assuming the existence of projection operators such that $P_1 + P_2 = 1$, $P_i = P_i^\dagger$, $P_i^2 = P_i$, $P_i \Psi_j = \delta_{ij} \Psi_j$, we can rewrite

$$\begin{aligned} E\Psi_1 &= P_1 H P_1 \Psi_1 + P_1 H P_2 \Psi_2 \\ E\Psi_2 &= P_2 H P_2 \Psi_2 + P_2 H P_1 \Psi_1 \end{aligned}$$

Defining $P_i H P_i = H_i$ and for $i \neq j$, $P_i H P_j = V_{ij}$ we see that our equations are in the form

$$\begin{aligned} E\Psi_1 &= H_1 \Psi_1 + V_{12}\Psi_2 \\ E\Psi_2 &= H_2 \Psi_2 + V_{21}\Psi_1 \end{aligned}$$

These are the coupled-channel equations. While such a derivation is formally very simple, in practice, the projection operators are notoriously difficult to handle. The usual procedure of actually writing down the equations is via the calculation of matrix elements. This is the method we will use ourselves. However in our case, formally, the projection operators are very simple and we can write them down as

$$1_{\mathbb{R}} \otimes 1_S \otimes 1_T = \left(\sum_i P_{ii}\right) \otimes \left(\sum_j |\phi_j\rangle\langle\phi_j|\right) \otimes \left(\sum_k |\Gamma_k\rangle\langle\Gamma_k|\right)$$

where the P_{ii} are our projection operators from chapter 2, the $|\phi_i\rangle$ are the spin states[1] and $|\Gamma\rangle$ are the isospin states.

10.2 Variational Principle

As mentioned above, the projection operator method is not a practical way of deriving coupled-channel equations. However, the variational principle does yield multi-channel equations in a straightforward manner. We will define a channel to be labeled by a spatial symmetry and a spin and isospin part, i.e. each channel wavefunction can be written as $\Psi_i = \psi_i \phi_i \gamma_i$, where ψ_i, ϕ_i and γ_i are the spatial, spin and isospin parts of the channel[2]. As an example let us assume that we have only two channels and expand our wavefunction Φ as

$$\Phi = \Psi_1 + \Psi_2$$

[1]For spin and isospin, we are merely using the property of completeness i.e. $1 = \sum_j |j\rangle\langle j|$.

[2]We will explicitly define our channels for the 2, 3 and 4 body cases later on in the chapter.

The coupled-channel equations are simply derived from

$$\delta E = \delta \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = 0 \tag{10.1}$$

Since Φ is complex we can vary $|\Phi\rangle$ and $\langle \Phi|$ independently, i.e.

$$E + \delta E = \frac{\langle \sum_i (\psi_i + \delta\psi_i)\phi_i\gamma_i | H | \sum_j \psi_j\phi_j\gamma_j \rangle}{\langle \sum_k (\psi_k + \delta\psi_k)\phi_k\gamma_k | \sum_l \psi_l\phi_l\gamma_l \rangle}$$

We know that ψ_1 and ψ_2 can be varied independently and for simplicity assume $\langle \delta\psi_1 | \psi_2 \rangle = \langle \delta\psi_2 | \psi_1 \rangle = 0$. Then we can easily show that Equation 10.1 reduces to the set of coupled-channel equations

$$\begin{aligned} E|\psi_1\rangle &= H_{11}|\psi_1\rangle + H_{12}|\psi_2\rangle \\ E|\psi_2\rangle &= H_{22}|\psi_2\rangle + H_{21}|\psi_1\rangle \end{aligned}$$

where $H_{ij} = \langle \phi_i\gamma_i | H | \phi_j\gamma_j \rangle$.

10.3 Channel Definitions

In this section we explicitly define our channels. Later on in the chapter we will see that while the number of channels multiplies very quickly with the number of nucleons, there is no channel-coupling between the symmetric and antisymmetric channels. This significantly reduces the numerical work that would be required to solve any given problem.

10.3.1 Two-body channels

The deuteron is the only stable two-body bound state with $T = 0$ and $S = 1$. This means that the spatial symmetry is $\square\square$. The relevant wavefunction is

$$\Psi_1 = \psi(11)\phi(11)\Gamma(21)$$

where $\phi(11)$ is the symmetric spin and $\Gamma(21)$ the antisymmetric isospin part[3]. We number the channels as

channel	*definition*
1	$\psi(11), M_S = 1$
2	$\psi(11), M_S = 0$
3	$\psi(11), M_S = -1$

Table 10.1: Definition of two-body channels

10.3.2 Three-body channels

From chapter 8, we know that our wavefunctions are

$$
\begin{aligned}
S &= \tfrac{1}{2} \\
\Psi_1 &= \psi_1(111)\frac{1}{\sqrt{2}}[\alpha^s\beta^a - \alpha^a\beta^s] \\
\Psi_2 &= \psi_2(321)\frac{1}{\sqrt{2}}[\alpha^s\beta^s + \alpha^a\beta^a] \\
\Psi_3 &= -\frac{1}{2}\psi_3(211)[\alpha^s\beta^a + \alpha^a\beta^s] - \frac{1}{2}\psi_3(121)[\alpha^s\beta^s - \alpha^a\beta^a] \\
S &= \tfrac{3}{2} \\
\Psi_4 &= \frac{1}{\sqrt{2}}\left[\psi_4(211)\bar{\phi}\beta^a - \psi_4(121)\bar{\phi}\beta^s\right]
\end{aligned}
$$

The only difference between these and the wavefunctions from chapter 8 is that now we have a subscript on the spatial wavefunction denoting which antisymmetric wavefunction it is derived from. This is convenient for labeling our channels.

Next we define our channels for $M_T = \frac{1}{2}$. Since the strong force does not distinguish between $M_T = \frac{1}{2}$ and $M_T = -\frac{1}{2}$, exactly the same channels can be used for $M_T = -\frac{1}{2}$. We number the channels as shown in Table 10.2.

It is important to note that there is *no channel mixing between the symmetric channels of column 1 and the antisymmetric channels of column 2* . Now we can see how group theory

[3]The symbols within the braces are the Yamanouchi symbols.

channel	*definition*	*channel*	*definition*
1	$\psi_1(111), M_S = \frac{1}{2}$	9	$\psi_2(321) M_S = \frac{1}{2}$
2	$\psi_1(111), M_S = -\frac{1}{2}$	10	$\psi_1(321) M_S = -\frac{1}{2}$
3	$\psi_3(211), M_S = \frac{1}{2}$	11	$\psi_3(121), M_S = \frac{1}{2}$
4	$\psi_3(211), M_S = -\frac{1}{2}$	12	$\psi_3(121), M_S = -\frac{1}{2}$
5	$\psi_4(211), M_S = \frac{3}{2}$	13	$\psi_4(121), M_S = \frac{3}{2}$
6	$\psi_4(211), M_S = \frac{1}{2}$	14	$\psi_4(121), M_S = \frac{1}{2}$
7	$\psi_4(211), M_S = -\frac{1}{2}$	15	$\psi_4(121), M_S = -\frac{1}{2}$
8	$\psi_4(211), M_S = -\frac{3}{2}$	16	$\psi_4(121), M_S = -\frac{3}{2}$

Table 10.2: Definition of three-body channels

cleanly separates out the channels and reduces what could have been a 16×16 matrix to two 8×8 matrices.

10.3.3 Four-body channels

From chapter 9, we know that our four-body wavefunctions are:

S = 0

$$\begin{aligned}
\Psi_1 &= \psi_1(1111)\frac{1}{\sqrt{2}}[\phi^s\Gamma^a - \phi^a\Gamma^s] \\
\Psi_2 &= \psi_2(4321)\frac{1}{\sqrt{2}}[\phi^s\Gamma^s + \phi^a\Gamma^a] \\
\Psi_3 &= -\frac{1}{2}\psi_3(2211)[\phi^s\Gamma^a + \phi^a\Gamma^s] - \frac{1}{2}\psi_3(2121)[\phi^s\Gamma^s - \phi^a\Gamma^a]
\end{aligned}$$

S = 1

$$
\begin{aligned}
\Psi_4 &= \frac{1}{\sqrt{6}}\psi_4(2111)\,[\beta^s\Gamma^a - \gamma^a\Gamma^s] + \\
&\quad \frac{1}{2\sqrt{3}}\psi_4(1211)\left[\sqrt{2}\alpha^s\Gamma^a + \beta^s\Gamma^a + \gamma^a\Gamma^s\right] + \\
&\quad \frac{1}{2\sqrt{3}}\psi_4(1121)\left[-\sqrt{2}\alpha^s\Gamma^s + \beta^s\Gamma^s - \gamma^a\Gamma^a\right] \\
\Psi_5 &= \frac{1}{2\sqrt{3}}\psi_5(3211)\left[\sqrt{2}\alpha^s\Gamma^a - \beta^s\Gamma^a - \gamma^a\Gamma^s\right] - \\
&\quad \frac{1}{2\sqrt{3}}\psi_5(3121)\left[\sqrt{2}\alpha^s\Gamma^s + \beta^s\Gamma^s - \gamma^a\Gamma^a\right] + \\
&\quad \frac{1}{\sqrt{6}}\psi_5(1321)\,[\beta^s\Gamma^s + \gamma^a\Gamma^a]
\end{aligned}
$$

S = 2

$$
\Psi_6 = \frac{1}{\sqrt{2}}\left[\psi_6(2211)\bar{\phi}\Gamma^a - \psi - 6(2121)\bar{\phi}\Gamma^s\right]
$$

where the subscripts on the spatial wavefunctions again denote which antisymmetric wavefunction it was derived from. We number the channels as given in Table 10.3. *Again the sixteen symmetric channels of the first column do not couple to any of the antisymmetric channels of the second column.*

channel	*definition*	*channel*	*definition*
1	$\psi_1(1111), M_S = 0$	17	$\psi_2(4321), M_S = 0$
2	$\psi_3(2211), M_S = 0$	18	$\psi_3(2121) M_S = 0$
3	$\psi_4(2111), M_S = 1$	19	$\psi_4(1121), M_S = 1$
4	$\psi_4(2111), M_S = 0$	20	$\psi_4(1121), M_S = 0$
5	$\psi_4(2111), M_S = -1$	21	$\psi_4(1121), M_S = -1$
6	$\psi_4(1211), M_S = 1$	22	$\psi_5(3121), M_S = 1$
7	$\psi_4(1211), M_S = 0$	23	$\psi_5(3121), M_S = 0$
8	$\psi_4(1211), M_S = -1$	24	$\psi_5(3121), M_S = -1$
9	$\psi_5(3211), M_S = 1$	25	$\psi_5(1321), M_S = 1$
10	$\psi_5(3211), M_S = 0$	26	$\psi_5(1321), M_S = 0$
11	$\psi_5(3211), M_S = -1$	27	$\psi_5(1321), M_S = -1$
12	$\psi_6(2211), M_S = 2$	28	$\psi_6(2121), M_S = 2$
13	$\psi_6(2211), M_S = 1$	29	$\psi_6(2121), M_S = 1$
14	$\psi_6(2211), M_S = 0$	30	$\psi_6(2121), M_S = 0$
15	$\psi_6(2211), M_S = -1$	31	$\psi_6(2121), M_S = -1$
16	$\psi_6(2211), M_S = -2$	32	$\psi_6(2121), M_S = -2$

Table 10.3: Definition of four-body channels

10.4 Three-body Coupled-channel Equations

The channels are defined above in section 10.3.2. As a representative we only give one 8×8 block of the coupled-channel matrix. Please note that

- The kinetic energy part is not explicitly written, but it does appear in all the diagonal terms (of the form $H_{i,i}$).

- $H_{i,j} = 3 \cdot H'_{i,j}$.

Hence the coupled-channel operator will be of the form

$$3 \cdot H'_{i,j} + \delta_{i,j} \sum_k -\frac{\hbar^2}{2m_k} \hat{\nabla}_k^2$$

$$H'_{1,1} = \frac{-\left(\left(L_x{}^2 + L_y{}^2 + L_z{}^2\right)\left(3\,y_s^e - y_t^e\right)\right)}{3} + \frac{L_z\,y_t^e}{3} - \frac{3\left(y_s^e + y_t^e\right)}{2}$$

$$H'_{1,2} = \frac{L_-\,y_t^e}{3}$$

$$H'_{1,3} = \frac{-3\left(y_s^e - y_t^e\right)}{2\sqrt{2}} - \frac{L_z\,y_t^e}{3\sqrt{2}} - \frac{\left(L_x{}^2 + L_y{}^2 + L_z{}^2\right)\left(3\,y_s^e + y_t^e\right)}{3\sqrt{2}}$$

$$H'_{1,4} = \frac{-\left(L_-\,y_t^e\right)}{3\sqrt{2}}$$

$$H'_{1,5} = \frac{-\left(L_+\,y_t^e\right)}{2\sqrt{6}} + \frac{\left(L_z\,L_+ + L_+\,L_z\right)\,y_t^e}{2\sqrt{6}} + \frac{3\sqrt{\frac{3}{2}}\,(\mathrm{i}y + x)\,y_t^e\,z}{r^2}$$

$$H'_{1,6} = \frac{L_z\,y_t^e}{3\sqrt{2}} + \frac{\left(L_x{}^2 + L_y{}^2 - 2\,L_z{}^2\right)\,y_t^e}{3\sqrt{2}} + \frac{3\,y_t^e\left(x^2 + y^2 - 2\,z^2\right)}{\sqrt{2}\,r^2}$$

$$H'_{1,7} = \frac{L_-\,y_t^e}{6\sqrt{2}} - \frac{\left(L_z\,L_- + L_-\,L_z\right)\,y_t^e}{2\sqrt{2}} + \frac{9\,(\mathrm{i}y - x)\,y_t^e\,z}{\sqrt{2}\,r^2}$$

$$H'_{1,8} = \frac{L_-\,y_t^e}{6\sqrt{2}} - \frac{\left(L_z\,L_- + L_-\,L_z\right)\,y_t^e}{2\sqrt{2}} + \frac{9\,(\mathrm{i}y - x)\,y_t^e\,z}{\sqrt{2}\,r^2}$$

$$H'_{2,2} = \frac{-\left(\left(L_x{}^2 + L_y{}^2 + L_z{}^2\right)\left(3\,y_s^e - y_t^e\right)\right)}{3} - \frac{L_z\,y_t^e}{3} - \frac{3\left(y_s^e + y_t^e\right)}{2}$$

$$H'_{2,3} = \frac{-\left(L_+\,y_t^e\right)}{3\sqrt{2}}$$

$$H'_{2,4} = \frac{L_z\,y_t^e}{3\sqrt{2}} - \frac{\left(L_x{}^2 + L_y{}^2 + L_z{}^2\right)\left(3\,y_s^e + y_t^e\right)}{3\sqrt{2}} + \frac{-3\,y_s^e + 3\,y_t^e}{2\sqrt{2}}$$

$$H'_{2,5} = \frac{L_+^{\,2}\, y_t^e}{\sqrt{6}} + \frac{3\sqrt{\frac{3}{2}}\,(iy + x)^2\, y_t^e}{r^2}$$

$$H'_{2,6} = \frac{-\left(L_+\, y_t^e\right)}{6\sqrt{2}} - \frac{\left(L_z L_+ + L_+ L_z\right) y_t^e}{2\sqrt{2}} - \frac{9\,(iy + x)\, y_t^e\, z}{\sqrt{2}\, r^2}$$

$$H'_{2,7} = \frac{L_z\, y_t^e}{3\sqrt{2}} - \frac{\left(L_x^{\,2} + L_y^{\,2} - 2L_z^{\,2}\right) y_t^e}{3\sqrt{2}} - \frac{3\, y_t^e \left(x^2 + y^2 - 2z^2\right)}{\sqrt{2}\, r^2}$$

$$H'_{2,8} = \frac{L_-\, y_t^e}{2\sqrt{6}} + \frac{\left(L_z L_- + L_- L_z\right) y_t^e}{2\sqrt{6}} + \frac{3\sqrt{\frac{3}{2}}\,(-iy + x)\, y_t^e\, z}{r^2}$$

$$H'_{3,3} = \frac{-\left(\left(L_x^{\,2} + L_y^{\,2} + L_z^{\,2}\right)\left(3\, y_s^e - y_t^e\right)\right)}{6} + \frac{L_z\, y_t^e}{6} - \frac{3\left(y_s^e + y_t^e\right)}{4}$$

$$H'_{3,4} = \frac{L_-\, y_t^e}{6}$$

$$H'_{3,5} = \frac{L_+\, y_t^e}{4\sqrt{3}} - \frac{\left(L_z L_+ + L_+ L_z\right) y_t^e}{4\sqrt{3}} - \frac{3\sqrt{3}\,(iy + x)\, y_t^e\, z}{2\, r^2}$$

$$H'_{3,6} = \frac{-\left(L_z\, y_t^e\right)}{6} - \frac{\left(L_x^{\,2} + L_y^{\,2} - 2L_z^{\,2}\right) y_t^e}{6} - \frac{3\, y_t^e \left(x^2 + y^2 - 2z^2\right)}{2\, r^2}$$

$$H'_{3,7} = \frac{-\left(L_-\, y_t^e\right)}{12} + \frac{\left(L_z L_- + L_- L_z\right) y_t^e}{4} - \frac{9\,(iy - x)\, y_t^e\, z}{2\, r^2}$$

$$H'_{3,8} = \frac{L_-^{\,2}\, y_t^e}{2\sqrt{3}} + \frac{3\sqrt{3}\,(iy - x)^2\, y_t^e}{2\, r^2}$$

$$H'_{4,4} = \frac{-\left(\left(L_x^{\,2} + L_y^{\,2} + L_z^{\,2}\right)\left(3\, y_s^e - y_t^e\right)\right)}{6} - \frac{L_z\, y_t^e}{6} - \frac{3\left(y_s^e + y_t^e\right)}{4}$$

$$H'_{4,5} = \frac{-\left(L_+^{\,2}\, y_t^e\right)}{2\sqrt{3}} - \frac{3\sqrt{3}\,(iy + x)^2\, y_t^e}{2\, r^2}$$

$$H'_{4,6} = \frac{L_+ y_t^e}{12} + \frac{(L_z L_+ + L_+ L_z) y_t^e}{4} + \frac{9\,(iy + x)\, y_t^e z}{2r^2}$$

$$H'_{4,7} = \frac{-(L_z y_t^e)}{6} + \frac{(L_x{}^2 + L_y{}^2 - 2L_z{}^2) y_t^e}{6} + \frac{3 y_t^e (x^2 + y^2 - 2z^2)}{2r^2}$$

$$H'_{4,8} = \frac{-(L_- y_t^e)}{4\sqrt{3}} - \frac{(L_z L_- + L_- L_z) y_t^e}{4\sqrt{3}} + \frac{3\sqrt{3}\,(iy - x)\, y_t^e z}{2r^2}$$

$$H'_{5,5} = \frac{-3 y_t^e}{2} + \frac{(L_x{}^2 + L_y{}^2) y_t^e}{2} + \frac{L_z y_t^e}{2} + \frac{3 y_t^e (x^2 + y^2 - 2z^2)}{2r^2}$$

$$H'_{5,6} = \frac{L_- y_t^e}{2\sqrt{3}} - \frac{(L_z L_- + L_- L_z)\,, y_t^e}{2\sqrt{3}} + \frac{3\sqrt{3}\,(iy - x)\, y_t^e z}{r^2}$$

$$H'_{5,7} = \frac{-(L_-{}^2 y_t^e)}{2\sqrt{3}} - \frac{3\sqrt{3}\,(iy - x)^2 y_t^e}{2r^2}$$

$$H'_{5,8} = 0$$

$$H'_{6,6} = \frac{-3 y_t^e}{2} + \frac{L_z y_t^e}{6} + \frac{(L_x{}^2 + L_y{}^2 + 4L_z{}^2) y_t^e}{6} - \frac{3 y_t^e (x^2 + y^2 - 2z^2)}{2r^2}$$

$$H'_{6,7} = \frac{L_- y_t^e}{3}$$

$$H'_{6,8} = \frac{-(L_-{}^2 y_t^e)}{2\sqrt{3}} - \frac{3\sqrt{3}\,(iy - x)^2 y_t^e}{2r^2}$$

$$H'_{7,7} = \frac{-3 y_t^e}{2} - \frac{L_z y_t^e}{6} + \frac{(L_x{}^2 + L_y{}^2 + 4L_z{}^2) y_t^e}{6} - \frac{3 y_t^e (x^2 + y^2 - 2z^2)}{2r^2}$$

$$H'_{7,8} = \frac{L_- y_t^e}{2\sqrt{3}} + \frac{(L_z L_- + L_- L_z) y_t^e}{2\sqrt{3}} - \frac{3\sqrt{3}\,(iy - x)\, y_t^e z}{r^2}$$

$$H'_{8,8} = \frac{-3 y_t^e}{2} + \frac{(L_x{}^2 + L_y{}^2) y_t^e}{2} - \frac{L_z y_t^e}{2} + \frac{3 y_t^e (x^2 + y^2 - 2z^2)}{2r^2}$$

10.5 Four-body Coupled-channel Equations

Note that in this section, we only give a representative sample of the equations because the number of channels is very large. Please note that

- The kinetic energy part is not explicitly written, but it does appear in all the diagonal terms (of the form $H_{i,i}$).

- $H_{i,j} = 6 \cdot H'_{i,j}$.

Hence the coupled-channel operator will be of the form

$$6 \cdot H'_{i,j} + \delta_{i,j} \sum_k -\frac{\hbar^2}{2m_k} \vec{\nabla}_k^2$$

$$\begin{aligned} H'_{1,1} &= \frac{-\left(\left(Lx^2 + Ly^2 + L_z{}^2\right)\left(3\,y_s^e - y_t^e\right)\right)}{3} - \frac{3\left(y_s^e + y_t^e\right)}{2} \\ H'_{1,2} &= \frac{-3\left(y_s^e - y_t^e\right)}{2\sqrt{2}} - \frac{\left(Lx^2 + Ly^2 + L_z{}^2\right)\left(3\,y_s^e + y_t^e\right)}{3\sqrt{2}} \end{aligned}$$

$$\begin{aligned} H'_{1,3} &= \frac{-\left(L_+\,y_t^e\right)}{3\sqrt{6}} \\ H'_{1,4} &= \frac{L_z\,y_t^e}{3\sqrt{3}} \\ H'_{1,5} &= \frac{L_-\,y_t^e}{3\sqrt{6}} \\ H'_{1,6} &= \frac{-\left(L_+\,y_t^e\right)}{3\sqrt{3}} \end{aligned}$$

$$H'_{1,7} = \frac{\sqrt{\frac{2}{3}}\, L_z\, y_t^e}{3}$$

$$H'_{1,8} = \frac{L_-\, y_t^e}{3\sqrt{3}}$$

$$H'_{1,9} = 0$$

$$H'_{1,10} = 0$$

$$H'_{1,11} = 0$$

$$H'_{1,12} = \frac{-\left(L_+^{\,2}\, y_t^e\right)}{2\sqrt{3}} - \frac{3\sqrt{3}\,(iy + x)^2\, y_t^e}{2\,r^2}$$

$$H'_{1,13} = \frac{\left(L_z L_+ + L_+ L_z\right) y_t^e}{2\sqrt{3}} + \frac{3\sqrt{3}\ (iy + x)\ y_t^e\, z}{r^2}$$

$$H'_{1,14} = \frac{\left(Lx^2 + Ly^2 - 2\,L_z^{\,2}\right) y_t^e}{3\sqrt{2}} + \frac{3\, y_t^e\, \left(x^2 + y^2 - 2\,z^2\right)}{\sqrt{2}\,r^2}$$

$$H'_{1,15} = \frac{-\left(\left(L_z L_- + L_- L_z\right) y_t^e\right)}{2\sqrt{3}} + \frac{3\sqrt{3}\ (iy - x)\ y_t^e\, z}{r^2}$$

$$H'_{1,16} = \frac{-\left(L_-^{\,2}\, y_t^e\right)}{2\sqrt{3}} - \frac{3\sqrt{3}\,(iy - x)^2\, y_t^e}{2\,r^2}$$

$$H'_{2,2} = \frac{-\left(\left(Lx^2 + Ly^2 + L_z^{\,2}\right)\left(3\, y_s^e - y_t^e\right)\right)}{6} - \frac{3\,\left(y_s^e + y_t^e\right)}{4}$$

$$H'_{2,3} = \frac{L_+\, y_t^e}{6\sqrt{3}}$$

$$H'_{2,4} = \frac{-\left(L_z\, y_t^e\right)}{3\sqrt{6}}$$

$$H'_{2,5} = \frac{-\left(L_-\, y_t^e\right)}{6\sqrt{3}}$$

$$
\begin{aligned}
H'_{2,6} &= \frac{L_+ y_t^e}{3\sqrt{6}} \\
H'_{2,7} &= \frac{-\left(L_z y_t^e\right)}{3\sqrt{3}} \\
H'_{2,8} &= \frac{-\left(L_- y_t^e\right)}{3\sqrt{6}} \\
H'_{2,9} &= 0 \\
H'_{2,10} &= 0 \\
H'_{2,11} &= 0 \\
H'_{2,12} &= \frac{{L_+}^2 y_t^e}{2\sqrt{6}} + \frac{3\sqrt{\frac{3}{2}}(iy+x)^2 y_t^e}{2r^2}
\end{aligned}
$$

$$
\begin{aligned}
H'_{2,13} &= \frac{-\left(\left(L_z L_+ + L_+ L_z\right) y_t^e\right)}{2\sqrt{6}} - \frac{3\sqrt{\frac{3}{2}}\,(iy+x)\, y_t^e z}{r^2} \\
H'_{2,14} &= \frac{-\left(\left(Lx^2 + Ly^2 - 2{L_z}^2\right) y_t^e\right)}{6} - \frac{3 y_t^e \left(x^2+y^2-2z^2\right)}{2r^2} \\
H'_{2,15} &= \frac{\left(L_- L_z + L_z L_-\right) y_t^e}{2\sqrt{6}} - \frac{3\sqrt{\frac{3}{2}}\,(iy-x)\, y_t^e z}{r^2} \\
H'_{2,16} &= \frac{{L_-}^2 y_t^e}{2\sqrt{6}} + \frac{3\sqrt{\frac{3}{2}}(iy-x)^2 y_t^e}{2r^2}
\end{aligned}
$$

10.6 Difficulty with the Brute Force Method

In this section, we show why, even with the brute force method, the democratization of the coupled-channel equations for the H-J is not easy. The reason has to do with the form of H-J, which is parameterized in terms of even-singlet, even-triplet, odd-singlet and and odd-triplet interactions. We discuss a particular 3-body example to show why such a parameterization, leads to complications in the construction of democratized coupled-channel equations.

10.6.1 Three-body example

As an example, let us calculate

$$\langle\Psi_1|\sum_{i<j}\vec{\tau}_i\cdot\vec{\tau}_j\theta_{ij}|\Psi_3\rangle$$

The brute force method is based on the fact that in order to calculate a matrix element for the ij part of the H-J potential[4], we need to expand our wavefunctions in terms of a basis which gives special status to particles i and j. The reason is that the H-J is parameterized in terms of even-singlet, even-triplet, odd-singlet and odd-triplet terms, and to calculate the matrix element, we need to know the coupling between particles i and j. As an example, let us calculate

$$\langle\Psi_1|\sum_{i<j}\vec{\tau}_i\cdot\vec{\tau}_j\theta_{ij}|\Psi_3\rangle$$

where Ψ_i are the three-body wavefunctions of chapter 8, with $M_S = M_T = 1/2$. Since we are using the brute force method, we will not utilize the Lemma in section 7.4, which gives a factor of $n(n-1)/2$ for matrix elements. So we have to calculate

$$\begin{aligned}\langle\Psi_1|\sum_{i<j}\vec{\tau}_i\cdot\vec{\tau}_j\theta_{ij}|\Psi_3\rangle &= \langle\Psi_1|\vec{\tau}_1\cdot\vec{\tau}_2\theta_{12}|\Psi_3\rangle + \langle\Psi_1|\vec{\tau}_1\cdot\vec{\tau}_3\theta_{13}|\Psi_3\rangle + \langle\Psi_1|\vec{\tau}_2\cdot\vec{\tau}_3\theta_{23}|\Psi_3\rangle \\ &= A+B+C\end{aligned}$$

We have already calculated A in chapter 8. Now we will try to compute B. As a particular example of θ_{13} we can assume that

$$\vec{\tau}_1\cdot\vec{\tau}_3\theta_{13} = \vec{\tau}_1\cdot\vec{\tau}_3\vec{\sigma}_1\cdot\vec{\sigma}_3 y_C^*(r_{13})$$

where the $*$ stands for even-singlet(*es*), even-triplet(*et*), odd-singlet(*os*) or odd-triplet(*ot*). Thus, in order to know which value of y_C^* to use, we need to know, which states we are coupling. However, the wavefunctions are given in terms of states which are *es*, *et*, *os* or *ot* only for particles 1 and 2. In order to proceed, we would need to expand our original

[4]By the ij part we mean V_{ij} in $H = \sum_{k<l} V_{kl}$.

wavefunctions, Ψ_1 and Ψ_3, in terms of wavefunctions with special status given to particles 1 and 3. This can be easily accomplished by choosing a basis of functions which diagonalizes the matrix representing the (13) permutation in the standard Young-Yamanouchi representation. The results are

$$\begin{aligned} f(211) &= \frac{\sqrt{3}}{2} f^a_{13} + \frac{1}{2} f^s_{13} \\ f(121) &= \frac{1}{2} f^a_{13} - \frac{\sqrt{3}}{2} f^a_{13} \end{aligned}$$

where, for example, $f(211)$ can represent a space(ψ), spin(ϕ) or isospin(γ) wavefunction, with Yamanouchi symbol 211 and f^a_{13} is antisymmetric and f^s_{13} is symmetric under the exchange of particles 1 and 3. By an explicit computation we can easily see that for spin wavefunctions

$$\begin{aligned} \phi^s_{13} &= -\phi(s_1 s_3(s_{13} = 1) s_2 s_{123} = \frac{1}{2}) \\ \phi^a_{13} &= \phi(s_1, s_3(s_{13} = 0) s_2 s_{123} = \frac{1}{2}) \end{aligned}$$

Similarly for isospin wavefunctions

$$\begin{aligned} \gamma^s_{13} &= -\gamma(t_1 t_3(t_{13} = 1) t_2 t_{123} = \frac{1}{2}) \\ \gamma^a_{13} &= \gamma(t_1, t_3(t_{13} = 0) t_2 t_{123} = \frac{1}{2} \end{aligned}$$

Now we can go ahead and compute the matrix element to be

$$\langle \Psi_1 | \vec{\tau}_1 \cdot \vec{\tau}_3 \vec{\sigma}_1 \cdot \vec{\sigma}_3 y^*_C(r_{13}) | \Psi_3 \rangle = \frac{1}{2\sqrt{2}} \int \psi(111)^* [-3y^{et}_C + 3y^{es}] \psi^s_{13}$$

A completely analogous calculation for V_{23} yields,

$$\langle \Psi_1 | \vec{\tau}_2 \cdot \vec{\tau}_3 \vec{\sigma}_2 \cdot \vec{\sigma}_3 y^*_C(r_{23}) | \Psi_3 \rangle = \frac{1}{2\sqrt{2}} \int \psi(111)^* [-3y^{et}_C(r_{23}) + 3y^{es}(r_{23})] \psi^s_{23}$$

However, to derive the coupled-channel equations, we need the integral to be between

wavefunctions which have special symmetry properties under the exchange of particles 1 and 2. We can then expand the spatial wavefunction ψ^s_{13} in terms of $\psi(211)$ and $\psi(121)$ to get the final answer to be

$$\langle\Psi_1|\vec{\tau}_1\cdot\vec{\tau}_3\vec{\sigma}_1\cdot\vec{\sigma}_3 y^*_C(r_{13})|\Psi_3\rangle = \frac{1}{2\sqrt{2}}\int \psi(111)^*[-3y^{et}_C(r_{13})+3y^{es}_C(r_{13})]\left(\frac{1}{2}\psi(211)-\frac{\sqrt{3}}{2}\psi(121)\right)$$

Similarly, we can expand

$$\psi^s_{23} = \frac{1}{2}\psi(211)+\frac{\sqrt{3}}{2}\psi(121)$$

to yield

$$\langle\Psi_1|\vec{\tau}_2\cdot\vec{\tau}_3\vec{\sigma}_2\cdot\vec{\sigma}_3 y^*_C(r_{23})|\Psi_3\rangle = \frac{1}{2\sqrt{2}}\int \psi(111)^*[-3y^{et}_C(r_{23})+3y^{es}(r_{23})]\left(\frac{1}{2}\psi(211)+\frac{\sqrt{3}}{2}\psi(121)\right)$$

However, these expansions, do not yield the coupled-channel equations, because we have now mixed the symmetries of the various channels i.e. we are getting coupling between symmetric and antisymmetric channels. If we go back and look at the derivation of the coupled-channel equations, it is clear that we need, in this example, for our coupled-channel operator to be only operating upon $\psi(211)$ (since that is the spatial channel-wavefunction). However, we are getting both the $\psi(211)$ and $\psi(121)$ terms. Hence, in general, for these coupled-channel equations, there does not seem to be a simple way of treating all the particles on an equal footing.

10.7 Ground-state Coupled-channel Equations

As we saw in the previous section, that there are difficulties with trying to treat all particles on an equivalent footing in the coupled-channel equations. However, the ground-state case is very simple, because the ground-state spatial wavefunctions belong to the trivial representation of the symmetric group. Hence the democratization process, is straight-forward.

The algorithm is simply to assert that for channels α and β,

$$\frac{n(n-1)}{2}V_{\alpha,\beta}(1,2) = \sum_{i<j} V_{\alpha,\beta}(i,j)$$

where $V_{\alpha,\beta}(12)$ was the coupled-channel operator for the non-democratized version of the coupled-channel equations.

10.7.1 Two-body equations

Then the diagonal parts of the coupled-channel equations can be written as

$$\begin{aligned}
H_{11} &= -\frac{\hbar^2}{2M_1}\nabla_1^2 - \frac{\hbar^2}{2M_2}\nabla_2^2 - 3y_C^{et} - 3y_T^{et}\frac{2z^2 - x^2 - y^2}{r^2} \\
&\quad + y_{LS}^{et}L_z + y_{LL}^{et}(L_x^2 + L_y^2) \\
H_{22} &= -\frac{\hbar^2}{2M_1}\nabla_1^2 - \frac{\hbar^2}{2M_2}\nabla_2^2 - 3y_C^{et} - 3y_T^{et}\frac{2x^2 + 2y^2 - 4z^2}{r^2} \\
&\quad + 2y_{LL}^{et}L_z^2 \\
H_{33} &= -\frac{\hbar^2}{2M_1}\nabla_1^2 - \frac{\hbar^2}{2M_2}\nabla_2^2 - 3y_C^{et} - 3y_T^{et}\frac{2z^2 - x^2 - y^2}{r^2} \\
&\quad - y_{LS}^{et}L_z + y_{LL}^{et}(L_x^2 + L_y^2)
\end{aligned}$$

The off-diagonal terms can also be simply written down as

$$\begin{aligned}
H_{12} &= y_T^{et}3\sqrt{2}\frac{(x-iy)z}{r^2} + y_{LS}^{et}\frac{L_-}{\sqrt{2}} - y_{LL}^{et}\frac{1}{\sqrt{2}}(L_zL_- + L_-L_z) \\
H_{13} &= y_T^{et}3\frac{(x-iy)^2}{r^2} - y_{LL}^{et}L_-^2 \\
H_{23} &= -y_T^{et}3\sqrt{2}\frac{(x-iy)z}{r^2} - y_{LS}^{et}\frac{L_-}{\sqrt{2}} + y_{LL}^{et}\frac{1}{\sqrt{2}}(L_zL_- + L_-L_z)
\end{aligned}$$

10.7.2 Three-body equations

$$
\begin{aligned}
H_{11} &= \sum_i -\frac{\hbar^2}{2M_i}\nabla_i^2 - \sum_{i<j}\frac{3}{2}\left(y_C^{es}(r_{ij}) + y_C^{et}(r_{ij})\right) + \\
&\quad \sum_{i<j}\frac{1}{3}y_{LS}^{et}(r_{ij})L_z(ij) - \sum_{i<j}\frac{1}{3}(3y_{LL}^{es}(r_{ij}) - y_{LL}^{et}(r_{ij}))\vec{L}(ij)^2 \\
H_{12} &= \sum_{i<j}\frac{1}{3}y_{LS}^{et}(r_{ij})L_-(ij) \\
H_{22} &= \sum_i -\frac{\hbar^2}{2M_i}\nabla_i^2 - \sum_{i<j}\frac{3}{2}(y_C^{es}(r_{ij}) + y_C^{et}(r_{ij})) - \\
&\quad \sum_{i<j}\frac{1}{3}y_{LS}^{et}(r_{ij})L_z(ij) - \sum_{i<j}\frac{1}{3}(3y_{LL}^{es}(r_{ij}) - y_{LL}^{et}(r_{ij}))\vec{L}(ij)^2
\end{aligned}
$$

where $L_z(ij)$, $\vec{L}(ij)$ etc. refer to the relevant angular momentum between particles i and j.

10.7.3 Four-body equations

The diagonal part of the Hamiltonian for the ground state is

$$
H_{11} = \sum_i -\frac{\hbar^2}{2M_i}\nabla_i^2 - \sum_{i<j}\frac{1}{3}(3y_{LL}^{es}(r_{ij}) - y_{LL}^{et}(r_{ij}))\vec{L}(ij)^2 - \sum_{i<j}\frac{3}{2}(y_C^{es}(r_{ij}) + y_C^{et}(r_{ij}))
$$

Chapter 11

Photodisintegration Of The Deuteron

In this chapter, we begin to explore the simplest of phonon-coupled nuclear reactions: photodisintegration of a deuteron, which is embedded in a lattice with one highly excited phonon mode. The problem of phonon-coupled reactions is a complicated one, and the work in this chapter is of a very preliminary nature. This should be regarded as a report of progress-to-date, rather than a finished result.

Interest in the photodisintegration of the deuteron started early on in nuclear physics [3, 8, 26, 66]. As a two-body problem, it is reasonably straight-forward to solve it in the center-of-mass (COM) frame[1]. We will, instead, work in the laboratory frame, because we want to look at the effects of the lattice on this reaction. This also allows us to make a connection with the thermal neutron scattering literature.

We will begin by calculating the vacuum differential cross-section. After the vacuum calculation, we compute the phonon-coupled matrix element. For this calculation, we assume that the neutron is ejected from the lattice, but the proton stays on as a part of the condensed matter environment. This assumption is required for two reasons

1. We want to make a connection with other phonon-coupled reactions that are of interest to us. These reactions are characterized by a change of phonon mode structure due to a Duschinsky [22] type mass effect e.g. $^4He \rightarrow^3 He + n$. We get a similar

[1]Center-of-mass frame is defined to be the frame in which the sum of initial momenta = 0.

mass-change effect in the photodisintegration of the deuteron, when the proton is left behind in the lattice.

2. At the moment, we do not have a way of analyzing the general case in which the proton may or may not leave the lattice.

We will show that an experiment will satisfy this assumption provided

- Energy of the incoming photon is matched to the binding energy of the deuteron.
- The emerging neutrons are nearly collinear with the incoming photon.
- We measure the energy-resolved differential cross-section.

However, in our first attempt in section 11.2, we will not calculate the energy-resolved differential cross-section, but merely the interaction matrix element. Since this work is of a preliminary nature, this computation gives us a feel for what happens in a condensed matter environment[2] However, in section 11.4, we do begin to calculate the energy-resolved forward differential cross-section. Unfortunately, due to time constraints, we were unable to complete the calculation.

Before going ahead and discussing our results, we would like to enumerate the various ways in which these calculations are incomplete. These are

1. The lattice changes by the conversion of a deuteron to a proton, and hence the initial lattice modes are different from the final lattice modes. This means that the initial thermal modes project into the final highly excited phonon mode and the initial highly excited mode projects into the final thermal phonon modes. This mode-mixing has not been properly taken into account.

2. Experimentally, we cannot initialize the lattice in an eigenstate of the highly excited phonon mode. However, we can put the lattice into a classical state. Hence we should repeat these phonon-coupled calculations with classical states instead of eigenstates.

[2]As discussed later on, this result, along with the vacuum density of states and an energy conserving delta function, should give the energy-resolved differential cross-section.

3. We calculate the energy-resolved differential cross-section in two ways:

   - In section 11.2, we calculate the interaction matrix element. This can be combined with the density of states[3] and an energy conserving Dirac delta function[4] to give the energy-resolved differential cross-section.
   - In section 11.4, we explicitly calculate the energy-resolved differential cross-section. This second method clearly shows how the Debye-Waller factor shows up in the first calculation in section 11.2.

   However, we do not prove that these two methods yield the same result.

4. We do not compute the angular momentum exchanged in this reaction. Exchange of angular momentum is one of the cornerstones of the Unified Model. By using this experiment, we should try and improve our understanding of angular momentum coupling.

11.1 Vacuum Photodisintegration of the Deuteron

We will assume that the deuteron is at rest in the laboratory frame. Suppose the photon has momentum $\vec{K}_0$, and frequency ω_0. It hits a deuteron, which disintegrates into a proton with momentum $\vec{K}_p$ and a neutron with momentum $\vec{K}_n$. We will assume that the binding energy of the deuteron is E_b ($E_b > 0$), the mass of the neutron is M_n and mass of the proton is M_p.

The differential cross-section is given by the golden rule

$$d\sigma = \frac{2\pi}{\hbar} |\langle f|V_{int}|i\rangle|^2 \rho(E_f) \frac{L^3}{c}$$

This calculation is broken into two parts: the calculation of

- density of states, $\rho(E_f)$.

[3] We can use the vacuum density of states calculated in subsection 11.1.1. The reason for this is explained in section 11.2.

[4] It is well-known [92] that to convert a two-body differential cross-section to an energy-resolved differential cross-section, we only need to add an energy conserving delta function.

- interaction matrix element, $\langle f|V_{int}|i\rangle$.

11.1.1 Density of states

The equations for momentum and energy conservation are

$$\begin{aligned} \vec{K}_0 &= \vec{K}_p + \vec{K}_n \\ E_i = \hbar\omega_0 - E_b &= \frac{\hbar^2 K_p^2}{2M_p} + \frac{\hbar^2 K_n^2}{2M_n} = E_f \end{aligned} \tag{11.1}$$

We can plug $\vec{K}_p = \vec{K}_0 - \vec{K}_n$ into the energy equation to get the expression for the final energy, E_f

$$E_f = \frac{\hbar^2 K_n^2}{2M_n} + \frac{\hbar^2 K_0^2}{2M_p} + \frac{\hbar^2 K_n^2}{2M_p} - \frac{2\hbar^2 K_0 K_n}{2M_p}\cos\theta$$

where θ is the angle between the *incoming* photon and *outgoing* neutron. Then the density of states can easily be calculated to be

$$\rho(E_f) = \left(\frac{L}{2\pi}\right)^3 \int \delta(E_f - \frac{\hbar^2 K_n^2}{2M_n} - \frac{\hbar^2 K_0^2}{2M_p} - \frac{\hbar^2 K_n^2}{2M_p} + \frac{2\hbar^2 K_0 K_n}{2M_p}\cos\theta) K_n^2 dK_n d\Omega$$

Defining unitless parameters $\xi = K_n/K_0$ and $\gamma = M_n/M_p$, we get

$$\rho(E_f) = \left(\frac{L}{2\pi}\right)^3 \frac{2M_n K_0}{\hbar^2} \frac{1}{1+\gamma} \int \delta(f(\xi))\xi^2 d\xi d\Omega$$

where

$$\begin{aligned} f(\xi) &= \xi^2 - \frac{2\gamma u}{1+\gamma} - \frac{\alpha - \gamma}{1+\gamma} \\ \alpha &= \frac{2M_n E_f}{\hbar^2 K_0^2} \\ \cos\theta &= u \end{aligned}$$

Since we want to figure out the explicit form of $\rho(E_f)$, we need to know, when do the two

roots of the quadratic expression inside the delta function, contribute. Thus, denoting $\xi_0^{\pm}$ to be the two roots of $f(\xi)$, it is easy to see that

$$(1+\gamma)\xi_0^{\pm} = \gamma u \pm \sqrt{\gamma^2 u^2 + (\alpha - \gamma)(1+\gamma)} \tag{11.2}$$

Using Equation 11.1 and the fact that $\gamma \approx 1$, we can see that

$$\frac{\hbar^2 K_0^2}{2M_n} = E_f + 2\frac{K_p K_n \hbar^2}{2M_n}\cos\eta$$

where η is the angle between the *outgoing* proton and neutron. Hence

$$\frac{E_f}{\hbar^2 K_0^2/2M_n} = 1 - 2\frac{K_p K_n}{K_0^2}\cos\eta$$

Now from the Equation 11.2, we can see that whether both roots contribute depends on $\cos\eta$ i.e.

$$\cos\eta > 0 \rightarrow \alpha < 1 \rightarrow \alpha - \gamma < 0$$

$$\cos\eta < 0 \rightarrow \alpha > 1 \rightarrow \alpha - \gamma > 0$$

So when $\alpha - \gamma < 0$, both the roots contribute and when $\alpha - \gamma > 0$, only ξ_0^+ contributes.

Hence, when $\cos\eta < 0$, then

$$\rho(E_f) = \left(\frac{L}{2\pi}\right)^3 \frac{2M_n K_0}{\hbar^2}\frac{1}{1+\gamma}\left[\frac{\xi_0^{+^2}}{|f'(\xi_0^+)|^2} + \frac{\xi_0^{-^2}}{|f'(\xi_0^-)|^2}\right]d\Omega$$

and when $\cos\eta > 0$, then

$$\rho(E_f) = \left(\frac{L}{2\pi}\right)^3 \frac{2M_n K_0}{\hbar^2}\frac{1}{1+\gamma}\left[\frac{\xi_0^{+^2}}{|f'(\xi_0^+)|^2}\right]d\Omega$$

This finishes our calculation of the laboratory frame density of states. In order to compute the differential cross-section we need to calculate the interaction matrix element $\langle f|V|i\rangle$. This is done in the next subsection.

11.1.2 Interaction matrix element

We can divide the interaction into the photoelectric part and the photomagnetic part and calculate each one separately. This is done because it is well known [26, 79] that

- The photoelectric and photomagnetic matrix elements do not interfere with each other.

- While at high energies the photoelectric part is dominant, at threshold, the photomagnetic part is also very important.

Photoelectric part

In this section we will assume that $M_n = M_p = M$. This is not a new assumption, since in the previous subsection, we assumed that $\gamma \approx 1$. Using

$$\vec{A}(\vec{r}_0) = \sum_{\vec{K}\lambda} \sqrt{\frac{2\pi\hbar c^2}{L^3\omega_k}} \left[a_{\vec{K},\lambda} e^{i\vec{K}.\vec{r}_0} + a^{\dagger}_{\vec{K},\lambda} e^{-i\vec{K}.\vec{r}_0} \right] \vec{\epsilon}_{\vec{K},\lambda}$$

the photoelectric part of V_{int} can be written as

$$V^{pe}_{int} = -\sum_{\alpha} \frac{e_\alpha}{M_\alpha c} \vec{p}_\alpha . \vec{A}(\vec{r}_\alpha)$$

where *pe* stands for the photoelectric part. Hence we wish to calculate the following matrix element

$$\langle f|V^{pe}_{int}|i\rangle = \frac{i\hbar e}{Mc} \sqrt{\frac{2\pi\hbar c^2}{L^3\omega_0}} \vec{\epsilon}_{K_0,\vec{\lambda}_0} \cdot \int \Psi_{pn} \vec{\nabla} e^{i\vec{K}_0.\vec{r}_p} \Psi_d$$

We will use the definitions

$$\begin{aligned}
\vec{R}_{cm} &= \frac{\vec{r}_p + \vec{r}_n}{2} \\
\vec{r} &= \vec{r}_n - \vec{r}_p \\
\vec{K}_f &= \vec{K}_p + \vec{K}_n \\
\vec{k} &= \frac{\vec{K}_n - \vec{K}_p}{2}
\end{aligned}$$

As a first approximation, a plane-wave approximation is used for the proton-neutron part i.e.

$$\Psi_{pn} = \frac{1}{L^3} e^{i\vec{K}_f \cdot \vec{R}_{cm}} e^{i\vec{k}\cdot\vec{r}} \otimes |\chi_S^{m_s}\rangle$$

where $|\chi_S^{m_s}\rangle$ can either be a triplet or a singlet. However a deuteron is only found in a spin triplet, so the deuteron wavefunction is [5]

$$\Psi_d(\vec{r}_p, \vec{r}_n) = \left[\frac{\beta}{2\pi}\right]^{1/2} \frac{e^{-\beta r}}{r} \frac{1}{L^{3/2}} \otimes |\chi_1^{m_{s'}}\rangle$$

Since $-i\hbar\nabla_{\vec{r}_p} = -\frac{i\hbar}{2}\nabla_{\vec{R}_{cm}} + i\hbar\nabla_{\vec{r}}$ and $\vec{\epsilon}_{\vec{K}_0,\lambda_0}.\vec{K}_0 = 0$ [6], we see that

$$\begin{aligned}
&\langle f|V_{int}^{pe}|i\rangle = \\
&\frac{-ie\hbar}{Mc}\sqrt{\frac{2\pi\hbar c^2}{L^3\omega_0}}\delta(\vec{K}_0 - \vec{K}_f)\frac{\vec{\epsilon}_{\vec{K}_0,\lambda_0}}{L^{3/2}} \cdot \langle \chi_1^{m_s}|\chi_S^{m_{s'}}\rangle \int e^{-i\left(\vec{k}+\frac{\vec{K}_0}{2}\right)\cdot\vec{r}} \nabla_{\vec{r}} \left[\frac{\beta}{2\pi}\right]^{1/2} \frac{e^{-\beta r}}{r} d\vec{r}
\end{aligned}$$

So for the photoelectric part, the initial and final spin wavefunctions have to be the same.

[5] There are some issues here with normalization since the relative wavefunction of the deuteron wants to be normalized in a sphere of radius R, and the COM motion is a plane wave normalized in a cube. So the factor of $\sqrt{(\gamma/(2\pi)}$ is actually $\sqrt{\gamma/(2\pi(1-e^{-2\beta R}))}$. We will assume that when R or L is large, there is essentially no difference between the two approaches.

[6] Actually we do not need this fact here, since we have assumed the deuteron to be at rest. If the deuteron had some initial momentum, then this fact would be relevant and we would get the same results except that the delta function would contain the initial momentum of the deuteron, as it should for conservation of linear momentum.

Since the deuteron is initially at rest

$$\vec{k} + \frac{\vec{K}_0}{2} = \vec{K}_n$$

Usually the $\vec{r}$ integral is carried out by doing a partial integration, resulting in $\vec{K}_n \cdot \vec{\epsilon}_{\vec{K}_0,\lambda_0}$ outside the integration sign, and getting the answer to be

$$\langle f|V_{int}^{pe}|i\rangle = \frac{-i\hbar e}{Mc}\sqrt{\frac{2\pi\hbar c^2}{L^3\omega_0}}\delta(\vec{K}_0 - \vec{K}_f)\frac{\vec{\epsilon}_{\vec{K}_0,\lambda_0}}{L^{3/2}}.\vec{K}_n \int e^{-i\vec{K}_n\cdot\vec{r}}\left[\frac{\beta}{2\pi}\right]^{1/2}\frac{e^{-\beta r}}{r}d\vec{r}$$

Now assuming $\vec{K}_0 = K_0\hat{z}$, $\vec{K}_n.\vec{\epsilon}_{\vec{K}_0,\lambda_0} = K_n \sin\theta\cos\phi$, where ϕ is the angle between the projection of $\vec{K}_n$ onto the $x-y$ plane and $\vec{\epsilon}_{\vec{K}_0,\lambda_0}$. So in the end, the total result is [7]

$$\langle f|V_{int}^{pe}|i\rangle = \frac{-i\hbar e}{Mc}\sqrt{\frac{2\pi\hbar c^2}{L^3\omega_0}}\delta(\vec{K}_i - \vec{K}_f)\frac{1}{L^{3/2}}K_n \sin\theta\cos\phi\, I(K_n)$$

where

$$I(K_n) = \int\left[\frac{\beta}{2\pi}\right]^{1/2} e^{-i\vec{K}_n\cdot\vec{r}}\frac{e^{-\beta r}}{r}d\vec{r}$$

only depends on the magnitude of $\vec{K}_n$.

Photomagnetic part

The photomagnetic part of the interaction allows spins to change. The magnetic field is given by

$$\vec{H}(\vec{r},t) = \sum_{\vec{K},\lambda} i\sqrt{\frac{2\pi\hbar c^2}{L^3\omega_K}}\left[a_{\vec{K},\lambda}e^{i\vec{K}.\vec{r}} - a^{\dagger}_{\vec{K},\lambda}e^{-i\vec{K}.\vec{r}}\right](\vec{K}\times\vec{\epsilon}_{\vec{K},\lambda})$$

Then

$$V_{int}^{pm} = -\vec{\mu}_p.\vec{H}(\vec{r}_p,t) - \vec{\mu}_n.\vec{H}(\vec{r}_n,t)$$

[7] If we assume that light is unpolarized, the ϕ averaging will give us a factor of $\frac{1}{2}$ in the differential cross-section expression.

where *pm* stands for the photomagnetic part, and

$$\begin{aligned}
\mu_0 &= \frac{e\hbar}{2Mc} \\
\vec{\mu}_p &= \frac{\mu_0 g_p}{2}\vec{\sigma}_p \\
\vec{\mu}_n &= \frac{\mu_0 g_n}{2}\vec{\sigma}_n \\
\vec{R}_{cm} &= \frac{\vec{r}_p + \vec{r}_n}{2} \\
\vec{r} &= \vec{r}_n - \vec{r}_p
\end{aligned}$$

Now,

$$\langle f|V_{int}^{pm}|i\rangle = -i\sqrt{\frac{2\pi\hbar c^2}{L^3\omega_0}}\frac{e\hbar}{Mc}(\vec{K}_0 \times \vec{\epsilon}_{\vec{K}_0,\lambda_0}).\frac{1}{2}\int \Psi_{pn}\left[\frac{g_p}{2}\vec{\sigma}_p e^{i\vec{K}_0\cdot\vec{r}_p} + \frac{g_n}{2}\vec{\sigma}_n e^{i\vec{K}_0\cdot\vec{r}_n}\right]\Psi_d$$

In this form the prefactor is the same as in the photoelectric case, so that now we can ignore the constants and focus on the important residual matrix elements

$$W_{ij} = \frac{1}{2}\int \Psi_{pn}\left[\frac{g_p}{2}\vec{\sigma}_p e^{i\vec{K}_0\cdot\vec{r}_p} + g_n\vec{\sigma}_n e^{i\vec{K}_0\cdot\vec{r}_n}\right]\Psi_d$$

where ij can stand for st or tt, denoting a singlet-triplet or a triplet-triplet transition. We will denote the spatial parts by ψ_{pn} and ψ_d. There are two types of possibilities: the triplet $\rightarrow$ singlet transition or the triplet $\rightarrow$ triplet transitions. We can use the fact (which can easily be verified by a direct computation) that

$$\begin{aligned}
\langle S=1, m_s|\vec{\sigma}_p|S'=1, m_{s'}\rangle &= \langle S=1, m_s|\vec{\sigma}_n|S'=1, m_{s'}\rangle \\
\langle S=0, m_s|\vec{\sigma}_p|S'=1, m_{s'}\rangle &= -\langle S=0, m_s|\vec{\sigma}_n|S'=1, m_{s'}\rangle
\end{aligned}$$

This simple observation allows us to write our triplet-triplet and singlet-triplet transitions

as W_{tt} and W_{st} where

$$W_{tt} = \frac{-i}{2}(\vec{K}_0 \times \vec{\epsilon}_{\vec{K}_0,\lambda_0}).\langle\chi_1^{m_s}|\vec{\sigma}_n|\chi_1^{m_{s'}}\rangle\left[\frac{g_p}{2}\int\psi^*_{pn}e^{i\vec{K}_0.\vec{r}_p}\psi_d + \frac{g_n}{2}\int\psi^*_{pn}e^{i\vec{K}_0.\vec{r}_n}\psi_d\right]$$

$$W_{st} = \frac{-i}{2}(\vec{K}_0 \times \vec{\epsilon}_{\vec{K}_0,\lambda_0}).\langle\chi_0^{m_s}|\vec{\sigma}_n|\chi_1^{m_{s'}}\rangle\left[\frac{g_p}{2}\int\psi^*_{pn}e^{i\vec{K}_0.\vec{r}_p}\psi_d - \frac{g_n}{2}\int\psi^*_{pn}e^{i\vec{K}_0.\vec{r}_n}\psi_d\right]$$

Simplifying, we get the results that

$$W_{tt} = \frac{-i}{2}(\vec{K}_0 \times \vec{\epsilon}_{\vec{K}_0,\lambda_0}).\langle\chi_1^{m_s}|\vec{\sigma}_n|\chi_1^{m_{s'}}\rangle\frac{1}{L^{3/2}}\left[\frac{\beta}{2\pi}\right]^{1/2}\delta(\vec{K}_0 - \vec{K}_f)$$
$$\left[\frac{g_p}{2}\int e^{-i\left(\vec{k}+\frac{\vec{K}_0}{2}\right).\vec{r}}\frac{e^{-\beta r}}{r} + \frac{g_n}{2}\int e^{-i\left(\vec{k}-\frac{\vec{K}_0}{2}\right).\vec{r}}\frac{e^{-\beta r}}{r}\right]$$

$$W_{st} = \frac{-i}{2}(\vec{K}_0 \times \vec{\epsilon}_{\vec{K}_0,\lambda_0}).\langle\chi_0^0|\vec{\sigma}_n|\chi_1^{m_{s'}}\rangle\frac{1}{L^{3/2}}\left[\frac{\beta}{2\pi}\right]^{1/2}\delta(\vec{K}_0 - \vec{K}_f)$$
$$\left[-\frac{g_p}{2}\int e^{-i\left(\vec{k}+\frac{\vec{K}_0}{2}\right).\vec{r}}\frac{e^{-\beta r}}{r} + \frac{g_n}{2}\int e^{-i\left(\vec{k}-\frac{\vec{K}_0}{2}\right).\vec{r}}\frac{e^{-\beta r}}{r}\right]$$

Now, we need to average over the initial spins and photon polarizations and sum over the final spins(we will see photon averaging is trivial, so that it does not matter whether we consider a polarized or an unpolarized beam). Then using

$$V_{st} = \frac{-i}{2}(\vec{K}_0 \times \vec{\epsilon}_{\vec{K}_0,\lambda_0}).\langle\chi_0^0|\vec{\sigma}_n|\chi_1^{m_{s'}}\rangle$$

$$V_{tt} = \frac{-i}{2}(\vec{K}_0 \times \vec{\epsilon}_{\vec{K}_0,\lambda_0}).\langle\chi_1^{m_s}|\vec{\sigma}_n|\chi_1^{m_{s'}}\rangle$$

we can see that

$$|V_{st}|^2_{avg} = \frac{1}{3}\cdot\frac{1}{2\pi}\int_0^{2\pi}\sum_{m_{s'}}\left[|V_{st}|^2\right]d\phi$$

$$= \frac{1}{4}\cdot\frac{1}{3}\cdot\frac{1}{2\pi}\int_0^{2\pi}\sum_{m_{s'}}K_0^2\cos\phi^2|\langle\chi_0^0|(\sigma_n)_x|\chi_1^{m_{s'}}\rangle|^2 + K_0^2\sin\phi^2|\langle\chi_0^0|(\sigma_n)_y|\chi_1^{m_{s'}}\rangle|^2$$

Since $|\langle\chi_0^0|(\sigma_n)_x|\chi_1^{m_{s'}}\rangle| = |\langle\chi_0^0|(\sigma_n)_y|\chi_1^{m_{s'}}\rangle|$, the ϕ integration is trivial. That $\sum_{m_{s'}}|\langle\chi_0^0|(\sigma_n)_x|\chi_1^{m_{s'}}\rangle|^2 = 1$, can be easily verified. Hence we can say that

$$|V_{st}|^2_{avg} = \frac{K_0^2}{12}$$

A similar calculation for $|V_{tt}|_{avg}$ can be carried out, with the difference being, that we have to sum over the three final m_s states. The result can be easily calculated to be

$$|V_{tt}|^2_{avg} = \frac{K_0^2}{6}$$

11.1.3 Summary of results

For vacuum photodisintegration the results of our calculations are

$$\begin{aligned}
|\langle f|V^{pe}|i\rangle| &= \frac{|V_0|}{L^{3/2}}\delta(\vec{K}_0 - \vec{K}_f)K_n \sin\theta\cos\phi I(K_n) \\
|\langle f|V^{pm}_{st}|i\rangle| &= \frac{|V_0|}{2L^{3/2}}\delta(\vec{K}_0 - \vec{K}_f)K_0\sqrt{\frac{1}{3}}\left[-\frac{g_p}{2}I(K_n) + \frac{g_n}{2}I(K_p)\right] \\
|\langle f|V^{pm}_{tt}|i\rangle| &= \frac{|V_0|}{2L^{3/2}}\delta(\vec{K}_0 - \vec{K}_f)K_0\sqrt{\frac{2}{3}}\left[\frac{g_p}{2}I(K_n) + \frac{g_n}{2}I(K_p)\right]
\end{aligned}$$

where

$$V_0 = \frac{i\hbar e}{Mc}\sqrt{\frac{2\pi\hbar c^2}{L^3\omega_0}}$$

Note that in the case of the magnetic calculation, we are off by a factor of 2 as compared to [79]. We have not been able to resolve this.

11.2 Phonon-coupled Photodisintegration of the Deuteron

As in the previous section, the photoelectric and photomagnetic matrix elements are again separately calculated. If we can ensure that no thermal phonon modes are excited, then we can still use the vacuum density of states for the calculation of the differential cross-section. This can be done by introducing a Debye-Waller factor in the computation. The details are

given in subsection 11.2.2. However, now we have to deal with two very different pictures: a phonon-coupling which is non-local, and a photon-deuteron interaction which is local. This presents a problem, which needs to be further discussed.

11.2.1 Local and non-local pictures

In this calculation, we have a local picture of the interaction between a deuteron and a gamma ray and a non-local picture of phonon modes. Such a mixing of local and non-local pictures is very difficult to deal with. However, we can make an approximation [36], that if we are dealing with thermal phonon modes and one highly excited phonon mode, the highly excited phonon mode can be separated out and the rest can still be approximately treated as a local coordinate i.e.

$$\vec{r}_p^{\,f} = \overline{\vec{r}}_p^{\,f} + \vec{u}_p\hat{q} \tag{11.3}$$

where the highly excited phonon mode is isolated and appears as $\vec{u}_p\hat{q}$. The contribution of all other modes make up the residual coordinate, $\overline{\vec{r}}_p^{\,f}$. *Note that Equation 11.3 is exact. The approximation is in the interpretation of the residual coordinate,* $\overline{\vec{r}}_p^{\,f}$*, as a coordinate vector.* However for Equation 11.3 to be valid, the proton has to stay within the lattice. This means that nearly all of the gamma momentum has to be taken up by the neutron.

For the neutron to carry nearly all the photon momentum, it is clear that the photon has to have energy that is matched to the binding energy, $E_b \approx 2.2MeV$, of the deuteron i.e we are interested in the threshold photodisintegration of the deuteron; if the energy is lower, the deuteron will not disintegrate and a higher energy will force both the proton and the neutron to leave the lattice. However, even with this energy matching, we are not guaranteed that the proton will stay within the lattice. A simple calculation can be done to find out the angular range within which the proton stays behind. The photon comes in with a momentum $\hbar\vec{K}_0$. The neutron flies off with momentum $\vec{K}_n$ at an angle θ and the proton moves with a momentum $\vec{K}_p$ at an angle β. By conservation of energy and momentum,

$$\begin{aligned} \hbar K_0 &= MV_n \cos\theta + MV_p \cos\beta \\ MV_n \sin\theta &= MV_p \sin\beta \\ E_0 - E_b &= E_p + E_n \end{aligned}$$

where V_p and V_n are speeds of the proton and neutron, $E_b(> 0)$ is the binding energy of the deuteron and E_0, E_p, E_n are the energies of the photon, proton and neutron respectively. Using these equations we can write down a quadratic equation for E_p in terms of θ, namely

$$\begin{aligned} 0 = {} & 16M^2E_p^2 + 8E_p\left[-\frac{ME_0^2}{c^2}\sin\theta^2 - 2M^2(E_0 - E_b)\right] + \left[\frac{E_0^4}{c^4} + 4M^2(E_0 - E_b)^2 + \right. \\ & \left. \frac{8ME_0^2}{c^2}(E_0 - E_b)\sin\theta^2 - \frac{4ME_0^2}{c^2}(E_0 - E_b)\right] \end{aligned} \tag{11.4}$$

By solving this quadratic equation, we can see that if we want the proton energy to be less than, say $50\,meV$ (to make sure that the proton stays within the lattice), then the angle has to be on the order of 0.01 degrees. However, we should be careful, because, due to the quadratic nature of Equation 11.4, for a given angle, we will get two solutions. Hence even when the angle is 0.01, we would get very low energy neutrons, with the protons flying off with nearly the photon momentum. In order to eliminate this situation, we would need to do an energy resolved cross-section. *Thus we should calculate the energy-resolved differential cross-section in the forward direction,* $\theta \approx 0$. The interaction matrix element is an important part of such a calculation, and as a first attempt, it is calculated next.

11.2.2 Detailed calculation

Photoelectric part

While the interaction is the same as in the vacuum case, the wavefunctions have to account for the presence of the lattice. Hence we will use

$$\begin{aligned} |\Psi_i> &= |1\rangle_\gamma |n\rangle |\bar{\Phi}_L^i\rangle \Psi_d(\vec{r}^i) \\ |\Psi_f> &= |0\rangle_\gamma |n'\rangle |\bar{\Phi}_L^f\rangle \frac{e^{i\vec{K}_n.\vec{r}_n}}{L^{3/2}} \\ V_{int}^{pe} &= V_0 e^{-iS_D} \nabla_{\vec{r}_p^i}.\vec{\epsilon}_{\vec{K}_0,\lambda_0} e^{i\vec{K}_0.\vec{r}_p^i} a_{\vec{K}_0,\lambda_0} \end{aligned}$$

where

$|n\rangle$ = Intial eigenstate of the highly excited phonon mode

$|n'\rangle$ = Final eigenstate of the highly excited phonon mode

$|\bar{\Phi}_L^i\rangle$ = All the initial thermal phonon modes

$|\bar{\Phi}_L^f\rangle$ = All the final thermal phonon modes

e^{-iS_D} = Duschinsky operator which converts the initial lattice into the final lattice

and the superscripts i and f on, for example $\vec{r}_p^i$ or $\vec{r}_p^f$, refer to the initial lattice or final lattice coordinates. Using $\vec{r}_n^f = \vec{r}^f + \vec{r}_p^f$, we can see that

$$\langle f|V_{int}^{pe}|i\rangle = \frac{V_0}{L^{3/2}}\vec{\epsilon}_{\vec{K}_0,\lambda_0} \cdot \int \langle \bar{\Phi}_L^f, n'|e^{-i\vec{K}_n.(\vec{r}^f+\vec{r}_p^f)} e^{i\vec{K}_0.\vec{r}_P^f} e^{-i\hat{S}_d} \nabla_{\vec{r}_p^f} \psi_d(\vec{r}^i)|\bar{\Phi}_L^i, n\rangle d^3\vec{r}^i$$

Since COM motion does not contribute (because the deuteron is stationary), we can just replace $\nabla_{\vec{r}_p^i} = -\nabla_{\vec{r}^i}$. Let us denote $-\nabla_{\vec{r}^i}\psi_d(\vec{r}^i) = \vec{\xi}(\vec{r}^i)$. Then we can see that

$$\begin{aligned} \langle f|V_{int}^{pe}|i\rangle &= \frac{V_0}{L^{3/2}}\vec{\epsilon}_{\vec{K}_0,\lambda_0}. \int \langle \bar{\Phi}_L^f, n|e^{i(\vec{K}_0-\vec{K}_n).\vec{r}_P^f} e^{-i\hat{S}_D} e^{-i\vec{K}_n.\vec{r}^i} \xi(\vec{r}^i)|\bar{\Phi}_L^i, n'\rangle d^3\vec{r}^i \\ &= \frac{V_0}{L^{3/2}}\vec{\epsilon}_{\vec{K}_0,\lambda_0}.\langle \bar{\Phi}_L^f, n'|e^{i(\vec{K}_0-\vec{K}_n).\vec{r}_P^f} e^{-i\hat{S}_D}|\hat{\Phi}_L^i, n\rangle \int e^{-i\vec{K}_n.\vec{r}^i}\vec{\xi}(\vec{r}^i)d^3\vec{r}^i \end{aligned}$$

By partial integration, $-\int e^{-i\vec{K}_n\cdot\vec{r}^i}\nabla_{\vec{r}^i}\psi_d(\vec{r}^i) = i\vec{K}_n\cdot\int e^{-i\vec{K}_n\cdot\vec{r}^i}\psi_d(\vec{r}^i)d^3\vec{r}^i = i\vec{K}_n\cdot I(K_n)$ [8]. Hence we conclude

$$\langle f|V_{int}^{pe}|i\rangle = \frac{iV_0}{L^{3/2}}\vec{\epsilon}_{\vec{K}_0,\lambda_0}.\vec{K}_n I(K_n)\langle\bar{\Phi}_L^f, n'|e^{i(\vec{K}_0-\vec{K}_n).\vec{r}_p^f}e^{-i\hat{S}_D}|\bar{\Phi}_L^i, n\rangle$$

Now, we use the expansion that we talked about in the beginning of this section, namely

$$\vec{r}_p^f = \bar{\vec{r}}_p^f + \vec{u}_p\hat{q}$$

Then we can say

$$\langle f|V_{int}^{pe}|i\rangle = \frac{iV_0}{L^{3/2}}\vec{\epsilon}_{\vec{K}_0,\lambda_0}.\vec{K}_n I(K_n)\langle\Phi_L^f|e^{i(\vec{K}_0-\vec{K}_n).\bar{\vec{r}}_p^f}e^{-i\hat{S}_D}|\bar{\Phi}_L^i\rangle\langle n|e^{i(\vec{K}_0-\vec{K}_n).\vec{u}_p\hat{q}}|n'\rangle$$

Please note that

$$\langle\bar{\Phi}_L^f, n'|e^{i(\vec{K}_0-\vec{K}_n).\vec{r}_p^f}e^{-i\hat{S}_D}|\bar{\Phi}_L^i, n\rangle = \langle\Phi_L^f|e^{i(\vec{K}_0-\vec{K}_n).\bar{\vec{r}}_p^f}e^{-i\hat{S}_D}|\bar{\Phi}_L^i\rangle\langle n|e^{i(\vec{K}_0-\vec{K}_n).\vec{u}_p\hat{q}}|n'\rangle$$

is the no mode-mixing approximation that we talked about at the beginning of the chapter. Let the light be x-polarized. Then $\vec{K}_n.\vec{\epsilon}_{\vec{K}_0,\lambda} = K_n\sin\theta\cos\phi$. So

$$\langle f|V_{int}^{pe}|i\rangle = \frac{iV_0}{L^{3/2}}K_n\sin\theta\cos\phi I(K_n)e^{-W}\langle n'|e^{i(\vec{K}_0-\vec{K}_n).\vec{u}_p\hat{q}}|n\rangle$$

where $e^{-W} = \langle\Phi_L^f|e^{i(\vec{K}_0-\vec{K}_n).\bar{\vec{r}}_p^f}e^{-i\hat{S}_D}|\bar{\Phi}_L^i\rangle$, being the square root of the Debye-Waller factor, is the square root of probability that we are not exchanging any thermal phonons[9]. Now we only focus on the $\langle n'|e^{i(\vec{K}_0-\vec{K}_n).\vec{u}_p\hat{q}}|n\rangle$ part. Define $\vec{K}_0 - \vec{K}_n = \vec{K}$ and $\vec{K}.\vec{u}_p = K u_p\cos\eta = \nu$. The $\langle n'|e^{i\nu\hat{q}}|n\rangle$ can be easily evaluated in terms of Laguerre polynomials. The complete answers are, that going from an initial state, $|i\rangle$, which contains n phonons to a final state $|f\rangle$ of $n + 2p$ phonons, the matrix element

[8] This only depends on the magnitude of $\vec{K}_n$

[9] Note that we know that averaging over polarizations (i.e. averaging over ϕ) will give us a factor of $\sqrt{\frac{1}{2}}$.

$$\langle f|V_{int}^{pe}|i\rangle = \frac{iV_0}{L^{3/2}} K_n \sin\theta\cos\phi I(K_n) e^{-W} \left(\left[\frac{\alpha}{\pi^{1/2} 2^{n+2p} (n+2p)!} \right]^{1/2} \left[\frac{\alpha}{\pi^{1/2} 2^n n!} \right]^{1/2} \frac{2 \cdot 2^{n-1/2}}{\alpha} \sqrt{\frac{\pi}{2}} n! (-1)^p b^{2p} e^{-b^2/4} L_n^{2p}\left(\frac{b^2}{4}\right) \right)$$

Similarly, in going from a state with n phonons to a state with $n + 2p + 1$ phonons, we get

$$\langle f|V_{int}^{pe}|i\rangle = \frac{iV_0}{L^{3/2}} K_n \sin\theta\cos\phi I(K_n) e^{-W} \left(\pm i \left[\frac{\alpha}{\pi^{1/2} 2^{n+2p+1} (n+2p+1)!} \right]^{1/2} \left[\frac{\alpha}{\pi^{1/2} 2^n n!} \right]^{1/2} \frac{2 \cdot 2^n}{\alpha} \sqrt{\frac{\pi}{2}} n! (-1)^p b^{2p+1} e^{-b^2/4} L_n^{2p+1}\left(\frac{b^2}{4}\right) \right)$$

In the above equation the $\pm$ depends on the sign of b where (in both the equations) $b = \nu/\alpha = Ku_p \cos\eta/\alpha$ where $\vec{K} = \vec{K}_0 - \vec{K}_n$, $\vec{K}.\vec{u}_p = Ku_p \cos\eta$.

Photomagnetic Part

The photomagnetic part can be evaluated using the results from the vacuum calculation and the phonon-coupled photoelectric part. The complete answers are given in the next section.

11.3 Results

The entire matrix element $\langle f|V_{int}|i\rangle$ can be broken up into three non-interfering parts, namely the photoelectric part, the singlet-triplet photomagnetic and the triplet-triplet photomagnetic part. The results are [10]

[10] In the state vectors, we are explicitly writing down the excitation of the phonon mode and the spin of the initial and final states.

In the vacuum

$$\begin{aligned}
\langle f, S|V_{int}^{pe}|i, S\rangle &= \frac{V_0}{L^{3/2}}\delta^{(3)}(\vec{K}_0 - \vec{K}_f)K_n \sin\theta\cos\phi I(K_n) \\
\langle f, S=0|V_{int}^{pm}|i, S=1\rangle &= \frac{V_0}{2L^{3/2}}\delta(\vec{K}_0 - \vec{K}_f)\frac{K_0}{\sqrt{3}}\left[-\frac{g_p}{2}I(K_n) + \frac{g_n}{2}I(K)\right] \\
\langle f, S=1|V_{int}^{pm}|i, n, S=1\rangle &= \frac{V_0}{2L^{3/2}}\delta(\vec{K}_0 - \vec{K}_f)K_0\sqrt{\frac{2}{3}}\left[\frac{g_p}{2}I(K_n) + \frac{g_n}{2}I(K)\right]
\end{aligned}$$

In the lattice

$$\begin{aligned}
\langle f, n', S|V_{int}^{pe}|i, n, S\rangle &= \frac{V_0}{L^{3/2}}e^{-W}K_n \sin\theta\cos\phi I(K_n)\langle n'|e^{i\vec{K}.\vec{u}_p\hat{q}}|n\rangle \\
\langle f, n', S=0|V_{int}^{pm}|i, n, S=1\rangle &= \frac{V_0}{2L^{3/2}}e^{-W}\frac{K_0}{\sqrt{3}}\left[-\frac{g_p}{2}I(K_n) + \frac{g_n}{2}I(K)\right]\langle n'|e^{i.\vec{u}_p\hat{q}}|n\rangle \\
\langle f, n', S=1|V_{int}^{pm}|i, n, S=1\rangle &= \frac{V_0}{2L^{3/2}}e^{-W}K_0\sqrt{\frac{2}{3}}\left[\frac{g_p}{2}I(K_n) + \frac{g_n}{2}I(K)\right]\langle n'|e^{i.\vec{u}_p\hat{q}}|n\rangle
\end{aligned}$$

where $\vec{K} = \vec{K}_0 - \vec{K}_n$. The matrix element $\langle n'|e^{i.\vec{u}_p\hat{q}}|n\rangle$ can be split into two parts depending on whether the difference in the phonon excitation between initial and final states is even or odd i.e.

$$\langle n+2p|e^{i.\vec{u}_p\hat{q}}|n\rangle = \left[\frac{\alpha}{\pi^{1/2}2^{n+2p}(n+2p)!}\right]^{1/2}\left[\frac{\alpha}{\pi^{1/2}2^n n!}\right]^{1/2}\frac{2\cdot 2^{n-1/2}}{\alpha}\sqrt{\frac{\pi}{2}}n!(-1)^p b^{2p}e^{-b^2/4}L_n^{2p}(\frac{b^2}{4})$$

$$\langle n+2p|e^{i.\vec{u}_p\hat{q}}|n\rangle = \pm i\left[\frac{\alpha}{\pi^{1/2}2^{n+2p+1}(n+2p+1)!}\right]^{1/2}\left[\frac{\alpha}{\pi^{1/2}2^n n!}\right]^{1/2}\frac{2\cdot 2^n}{\alpha}\sqrt{\frac{\pi}{2}}n!(-1)^p b^{2p+1}e^{-b^2/4}L_n^{2p+1}(\frac{b^2}{4})$$

with $b = \frac{\nu}{\alpha} = \frac{Ku_p\cos\eta}{\alpha}$ where $\vec{K} = \vec{K}_0 - \vec{K}_n$, $\vec{K}.\vec{u}_p = Ku_p\cos\eta$.

11.4 Thermal Averaging

From thermal neutron scattering literature [62, 92] and our own calculations, we know that in order to calculate an experimentally measurable quantity, we need

- An energy resolved differential cross-section.
- Thermal averaging.
- A classical state of the highly excited phonon mode.

In this section we will be able to accomplish the first two of the three tasks. Due to time constraints, we were not able to use classical states for the highly excited phonon mode; instead we will settle for the eigenstates.

$$\left(\frac{d\sigma}{d\Omega}\right)_{\lambda\to\lambda'} = \frac{1}{\Phi_{inc}}\frac{1}{d\Omega}\sum_{\vec{k}'\in d\Omega} W_{\vec{K}_0,\lambda\to\vec{K}_n,\lambda'}$$

where

$$\begin{aligned}
\sum_{\vec{K}_n\in d\Omega} W_{\vec{K}_0,\lambda\to\vec{K}_n,\lambda'} &= \frac{2\pi}{\hbar}\rho_{\vec{K}_n}\left|\langle\Psi_f|V|\Psi_i\rangle\right|^2 \\
|\Psi_i\rangle &= |1\rangle_\gamma \otimes |\lambda\rangle \otimes \Psi_d \\
|\Psi_f\rangle &= |0\rangle_\gamma \otimes |\lambda'\rangle \otimes \Psi_n \\
\Phi_{inc} &= \text{The incoming flux}
\end{aligned}$$

Here

$$\begin{aligned}
\Psi_d &= \left[\frac{\beta}{2\pi}\right]^{1/2}\frac{e^{-\beta r}}{r}\frac{e^{i\vec{K}_i\cdot\vec{R}_{cm}}}{L^{3/2}}\otimes|\chi_1^{m_s}\rangle \\
\Psi_n &= \frac{1}{L^{3/2}}e^{i\vec{K}_n\cdot\vec{r}_n}\otimes|\chi_S^{m_s}\rangle
\end{aligned}$$

It is important to note that the COM coordinate of the deuteron is a part of the lattice, λ. Here λ and λ' refer to the initial and final state of the lattice. Now the neutron density of

states and Φ_{inc} can easily be calculated to be

$$\begin{aligned} \rho_{\vec{K}_n} &= \frac{L^3}{(2\pi)^3} K_n \frac{m}{\hbar^2} d\Omega \\ \Phi_{inc} &= \frac{c}{L^3} \end{aligned}$$

Hence we can put everything together as

$$\left(\frac{d\sigma}{d\Omega}\right)_{\lambda\to\lambda'} = \frac{L^6 K_n M}{c\hbar^3(2\pi)^2} |\langle \vec{K}_n, \lambda' | V | \vec{K}_0, \lambda \rangle|^2$$

Now for a two-body reaction it is well-known [92] that

$$\left(\frac{d^2\sigma}{d\Omega dE_n}\right)_{\lambda\to\lambda'} = \left(\frac{d\sigma}{d\Omega}\right)_{\lambda\to\lambda'} \delta(E_{initial} - E_{final})$$

where $(E_b > 0)$

$$\begin{aligned} E_{initial} &= E_\lambda + E_0 - E_b \\ E_{final} &= E_{\lambda'} + E_n \end{aligned}$$

Using the wavefunctions, it can be seen that

$$\langle \Psi_f | V_{int} | \Psi_i \rangle = i \frac{V_o}{L^{3/2}} \vec{\epsilon}.\vec{K}_n I(K_n) \langle \lambda' | e^{i\vec{K}.\vec{r}_p^f} e^{-iS_D} | \lambda \rangle$$

and hence

$$\left(\frac{d^2\sigma}{d\Omega dE_n}\right)_{\lambda\to\lambda'} = \frac{L^3 K_n M}{c\hbar^3(2\pi)^2} |V_o I(K_n)|^2 |\vec{\epsilon}_{\vec{K}_0,\lambda_0}.\vec{K}_n|^2 \left|\langle \lambda' | e^{i\vec{K}.\vec{r}_p^f} e^{-iS_D} | \lambda \rangle\right|^2 \delta(E_f - E_i)$$

Now $E_f - E_i = E_\lambda - E_{\lambda'} + \hbar\omega$ where $\hbar\omega = E_0 - E_b - E_n$. We can use the expansion

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk$$

to rewrite

$$\left(\frac{d^2\sigma}{d\Omega dE_n}\right)_{\lambda\to\lambda'} = \frac{L^3K_nM}{c\hbar^3(2\pi)^2}|V_oI(K_n)|^2|\vec{\epsilon}_{\vec{K}_0,\lambda_0}.\vec{K}_n|^2\int\langle\lambda|e^{-i\vec{K}.\vec{r}_p^f}e^{iS_D}|\lambda'\rangle\langle\lambda'|e^{i\frac{Ht}{\hbar}}e^{i\vec{K}.\vec{r}_p^f}e^{-iS_D}e^{-i\frac{Ht}{\hbar}}|\lambda\rangle e^{-i\omega t}dt$$

We then need to average over the thermal phonon modes and sum over all the possible final-state modes (including the thermal phonon modes and the highly excited phonon mode). We can use the fact that

$$|\lambda\rangle = |\overline{\Phi}_L^f, n\rangle$$
$$|\lambda'\rangle = \overline{\Phi}_L^i, n'\rangle$$

to see that

$$\left(\frac{d^2\sigma}{d\Omega dE_n}\right) = \sum_{\overline{\Phi}_L^f,\lambda'} p_{\overline{\Phi}_L^f}\left(\frac{d^2\sigma}{d\Omega dE_n}\right)_{\lambda\to\lambda'}$$

where the summation $\overline{\Phi}_L^f$ does not include the highly excited phonon mode and

$$p_{\overline{\Phi}_L^f} = \frac{e^{-E_{\overline{\Phi}_L^f}\beta}}{\mathcal{Z}}$$

with $\mathcal{Z}$ being the partition function. Also, in the Boltzmann factor, $E_{\overline{\Phi}_L^f}$ will include the energies of all the phonon modes except the highly excited one.

$$\begin{aligned}
\left(\frac{d^2\sigma}{d\Omega dE_n}\right) &= \sum_{\overline{\Phi}_L^f,\lambda'} \frac{e^{-E_{\overline{\Phi}_L^f}\beta}}{\mathcal{Z}} \frac{L^3K_nM}{c\hbar^3(2\pi)^2}|V_oI(K_n)|^2|\vec{\epsilon}_{\vec{K}_0,\lambda_0}.\vec{K}_n|^2 \\
&\quad \int \langle\lambda|e^{-i\vec{K}.\vec{r}_p^f}e^{iS_D}|\lambda'\rangle\langle\lambda'|e^{i\frac{Ht}{\hbar}}e^{i\vec{K}.\vec{r}_p^f}e^{-iS_D}e^{-i\frac{Ht}{\hbar}}|\lambda\rangle e^{-i\omega t}dt \\
&= \frac{L^3K_nM}{c\hbar^3(2\pi)^2}|V_oI(K_n)|^2|\vec{\epsilon}_{\vec{K}_0,\lambda_0}.\vec{K}_n|^2 \sum_{\overline{\Phi}_L^i} \frac{e^{-E_{\overline{\Phi}_L^f}\beta}}{\mathcal{Z}} \\
&\quad \int \sum_{\overline{\Phi}_L^f,n'} \langle\overline{\Phi}_L^i, n|e^{iS_D}e^{-i\vec{K}.\vec{r}_p^f(t=0)}|\overline{\Phi}_L^f, n'\rangle\langle\overline{\Phi}_L^f, n'|e^{i\vec{K}.\vec{r}_p^f(t)}e^{-iS_D}|\overline{\Phi}_L^i, n\rangle e^{-i\omega t}dt \\
&= \frac{L^3K_nM}{c\hbar^3(2\pi)^2}|V_oI(K_n)|^2|\vec{\epsilon}_{\vec{K}_0,\lambda_0}.\vec{K}_n|^2 \sum_{\overline{\Phi}_L^i} \frac{e^{-E_{\overline{\Phi}_L^f}\beta}}{\mathcal{Z}} \\
&\quad \int \sum_{\overline{\Phi}_L^f,n'} \langle\overline{\Phi}_L^i, n|e^{iS_D}e^{-i\vec{K}.\vec{r}_p^f(t=0)}|\overline{\Phi}_L^f, n'\rangle\langle\overline{\Phi}_L^f, n'|e^{i\vec{K}.\vec{r}_p^f(t)}e^{-iS_D}|\overline{\Phi}_L^i, n\rangle e^{-i\omega t}dt
\end{aligned}$$

This expression is very difficult to evaluate exactly. However, we make an approximation, whose validity still needs to be tested. We will make the claim that

$$\int \langle\overline{\Phi}_L^f, n'|e^{i\vec{K}.\vec{r}_p^f(t)}e^{-iS_D}|\overline{\Phi}_L^i, n\rangle e^{-i\omega t}dt = \int \langle\overline{\Phi}_L^f|e^{i\vec{K}.\vec{\bar{r}}_p^f(t)}e^{-iS_D}|\overline{\Phi}_L^i\rangle\langle n'|e^{i\vec{K}.\vec{u}_p\hat{q}(t)}|n\rangle e^{-i\omega t}dt$$

where we have used the expansion

$$\vec{r}_p^f(t) = \vec{\bar{r}}_p^f(t) + \vec{u}_p\hat{q}(t)$$

Now we can approximate the thermal phonon average by a Debye-Waller factor e^{-2W} to get

$$\left(\frac{d^2\sigma}{d\Omega dE_n}\right) = \frac{L^3K_nM}{c\hbar^3(2\pi)^2}|V_oI(K_n)|^2|\vec{\epsilon}_{\vec{K}_0,\lambda_0}.\vec{K}_n|^2e^{-2W} \sum_{n'} \int \langle n|e^{-i\vec{K}.\vec{u}_p\hat{q}(0)}|n'\rangle\langle n'|e^{i\vec{K}.\vec{u}_p\hat{q}(t)}|n\rangle e^{-i\omega t}dt$$

where

$$e^{-2W} = \sum_{\overline{\Phi}_L^i,\overline{\Phi}_L^f} \frac{e^{-E_{\overline{\Phi}_L^f}\beta}}{\mathcal{Z}} \langle\overline{\Phi}_L^i|e^{iS_D}e^{-i\vec{K}.\vec{\bar{r}}_p^f(t=0)}|\overline{\Phi}_L^f\rangle\langle\overline{\Phi}_L^f|e^{i\vec{K}.\vec{\bar{r}}_p^f(t)}e^{-iS_D}|\overline{\Phi}_L^i\rangle$$

Using $\sum_{n'} |n'\rangle\langle n'| = 1$, we can see that

$$\left(\frac{d^2\sigma}{d\Omega dE_n}\right) = \frac{L^3 K_n M}{c\hbar^3(2\pi)^2}|V_o I(K_n)|^2|\vec{\epsilon}_{\vec{K}_0,\lambda_0}.\vec{K}_n|^2 e^{-2W}\int \langle n|e^{-i\vec{K}.\vec{u}_p\hat{q}(0)}e^{-i\vec{K}.\vec{u}_p\hat{q}(t)}|n\rangle e^{-i\omega t}dt$$

This calculation very clearly shows how we get the Debye-Waller factor in the previous calculation, where it was inserted by hand. However, given the time constraints, we were unable to take this calculation further and get a concrete result and compare with the work of section 11.2.

Chapter 12

Coherence Factors In N-level Atoms

This chapter is somewhat different from the rest of the thesis, both in terms of physical motivation and mathematical sophistication. It deals with the phenomenon of *superradiance*, which is the spontaneous emission of a coherent system of atoms. It was originally introduced by Dicke [21]. The superradiant 2-level atomic problem is very well understood [83]. With the help of group theory, a significant amount of research has been done to understand superradiance in three and N-level systems [15, 50, 56, 63, 74, 75, 90]. This chapter focuses on a different aspect as compared to these works. Our objective is to find out whether it is possible to understand coherence effects in N-level atoms, in terms of such effects in 2-level atoms. We will see, that while this is indeed possible for the completely symmetric state, for lower symmetry states, such a simple description cannot be achieved.

It should be mentioned here, that in this thesis, we have not discussed all the mathematical ideas used in this chapter e.g. *Cartan subalgebras*, *weight spaces* etc. These concepts belong to the theory of complex semisimple Lie algebras [31, 47], which is far beyond what we discussed in chapters 2 and 3. However, the result which we present at the end, at least for the symmetric case, is delightfully simple.

We will first discuss the 2-level problem. While this can be understood in terms of the usual angular momentum techniques, we will also develop the Lie algebra point of view. Such a perspective makes the generalization to the 3-level and N-level system seem much

more natural. We then go on to discuss representation theory of the Lie algebra $\mathfrak{sl}(3,\mathbb{C})$, which is used to study the three-level problem. We then give a brief outline showing how to generalize to the N-level case. We finish the chapter by discussing why the lower symmetry states are not easy to understand in terms of two-level systems.

12.1 Physical Motivation

Within the realm of physics, there are many kinds of coherence that are of interest in different fields. One of the earliest such examples from classical physics is the case of radiating antennas. If two identical antennas are widely separated (by many wavelengths of the radiated electromagnetic waves), then the total radiated power will be close to twice the radiated power from a single antenna in isolation. If the two antennas are brought very close together and made to oscillate in phase, then the total radiated power will approach four times that of a single antenna in isolation. We understand this effect classically in terms of the electric and magnetic fields, which double in strength as the antenna is "doubled". The radiated power is proportional to the product of the fields, and this leads to an increase of a factor of four over what a single antenna radiates.

Atoms and nuclei act as antennas on a microscopic scale in radiative decay. If two well-separated identical excited atoms decay, the total power radiated is again roughly twice that for a single decaying atom. The same two atoms, if placed within a fraction of a wavelength and radiate in phase, emit roughly four times as much power as a single atom in isolation. This implies that they will also decay roughly twice as fast. This effect is called Dicke superradiance.

Dicke superradiance has been observed experimentally in many systems, including spin systems in the 1950s and optical systems in the 1970s. In optical experiments, atoms are prepared initially in excited states by an optical π-pulse, and then the coherent decay of the system is observed. The coherent decay of the system of atoms leads to a "burst" of optical radiation which is emitted as the atoms decay collectively. Enhancements of many orders of magnitude in the decay rate have been observed in such experiments.

12.1.1 Link to the phonon-coupled Unified Model

The fundamental idea behind superradiance is that when the coupling between the atoms and the resonant electric field is strong, the interaction has to to take into account the entire system at once. This is very similar to the Phonon-coupled Unified Model, in which nuclei are strongly coupled to a highly excited phonon mode; the system has to be treated as a whole and the various nuclei cannot be treated independently. Thus a similar kind of coherent enhancement is expected in the Unified Model.

12.2 Two-Level Atoms

We begin by reviewing Dicke states in the case of two-level systems. Consider a 2-level atom, with energy levels $|a\rangle$ and $|b\rangle$.

12.2.1 Two atoms

If there are two such atoms, we are working in a 4-dimensional space. The natural direct product basis is $|a, a\rangle, |a, b\rangle, |b, a\rangle, |b, b\rangle$. However, it is conceptually and computationally much better to use a different basis: namely, the three symmetric states

$$|b, b\rangle, \ \frac{1}{\sqrt{2}}(|a, b\rangle + |b, a\rangle), \ |a, a\rangle$$

and the antisymmetric state

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

The decay (electric dipole transition) is determined by the matrix element of

$$\langle\alpha|\sigma(1) + \sigma(2)|\beta\rangle$$

where the $\sigma(j) = \frac{1}{\sqrt{2}}[\sigma_x(j) - i\sigma_y(j)]$ (σ_x, σ_y are Pauli matrices). It is easy to see that since there can be no transitions between symmetric and antisymmetric states, the antisymmetric state cannot decay[1]; it is *subradiant.*

In the abstract notation of Appendix A, i.e. we are decomposing $V \otimes V$ as

$$V \otimes V = Sym^2 V \oplus \Lambda^2 V$$

where V represents the 2-dimensional space spanned by $|a\rangle$ and $|b\rangle$, $Sym^2 V$ represents symmetric tensors and $\Lambda^2 V$ the antisymmetric tensors.

12.2.2 Three atoms

With three atoms, we are in a 8-dimensional space. The Dicke states are well known [83]. They are

$$\begin{aligned}
|3\rangle &= |aaa\rangle \\
|2\rangle &= 1/\sqrt{3}(|aab\rangle + |aba\rangle + |baa\rangle) \\
|1\rangle &= 1/\sqrt{3}(|bba\rangle + |bab\rangle + |abb\rangle) \\
|0\rangle &= |bbb\rangle \\
|2'\rangle &= 1/\sqrt{6}(|aab\rangle + |aba\rangle - 2|baa\rangle) \\
|1'\rangle &= 1/\sqrt{6}(|bba\rangle + |bab\rangle - 2|abb\rangle) \\
|2''\rangle &= 1/\sqrt{2}(|aab\rangle - |aba\rangle) \\
|1''\rangle &= 1/\sqrt{2}(|bba\rangle - |bab\rangle)
\end{aligned}$$

One can see by explicit computation that for Dicke states:

1. The matrix elements are zero between states of different symmetry.

[1]These selection rules are a consequence of the Wigner-Eckart theorem for $S(2)$.

2. The decay rates are higher among symmetric states as compared to states of lower symmetry.

In fact the first one is a direct consequence of the Wigner-Eckart theorem (as applied to $S(3)$) and the second effect is a manifestation of superradiance. Typically the superradiant decay rate of the maximally symmetric state grows as N^2, where N is the number of atoms.

As for two particles, in the notation of Appendix A, we are merely decomposing $V \otimes V \otimes V$ as

$$V^{\otimes 3} = V^{\square\square\square} \oplus V^{\square\!\square} \oplus V^{\square\!\square}$$

Before we begin to discuss representation theory of Lie algebras, we want to highlight some of the interesting mathematical properties of Dicke states. This will help us in our generalization to N-level atoms.

12.2.3 Group theoretical properties of Dicke states

There are several group theory properties that are of interest to us:

- The unprimed states form a 4-dimensional irreducible representation of $\mathfrak{sl}(2, \mathbb{C}) = \{2 \times 2 \text{ complex traceless matrices}\}$.
- The primed states and the double primed states form (isomorphic) 2-dimensional irreducible representations of $\mathfrak{sl}(2, \mathbb{C})$.
- $|3\rangle, |2\rangle, |1\rangle, |0\rangle$ (each state individually) forms the trivial representation of $S(3)$. Similarly $\{|2'\rangle, |2''\rangle\}$ and $\{|1'\rangle, |1''\rangle\}$ form two (isomorphic) 2-dimensional irreducible representations of $S(3)$. However, The "sign representation" of $S(3)$ is missing.

We can see that representation theory provides us insights into the structure of Dicke states, otherwise not easily obtainable. From the above-mentioned properties, we can deduce that

the important groups are

$$\begin{aligned} S(d) &= \{\text{Group of permutatations of } d \text{ objects}\} \\ \mathfrak{sl}(n,\mathbb{C}) &= \{\text{Lie algebra of } n \times n \text{ traceless matrices}\} \end{aligned}$$

However, using the Weyl Unitary trick [31], we know that there are natural bijective correspondences between the complex linear representations of $\mathfrak{sl}(n,\mathbb{C})$, real linear representations of $\mathfrak{su}(n)$ and the real analytic representations of $SU(n)$ where

$$\begin{aligned} \mathfrak{su}(n) &= \{\text{Lie algebra of } n \times n \text{ anti-hermitian traceless matrices}\} \\ SU(n) &= \{\text{Lie Group of unitary } n \times n \text{ matrices of determinant } 1\} \end{aligned}$$

Before we begin to study these objects, it is best to discuss angular momentum algebra, both from the familiar physicists perspective and from the Lie algebra point of view. This will help us understand terminology and the theorems that will be needed.

12.3 Representation Theory of $\mathfrak{sl}(2,\mathbb{C})$

12.3.1 The physicist's way

From quantum mechanics we know that angular momentum operators, J_i, generate irreducible representations of $SU(2)$ via $\exp\frac{-i\vec{J}.\hat{\vec{\theta}}}{\hbar}$. These operators infinitesimally satisfy the following relations

$$[J_i, J_j] = i\epsilon_{ijk}J_k$$

with the usual

$$\begin{aligned} J_z|j,m\rangle &= \hbar m|j,m\rangle \\ J_+|j,m\rangle &= \hbar\sqrt{(j-m)(j+m+1)}|j,m+1\rangle \\ J_+|j,m\rangle &= \hbar\sqrt{(j+m)(j-m+1)}|j,m-1\rangle \end{aligned}$$

While the J_i are Hermitian operators, the J_+ and J_- are not.

12.3.2 The mathematician's way

As mentioned in subsection 12.2.3, $\mathfrak{su}(2)$ consists of anti-hermitian traceless matrices. From general Lie theory it is known that the exponential map is the critical link between any Lie algebra $\mathfrak{g}$ and its Lie group G. In the case of Lie subgroups of $GL(n, \mathbb{C})$, the exponential map is just the matrix exponential. It can be checked by direct computation that anti-hermitian traceless matrices exponentiate to special unitary matrices. Hence, as expected, the matrix exponential is the link between $\mathfrak{su}(2)$ to $SU(2)$. Since mathematicians have no reason to prefer hermitian over anti-hermitian operators[2], they use anti-hermitian matrices for $\mathfrak{su}(2)$.

Using

$$X_1 = \frac{i}{2}\sigma_1 \quad X_2 = -\tfrac{i}{2}\sigma_2 \quad X_3 = \frac{i}{2}\sigma_3$$

where the σ_i are the Pauli matrices. With these definitions we get the commutation relation

$$[X_i, X_j] = \epsilon_{ijk} X_k$$

where ϵ_{ijk} is the usual Levi-Civita tensor. Since $\mathfrak{sl}(2, \mathbb{C}) = \mathbb{C} \otimes_{\mathbb{R}} \mathfrak{su}(2) = \mathfrak{su}(2) \oplus i\mathfrak{su}(2)$, any complex representation of $\mathfrak{su}(2)$ bijectively corresponds to a complex representation of $\mathfrak{sl}(2, \mathbb{C})$. A convenient basis for $\mathfrak{sl}(2, \mathbb{C})$ is

$$X = -i(X_1 - iX_2) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

[2]Unlike the physicists, for whom hermitian operators correspond to physical observables.

$$Y = -i(X_1 + iX_2) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$H = -iX_3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Mathematicians normally use $H = -2iX_3$, but we will adhere to the above defined value to make the connection with the physicists.

With these definitions, the commutation relations look like

$$\begin{aligned} [H, X] &= X \\ [H, Y] &= -Y \\ [X, Y] &= 2H \end{aligned}$$

The above are the commutation relations for the raising and lowering operators of angular momentum (provided we normalize $\hbar = 1$). If we think of $H \to J_z$, $X \to J_+$ and $Y \to J_-$, then we can rewrite the above equations as

$$\begin{aligned} [J_z, J_+] &= \hbar J_+ \\ [J_z, J_-] &= -\hbar J_- \\ [J_+, J_-] &= 2\hbar J_z \end{aligned}$$

We can now proceed exactly as in any modern quantum mechanics text [81] to get the matrix elements of X or Y. However, keeping in mind our generalization to $\mathfrak{sl}(n, \mathbb{C})$, we introduce some ideas from the theory of Lie algebras.

Let V be an irreducible representation of $\mathfrak{sl}(2, \mathbb{C})$. Then

$$V = \bigoplus_{\alpha} V_{\alpha}$$

where $\alpha \in \mathbb{C}$ s.t.

$$H\, v = \alpha\, v, \ \forall v \in V$$

H generates a subalgebra, $\mathfrak{h}$, which is called the *Cartan subalgebra*, α are called the *weights* and V_{α} are called the *weight spaces*.

Consider the *standard representation* V of $\mathfrak{sl}(2, \mathbb{C})$ on $\mathbb{C}^2$. If

$$x = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad y = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

then

$$H\, x = \frac{x}{2} \ , \ \ H\, y = -\frac{y}{2}$$

Hence we can conclude

$$V = V_{-1/2} \oplus V_{1/2}$$

where $V_{-1/2}$ is spanned by y and $V_{1/2}$ is spanned by x. The representation $Sym^{(n)}V$, which is a completely general algebraic construction, will feature prominently in the rest of the chapter. It is the quotient of $V^{\otimes n}$ by the subspace generated by all $v_1 \otimes \cdots \otimes v_n - v_{\sigma(1)} \otimes \cdots \otimes v_{\sigma(n)}$, where σ is any permutation of $\{1, \cdots, d\}$, where d = dim V. We can also think of $Sym^{(n)}V \subset V^{\otimes n}$ by mapping $v_1 v_2 \cdots v_n \mapsto \sum_{\sigma \in S(n)} v_{\sigma(1)} \otimes \cdots \otimes v_{\sigma(n)}$.

Consider $Sym^{(2)}V$. This has basis $\{x^2, y^2, xy\}$. Then

$$\begin{aligned} H(x.x) &= x.H(x) + H(x).x = x.x \\ H(x.y) &= xH(y) + H(x).y = 0 \\ H(y.y) &= yH(y) + H(y).y = -y.y \end{aligned}$$

Hence $W = Sym^{(2)}V = \mathbb{C}y^2 \oplus \mathbb{C}xy \oplus \mathbb{C}x^2 = W_{-1} \oplus W_0 \oplus W_1$. More generally $Sym^{(m)}V$ has basis $\{x^m, x^{m-1}y, \cdots, y^m\}$. Then

$$Hx^{m-k}y^k = \frac{m-2k}{2}x^{m-k}y^k$$

The eigenvalues of Sym^mV are $\{-m/2, -m/2 + 1, \cdots, m/2\}$. These are exactly the same results we get from quantum mechanics. In fact, *any irreducible representation of* $\mathfrak{sl}(2, \mathbb{C})$ *is a symmetric power,* $Sym^{(m)}V$ *of the standard representation* $V \simeq \mathbb{C}^2$.

By analogy to two-level systems, we know that when we will try to generalize to the three-level systems, we will need to understand the representation theory of $\mathfrak{sl}(3, \mathbb{C})$.

12.4 Representation Theory of $\mathfrak{sl}(3, \mathbb{C})$

Concretely, for $\mathfrak{sl}(3, \mathbb{C})$, we will be using the basis

$$E_{12} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad E_{13} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$E_{23} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \quad E_{21} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$E_{31} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad E_{32} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

$$H_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad H_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Note that E_{ij} are precisely what are commonly accepted as the raising and lowering operators. The H_i's generate what is called a *Cartan subalgebra* and denoted by $\mathfrak{h}$.

For $\mathfrak{sl}(3, \mathbb{C})$, we have to generalize our theory of $\mathfrak{sl}(2, \mathbb{C})$. The role of $H \subset \mathfrak{sl}(2, \mathbb{C})$, is now played by the Cartan subalgebra of all diagonal matrices $\mathfrak{h}$ in $\mathfrak{sl}(3, \mathbb{C})$. Let V be a representation of $\mathfrak{sl}(3, \mathbb{C})$. Using the fact that commuting diagonalizable matrices are simultaneously diagonalizable, we can decompose V as

$$V = \bigoplus_{\alpha} V_\alpha$$

where $v \in V_\alpha$ is an eigenvector (in the generalized sense) for every $H \in \mathfrak{h}$ i.e.

$$H\, v = \alpha(H)\, v$$

where $\alpha \in \mathfrak{h}^*$ (i.e. α is a linear map from $\alpha : \mathfrak{h} \to \mathbb{C}$).

Any Lie algebra acts on itself by the *adjoint action* i.e. $H.Y = [H, Y]$. This action is usually written as $H.Y = ad(H)Y$. Under this adjoint action,

$$\mathfrak{sl}(3, \mathbb{C}) = \mathfrak{h} \bigoplus_{\alpha \in \mathfrak{h}^*} \left(\oplus \mathfrak{g}_\alpha \right)$$

$$[H, Y] = ad(H)Y = \alpha(H)Y \quad H \in \mathfrak{h},\ Y \in \mathfrak{g}_\alpha$$

α are called the *roots* and the $\mathfrak{g}_\alpha$ are called the *root spaces*. Let D be any diagonal matrix. Then

$$\left[D, E_{ij}\right] = (L_i - L_j)(D)E_{ij} \tag{12.1}$$

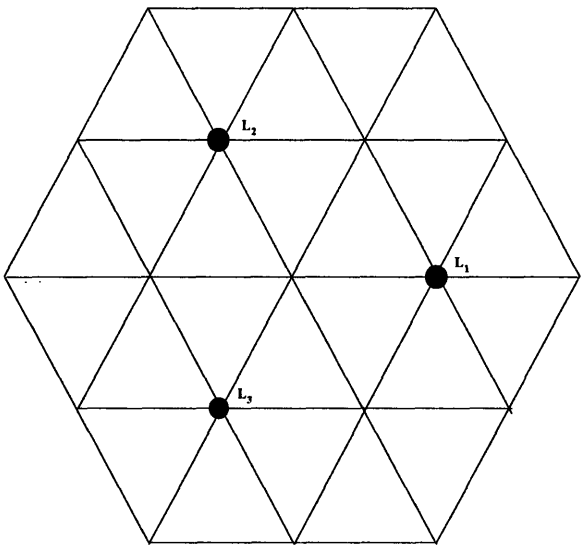


Figure 12-1: Root diagram of $\mathfrak{sl}(3, \mathbb{C})$

where

$$L_i \begin{pmatrix} a_1 & & \\ & a_2 & \\ & & a_3 \end{pmatrix} = a_i$$

$$\mathfrak{h} = \left\{ \begin{pmatrix} a_1 & & \\ & a_2 & \\ & & a_3 \end{pmatrix} ; a_1 + a_2 + a_3 = 0 \right\}$$

$$\mathfrak{h}^* = \mathbb{C}\{L_1, L_2, L_3\} / (L_1 + L_2 + L_3 = 0)$$

The root diagram is drawn in Figure 12-1.

Hence by Equation 12.1 we can see that the linear functionals $\alpha \in \mathfrak{h}^*$ appearing in the direct sum decomposition are $L_i - L_j$, where the space $\mathfrak{g}_{L_i - L_j}$ is generated by E_{ij}.

Now if V is a representation of $\mathfrak{sl}(3, \mathbb{C})$, then we already know that

$$V = \bigoplus_{\alpha} V_{\alpha}$$

A simple calculation reveals that

$$HXv = XHv + [H, X]v = (\alpha(H) + \beta(H))Xv \;\; X \in \mathfrak{g}_\alpha, \;\; V \in V_\beta$$

Hence Xv is again an eigenvector for the action of $\mathfrak{h}$, with eigenvalue $\alpha + \beta$. In other words

$$\mathfrak{g}_\alpha : \; V_\beta \rightarrow V_{\alpha+\beta}$$

For each root α, $\mathfrak{g}_\alpha$, $\mathfrak{g}_{-\alpha}$ and $[\mathfrak{g}_\alpha, \mathfrak{g}_{-\alpha}]$ generate a Lie subalgebra $\mathfrak{s}_\alpha \simeq \mathfrak{sl}(2, \mathbb{C})$. This subalgebra which gets attached to each root, will play a crucial role in our application. Then $\oplus_n V_{\beta+n\alpha}$ forms a representation of $\mathfrak{s}_\alpha \simeq \mathfrak{sl}(2, \mathbb{C})$. Now it is clear that $\mathfrak{g}_\alpha$, $\mathfrak{g}_{-\alpha}$ are precisely the raising and lowering operators of quantum mechanics.

12.5 Three-Level Atoms

Having developed some expertise in representation theory of $\mathfrak{sl}(3, \mathbb{C})$, we can now try to use it to understand coherence effects in three-level atoms. We compute the matrix elements of the maximally symmetric state since it is probably the most important[3] of all the symmetry-adapted states. Our intuition also suggests that these symmetric-state matrix elements should be the easiest to calculate as well. As the following calculations show, this indeed turns out to be true.

12.5.1 Highest symmetry state

Consider V an irreducible representation of $\mathfrak{sl}(n\mathbb{C})$. Then we know from the theorem in Appendix A that

$$V^{\otimes n} = \bigoplus_\lambda \mathbb{S}_\lambda V^{\otimes m_\lambda}$$

Hence the highest symmetry states are precisely those corresponding to $Sym^{(n)}V$. We al-

[3]It controls the decay rate in a superradiant system

ready know that

$$Sym^{(n)}V = \bigoplus_{\beta} V_{\beta}$$

The remarkable property of $Sym^{(n)}V$ is that all the weight spaces have dimension 1. This fact will turn out to be very important in simplifying our answer for the N-level system.

If we consider the action of $\mathfrak{s}_{\alpha} \simeq \mathfrak{sl}(2, \mathbb{C})$ on any weight space V_{β} then $\oplus_n V_{\beta+n\alpha}$ forms an irreducible representation (since all weight spaces are 1-dimensional) of $\mathfrak{sl}(2, \mathbb{C})$. And we know the matrix elements of the raising and lowering operators for the irreducible representations of $\mathfrak{sl}(2, \mathbb{C})$.

A concrete example: $Sym^{(2)}V$

The weights for $Sym^{(2)}V$ are $\{2L_1, 2L_2, 2L_3, L_1 + L_2, L_1 + L_3, L_2 + L_3\}$. The weight diagram is drawn in Figure 12-2.

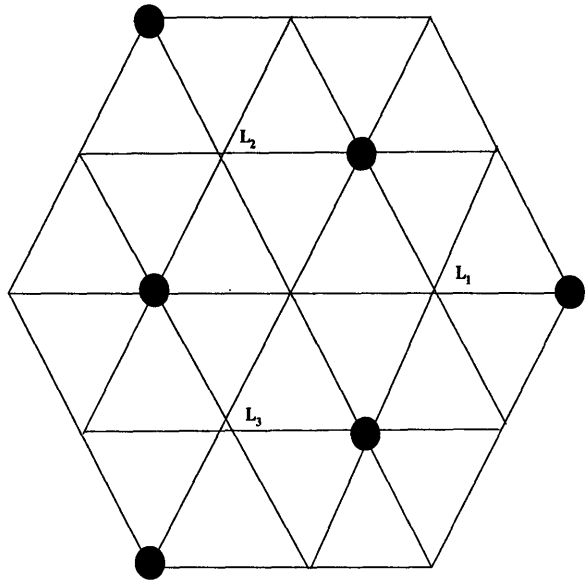


Figure 12-2: Weight diagram for $Sym^{(2)}V$

In the theory of semisimple Lie algebras, we can define *positive roots* and *simple roots* which lead to the concept of *the highest weight.* We will not go into any details, but will merely state that for our purposes $2L_1$ is the highest weight and the $L_i - L_j$, $i < j$ are the positive roots. As mentioned in the section 12.4 the $\mathfrak{g}_{L_i - L_j} = \mathbb{C}E_{ij}$ maps the weight spaces

as shown in Figure 12-3. We now think of an atom with 3-levels (corresponding to $\mathfrak{sl}(3, \mathbb{C})$).

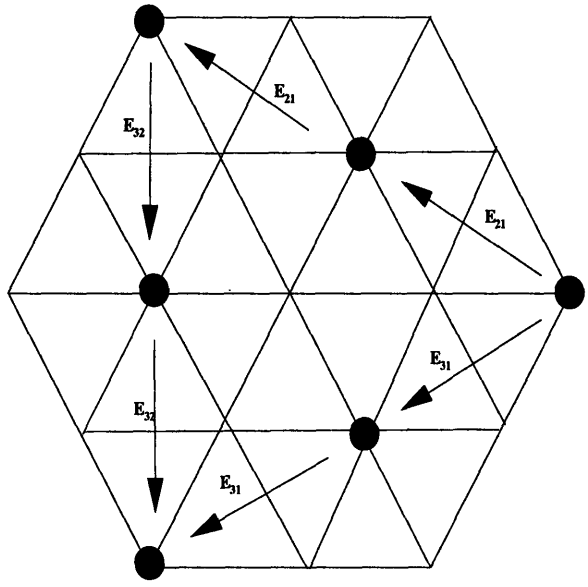


Figure 12-3: Raising and lowering operators

Since we are dealing with $Sym^{(2)}V$, this means that there are 2 bosons to deal with. We will use the convention that the highest weight space corresponds to both the particles being in the highest energy level i.e. to $(n_1 = 2, n_2 = 0, n_3 = 0)$. The precise correspondence that we use is shown in Figure 12-4.

As already mentioned the {(2, 0, 0), (1, 1, 0), (0, 2, 0)} states form a 3-dimensional irreducible representation of $\mathfrak{sl}(2, \mathbb{C})$. The $\mathfrak{sl}(2, \mathbb{C})$ is generated by $\{\mathfrak{g}_{L_2-L_1}, \mathfrak{g}_{L_1-L_2}, \mathfrak{h}_{L_2-L_1}\}$ where $\mathfrak{h}_{L_2-L_1} = [\mathfrak{g}_{L_2-L_1}, \mathfrak{g}_{L_1-L_2}] \in \mathfrak{h}$. Hence we know for example that

$$\begin{aligned} E_{21}|2, 0, 0\rangle &= \sqrt{2}|1, 1, 0\rangle \\ E_{21}|1, 1, 0\rangle &= \sqrt{2}|0, 2, 0\rangle \\ E_{21}|2, 0, 0\rangle &= 0 \end{aligned}$$

corresponding to J_+ and for $j = 1$ and

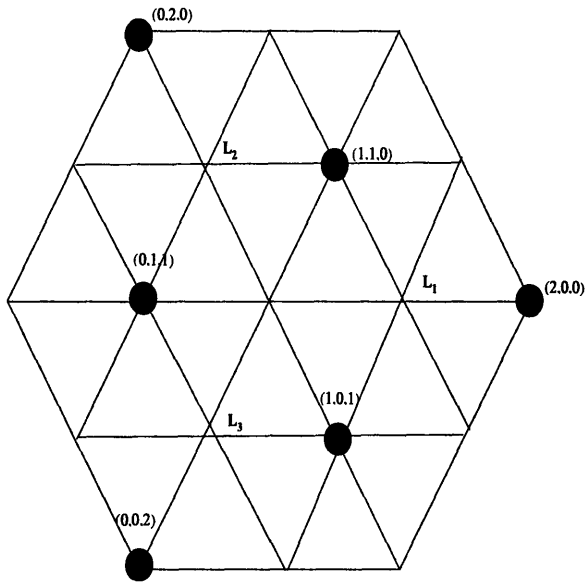


Figure 12-4: Correspondence between occupation of energy levels and weights

$$
\begin{aligned}
E_{12}|2, 0, 0\rangle &= 0 \\
E_{12}|1, 1, 0\rangle &= \sqrt{2}|2, 0, 0\rangle \\
E_{12}|0, 2, 0\rangle &= \sqrt{2}|1, 1, 0\rangle
\end{aligned}
$$

corresponding to J_- for $j = 1$.

Similarly $\{(1, 1, 0), (0, 1, 1)\}$ correspond to a 2-dimensional (i.e. $j = 1/2$) representation of $\mathfrak{sl}(2, \mathbb{C})$. In this case the $\mathfrak{sl}(2, \mathbb{C})$ is generated by $\{\mathfrak{g}_{L_3-L_1}, \mathfrak{g}_{L_1-L_3}, \mathfrak{h}_{L_3-L_1}\}$ where $\mathfrak{h}_{L_3-L_1} = [\mathfrak{g}_{L_3-L_1}, \mathfrak{g}_{L_1-L_3}] \in \mathfrak{h}$. Hence e.g.

$$
\begin{aligned}
E_{31}|1, 1, 0\rangle &= |0, 1, 1\rangle \\
E_{31}|0, 1, 1\rangle &= 0
\end{aligned}
$$

E_{21}	$j_{21} = \frac{n_2+n_3}{2}$	$m_{21} = \frac{n_3-n_2}{2}$
E_{31}	$j_{31} = \frac{n_1+n_3}{2}$	$m_{31} = \frac{n_3-n_1}{2}$
E_{32}	$j_{32} = \frac{n_1+n_2}{2}$	$m_{32} = \frac{n_2-n_1}{2}$

Table 12.1: Correspondence between level occupation in a three-level system and angular momentum

for J_+ and

$$\begin{aligned} E_{13}|0,1,1\rangle &= |1,1,0\rangle \\ E_{13}|1,1,0\rangle &= 0 \end{aligned}$$

corresponding to J_-.

12.5.2 Summary

Thus with $n = n_1 + n_2 + n_3$, we can construct a 1-1 correspondence between angular momentum eigenstates and the occupation of the highest symmetry state in a three-level system. This is defined in Table 12.1. If we wish to calculate the matrix element for the lowering operator from state $(n-1,1,0)$ to $(n-2,2,0)$, then this corresponds to E_{21} with $j_{21} = n$ and $m_{21} = n-2$. Hence,

$$E_{21}|n-1,1,0\rangle = \sqrt{(j_{21}+m_{21})(j_{21}-m_{21}+1)}|n-2,2,0\rangle$$

We can, in principle, generalize the above result for the three-level symmetric case, to the N-level symmetric case.

12.5.3 $Sym^{(m)}V$ for $\mathfrak{sl}(n,\mathbb{C})$

It is hard to draw weight diagrams even for $\mathfrak{sl}(4,\mathbb{C})$, and impossible for higher n. However, the basic fact that the weight spaces are 1-dimensional still holds true for $Sym^{(m)}V$ of $\mathfrak{sl}(n,\mathbb{C})$. This was the critical fact that let us consider "1-dimensional subspaces" of the

weight diagram as irreducible representations of $\mathfrak{sl}(2, \mathbb{C})$. The $\mathfrak{sl}(2, \mathbb{C})$ subalgebra associated to each root is still generated by $\{\mathfrak{g}_{L_j-L_i}, \mathfrak{g}_{L_i-L_j}, \mathfrak{h}_{L_j-L_i}\}$ where $\mathfrak{h}_{L_j-L_i} = [\mathfrak{g}_{L_j-L_i}, \mathfrak{g}_{L_i-L_j}]$. The highest weight is still mL_1, and it corresponds to "m particles in the highest energy level (with n levels in all)". Any consistent set of conventions for lowering operators can be made, with the relevant angular momentum still defined by $j = \frac{n_k+n_l}{2}$, $m = \frac{n_k-n_l}{2}$, $k > l$.

12.5.4 Mixed symmetry states

The mixed symmetry states are relatively difficult to understand in terms of this simple 2-level picture. This becomes apparent in the simplest of cases. This problem does not occur in $\mathfrak{sl}(2, \mathbb{C})$ since all the irreducible representations are given by $Sym^{(m)}V$, and we know the weight spaces have dimension 1. However, let us consider $\mathfrak{sl}(3, \mathbb{C})$. The irreducible representation $\Gamma_{1,1}$, has a weight diagram which is drawn in Figure 12-5. The vector spaces are labeled by integers, with the zero weight space, V_0, assigned the numeral 0.

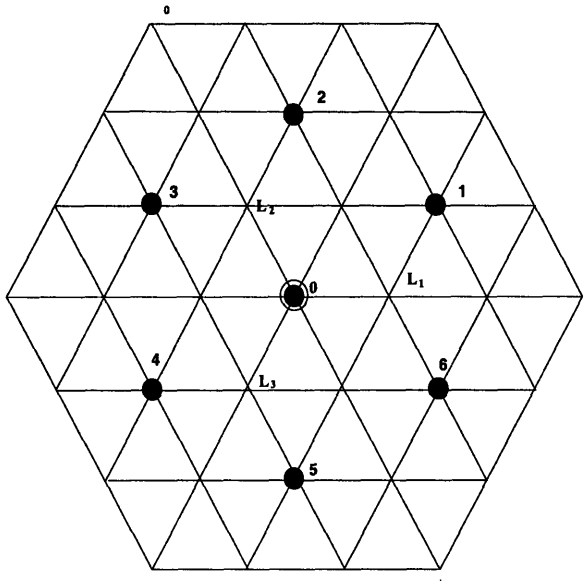


Figure 12-5: The problem with $\Gamma_{1,1}$

The circle around V_0 denotes the fact that there are two linearly independent vectors in V_0. This causes our simple method to breakdown. The fundamental problem is that when we want to calculate the matrix elements of the raising/lowering operators in the transitions

$3 \rightarrow 0 \rightarrow 2$, the vector in the 0 which forms a 3-dimensional irreducible representation of $\mathfrak{sl}(2, \mathbb{C})$ in the 3, 0, 6 sequence is *linearly independent* of the vector which forms a 3-dimensional irreducible representation of $\mathfrak{sl}(2, \mathbb{C})$ in the 2, 0, 5 sequence.

This problem of linear independence appears in all the mixed symmetry representations. As we have seen, this makes it hard to use the two-level formalism to understand the N-level problem. While it is true that in a particular case, by explicit computation, we can figure out the effects of this linear independence, there do not seem to be useful, general results for the N-level mixed symmetry problem.

Chapter 13

Conclusions

In this chapter we summarize the main contributions of this thesis and outline some possible directions for future research.

13.1 Summary of Contributions

In this thesis, we have

- explicitly constructed all the channels for the three and four-body nuclear problems.
- found a simple method for constructing symmetry-adapted spin/isospin states.
- formally calculated matrix elements for the Hamada-Johnston potential.
- identified a possible generalization of Racah's method.
- devised a systematic way of calculating matrix elements with correlated wavefunctions.
- derived the democratized coupled-channel equations for the Hamada-Johnston for the three and four-body ground-state problems.
- analyzed phonon-coupled photodisintegration.

- introduced a simple method of thinking about N-particle coherence problems.

The main objective for undertaking this research was to allow realistic nuclear potentials to be used in the Unified Model. However, this research can have a broader impact on the field of phonon-coupled nuclear reactions. This is because progress in condensed-matter nuclear reactions requires collaboration from various disciplines. The coupled-channel equations open up this field to atomic physicists, applied mathematicians etc.

13.2 Future Directions

The coupled-channel equations could be used to

- develop pedagogic applications to few-body vacuum nuclear physics. Nuclear physics is a daunting subject, and the coupled-channel equations could be used to simplify presentation of the few-body nuclear problem. Apart from ground-state calculations, these equations could be used to study excited state spectra of few-body nuclei or d-d fusion reaction cross-sections.

- realistically compute the predictions of the Unified Model. This could include an attempt to explain the Kasagi experiment[38] or calculate d-d fusion reaction cross-section in a lattice.

There are certain aspects of the research which are left unfinished. These are to

- democratize the coupled-channel equations.

- complete the phonon-coupled photodisintegration.

- understand why the phases of the Clebsch-Gordan and the projection operator approach are the same.

- figure out whether a generalization of the Clebsch-Gordan approach to arbitrary $SU(2)$ (or even $SU(n)$) representations is possible.

The democratization of the coupled-channel equations is crucial because without it, numerical computations will be difficult. It is also important to understand the phenomenon of phonon-coupled photodisintegration, as it is the simplest possible condensed matter nuclear reaction. A better comprehension of this basic reaction is a prerequisite to understand the more complex phonon-coupled nuclear reactions. Hence both these projects should be undertaken as soon as possible. The last two aspects of unfinished research require some leisure time, and if possible, would be fun and satisfying to understand.

Appendix A

Representation Theory And Symmetric Polynomials

A.1 Introduction

The material in this appendix is not really required for understanding any part of the thesis. The reason for including this material is to give the reader an idea of the amazing interaction between representation theory of the symmetric and general linear groups, symmetric polynomials and combinatorics. It is obvious that these few pages are certainly insufficient to do any justice to the above mentioned subjects. Unfortunately, we also cannot follow the example-based procedure, adopted in chapters 2 and 3 for learning group theory, because most physicists are not already familiar with the objects discussed in this appendix. The motivation for including this appendix is only to pique the interest of the reader into reading the mathematics literature which expounds these results in great detail and from where most of this discussion has been taken [30, 31, 35].

This appendix is mainly about the celebrated *Littlewood-Richardson* rule. This rule can come in various forms. The principle ones are

- Multiplication in the *plactic monoid.*

- Multiplication of *Schur polynomials*.
- Product in the *Grothendeik group* of irreducible representations of $S(m)$.
- Tensor products of irreducible representations of $GL(n, \mathbb{C})$.

where $GL(n, \mathbb{C})$ are invertible complex $n \times n$ matrices, the plactic monoid is a construct from combinatorics and Schur polynomials are some symmetric polynomials. On the surface, all these four objects seem to be very different, and one does wonder, what, if anything, can these objects have in common with each other. The beauty of the subject arises from the very fact that the Littlewood-Richardson rule unites these ostensibly disparate fields of mathematics.

Towards the end of the appendix, we make some remarks about representations of $SU(n)$ and $SL(n, \mathbb{C})$. This is intended to clarify why physicists, when dealing with representations of $SU(n)$, can (and in fact do)use the mathematics associated with $SL(n, \mathbb{C})$ representations.

A note of warning is that the term Young tableaux used here is different from the one used in chapter 3. This is done because there are some differences in terminology in the mathematics and physics literature.

We should first define all the groups that we will be discussing in this appendix.

- $S(m)$ = Permutations of $\{1, \ldots, m\}$.
- $GL(n, \mathbb{C})$ = Invertible complex $n \times n$ matrices.
- $SL(n, \mathbb{C})$ = Complex $n \times n$ matrices of determinant 1. This is a complex Lie group.
- $\mathfrak{sl}(n, \mathbb{C})$ = traceless $n \times n$. matrices. This is the Lie Algebra of $SL(n, \mathbb{C})$.
- $SU(n)$ = $n \times n$ matrices of determinant 1 such that $A^\dagger A = I$. This is a *real* Lie group (although the matrices have complex entries!) since its Lie algebra is defined over $\mathbb{R}$ and not over $\mathbb{C}$.
- $\mathfrak{su}(n)$ = traceless, anti-hermitian $n \times n$ matrices. This is the Lie algebra of $SU(n)$.

- Symmetric polynomials in m variables. This needs a bit of explanation. $S(m)$ acts naturally on the polynomial ring $R[X_1, \ldots X_m]$ where $R = \mathbb{Z}$ or $\mathbb{Q}$ by $\sigma(X_i) = X_{\sigma(i)}$ for $\sigma \in S(n)$. All polynomials invariant under $S(m)$ are called symmetric polynomials. In fact it is clear that symmetric polynomials form a graded (by the degree of the polynomial) ring.

$$\Lambda_m = \oplus_d \Lambda_m^d$$

$$f(X_1, \ldots, X_m) \in \Lambda_m^d \Leftrightarrow f(X_1, \ldots X_m) = \sum_{|\alpha|=d} c_\alpha X^\alpha$$

where $X^\alpha = X_1^{\alpha_1} \ldots X_m^{\alpha_m}$ with $|\alpha| = \alpha_1 + \ldots + \alpha_m$.

A.2 Representation Theory of the Symmetric Group

Young diagram is a collection of boxes, arranged in left-justified rows, with weakly decreasing number of boxes in each row. A *partition* of m is a sequence of weakly decreasing non-negative integers $(\lambda_1, \lambda_2, \ldots \lambda_m)$ such that $\sum \lambda_i = 1$. It is clear that partitions of m are equivalent to Young diagrams with m boxes. e.g.  corresponds to $\lambda = (4, 3, 3, 2) = (4, 3^2, 2)$. Sometimes the notation $\lambda \vdash m$ or $|\lambda| = m$ is used.

Apart from the convenience of a graphical representation, the reason for introducing the Young diagram is to put something in the boxes. Any way of placing positive integers in each box will be called a

- *numbering*, if the entries are all distinct.
- *filling*, if the entries are not distinct.

A *tableau* is a filling that is

1. Weakly increasing in each row.
2. Strictly increasing in each column

λ is called the shape of the tableau T. A *standard tableau* is a tableau which is a numbering. We can transpose a Young diagram by flipping it along the diagonal e.g.  →  .

A.2.1 A preview of symmetric polynomials

To any numbering of T of a Young diagram we associate a monomial X^T which is a product of the variables X_i corresponding to the i's that occur in T. e.g. if  contains two 1's, two 2's, one 3 and one 5 then,  → $X_1^2X_2^2X_3X_5$. Associated to each partition λ and integer m such that λ has at most m rows, there is a very important symmetric polynomial called the *Schur polynomial* which is defined as

$$s_\lambda(X_1, \ldots, X_n) = \sum X^T$$

where the sum is over all tableau of shape λ using $1, \ldots, m = [m]$. It turns out the s_λ are symmetric polynomials and form a basis of the ring of symmetric polynomials.

The Schur polynomial corresponding to the Young diagram of $\lambda = (n)$ is called the n^{th} *completely symmetric polynomial.* It is the sum of all distinct monomials of degree n in the variables $X_1 \ldots X_m$. It is denoted by $h_n(X_1, \ldots, X_m) = h_n(X)$. Similarly the Schur polynomial corresponding to $\lambda = (1^n)$, is called the n^{th} *elementary symmetric polynomial.* This polynomial is the sum of all monomials $X_{i_1}, \ldots, X_{i_n}$ for all strictly increasing sequences i.e. $1 \leq i_1 < i_2 \ldots < i_n \leq m$ and is denoted by $e_n(X_1, \ldots, X_n) = e_n(X)$. It is clear that e_i and h_i are symmetric polynomials. The first few polynomials are given by

$$h_1 = e_1 = X_1 + X_2 + \ldots + X_m$$

$$h_2 = \sum_{i \leq j} X_i X_j$$

$$e_2 = \sum_{i < j} X_i X_j$$

There are some beautiful identities dating back to the nineteenth century in the ring Λ_m. They can be proved by brute-force techniques. However, it is much easier to follow the

somewhat circuitous path of the *plactic monoid* which was developed in the latter half of the twentieth century.

A.2.2 Plactic monoid

Before we explain what a plactic monoid is, we need to give some other preliminary explanations. First we give the *Schensted Row-insertion Algorithm.* Given a tableau T and a positive integer x, we construct a new tableau denoted by $T \leftarrow x$. The algorithm is: if x is at least as large as all the entries in the first row of T, simply add x in a new box to the end of the first row. If not, find the left-most entry in the first row that is strictly larger than x. Put x in the box of this entry, and remove ("bump") the entry. Take this entry that was bumped from the first row, and repeat the process on the second row. Keep going until the bumped entry can be put at the end of the row it is bumped into, or until it is bumped out at the bottom, in which case it forms a new row with one entry [1] It turns out that we again get a tableau with one more box.

This algorithm can be used to define the *product tableau* $T.U$ of two tableau T and U. The algorithm is to start with T and row-insert the left-most entry in the bottom row of U into T. Row-insert into the result, the next entry of the bottom row of U, and continue until all entries in the bottom row of U have been inserted. Then insert, in order, the entries of the next to last row, left to right, and continue with other rows until all entries of U have been inserted i.e. if we list entries of U in order from left to right and bottom to top, we get the sequence $x_1, x_2, \ldots, x_s$ then

$$T.U = ((((\ldots(T \leftarrow x_1) \leftarrow x_2) \leftarrow \ldots) \leftarrow x_{s-1}) \leftarrow x_s)$$

(see pages 11-12 [30]).

Theorem. *The product operation makes the set of tableau an associative monoid. The empty tableau is a unit in this monoid* $\phi.T = T.\phi = T$.

Proof. See pages 30-35 [30] .

[1] See page 7, [30] from where this description is copied and the example there.

This is called the *plactic monoid* (this is actually called the monoid of tableau and another monoid, isomorphic to the monoid of tableau, is called the plactic monoid. See page 23 [30]). A monoid has an associated *group ring*. For the monoid of tableau with entries in $[m]$ we denote this *tableau ring* by $R_{[m]}$. This is a free $\mathbb{Z}$-module, with basis, the tableau with entries in $[m] = \{1, \ldots, m\}$. There is a natural ring homomorphism from

$$R_{[m]} \to \mathbb{Z}[X_1, \ldots, X_m]$$

which maps $T \to X^T$, where $X^T$is the product of variables X_i, each occurring as many times in X^T as i occurs in T. It turns out that it is easier to prove certain identities in $R_{[m]}$ and carry them over, by the ring homomorphism to $\mathbb{Z}[X_1, \ldots, X_m]$. This is the reason why we introduced the plactic monoid in the first place.

A.2.3 Some useful identities in $R_{[m]}$

Let $S_\lambda = S_\lambda[m]$ be the sum of all tableau of shape λ with entries in $[m]$.

Lemma 1.

$$S_\lambda . S_{(p)} = \sum_\mu S_\mu$$

where the sum is over all μ's that are obtained from λ by adding p boxes, with no two in the same column. Similarly

$$S_\lambda . S_{(1^p)} = \sum_\mu S_\mu$$

where the sum is over all μ's that are obtained by adding p boxes to λ, with no two in the same column.

Proof. See page 24 [30] .

A tableau T has *content* $\mu = (\mu_1, \ldots \mu_l)$if its entries consist of u_1 $1's$, u_2 $2's$ etc. up to u_l $l's$. Let λ be a partition of n and $\mu = (\mu_1, \ldots, \mu_l)$ a sequence of non-negative integers. Then define $K_{\lambda\mu} \doteq$ number of tableau of shape λ with content μ.

Lemma 2.

$$S_{(\mu_1)} \cdot S_{(\mu_2)} \ldots S_{(\mu_l)} = \sum_{\lambda} K_{\lambda\mu} S_{\lambda}$$

$$S_{(1^{\mu_1})} \ldots S_{(1^{\mu_l})} = \sum_{\lambda} K_{\tilde{\lambda}\mu} S_{\lambda}$$

where $\tilde{\lambda}$ *is conjugate to* λ.

Proof. See pages 25-26 [30] .

Littlewood-Richardson Rule 1.

$$S_{\lambda} \cdot S_{\mu} = \sum_{\nu} c_{\lambda\mu}^{\nu} S_{\nu}$$

Proof. See page 63 [30] .

The $c_{\lambda\mu}^{\nu}$ are non-negative integers called the Littlewood-Richardson integers.

A.2.4 More symmetric polynomials

We have the ring homomorphism

$$R_{[m]} \to \mathbb{Z}[X_1, \ldots X_n]$$

mapping $T \mapsto X^T$. Under this homomorphism

$$S_{\lambda} \mapsto s_{\lambda}(X_1, \ldots X_m)$$

$$S_{(p)} \mapsto h_p(X_1, \ldots, X_m)$$

$$S_{(1^p)} \mapsto e_p(X_1, \ldots, X_m)$$

and our results of the previous subsection transfer over to the ring of symmetric polynomials. Hence we have the following lemma.

Lemma 3.

$$s_\lambda(X_1, \ldots, X_m)h_p(X_1, \ldots, X_m) = \sum_\mu s_\mu(X_1, \ldots, X_m)$$

$$s_\lambda(X_1, \ldots, X_m)e_p(X_1, \ldots, X_m) = \sum_\mu s_\mu(X_1, \ldots, X_m)$$

Littlewood-Richardson Rule 2.

$$s_\lambda s_\mu = \sum_\nu c_{\lambda\mu}^\nu s_\nu$$

Although the theorem follows from the corresponding theorem in $R_{[m]}$, there is an elegant, direct proof given by Stembridge [96] . The reader is strongly urged to look at it. In fact as a corollary to Stembridge's Theorem we get an alternative definition of Schur polynomials (which was the original one given by Jacobi).

Corollary.

$$s_\lambda = \frac{|X_j^{\lambda_i+m-i}|}{|X_j^{m-i}|}$$

where $|a_{i,j}|$ = *determinant of a* $m \times m$ *matrix.*

For a partition λ define

$$h_\lambda = h_{\lambda_1}h_{\lambda_2}\ldots h_{\lambda_m}$$

$$e_\lambda = e_{\lambda_1}e_{\lambda_2}\ldots e_{\lambda_m}$$

We also define a new basis by m_λ = sum of all distinct monomials obtained from $X_1^{\lambda_1}\ldots X_m^{\lambda_m}$ by permuting all variables e.g.

$$m_{(2,1)} = \sum_{i\neq j} X_i^2 X_j$$

Theorem. *The following are bases over* $\mathbb{Z}$ *of the homogeneous polynomials of degree n in m variables.*

1. $\{m_\lambda : \lambda$ *a partition of n with at most m rows* $\}$

2. $\{s_\lambda : \lambda$ *a partition of n with at most m rows* $\}$

3. $\{e_\lambda : \lambda$ *a partition of n with at most m columns* $\}$

4. $\{h_\lambda : \lambda$ *a partition of n with at most m columns* $\}$

5. $\{h_\lambda : \lambda$ *a partition of n with at most m rows* $\}$

Proof. See pages 73-74 of [30] .

For many useful identities relating to these and other symmetric polynomials, a good starting point would be pages 72-78 of [30] . It is somewhat difficult to keep track of the number of variables m. Either we can assume they are "sufficiently large" or use something slightly more fancy (see page 77 of [30]). In either case, we now drop m and get our ring of symmetric functions as

$$\Lambda = \oplus_{n=0}^{\infty} \Lambda_n$$

where n is the degree of the symmetric polynomial.

Since the Schur functions form a a basis of Λ_n, we can put an inner product on Λ_n by requiring that s_λ form an orthonormal basis i.e. $< s_\lambda, s_\mu >= \delta_{\lambda\mu}$

A.2.5 Construction of the representations

Let T be a numbering. $S(m)$ acts on the set of numberings with $\sigma \in S(m)$ mapping $T \mapsto \sigma T$, where σT is a numbering that puts $\sigma(i)$ in the box in which T puts i. For any numbering T, we have a subgroup $R(T)$ of $S(m)$ which consists of those permutations that permute entries of each row among themselves. Analogously we can define the column group $C(T)$.

$$R(T) \cong S(\lambda_1) \times S(\lambda_2) \times \ldots \times S(\lambda_m)$$

$$C(T) \cong S(\tilde{\lambda_1}) \times S(\tilde{\lambda_2}) \times \ldots \times S(\tilde{\lambda_m})$$

where $\tilde{\lambda}$ is conjugate to λ.

Now for any given partition λ, let us fix a standard tableau T[2]. We can then define $a_\lambda, b_\lambda, c_\lambda \in \mathbb{C}$ by

$$\begin{aligned} a_\lambda &= \sum_{p \in R(T)} p \\ b_\lambda &= \sum_{q \in C(T)} (sgn\ q) q \\ c_\lambda &= a_\lambda b_\lambda \end{aligned}$$

Let $A = \mathbb{S}(m)$. We can define $S^\lambda = A\, b_\lambda a_\lambda \simeq A c_\lambda$ and $M^\lambda = A a_\lambda$. Clearly $S^\lambda \subset M^\lambda$. In fact one can show that

Theorem. *For each partition λ of n, S^λ is an irreducible representation of $S(n)$. Every irreducible representation of $S(n)$ is isomorphic to exactly one S^λ.*

Let R_n be the free Abelian group on isomorphism classes of irreducible representations of $S(n)$ i.e. $[V] \in R_n \to [V] = \sum m_\lambda [S^\lambda]\ m_\lambda \in \mathbb{Z}$ where $[V]$ denotes isomorphism class of V, a representation of $S(n)$. Define

$$R = \oplus_{n=0}^{\infty} R_n \quad R_0 = \mathbb{Z}$$

Define a product on R

$$R_n \times R_m \to R_{n+m}$$

by

$$[V].[W] = [Ind_{S_n \times S_m}^{S_{n+m}} V \otimes W]$$

This product is associative and makes R into a commutative, associative, graded ring with unit. This is called the *Grothendeik group*. Now we can define a symmetric inner product on R_n by requiring $[S^\lambda]$ form an orthonormal basis. Since h_λ form a basis of Λ we can

[2]We could use the unique normal tableau.

define a ring homomorphism

$$\varphi : \Lambda \to R$$

sending $h_\lambda \mapsto [M^\lambda]$.

Theorem. *φ is a homomorphism of graded rings which preserves inner products and $\varphi(s_\lambda) = [S^\lambda]$.*

Proof. See page 91 of [30] .

This is the main result that now allows us to transfer what we know about symmetric functions to the irreducible representations of $S(m)$. Hence we get our third version of the celebrated *Littlewood-Richardson Rule*: this time it is for the irreducible representations of $S(m)$.

Littlewood-Richardson Rule 3.

$$S^\lambda . S^\mu \cong \oplus_\nu S^{\nu \oplus c^\nu_{\lambda\mu}}$$

Corollary.

$$S^\lambda \otimes \mathbb{U}_m \cong S^{\tilde{\lambda}}$$

where $\mathbb{U}_n$ is the alternating representation and $\tilde{\lambda}$ is conjugate to λ.

A.3 Schur-Weyl Duality

Consider $V^{\otimes m}$ where $V = \mathbb{C}^n$. $GL(V)$ and $S(m)$ act on $V^{\otimes m}$ in the obvious manner: let $g \in GL(V)$ and $\sigma \in S(m)$ then

$$g.v_1 \otimes v_2 \otimes \ldots v_n = gv_1 \otimes gv_2 \otimes \ldots gv_m$$

$$v_1 \otimes v_2 \otimes \ldots v_m.\sigma = v_{\sigma(1)} \otimes v_{\sigma(2)} \otimes \ldots v_{\sigma(m)}$$

These two actions of $S(n)$ and $GL(V)$ commute with each other[3]

[3]In fact $GL(V)$ and $S(n)$ are *commutants* of each other. This fact plays a very important role in Schur-Weyl

Let λ be a partition of m, and T a standard tableau with $C(T) \equiv c_\lambda$. Define the Schur module[4].

$$\mathbb{S}_\lambda V = Im(c_\lambda)$$

Theorem. *Let $n = \dim V$. Then*

1. *$\mathbb{S}_\lambda V$ is zero if $\lambda_{n+1} \neq 0$. If $\lambda = (\lambda_1 \geq \lambda_2 \ldots \lambda_n \geq 0)$ then $\dim \mathbb{S}_\lambda V = s_\lambda(1, 1, \ldots, 1)$.*

2. *Under the action of $GL(n, \mathbb{C}) \times S(m)$, the space of m-tensors over $\mathbb{C}^n$ decomposes*

$$V^{\otimes m} = \oplus \mathbb{S}_\lambda(V) \otimes S^\lambda$$

   where the sum is over all partitions of m with at most n parts.

3. *Each $\mathbb{S}_\lambda V$ is an irreducible representation of $GL(V)$.*

4. *For any $g \in GL(V)$*

$$\chi_{\mathbb{S}_\lambda V}(g) = s_\lambda(x_1, \ldots, x_n)$$

   where $x_1, \ldots, x_n$ are eigenvalues of g.

Proof. See pages 84-87 [31] and page 374 [35] .

Corollary. *Let $c \in \mathbb{C}S(m)$ and $(\mathbb{C}S(m)).\sigma = \oplus_\lambda V_\lambda^{\oplus r_\lambda}$ as representations of $S(m)$, there is a corresponding decomposition of $GL(V)$-spaces by*

$$V^{\otimes m}.c = \oplus_\lambda \mathbb{S}_\lambda^{\oplus r_\lambda}$$

Littlewood-Richardson Rule 4.

$$\mathbb{S}_\lambda V \otimes \mathbb{S}_\mu V \cong \oplus_\nu c_{\lambda\mu}^\nu \mathbb{S}_\nu V$$

---

duality vector space W. For any $S \subset End(W)$ we define

$$Comm(S) = \{x \in End(W) : xs = sx \text{ for all } s \in S\}$$

$Comm(S)$ is called the *commutant* of S. Let $W = V^{\otimes m}$, $\mathcal{A} = \rho(\mathbb{C}[GL(V)])$ and $\mathcal{B} = \pi(\mathbb{C}[S(n)])$ where ρ, π are representations of $GL(V)$ and $S(n)$ on $V^{\otimes m}$ described above.

[4]We can define the Schur module in an intrinsic way.

where $c^{\nu}_{\lambda\mu}$ are Littlewood-Richardson numbers.

A.3.1 Remarks

Since $\mathbb{S}_\lambda V$ is an irreducible representation of $GL(V)$, $\mathbb{S}_\lambda V$ is also an irreducible representation of $SL(V)$. By the correspondence between irreducible representations of connected Lie groups and their Lie algebras, we get an irreducible representation of $\mathfrak{sl}(n, \mathbb{C})$.

Theorem. *The representation $\mathbb{S}_\lambda V$ is the irreducible representation of $\mathfrak{sl}(n, \mathbb{C})$ with highest weight $\lambda_1 L_1 + \ldots + \lambda_n L_n$ where the* weight lattice *is given by*

$$\Lambda_W = \mathbb{Z}L_1, \ldots L_n / (\sum L_i = 0)$$

Proof. See page 223 of [31] .

By the *Theorem of Highest Weight*, we know that these are all the irreducible representations of $\mathfrak{sl}(n, \mathbb{C})$.

A.4 Some Comments on $SU(n)$ and $\mathfrak{sl}(n, \mathbb{C})$

Physicists are mostly interested in irreducible representations of $SU(n)$ and yet they use the representation theory of $\mathfrak{sl}(n, \mathbb{C})$. The reason is that there is a one-one correspondence between representations of the *real lie group* $SU(n)$ and the *complex lie algebra* $\mathfrak{sl}(n, \mathbb{C})$. This occurs via *Weyl's Unitary trick.*

Suppose we are given a complex representation ρ of $\mathfrak{sl}(n, \mathbb{C})$. Since

$$\mathfrak{sl}(n, \mathbb{C}) = \mathbb{C} \otimes \mathfrak{su}(n) = \mathfrak{su}(n) \oplus i\mathfrak{su}(n)$$

Restrict ρ to $\mathfrak{su}(n)$. ρ is still irreducible under $\mathfrak{su}(n)$. Since $\mathfrak{su}(n)$ is the Lie algebra of a simply connected Lie group $SU(n) \Rightarrow$ it lifts to a representation of $SU(n)$. Since $SU(n)$ is connected, this lifting is still irreducible.

Conversely, given an irreducible representation of $SU(n)$ it gives an irreducible representation of $\mathfrak{su}(n)$ (since $SU(n)$ is a connected Lie group) $\Rightarrow$ it extends to an irreducible representation of $\mathfrak{sl}(n, \mathbb{C})$.

Appendix B

Semi-Classical Matrix Element Calculation

This appendix should be considered as a supplement to sections 7.5 and 7.6. Here we discuss the classical method of calculating matrix elements in some detail and apply it to the spin and isospin parts of three-body wavefunctions. As explained at the beginning of chapter 7, in this method we

- Expand spin and isospin wavefunctions in terms of a basis with special symmetry properties under the exchange of the last two particles.
- Leave spatial wavefunctions in their original form (and hence it has no symmetry properties under exchange of last two coordinates).
- Evaluate matrix elements, with the results given in terms of multidimensional spatial integrals.

It should be emphasized, that this approach to calculating matrix elements cannot be applied to the H-J potential. The reason being, that in the H-J, the potential is dependent on the spatial symmetry and spin of the wavefunctions involved. When the matrix elements are calculated, we get (as shown in section 7.6) spurious couplings between states of even and odd spatial symmetry (the same applies to spin as well). Hence, in evaluating the

matrix elements, we do not know whether to use even-singlet, even-triplet, odd-singlet or odd-triplet values. However, this method can be applied to other potentials which are not given in terms of even-singlet, odd-singlet etc. parameters.

We will first give a proof of Equation 7.6 and then summarize the results. In the end we will show how to put everything together in order to explicitly calculate matrix elements.

B.1 Proof of Equation 7.6

Take our given wavefunction Ξ. Then

$$\begin{aligned}\Xi &= |[\tilde{\eta}]_R[\eta']_S[\eta'']_T\rangle \\ &= \frac{1}{\sqrt{d_\eta}} \sum_{[\tilde{Y}]} \Psi_n((\tilde{\eta}), [\tilde{Y}]) \sum_{[Y'],[Y'']} C((\eta')[Y'](\eta'')|(\eta)Y)\Phi_n((\eta'), [Y'], M_S)\Gamma_n((\eta''), [Y''], M_T)\end{aligned}$$

where

- d_η is the dimension of the representation (η).
- the C's are the Clebsch-Gordan coefficients of $S(n)$.
- (η), (η') and (η'') are the Young diagrams with corresponding Yamanouchi symbols $[Y]$, $[Y']$ and $[Y'']$.
- $(\tilde{\eta})$ and $[\tilde{Y}]$ are the conjugate Young diagram and Yamanouchi symbol to (η) and $[Y]$ respectively.
- Ψ_n, Φ_n and Γ_n are n-body space, spin and isospin wavefunctions.

Let the Yamanouchi symbols be given by $Y = pq\ y$, where p, q refer to the rows of particles n and $n-1$ and y is the remaining Yamanouchi symbol. Suppose we could write out each

of the space, spin and isospin wavefunctions as a product

$$\begin{aligned}
\Phi_n((\eta'),[p'q'y'],M_S) &= \sum_{s,s'....} \sigma_{\eta'_{p'q'}} \Phi_{n-2}((\eta'_{p'q'})[y'],M'_S)\phi_2([s]) \\
\Gamma_n((\eta''),[p''q''y''],M_S) &= \sum_{t,t''....} \tau_{\eta''_{p''q''}} \Gamma_{n-2}((\eta''_{p''q''})[y''],M''_S)\gamma_2([t]) \\
\Psi_n((\tilde{\eta}),[\tilde{p}\tilde{q}\tilde{y}] &= \sum_{r,r'....} \rho_{\tilde{\eta}_{\tilde{p}\tilde{q}}} \Psi_{n-2}((\tilde{\eta}_{\tilde{p}\tilde{q}})[\tilde{y}])\psi_2([r])
\end{aligned} \tag{B.1}$$

where ψ, ϕ, γ depend on the coordinates of the last two particles and are either symmetric or antisymmetric under transposition of particle labels and e.g. $\eta'_{p'q'}$ is the Young diagram we get by removing the boxes from η' containing particles n and $n-1$.

From Racah's factorization lemma [94] we know that

$$C([\eta'],p'q'y'[\eta''],p''q''y''|[\eta]pqy) = K_2([\eta],pq[\eta']p'q'|[\eta'']p''q'')C([\eta'_{p'q'}]y'[\eta''_{p''q''}]y''|[\eta_{pq}]y)$$

where K_2 is an isoscalar factor [94] of $S(n)$. After some algebra, we see that

$$\begin{aligned}
\Xi &= \frac{1}{n_\eta} \sum_{r,s,t,r'.....} \sum_{\tilde{p}\tilde{q}} \sum_{p'q'} \sum_{p''q''} \sqrt{n_{\eta_{pq}}} \sigma_{\eta'_{p'q'}} \tau_{\eta''_{p''q''}} \rho_{\tilde{\eta}_{\tilde{p}\tilde{q}}} K_2([\eta],pq[\eta']p'q'|[\eta'']p''q'') \\
&\quad \psi_2([r])\phi_2([s])\gamma_2([t])\Psi_{n-2}
\end{aligned}$$

Now, modulo the proof of Equation B.1, we have proved Equation 7.6. In the next section we use the diagonalized Young-Yamanouchi-Rutherford representation to prove Equation B.1.

B.2 Diagonalized Young-Yamanouchi-Rutherford Representation

As stated before, this method only works for product states. Hence it is not applicable to our correlated spatial wavefunctions. However, if we were dealing with angular momentum eigenstates, then Equation B.1 would be true, which in turn would imply Equation 7.6,

and hence we would get all the simplifications of the classical method as mentioned in section 7.4. However, in our case, we can only apply it to spin and isospin wavefunctions. Two facts will be used to break up a spin (or isospin) wavefunction into something which is symmetric or antisymmetric in the last two variables. The first is the change of order of angular momentum coupling [49]

$$\Phi(j_1^c, j_1^a, j_1^b(J_{ab}), J, M) = \sum_{J_{ac}} U(j_c j_a J j_b; J_{ac}, J_{ab}) \Phi(j_1^c, j_2^a, (J_{ac}), j_3^b, J, M)$$

where U is the Jahn U-coefficient which is related to the famous Racah W-coefficient by

$$U(abcd; ef) = \sqrt{(2c+1)(2f+1)} W(abcd; ef)$$

The other fact is that given a Young diagram $[f]$ with Young-Yamanouchi symbol $Y = pqy$ (with p and q representing the first two numbers and y the last $n-2$), then

$$\begin{aligned} |[\eta]\overline{pq}y\rangle &= \sqrt{\frac{\mu+1}{2\mu}} |[\eta]pqy\rangle + \sqrt{\frac{\mu-1}{2\mu}} |[\eta]qpy\rangle \\ |[\eta]\tilde{pq}y\rangle &= \sqrt{\frac{\mu-1}{2\mu}} |[\eta]pqy\rangle - \sqrt{\frac{\mu+1}{2\mu}} |[\eta]qpy\rangle \end{aligned}$$

provided $p < q$ where

- $\mu = c_n - c_{n-1} - (r_n - r_{n-1})$ where $c_i(r_i)$ is the column(row) of the the number i. It is called the *axial distance*. Here particles n and $n-1$ are in rows p and q respectively.

- $\overline{pq}(\tilde{pq})$ represents a wavefunction symmetric(antisymmetric) in the last two particles i.e. in n and $n-1$.

Let us see how these two facts allow us to expand a spin (or isospin) wavefunction of arbitrary symmetry in terms of wavefunctions, symmetric or antisymmetric in the last two variables. Following the method of Elliot, Hope and Jahn [25], we illustrate it via a concrete example.

B.2.1 An example

Consider the spin wavefunctions $\phi([\boxplus]121, S = \frac{1}{2}, M_S)$ and $\phi([\boxplus]211, S = \frac{1}{2}, M_S)$. By using the first fact, we can write these as

$$\begin{aligned}
\phi([\boxplus]121, S = \frac{1}{2}, M_S) &= \phi(s_a = \frac{1}{2}, s_b = \frac{1}{2}(S_{ab} = 0), s_c = \frac{1}{2}, S = \frac{1}{2}, M_S) \\
&= \sum_{S_{bc}} U(\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}; 0, S_{bc})\phi(s_a = \frac{1}{2}, s_b = \frac{1}{2}, s_c = \frac{1}{2}, S_{bc}, S = \frac{1}{2}, M_S) \\
&= -\frac{1}{2}\phi(s_a = \frac{1}{2}, s_b = \frac{1}{2}, s_c = \frac{1}{2}, (S_{bc} = 0), S = \frac{1}{2}, M_S) + \\
&\quad \frac{\sqrt{3}}{2}\phi(s_a = \frac{1}{2}, s_b = \frac{1}{2}, s_c = \frac{1}{2}(S_{bc} = 1), S = \frac{1}{2}, M_S)
\end{aligned}$$

$$\begin{aligned}
\phi([\boxplus]211, S = \frac{1}{2}, M_S) &= \phi(s_a = \frac{1}{2}, s_b = \frac{1}{2}(S_{ab} = 1), s_c = \frac{1}{2}, S = \frac{1}{2}, M_S) \\
&= \sum_{S_{bc}} U(\frac{1}{2}\frac{1}{2}\frac{1}{2}\frac{1}{2}; 1, S_{bc})\phi(s_a = \frac{1}{2}, s_b = \frac{1}{2}, s_c = \frac{1}{2}, S_{bc}, S = \frac{1}{2}, M_S) \\
&= \frac{\sqrt{3}}{2}\phi(s_a = \frac{1}{2}, s_b = \frac{1}{2}, s_c = \frac{1}{2}(S_{bc} = 0), S = \frac{1}{2}, M_S) + \\
&\quad \frac{1}{2}\phi(s_a = \frac{1}{2}, s_b = \frac{1}{2}, s_c = \frac{1}{2}(S_{bc} = 1), S = \frac{1}{2}, M_S) \qquad \text{(B.2)}
\end{aligned}$$

Note that since we are dealing with $SU(2)$, there is no need to write the total value of spin, since given the total number of particles, there is a one-one correspondence between the shape of the Young diagram and total spin i.e. given that ϕ belongs to the $[\boxplus]$ representation, we know that $S = \frac{1}{2}$. Also the M_S value is a constant in each equation, and the coefficients are independent of M_S. Thus, unless explicitly needed we will not carry these two labels.

For the Yamanouchi symbol 121, the axial distance $\mu = 2$ (in the statement of second fact $p < q$ for a Yamanouchi symbol pqy so we cannot use 211 here). By the second fact

$$\begin{aligned}
\phi([\boxplus]\overline{12}1) &= \frac{\sqrt{3}}{2}\phi([\boxplus], 121) + \frac{1}{2}\phi([\boxplus], 211) \\
\phi([\boxplus]\tilde{12}1) &= \frac{1}{2}\phi([\boxplus], 121) - \frac{\sqrt{3}}{2}\phi(\boxplus, 211)
\end{aligned}$$

Using this equation we can write

$$\begin{aligned}\phi([\square\square], 121) &= \frac{\sqrt{3}}{2}\phi([\square\square]\overline{12}1) + \frac{1}{2}\phi([\square\square]\tilde{12}1)\\ \phi([\square\square], 211) &= \frac{1}{2}\phi([\square\square]\overline{12}1) - \frac{\sqrt{3}}{2}\phi([\square\square]\tilde{12}1)\end{aligned} \tag{B.3}$$

Comparing Equations B.2 and B.3, we easily conclude that (dropping the Young diagram $\square\square$)

$$\begin{aligned}\phi(\overline{12}1) &= \phi(s_a = \frac{1}{2}, s_b = \frac{1}{2}, s_c = \frac{1}{2}(S_{bc} = 1), S = \frac{1}{2}, M_S)\\ \phi(\tilde{12}1) &= -\phi(s_a = \frac{1}{2}, s_b = \frac{1}{2}, s_c = \frac{1}{2}(S_{bc} = 0), S = \frac{1}{2}, M_S)\end{aligned}$$

In all the calculations that we do, we change this notation slightly and use

$$\begin{aligned}\phi([\square\square], 121) &= \frac{\sqrt{3}}{2}\phi([\square\square]\overline{12}1) - \frac{1}{2}\phi([\square\square]\tilde{12}1)\\ \phi([\square\square], 211) &= \frac{1}{2}\phi([\square\square]\overline{12}1) + \frac{\sqrt{3}}{2}\phi([\square\square]\tilde{12}1)\end{aligned} \tag{B.4}$$

and correspondingly change the sign of $\phi(\tilde{12}1)$ i.e.

$$\begin{aligned}\phi(\overline{12}1) &= \phi(s_a = \frac{1}{2}, s_b = \frac{1}{2}, s_c = \frac{1}{2}(S_{bc} = 1), S = \frac{1}{2}, M_S)\\ \phi(\tilde{12}1) &= \phi(s_a = \frac{1}{2}, s_b = \frac{1}{2}, s_c = \frac{1}{2}(S_{bc} = 0), S = \frac{1}{2}, M_S)\end{aligned}$$

With this, we have solved the problem of rewriting our total wavefunction in terms of spin/isospin wavefunctions which are symmetric or antisymmetric under the exchange of the last two particles.

B.3 Wavefunctions

Using Equation B.4, we can rewrite the three-body wavefunctions as

$$\begin{aligned}
\Psi_1 &= \psi(111)\frac{1}{\sqrt{2}}\left[\phi(\tilde{1}21)\Gamma(\overline{12}1) - \phi(\overline{12}1)\Gamma(\tilde{1}21)\right] \\
\Psi_2 &= \psi(321)\frac{1}{\sqrt{2}}\left[\phi(\overline{12}1)\Gamma(\overline{12}1)+\right] \\
\Psi_3 &= \frac{1}{2}\psi(211)\left[\frac{\sqrt{3}}{2}\phi(\tilde{1}21)\Gamma(\tilde{1}21) - \frac{1}{2}\phi(\tilde{1}21)\Gamma(\overline{12}1) - \frac{1}{2}\phi(\overline{12}1)\Gamma(\tilde{1}21) - \frac{\sqrt{3}}{2}\phi(\overline{12}1)\Gamma(\overline{12}1)\right] \\
&\quad -\frac{1}{2}\psi(121)\left[\frac{1}{2}\phi(\tilde{1}21)\Gamma(\tilde{1}21) + \frac{\sqrt{3}}{2}\phi(\tilde{1}21)\Gamma(\overline{12}1) + \frac{\sqrt{3}}{2}\phi(\overline{12}1)\Gamma(\tilde{1}21) - \frac{1}{2}\phi(\overline{12}1)\Gamma(\overline{12}1)\right] \\
\Psi_4 &= \frac{1}{\sqrt{2}}\left[\psi(211)\phi(111)\Gamma(121) - \psi(121)\phi(111)\Gamma(211)\right]
\end{aligned}$$

B.4 Matrix Elements

To reduce the length of the formulas, we will use the short hand

$$\begin{aligned}
\phi^s &= \phi(\overline{12}1) \\
\Gamma^s &= \Gamma(\overline{12}1) \\
\phi^a &= \phi(\tilde{1}21) \\
\Gamma^a &= \Gamma(\tilde{1}21) \\
\bar{\psi} &= \psi(111) \\
\tilde{\psi} &= \psi(321)
\end{aligned}$$

We also know that the operator V_{23}, with or without any isospin dependence, does not couple symmetric and antisymmetric states i.e.

$$\begin{aligned}
\langle\phi^a|V_{23}|\phi^s\rangle &= 0 \\
\langle\Gamma^a|V_{23}|\Gamma^s\rangle &= 0
\end{aligned}$$

This can be seen as a simple application of Wigner-Eckart theorem for the symmetric group. If one looks at the nuclear force, there seem to be two types of operators; one, isospin dependent, of the form $\vec{\tau}_2.\vec{\tau}_3\theta_{23}$ and the other, isospin independent, of the form θ_{23}, where θ_{23} contains spin and space terms only. We give the results of our calculations in the next couple of subsections.

B.4.1 Isospin dependent potentials

Using the fact that

$$\begin{aligned}\langle\Gamma^s(M_T)|\vec{\tau}_2.\vec{\tau}_3|\Gamma^s(M'_T)\rangle &= -3\,\delta_{M_S,M'_S}\\ \langle\Gamma^a(M_T)|\vec{\tau}_2.\vec{\tau}_3|\Gamma^a(M_T)\rangle &= \delta_{M_T,M'_T}\end{aligned}$$

we can start calculating the various matrix elements.

$$\langle\Psi_1(M_S,M_T)|\vec{\tau}_2.\vec{\tau}_3\theta|\Psi_1(M'_S,M'_T) = \frac{1}{2}\int\overline{\psi}^*\left[-3\langle\phi^s(M_S)|\theta|\phi^s(M'_S)\rangle + \langle\phi^a(M_S)|\theta|\phi^a(M'_S)\rangle\right]\overline{\psi}\delta_{M_T,M'_T}$$

$$\langle\Psi_1(M_S,M_T)|\vec{\tau}_2.\vec{\tau}_3\theta|\Psi_2(M'_S,M'_T)\rangle = 0$$

$$\begin{aligned}\langle\Psi_1(M_S,M_T)|\vec{\tau}_2.\vec{\tau}_3\theta|\Psi_3(M'_S,M'_T) = &\\ \frac{1}{2\sqrt{2}}\int\overline{\psi}^*\left[-\frac{3}{2}\langle\phi^s(M_S)|\theta|\phi^s(M'_S)\rangle - \frac{1}{2}\langle\phi^a(M_S)|\theta|\phi^a(M'_S)\rangle\right]\psi(211)\delta_{M_T,M'_T}&\\ -\frac{1}{2\sqrt{2}}\int\overline{\psi}^*\left[\frac{3\sqrt{3}}{2}\langle\phi^s(M_S)|\theta|\phi^s(M'_S)\rangle + \frac{\sqrt{3}}{2}\langle\phi^a|\theta|\phi^a\rangle\right]\psi(121)\delta_{M_T,M'_T}&\end{aligned}$$

$$\langle \Psi_1(M_S, M_T)|\vec{\tau}_2.\vec{\tau}_3\theta|\Psi_4(M'_S, M'_T) =$$
$$\frac{1}{2}\int \overline{\psi}^* \left[-\frac{3}{2}\langle \phi^s(M_S)|\theta|\overline{\phi}(M'_S)\rangle\right]\psi(211) - \frac{1}{2}\int \overline{\psi}^* \left[\frac{3\sqrt{3}}{2}\langle \phi^s(M_S)|\theta|\overline{\phi}(M'_S)\rangle\right]\psi(121)\delta_{M_T,M'_T}$$

$$\langle \Psi_2(M_S, M_T)|\vec{\tau}_2.\vec{\tau}_3\theta|\Psi_2(M'_S, M'_T) =$$
$$\frac{1}{2}\int \tilde{\psi}^* \left[\langle \phi^s(M_S)|\theta|\phi^s(M'_S)\rangle - 3\langle \phi^a(M_S)|\theta|\phi^a(M'_S)\rangle\right]\tilde{\psi}\delta_{M_T,M'_T}$$

$$\langle \Psi_2(M_S, M_T)|\vec{\tau}_2.\vec{\tau}_3\theta|\Psi_3(M'_S, M'_T) =$$
$$\frac{1}{2\sqrt{2}}\int \tilde{\psi}^* \left[-\frac{\sqrt{3}}{2}\langle \phi^s(M_S)|\theta|\phi^s(M'_S)\rangle - \frac{3\sqrt{3}}{2}\langle \phi^a(M_S)|\theta|\phi^a(M'_S)\rangle\right]\psi(211)\delta_{M_T,M'_T}$$
$$-\frac{1}{2\sqrt{2}}\int \tilde{\psi}^* \left[-\frac{1}{2}\langle \phi^s(M_S)|\theta|\phi^s(M'_S)\rangle - \frac{3}{2}\langle \phi^a|\theta|\phi^a\rangle\right]\psi(121)\delta_{M_T,M'_T}$$

$$\langle \Psi_2(M_S, M_T)|\vec{\tau}_2.\vec{\tau}_3\theta|\Psi_4(M'_S, M'_T) =$$
$$\frac{1}{2}\int \tilde{\psi}^* \left[\frac{\sqrt{3}}{2}\langle \phi^s(M_S)|\theta|\overline{\phi}(M'_S)\rangle\right]\psi(211) - \frac{1}{2}\int \tilde{\psi}^* \left[\frac{1}{2}\langle \phi^s(M_S)|\theta|\overline{\phi}(M'_S)\rangle\right]\psi(121)\delta_{M_T,M'_T}$$

$$\langle\Psi_3(M_S, M_T)|\vec{\tau}_2.\vec{\tau}_3\theta|\Psi_3(M'_S, M'_T) =$$
$$\frac{1}{4}\int \psi^*(211)\left[-2\langle\phi^a|\theta|\phi^a\rangle\right]\psi(211)\delta_{M_T,M'_T} -$$
$$\frac{1}{4}\int \psi^*(211)\left[-\sqrt{3}\langle\phi^a|\theta|\phi^a\rangle + \sqrt{3}\langle\phi^s|\theta|\phi^s\rangle\right]\psi(121) -$$
$$\frac{1}{4}\int \psi^*(121)\left[-\sqrt{3}\langle\phi^a|\theta|\phi^a\rangle + \sqrt{3}\langle\phi^s|\theta|\phi^s\rangle\right]\psi(211) +$$
$$\frac{1}{4}\int \psi^*(121)\left[-2\langle\phi^s|\theta|\phi^s\rangle\right]\psi(121)\delta_{M_T,M'_T}$$

$$\langle\Psi_3(M_S, M_T)|\vec{\tau}_2.\vec{\tau}_3\theta|\Psi_4(M'_S, M'_T) =$$
$$\frac{1}{2\sqrt{2}}\int \psi^*(211)\left[-\frac{3}{2}\langle\phi^s(M_S)|\theta|\bar{\phi}(M'_S)\rangle\right]\psi(211)\delta_{M_T,M'_T} -$$
$$\frac{1}{2\sqrt{2}}\int \psi^*(211)\left[\frac{\sqrt{3}}{2}\langle\phi^s(M_S)|\theta|\bar{\phi}(M'_S)\rangle\right]\psi(121)\delta_{M_T,M'_T} -$$
$$\frac{1}{2\sqrt{2}}\int \psi^*(121)\left[\frac{\sqrt{3}}{2}\langle\phi^s(M_S)|\theta|\bar{\phi}(M'_S)\rangle\right]\psi(211)\delta_{M_T,M'_T} +$$
$$\frac{1}{2\sqrt{2}}\int \psi^*(121)\left[-\frac{5}{2}\langle\phi^s(M_S)|\theta|\bar{\phi}(M'_S)\rangle\right]\psi(121)\delta_{M_T,M'_T}$$

$$\langle\Psi_4(M_S, M_T)|\vec{\tau}_2.\vec{\tau}_3\theta|\Psi_4(M'_S, M'_T) =$$
$$-\frac{1}{2}\int \psi^*(211)\left[\sqrt{3}\langle\bar{\phi}(M_S)|\theta|\bar{\phi}(M'_S)\rangle\right]\psi(121)\delta_{M_T,M'_T} -$$
$$\frac{1}{2}\int \psi^*(121)\left[\sqrt{3}\langle\bar{\phi}(M_S)|\theta|\bar{\phi}(M'_S)\rangle\right]\psi(211)\delta_{M_T,M'_T}$$
$$+\frac{1}{2}\int \psi^*(121)\left[-2\langle\bar{\phi}(M_S)|\theta|\bar{\phi}(M'_S)\rangle\right]\psi(121)\delta_{M_T,M'_T}$$

B.4.2 Isospin independent potentials

$$\langle \Psi_1(M_S, M_T)|\theta|\Psi_1(M'_S, M'_T) = \frac{1}{2}\int \overline{\psi}^* \left[\langle \phi^s(M_S)|\theta|\phi^s(M'_S)\rangle + \langle \phi^a(M_S)|\theta|\phi^a(M'_S)\rangle\right]\overline{\psi}\delta_{M_T,M'_T}$$

$$\langle \Psi_1(M_S, M_T)|\theta|\Psi_2(M'_S, M'_T)\rangle = 0$$

$$\langle \Psi_1(M_S, M_T)|\theta|\Psi_3(M'_S, M'_T) = \frac{1}{2\sqrt{2}}\int \overline{\psi}^* \left[\langle \phi^s(M_S)|\theta|\phi^s(M'_S)\rangle - \frac{1}{2}\langle \phi^a(M_S)|\theta|\phi^a(M'_S)\rangle\right]\psi(211)\delta_{M_T,M'_T} - \frac{1}{2\sqrt{2}}\int \overline{\psi}^* \left[\frac{-\sqrt{3}}{2}\langle \phi^s(M_S)|\theta|\phi^s(M'_S)\rangle + \frac{\sqrt{3}}{2}\langle \phi^a|\theta|\phi^a\rangle\right]\psi(121)\delta_{M_T,M'_T}$$

$$\langle \Psi_1(M_S, M_T)|\theta|\Psi_4(M'_S, M'_T) = \frac{1}{2}\int \overline{\psi}^* \left[\frac{1}{2}\langle \phi^s(M_S)|\theta|\overline{\phi}(M'_S)\rangle\right]\psi(211) - \frac{1}{2}\int \overline{\psi}^* \left[\frac{-\sqrt{3}}{2}\langle \phi^s(M_S)|\theta|\overline{\phi}(M'_S)\rangle\right]\psi(121)\delta_{M_T,M'_T}$$

$$\langle \Psi_2(M_S, M_T)|\theta|\Psi_2(M'_S, M'_T) = \frac{1}{2}\int \tilde{\psi}^* \left[\langle \phi^s(M_S)|\theta|\phi^s(M'_S)\rangle + \langle \phi^a(M_S)|\theta|\phi^a(M'_S)\rangle\right]\tilde{\psi}\delta_{M_T,M'_T}$$

$$\langle \Psi_2(M_S, M_T)|\theta|\Psi_3(M'_S, M'_T) =$$
$$\frac{1}{2\sqrt{2}} \int \tilde{\psi}^* \left[-\frac{\sqrt{3}}{2} \langle \phi^s(M_S)|\theta|\phi^s(M'_S)\rangle + \frac{\sqrt{3}}{2} \langle \phi^a(M_S)|\theta|\phi^a(M'_S)\rangle \right] \psi(211)\delta_{M_T,M'_T}$$
$$-\frac{1}{2\sqrt{2}} \int \tilde{\psi}^* \left[-\frac{1}{2} \langle \phi^s(M_S)|\theta|\phi^s(M'_S)\rangle + \frac{1}{2} \langle \phi^a|\theta|\phi^a\rangle \right] \psi(121)\delta_{M_T,M'_T}$$

$$\langle \Psi_2(M_S, M_T)|\theta|\Psi_4(M'_S, M'_T) =$$
$$\frac{1}{2} \int \tilde{\psi}^* \left[\frac{\sqrt{3}}{2} \langle \phi^s(M_S)|\theta|\bar{\phi}(M'_S)\rangle \right] \psi(211) - \frac{1}{2} \int \tilde{\psi}^* \left[\frac{1}{2} \langle \phi^s(M_S)|\theta|\bar{\phi}(M'_S)\rangle \right] \psi(121)\delta_{M_T,M'_T}$$

$$\langle \Psi_3(M_S, M_T)|\theta|\Psi_3(M'_S, M'_T) =$$
$$\frac{1}{4} \int \psi^*(211) \left[\langle \phi^a|\theta|\phi^a\rangle \right] + \langle \phi^s|\theta\phi^s\rangle \psi(211)\delta_{M_T,M'_T} +$$
$$\frac{1}{4} \int \psi^*(121) \left[\langle \phi^a|\theta|\phi^a\rangle + \langle \phi^s|\theta|\phi^s\rangle \right] \psi(121)\delta_{M_T,M'_T}$$

$$\langle \Psi_3(M_S, M_T)|\theta|\Psi_4(M'_S, M'_T) =$$
$$\frac{1}{2\sqrt{2}} \int \psi^*(211) \left[-\frac{1}{2} \langle \phi^s(M_S)|\theta|\bar{\phi}(M'_S)\rangle \right] \psi(211)\delta_{M_T,M'_T} -$$
$$\frac{1}{2\sqrt{2}} \int \psi^*(211) \left[\frac{-\sqrt{3}}{2} \langle \phi^s(M_S)|\theta|\bar{\phi}(M'_S)\rangle \right] \psi(121)\delta_{M_T,M'_T} -$$
$$\frac{1}{2\sqrt{2}} \int \psi^*(121) \left[\frac{-\sqrt{3}}{2} \langle \phi^s(M_S)|\theta|\bar{\phi}(M'_S)\rangle \right] \psi(211)\delta_{M_T,M'_T} +$$
$$\frac{1}{2\sqrt{2}} \int \psi^*(121) \left[\frac{1}{2} \langle \phi^s(M_S)|\theta|\bar{\phi}(M'_S)\rangle \right] \psi(121)\delta_{M_T,M'_T}$$

$$\langle\Psi_4(M_S, M_T)|\theta|\Psi_4(M'_S, M'_T) = \frac{1}{2}\int \psi^*(211)\left[\langle\bar{\phi}(M_S)|\theta|\bar{\phi}(M'_S)\right]\psi(211)\delta_{M_T,M'_T} + \frac{1}{2}\int \psi^*(121)\left[\langle\bar{\phi}(M_S)|\theta|\bar{\phi}(M'_S)\right]\psi(121)\delta_{M_T,M'_T}$$

In order to get the answers, we still need to know the actual matrix elements of the nuclear potential operators. These are tabulated in the next subsection.

B.4.3 Certain useful three-body matrix elements

In chapter 7, we have already calculated the two-body matrix elements. Using those results, we can calculate the three-body matrix elements of the various nuclear force operators. For the three-body case there are two core "building blocks" of our wavefunctions. These are labeled 's' and 'a', being symmetric or antisymmetric under permutations of particles 2 and 3. The symmetric wavefunction is

$$\begin{aligned}\phi_3^s(M_S) &= \phi_3(s'' = \frac{1}{2}; s_2 = \frac{1}{2}, s_3 = \frac{1}{2}, S_2 = 1; S = \frac{1}{2}, M_S) \\ &= \sum_{m_{s''}+M_{S_2}=M_S} C^{\frac{1}{2},M_S}_{\frac{1}{2},m_{s''};1,m_{S_2}} |s'' = \frac{1}{2}, m_{s''}\rangle \otimes |S_2 = 1, M_{S_2}\rangle \end{aligned} \tag{B.5}$$

And the antisymmetric wavefunction is

$$\begin{aligned}\phi_3^a(M_S) &= \phi_3(s'' = \frac{1}{2}; s_2 = \frac{1}{2}, s_3 = \frac{1}{2}, S_2 = 0; S = \frac{1}{2}, M_S) \\ &= \sum_{m_{s''}+M_{S_2}=M_S} C^{\frac{1}{2},M_S}_{\frac{1}{2},m_{s''};1,m_{S_2}} |s'' = \frac{1}{2}, m_{s''}\rangle \otimes |S_2 = 0, M_{S_2}\rangle \\ &= C^{\frac{1}{2},M_S}_{\frac{1}{2},M_S;S_2=0,M_{S_2}=0} |m_{s''} = M_S\rangle \otimes |M_{S_2} = 0\rangle \\ &= |m_{s''} = M_S\rangle \otimes |M_{S_2} = 0\rangle \end{aligned} \tag{B.6}$$

Now we need to calculate the three matrix elements $\langle\phi_3^s|\theta|\phi_3^s\rangle$, $\langle\phi_3^s|\theta|\phi_3^a\rangle$ and $\langle\phi_3^a|\theta|\phi_3^a\rangle$ where θ is one of the operators in the nuclear force. Without doing any calculations, we can say that

$$\langle\phi_3^s|\theta|\phi_3^a\rangle = 0$$

This is because θ is completely symmetric under the exchange of particles 2 and 3 which means that it only couples symmetric to symmetric and antisymmetric to antisymmetric. This is a simple application of the Wigner Eckart theorem as applied to the symmetric group. In order to do these calculations we will use the results of the last section. As an example, we work out the details of the V_T operator. The rest can be worked out in exactly the same way.

B.4.4 The detailed V_T example

We want to calculate the matrix elements of

$$S_{23} = [[\vec{\sigma}_2 \times \vec{\sigma}_3]^{(2)} \times Y^{(2)}]^{(0)} 2\sqrt{6\pi}$$

$$\begin{aligned}\langle\phi_3^a(M_S)|S_{23}|\phi_3^a(M_{S'})\rangle &= \langle m_{s''} = M_S| \otimes \langle M_{S_2} = 0|S_{23}|M_{S_2'} = 0\rangle \otimes |m_{s''} = M_{S'}\rangle \\ &= 0\end{aligned}$$

The ϕ_3^s can be computed by

$$\langle \phi_3^s(M_S)|S_{23}|\phi_3^s(M_{S'})\rangle =$$
$$\sum_{m_{s''}+M_{S_2}=M_S} C^{\frac{1}{2},M_S}_{\frac{1}{2};1,M_{S_2}} \langle m_{s''}| \otimes \langle M_{S_2}|S_{23}| \sum_{m'_{s''}+M_{S'_2}=M_{S'}} C^{\frac{1}{2}M_{S'}}_{\frac{1}{2},m'_{s''};1,M_{S'_2}} |m'_{s''}\rangle \otimes |M^{S'_2}\rangle$$
$$= \sum_{m_{s''}+M_{S_2}=M_S}^{m''_s+M'_{S_2}=M'_S} C^{\frac{1}{2},M_S}_{\frac{1}{2},m_{s''};1,M_{S_2}} \langle M_{S_2}, S_2 = 1|S_{23}|M'_{S_2}, S_2 = 1\rangle C^{\frac{1}{2},M'_S}_{\frac{1}{2}}, m_{s''}; 1, M'_{S_2}\rangle$$

The results are explicitly calculated as below:

$M_S = \frac{1}{2}, M'_S = \frac{1}{2}$

$$C^{1/2,1/2}_{1/2,1/2;1,0} C^{1/2,1/2}_{1/2,1/2,1,0} \langle 0|S_{23}|0\rangle + C^{1/2,1/2}_{1/2,-1/2;1,1} C^{1/2,1/2}_{1/2,-1/2;1,1} \langle 1|S_{23}|1\rangle =$$
$$\frac{1}{3}\frac{2x^2+2y^2-4z^2}{r^2} + \frac{2}{3}\frac{2z^2-x^2-y^2}{r^2} = 0$$

$M_S = \frac{1}{2}, M'_S = -\frac{1}{2}$

$$C^{1/2,1/2}_{1/2,1/2;1,0} C^{1/2,-1/2}_{1/2,1/2,1,-1} \langle 0|S_{23}|-1\rangle + C^{1/2,1/2}_{1/2,-1/2;1,1} C^{1/2,-1/2}_{1/2,-1/2;1,0} \langle 1|S_{23}|0\rangle =$$
$$\frac{1}{\sqrt{3}}\sqrt{\frac{2}{3}}(-3\sqrt{2})(x-iy)\frac{z}{r^2} + (-\sqrt{\frac{2}{3}})(-\frac{1}{\sqrt{3}})(3\sqrt{2})(x-iy)\frac{z}{r^2} = 0$$

$M_S = -\frac{1}{2}, M'_S = -\frac{1}{2}$

$$C^{1/2,-1/2}_{1/2,1/2;1,-1} C^{1/2,-1/2}_{1/2,1/2,1,-1} \langle -1|S_{23}|-1\rangle + C^{1/2,-1/2}_{1/2,-1/2;1,0} C^{1/2,-1/2}_{1/2,-1/2;1,0} \langle 0|S_{23}|0\rangle =$$
$$\frac{2}{3}\frac{2z^2-x^2-y^2}{r^2} + \frac{1}{3}\frac{2x^2+2y^2-4z^2}{r^2} = 0$$

B.4.5 Summary of results

Results for V_C

Using $\Theta = \vec{\sigma}_2.\vec{\sigma}_3$, we get

$$\begin{aligned}
\langle \phi_3^s(M_S)|\vec{\sigma}_2.\vec{\sigma}_3|\phi_3^s(M'_S)\rangle &= \delta_{M_S,M'_S} \\
\langle \phi_3^a(M_S)|\vec{\sigma}_2.\vec{\sigma}_3|\phi_3^a(M'_S)\rangle &= -3\delta_{M_S,M'_S} \\
\langle \phi_3^s(M_S)|\Theta|\bar{\phi}_3(M'_S)\rangle &= 0 \\
\langle \bar{\phi}_3(M_S)|\Theta|\bar{\phi}_3(M'_S)\rangle &= \delta_{M_S,M'_S}
\end{aligned}$$

Results for V_T

Using $\Theta = S_{23}$, we get

$$\begin{aligned}
\langle \phi_3^s(M_S)|S_{23}|\phi_3^s(M'_S)\rangle &= 0 \\
\langle \phi_3^a(M_S)|S_{23}|\phi_3^a(M'_S)\rangle &= 0 \\
\langle \phi_3^s(\frac{1}{2})|\Theta|\bar{\phi}_3(\frac{3}{2})\rangle &= \sqrt{6}(x+iy)\frac{z}{r^2} \\
\langle \phi_3^s(\frac{1}{2})|\Theta|\bar{\phi}_3(\frac{1}{2})\rangle &= \sqrt{2}\frac{x^2+y^2-2z^2}{r^2} \\
\langle \phi_3^s(\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{1}{2})\rangle &= -3\sqrt{2}(x-iy)\frac{z}{r^2} \\
\langle \phi_3^s(\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{3}{2})\rangle &= -\sqrt{6}\frac{(x-iy)^2}{r^2}
\end{aligned}$$

$$
\begin{aligned}
\langle \phi_3^s(-\frac{1}{2})|\Theta|\bar{\phi}_3(\frac{3}{2})\rangle &= \sqrt{6}\frac{(x+iy)^2}{r^2} \\
\langle \phi_3^s(-\frac{1}{2})|\Theta|\bar{\phi}_3(\frac{1}{2})\rangle &= -3\sqrt{2}(x+iy)\frac{z}{r^2} \\
\langle \phi_3^s(-\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{1}{2})\rangle &= \sqrt{2}\frac{2z^2-x^2-y^2}{r^2} \\
\langle \phi_3^s(-\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{3}{2})\rangle &= \sqrt{6}(x-iy)\frac{z}{r^2}
\end{aligned}
$$

$$
\begin{aligned}
\langle \bar{\phi}_3(\frac{3}{2})|\Theta|\bar{\phi}_3(\frac{3}{2})\rangle &= \frac{2z^2-x^2-y^2}{r^2} \\
\langle \bar{\phi}_3(\frac{3}{2})|\Theta|\bar{\phi}_3(\frac{1}{2})\rangle &= 2\sqrt{3}(x-iy)\frac{z}{r^2} \\
\langle \bar{\phi}_3(\frac{3}{2})|\Theta|\bar{\phi}_3(-\frac{1}{2})\rangle &= \sqrt{3}\frac{(x-iy)^2}{r^2} \\
\langle \bar{\phi}_3(\frac{3}{2})|\Theta|\bar{\phi}_3(-\frac{3}{2})\rangle &= 0 \\
\langle \bar{\phi}_3(\frac{1}{2})|\Theta|\bar{\phi}_3(\frac{1}{2})\rangle &= \frac{x^2+y^2-2z^2}{r^2} \\
\langle \bar{\phi}_3(\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{1}{2})\rangle &= 0
\end{aligned}
$$

$$
\begin{aligned}
\langle \bar{\phi}_3(\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{3}{2})\rangle &= \sqrt{3}\frac{(x-iy)^2}{r^2} \\
\langle \bar{\phi}_3(-\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{1}{2})\rangle &= \frac{x^2+y^2-2z^2}{r^2} \\
\langle \bar{\phi}_3(-\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{3}{2})\rangle &= -2\sqrt{3}(x-iy)\frac{z}{r^2} \\
\langle \bar{\phi}_3(-\frac{3}{2})|\Theta|\bar{\phi}_3(-\frac{3}{2})\rangle &= \frac{2z^2-x^2-y^2}{r^2}
\end{aligned}
$$

Results for V_{LS}

Using $\Theta = V_{LS}$

$$\begin{aligned}
\langle \phi_3^s(\frac{1}{2})|\vec{L}.\vec{S}|\phi_3^s(\frac{1}{2})\rangle &= \frac{4}{3}L_z \\
\langle \phi_3^s(\frac{1}{2})|\vec{L}.\vec{S}|\phi_3^s(\frac{-1}{2})\rangle &= \frac{4}{3}L_- \\
\langle \phi_3^s(-\frac{1}{2})|\vec{L}.\vec{S}|\phi_3^s(-\frac{1}{2})\rangle &= -\frac{4}{3}L_z \\
\langle \phi_3^a(M_S)|\vec{L}.\vec{S}|\phi_3^a(M'_S)\rangle &= 0 \\
\langle \phi_3^s(\frac{1}{2})|\Theta|\overline{\phi}_3(\frac{3}{2})\rangle &= \sqrt{\frac{2}{3}}L_+
\end{aligned}$$

$$\begin{aligned}
\langle \phi_3^s(\frac{1}{2})|\Theta|\overline{\phi}_3(\frac{1}{2})\rangle &= -2\frac{\sqrt{2}}{3}L_z \\
\langle \phi_3^s(\frac{1}{2})|\Theta|\overline{\phi}_3(-\frac{1}{2})\rangle &= -\frac{\sqrt{2}}{3}L_- \\
\langle \phi_3^s(\frac{1}{2})|\Theta|\overline{\phi}_3(-\frac{3}{2})\rangle &= 0
\end{aligned}$$

$$\begin{aligned}
\langle \phi_3^s(-\frac{1}{2})|\Theta|\overline{\phi}_3(\frac{3}{2})\rangle &= 0 \\
\langle \phi_3^s(-\frac{1}{2})|\Theta|\overline{\phi}_3(\frac{1}{2})\rangle &= \frac{\sqrt{2}}{3}L_+
\end{aligned}$$

$$\begin{aligned}
\langle \phi_3^s(-\frac{1}{2})|\Theta|\overline{\phi}_3(-\frac{1}{2})\rangle &= -2\frac{\sqrt{2}}{3}L_z \\
\langle \phi_3^s(-\frac{1}{2})|\Theta|\overline{\phi}_3(-\frac{3}{2})\rangle &= -\sqrt{\frac{2}{3}}L_-
\end{aligned}$$

$$
\begin{aligned}
\langle\bar{\phi}_3(\frac{3}{2})|\Theta|\bar{\phi}_3(\frac{3}{2})\rangle &= 2L_z \\
\langle\bar{\phi}_3(\frac{3}{2})|\Theta|\bar{\phi}_3(\frac{1}{2})\rangle &= \frac{2}{\sqrt{3}}L_- \\
\langle\bar{\phi}_3(\frac{3}{2})|\Theta|\bar{\phi}_3(-\frac{1}{2})\rangle &= 0 \\
\langle\bar{\phi}_3(\frac{3}{2})|\Theta|\bar{\phi}_3(-\frac{3}{2})\rangle &= 0 \\
\langle\bar{\phi}_3(\frac{1}{2})|\Theta|\bar{\phi}_3(\frac{1}{2})\rangle &= \frac{2}{3}L_z
\end{aligned}
$$

$$
\begin{aligned}
\langle\bar{\phi}_3(\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{1}{2})\rangle &= \frac{4}{3}L_- \\
\langle\bar{\phi}_3(\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{3}{2})\rangle &= 0 \\
\langle\bar{\phi}_3(-\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{1}{2})\rangle &= -\frac{2}{3}L_z \\
\langle\bar{\phi}_3(-\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{3}{2})\rangle &= \frac{2}{\sqrt{3}}L_- \\
\langle\bar{\phi}_3(-\frac{3}{2})|\Theta|\bar{\phi}_3(-\frac{3}{2})\rangle &= -2L_z
\end{aligned}
$$

Results for V_{LL}

Defining $\Theta = \vec{\sigma}_2.\vec{\sigma}_3 - \frac{1}{2}(\vec{\sigma}_2.\vec{L}\vec{\sigma}_3.\vec{L} + \vec{\sigma}_3.\vec{L}\vec{\sigma}_2.\vec{L})$, we get

$$
\begin{aligned}
\langle\phi^s_3(M_S = \frac{1}{2})|\Theta|\phi^s_3(M'_S = \frac{1}{2})\rangle &= \frac{2}{3}\vec{L}^2 \\
\langle\phi^s_3(M_S = \frac{1}{2})|\Theta|\phi^s_3(M'_S = \frac{-1}{2})\rangle &= 0 \\
\langle\phi^s_3(M_S = -\frac{1}{2})|\Theta|\phi^s_3(M'_S = -\frac{1}{2})\rangle &= \frac{2}{3}\vec{L}^2 \\
\langle\phi^a_3(M_S)|\Theta|\phi^a_3(M'_S)\rangle &= -2\vec{L}^2\delta_{M_S,M'_S} \\
\langle\phi^s_3(\frac{1}{2})|\Theta|\bar{\phi}_3(\frac{3}{2})\rangle &= -\frac{1}{\sqrt{6}}(L_+L_z + L_zL_+)
\end{aligned}
$$

$$\langle \phi_3^s(\frac{1}{2})|\Theta|\bar{\phi}_3(\frac{1}{2})\rangle = \frac{\sqrt{2}}{3}(2L_z^2 - L_x^2 - L_y^2)$$
$$\langle \phi_3^s(\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{1}{2})\rangle = \frac{1}{\sqrt{2}}(L_-L_z + L_zL_-)$$
$$\langle \phi_3^s(\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{3}{2})\rangle = \sqrt{\frac{2}{3}}L_-^2$$
$$\langle \phi_3^s(-\frac{1}{2})|\Theta|\bar{\phi}_3(\frac{3}{2})\rangle = -\sqrt{\frac{2}{3}}L_+^2$$

$$\langle \phi_3^s(-\frac{1}{2})|\Theta|\bar{\phi}_3(\frac{1}{2})\rangle = \frac{1}{\sqrt{2}}(L_+L_z + L_zL_+)$$
$$\langle \phi_3^s(-\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{1}{2})\rangle = \frac{\sqrt{2}}{3}(L_x^2 + L_y^2 - 2L_z^2)$$
$$\langle \phi_3^s(-\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{3}{2})\rangle = -\frac{1}{\sqrt{6}}(L_-L_z + L_zL_-)$$

$$\langle \bar{\phi}_3(\frac{3}{2})|\Theta|\bar{\phi}_3(\frac{3}{2})\rangle = L_x^2 + L_y^2$$
$$\langle \bar{\phi}_3(\frac{3}{2})|\Theta|\bar{\phi}_3(\frac{1}{2})\rangle = -\frac{1}{\sqrt{3}}(L_-L_z + L_zL_-)$$
$$\langle \bar{\phi}_3(\frac{3}{2})|\Theta|\bar{\phi}_3(-\frac{1}{2})\rangle = -L_-^2\frac{1}{\sqrt{3}}$$

$$\langle \bar{\phi}_3(\frac{3}{2})|\Theta|\bar{\phi}_3(-\frac{3}{2})\rangle = 0$$
$$\langle \bar{\phi}_3(\frac{1}{2})|\Theta|\bar{\phi}_3(\frac{1}{2})\rangle = \frac{1}{3}(4L_z^2 + L_x^2 + L_y^2)$$
$$\langle \bar{\phi}_3(\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{1}{2})\rangle = 0$$

$$
\begin{aligned}
\langle\bar{\phi}_3(\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{3}{2})\rangle &= -\frac{1}{\sqrt{3}}L_-^2 \\
\langle\bar{\phi}_3(-\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{1}{2})\rangle &= \frac{1}{3}(L_x^2+L_y^2+4L_z^2) \\
\langle\bar{\phi}_3(-\frac{1}{2})|\Theta|\bar{\phi}_3(-\frac{3}{2})\rangle &= \frac{1}{\sqrt{3}}(L_-L_z+L_zL_-) \\
\langle\bar{\phi}_3(-\frac{3}{2})|\Theta|\bar{\phi}_3(-\frac{3}{2})\rangle &= L_x^2+L_y^2
\end{aligned}
$$

B.5 Putting It All Together

Finally we can put everything together to get the answers we are looking for. We will explicitly do one example to explain the method of calculating nuclear force matrix elements.

The wavefunctions are

$$
\begin{aligned}
|\Psi_1(M_S,M_T)\rangle &= \psi([111])\frac{1}{\sqrt{2}}\left\{-\phi_3^s(M_S)\Gamma_3^a(M_T)+\phi_3^a(M_S)\Gamma_3^s(M_T)\right\} \\
|\Psi_2(M_S,M_T)\rangle &= \psi[321]\frac{1}{\sqrt{2}}\left\{\phi_3^s(M_S)\Gamma_3^s(M_T)+\phi_3^a(M_S)\Gamma_3^a(M_T)\right\} \\
|\Psi_3(M_S,M_T)\rangle &= \frac{\psi([211])}{2}\left\{\frac{\sqrt{3}}{2}\phi_3^a(M_S)\Gamma_3^a(M_T)-\frac{1}{2}\phi_3^a\Gamma_3^s-\frac{1}{2}\phi_3^s(M_S)\Gamma_3^a(M_T)\right. \\
&\quad \left.-\frac{\sqrt{3}}{2}\phi_3^s(M_S)\Gamma_3^s(M_T)\right\}-\frac{\psi([121])}{2}\left\{\frac{1}{2}\phi_3^a(M_S)\Gamma_3^a(M_T)+\frac{\sqrt{3}}{2}\phi_3^a(M_S)\Gamma_3^s(M_T)\right. \\
&\quad \left.+\frac{\sqrt{3}}{2}\phi_3^s(M_S)\Gamma_3^a(M_T)-\frac{1}{2}\phi_3^s(M_S)\Gamma_3^s(M_T)\right\}
\end{aligned}
$$

From Hamada Johnston we know

$$V_C = \vec{\sigma}_2.\vec{\sigma}_3\vec{\tau}_2.\vec{\tau}_3 y_C(r_{23})$$

Let us calculate $\langle\Psi_1(M_S,M_T)|V_C|\Psi_1(M_S',M_T')\rangle$ in detail.

$$
\begin{aligned}
&\langle \Psi_1(M_S, M_T)|V_C|\Psi_1(M'_S, M'_T)\rangle = \\
&\quad \langle \psi([111])\frac{1}{\sqrt{2}}\left\{-\phi_3^a(M_S)\Gamma_3^a(M_T) + \phi_3^a(M_S)\Gamma_3^s(M_T)\right\} \\
&\quad |\vec{\tau}_2.\vec{\tau}_3\vec{\sigma}_2.\vec{\sigma}_3 y_C(r_{23})|\psi([111])\frac{1}{\sqrt{2}}\left\{-\phi_3^a(M'_S)\Gamma_3^a(M'_T) + \phi_3^a(M'_S)\Gamma_3^s(M'_T)\right\}\rangle \\
= &\quad \int \psi^*([111])\psi([111])\frac{1}{2}y_C(r_{23})\left[\langle \phi_3^s(M_S)\Gamma_3^a(M_T)|\vec{\tau}_2.\vec{\tau}_3\vec{\sigma}_2.\vec{\sigma}_3|\right. \\
&\quad \left.\phi_3^s(M'_S)\Gamma_3^a(M'_T)\rangle + \left\langle \phi_3^a(M_S)\Gamma_3^s(M_T)|\vec{\tau}_2.\vec{\tau}_3\vec{\sigma}_2.\vec{\sigma}_3|\phi_3^a(M'_S)\Gamma_3^s(M'_T)\right\rangle\right] \\
= &\quad \int \psi^*([111])\psi([111])\frac{1}{2}y_C(r_{23})\left[(-3)(1) + (-3)(1)\right]\delta_{M_S,M'_S}\delta_{M_T,M'_T} \\
&\quad \int \psi^*([111])\psi([111])y_C(r_{23})(-3)\delta_{M_S,M'_S}\delta_{M_T,M'_T}
\end{aligned}
$$

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