1997


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ELECTRON SCATTERING STUDIES IN THE FRAMEWORK OF THE SYMPLECTIC SHELL MODEL

A Dissertation

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Doctor of Philosophy

in

The Department of Physics and Astronomy

by

Jutta Escher
Vordiplom, University of Bonn. 1988
M.S., Louisiana State University. 1993
May 1997
To Mark
My own plans are made. While I can, I sail east on the *Dawn Treader*. When she fails me, I paddle east in my coracle. When she sinks, I shall swim east with my four paws. And when I can swim no longer, if I have not reached Aslan’s country, or shot over the edge of the world in some vast cataract, I shall sink with my nose to the sunrise ...

- Reepicheep
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## Contents

Epigraph ........................................................................................................ iii

Acknowledgements ......................................................................................... iv

List of Tables .................................................................................................... ix

List of Figures ................................................................................................... x

Abstract ........................................................................................................... xi

Chapter

1 Introduction ....................................................................................................... 1

2 The Symplectic Model as an Extension of the SU(3) Model ......................... 5
   2.1 The SU(3) Model .......................................................................................... 5
      2.1.1 SU(3) model space ..................................................................................... 6
      2.1.2 Geometrical interpretation of the model space ........................................... 9
      2.1.3 SU(3) model Hamiltonians ....................................................................... 12
      2.1.4 Pseudospin and pseudo-SU(3) ................................................................. 16
      2.1.5 Effective charges and multishell correlations - the need for an extension 20
   2.2 The Symplectic Extension ........................................................................... 20
      2.2.1 Generators of the symplectic algebra ...................................................... 21
      2.2.2 Symplectic model space .......................................................................... 24
      2.2.3 Symplectic model Hamiltonians .............................................................. 27
      2.2.4 Symmetry-breaking and truncations in the symplectic model ................ 33
      2.2.5 Sample application for a light nucleus .................................................... 37
      2.2.6 Pseudo-symplectic extension ................................................................... 42

3 From a Bosonic Basis to a Fermion Realization ............................................ 45
   3.1 Symplectic Model in a Bosonic Basis .......................................................... 46
      3.1.1 Cartesian Scheme ....................................................................................... 47
      3.1.2 Spherical Scheme ..................................................................................... 49
      3.1.3 SU(3) Tensor Operators .......................................................................... 53
      3.1.4 SU(3) Tensor Products .......................................................................... 58
      3.1.5 Symplectic raising and lowering operators $B'$ and $B$ ............................ 61
      3.1.6 Matrix Elements of the $u(3) \otimes W_{cyb}$ Algebra ................................. 63
      3.1.7 Matrix Elements of the $sp(3,R)$ Algebra and the $K$-matrix .................. 67
   3.2 Symplectic Model in a Fermionic Basis ....................................................... 70
      3.2.1 Symplectic generators in terms of $b'$ and $b$ ......................................... 71
      3.2.2 Matrix Elements of $b'$ and $b$ ................................................................. 74
      3.2.3 Fermion creation and annihilation operators $a'$ and $a$ ......................... 76
3.2.4 Fermion realization of the symplectic algebra ........................................ 81
3.3 Recursion Relation ..................................................................................... 88
  3.3.1 Derivation ............................................................................................. 88
  3.3.2 Testing the recursion relation ................................................................. 96
  3.3.3 Some special relations for the SU(3) Racah coupling coefficients ......... 96
4 Electron Scattering ......................................................................................... 98
  4.1 Electron scattering as a probe of nuclear structure ................................. 98
  4.2 Quantities measured in electron scattering studies ....................................... 101
  4.3 Electron scattering and the symplectic shell model ..................................... 104
    4.3.1 Generator function method ................................................................. 105
    4.3.2 Boson second quantization formalism .................................................. 106
    4.3.3 Fermion second quantization approach ............................................... 107
  4.4 Electron scattering predictions in the symplectic model ............................ 108
    4.4.1 Longitudinal and transverse form factors ............................................ 109
  4.5 Application to $^{24}\text{Mg}$ .......................................................................... 112
    4.5.1 The calculation .................................................................................... 113
    4.5.2 Longitudinal form factors ..................................................................... 117
    4.5.3 Transverse form factors ....................................................................... 126
    4.5.4 Conclusions ......................................................................................... 133
5 Summary and Conclusion ............................................................................... 137

Bibliography ....................................................................................................... 139

Appendix
A Basic Elements of the Theory of Groups and Their Representations ............... 148
  A.1 Groups and Their Representations ............................................................ 149
  A.2 Lie Groups and Lie Algebras ...................................................................... 151
  A.3 Tensor Operators and the Wigner-Eckart Theorem ....................................... 155
B The Formalism of Second Quantization ............................................................. 158
  B.1 Many-particle states and many-particle Schrödinger equation .................... 159
  B.2 Symmetry requirements ............................................................................ 160
    B.2.1 Particle permutation symmetry ........................................................... 161
    B.2.2 Rotational invariance ........................................................................... 164
    B.2.3 Other symmetries ................................................................................ 164
  B.3 Occupation number formalism - Many-particle wave functions in second quantization 165
  B.4 Operators in second quantization ............................................................... 167
    B.4.1 Definitions ........................................................................................... 168
    B.4.2 Matrix elements of one and two body fermion operators in first quantized form 169
    B.4.3 One and two body operators in second quantized form .......................... 172
  B.5 Applications of the second quantization formalism to nuclear physics .......... 176
  B.6 Miscellaneous ............................................................................................ 176
C The SU(3) Scheme ......................................................................................... 179
  C.1 Basis States in the SU(3) Scheme ............................................................... 179
  C.2 Coupling and Recoupling Coefficients in the SU(3) Scheme ....................... 183
    C.2.1 SU(3) Wigner coefficients: Coupling of two SU(3) irreps ...................... 183
    C.2.2 SU(3) Racah Coefficients: Coupling of three SU(3) irreps .................... 190
    C.2.3 SU(3) 9-($\lambda_J$) coefficients: Coupling of four SU(3) irreps ................. 194
List of Tables

2.1 B(E2) strengths of $^{24}$Mg ................................................................. 40
2.2 Probabilities of the $^{24}$Mg ground band ............................................. 41
2.3 Energies and B(E2) strengths for $^{238}$U ............................................. 44
4.1 Hamiltonian parameters of symplectic calculations for $^{24}$Mg ............. 114
4.2 B(E2) transition strengths of $^{24}$Mg .................................................... 116
List of Figures

2.1 Traditional ($\beta\gamma$) plot .................................................................................. 11
2.2 Pseudo-SU(3) scheme .......................................................................................... 19
2.3 Symplectic extension of the Elliott SU(3) scheme ............................................. 23
2.4 Symplectic shell model space ............................................................................... 28
2.5 Energy spectrum of $^{24}$Mg ................................................................................ 39
4.1 Calculated energy spectra of $^{24}$Mg ................................................................. 115
4.2 Elastic form factor for $^{24}$Mg ............................................................................ 119
4.3 Inelastic form factor for the $0^+_1 \rightarrow 2^+_1$ transition ..................................... 121
4.4 Inelastic form factor for the $0^+_1 \rightarrow 2^+_2$ transition ..................................... 123
4.5 Inelastic form factor for the $0^+_1 \rightarrow 4^+_1$ transition ..................................... 124
4.6 Longitudinal form factor for the inelastic $0^+_1 \rightarrow 4^+_2$ transition. ............... 125
4.7 Transverse form factor for the $0^+_1 \rightarrow 2^+_1$ transition ................................... 129
4.8 Transverse form factor predictions from various models for the $0^+_1 \rightarrow 2^+_1$ transition ................................................................. 130
4.9 Transverse form factor for the transition to $2^+_2$ and $4^+_1$ ................................. 131
4.10 Predicted transverse form factor for the transition to $2^+_2$ and $4^+_1$ .................... 132
4.11 Transverse form factor for the $0^+_1 \rightarrow 4^+_2$ transition ................................... 134
4.12 Transverse form factor for the $0^+_1 \rightarrow 3^+_1$ transition ................................... 135
C.1 Breakup of the $U(4\Omega)$ model space ............................................................... 182

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Abstract

Electron scattering offers numerous advantages for studying nuclear structure: the weakness of the electromagnetic interaction, the precise knowledge of the reaction mechanism, the ability to vary independently the transferred momentum and energy, as well as the excellent spatial resolution that can be obtained with the point-like probing particles, have made this approach a valuable tool in nuclear physics. Scattering experiments provide crucial tests for the applicability and limitations of modern nuclear models and further our understanding of the nucleon-nucleon interaction and its modifications in nuclear matter. A microscopic theory for deformed nuclei, which takes proper account of the Exclusion Principle and of inter-shell couplings, is given by the symplectic shell model. In the context of electron scattering it provides a multi-shell realization of the nuclear shell model and allows for a careful study of the relevance of multi-shell correlations.

A detailed overview of the Elliott SU(3) model and its multi-$\hbar\omega$ extension, the symplectic shell model, is given. The expansion of electron scattering charge and current multipole operators in a second quantized fermion representation is reviewed. A fermion realization of the symplectic shell model, which complements the traditional bosonic representation, is developed. A recursive process is presented in which symplectic matrix elements of arbitrary one-body fermion operators between states of excitation $N\hbar\omega$ and $N'\hbar\omega$ in the same or in different symplectic bands are related back to valence shell matrix elements, which can be evaluated by standard shell model techniques. The formalism is employed to calculate electron scattering form factors for the deformed light nucleus $^{24}\text{Mg}$ in the symplectic shell model, and to discuss the significance of multi-shell correlations.
Chapter 1

Introduction

A long-standing goal of nuclear physics has been the development of a microscopic many-body theory that can account for the structure and interactions of nuclei in terms of a realistic nucleon-nucleon force. Electron scattering offers a variety of advantages for the study of nuclear structure: The weakness of the electromagnetic interaction relative to nuclear forces and the precise knowledge of the reaction mechanism, the ability to vary independently the momentum and energy transferred to the nucleus, as well as the excellent spatial resolution that can be obtained with the point-like probing particles, have made this approach a valuable tool in nuclear physics. Clearly, electron scattering experiments provide crucial tests for the applicability and limitations of modern nuclear models and hence further our understanding of the nucleon-nucleon interaction and its modifications in nuclear matter.

With the development of new accelerators and experimental techniques, a wide range of beam energies combined with high resolution have become available, thus allowing a detailed mapping of the charge and current densities in a variety of nuclei which exhibit properties ranging from single-particle to collective phenomena. An exciting prospect for a facility like the Thomas Jefferson Lab (formerly CEBAF for Continuous Electron Beam Accelerator Facility) in Newport News, Virginia, is the ability to make systematic investigations of the charge distribution and current...
flows in deformed nuclei which, due to the nature of the phenomena being studied, requires very high resolution data at high momentum transfer. In order to extract information about many-body aspects of the nucleus (e.g. modifications of the nucleon-nucleon interaction in the nuclear medium, the nature of short-range correlations, the importance of three-body forces in nuclei, etc.) as well as about the nucleon substructure, it is essential to have a thorough understanding of what can and cannot be explained within the framework of current microscopic theories, e.g. the nuclear shell model.

A microscopic theory for deformed nuclei, which takes proper account of the Exclusion Principle as well as of inter-shell couplings, has been suggested by Rosensteel and Rowe \[144, 145, 149\] and Castaños et al. \[23, 27\]: The symplectic shell model for light nuclei and its pseudo-symplectic extension for heavy nuclei, both based on the Sp(3,R) group symmetry of the harmonic oscillator, have been applied to a variety of collective phenomena. In the context of electron scattering, they provide a multi-shell realization of the nuclear shell model which then allows for a careful study of the relevance of multi-shell correlations. Once the influence of these correlations is known, a comparison of symplectic model predictions with scattering data will allow limits to be placed on the importance of other contributions (e.g. meson exchange currents), thus giving some guidance for the transition from an effective interaction picture to a more fundamental description of the nucleon-nucleon interaction in terms of quarks and gluons.

Some major ingredients necessary for a symplectic shell model treatment of electron scattering were developed by Draayer and co-workers: Second quantized fermion expressions for the charge and current multipole operators in terms of SU(3) tensors have been derived by Rochford and Draayer \[138\], and a computer code that provides SU(3) reduced matrix elements of the tensors within any shell has been developed by Bahri and Draayer \[6, 9\]. For a submodel of the Symplectic Shell Model, namely, the Elliott SU(3) model \[61, 62, 64, 65\], a study of light deformed nuclei has been performed, demonstrating the basic validity of this approach and, at the same time, stressing the need for an extension to the full symplectic calculation with multiple-shell correlations \[136\].
The objective of this dissertation project is to extend the previous study to include symplectic excitations and to investigate their effect on form factors and currents. In order to evaluate charge and current operators in the symplectic model space, matrix elements of one-body operators that connect different major shells are required. To this end a recursion formula is derived which relates symplectic matrix elements between different major oscillator shells back to valence shell matrix elements, which in turn can be computed with the help of Bahri's code. Computer algorithms which make use of this recursion formula and allow for a symplectic shell model analysis of electron scattering are developed. The new formalism is employed to evaluate longitudinal and transverse form factors for light (ds-shell) nuclei. In particular, the nucleus $^{24}$Mg is studied in detail and the results are compared to the single-shell calculations of Rochford and Draayer as well as to the alternative approaches.

Chapter 2 presents the SU(3) model and its multi-shell extension, the symplectic shell model. The relevant Hilbert spaces and typical Hamiltonians are introduced. Some representative applications, which can be found in the literature, are recaptured and discussed. Successes and limitations of both models are highlighted and possible extensions are pointed out.

In Chapter 3, we discuss two different realizations of the symplectic shell model. Starting (in Section 3.1) with the usual Cartesian representation of the symplectic algebra in terms of (bosonic) harmonic oscillator creation and annihilation operators, we make a transformation to a spherical basis and subsequently express the symplectic generators as SU(3) tensor operators. We then outline the method of Rosensteel and Rowe for the evaluation of matrix elements of these generators. While the important results and definitions of Section 3.1 can be found in the existing literature on the subject, we give additional details which should aide the understanding of the mathematical aspects of the model in general and of Sections 3.2 and 3.3 in particular. In Section 3.2 we make the transition from the well-known boson representation of the symplectic model to a new realization in terms of fermionic particle creation and annihilation operators. Commutation relations for various SU(3) coupled tensor products of these fermion operators are given as well.
Section 3.3 addresses the central problem of this dissertation project, the evaluation of symplectic matrix elements of arbitrary one-body operators. Here we present a recursive process in which symplectic matrix elements of arbitrary one-body operators between states of excitation $N\hbar\omega$ and $N'\hbar\omega$ in the same or in different symplectic bands are related back to valence shell matrix elements, which can be evaluated by standard shell model techniques. The step-by-step development of a fermionic realization of the symplectic model and the derivation of a recursion formula which allows for the evaluation of arbitrary one-body operators (such as nuclear charge and current multipole operators) in the symplectic model space have been the primary goals of this dissertation project and represent new contributions to the literature on the symplectic model.

In Chapter 4 we summarize the formalism that is usually employed to extract nuclear structure information from electron scattering experiments. We discuss previous efforts to describe electron scattering results in the framework of the symplectic model and its various submodels. In particular, the generator function method, the boson second quantization formalism, and the fermion second quantization approach are reviewed. We then employ the fermion second quantization formalism in conjunction with our findings from Section 3.3 to evaluate electron scattering form factors for $^{24}$Mg and discuss the results. Chapter 5 summarizes our findings and outlines possible extensions of the project.

An additional goal of this dissertation is to provide a general introduction to SU(3) and symplectic model calculations. This is the motivation for the detailed overview over these models in Chapter 2 and for the inclusion of the appendices. In Appendix A we give some basic elements of the theory of groups and their representations and in Appendix B we review the formalism of second quantization. Appendix C is a compilation of relations that are essential for analytic work in the SU(3) and symplectic schemes.
Chapter 2

The Symplectic Model as an Extension of the SU(3) Model

The symplectic shell model is a microscopic theory for the description of the nuclear many-body system. It takes proper account of the Pauli Exclusion Principle, makes use of the symmetries of the physical system under consideration, and provides a multi-shell realization of the nuclear shell model.

The symplectic model can be approached from different perspectives. The approach that we will take here is to view it as an extension of the Elliott SU(3) model. This has the advantage that many of the concepts which play an important role in the symplectic model can be discussed in the framework of the simpler SU(3) model. We will first review the SU(3) model, its model space, geometrical interpretation, Hamiltonians, and possible extensions. We will then summarize the basic ingredients of the symplectic model, introduce the generators of the symplectic algebra, symplectic basis states and discuss the relevant Hamiltonians. We will also mention several submodels and present a typical application of the symplectic model to a light, well-deformed, ds-shell nucleus.

2.1 The SU(3) Model

The SU(3) model (also called the Elliott model) is an algebraic theory which treats the nucleus microscopically as a many-fermion system and invokes special group symmetries associated with
collective behavior in an attempt to achieve a tractable microscopic description of nuclear phenomena [61, 62, 64, 65, 88]. It is based on the assumption that the motion of a nucleon under the influence of all others can be approximated - at least in lowest order - by its motion in an average central field and takes this field to be a three-dimensional harmonic oscillator potential. Many-particle wave functions, which have to be totally anti-symmetric in order to satisfy the Pauli Exclusion Principle, can be obtained by distributing the nucleons among the lowest available single-particle levels and constructing Slater determinants of the single-particle wave functions of the nucleons.

2.1.1 SU(3) model space

The SU(3) model simplifies the task of constructing the nuclear many-particle wave functions considerably by taking into account shell closures. Since the $\eta$-th harmonic oscillator shell is $\Omega = (\eta+1)(\eta+2)/2$-fold degenerate, it will hold up to $(\eta+1)(\eta+2)$ identical fermions $2(\eta+1)(\eta+2)$ in a spin-isospin formalism. Once such a major shell is occupied by the maximal possible number of particles, it is considered to be closed, i.e. it is treated as a part of the inert core which is presumed to be spherical and to not directly affect the single-particle motion. Thus, after having filled a number of low-lying shells, one has to consider only the first partially occupied oscillator shell, called the valence shell (analogously to atomic physics), and the nucleons in that shell, the valence particles. The totally anti-symmetric nuclear wave functions can then be written as Slater determinants of the single-particle wave functions of the valence nucleons.

The fact that the wave functions associated with a quantum mechanical system can be characterized by their invariance properties with respect to certain symmetry transformations may be employed to classify basis states for the physical system under investigation. Just as the orbital angular momentum, $L$, is used to describe the transformation properties of a wave function under the action of SO(3), the group of rotations in three-dimensional coordinate space, one can introduce other quantum labels which are associated with more general groups of transformation.
The symmetry group that is important in the Elliott model is $U(k\Omega)$, where $\Omega$ is the spatial degeneracy of the $s$-th oscillator shell and $k$ denotes the intrinsic degrees of freedom ($k = 2$ for an identical particle system with spin degrees of freedom and $k = 4$ in a spin-isospin formalism.) Separation of the full $k\Omega$ dimensional space into its space and spin (or spin-isospin) parts corresponds to the reduction of $U(k\Omega)$ to its subgroup $U(\Omega) \otimes U(k)$ (See Appendix C.1 for more details). Further classification of the basis states can be obtained through the irreducible representations (irreps) of subgroups of $U(\Omega)$ and $U(k)$. Elliott’s SU(3) furnishes a physically relevant subgroup of $U(\Omega)$. The generators of SU(3) are the three components of the orbital angular momentum operator, $L_\mu = \sum_s l_s (\mu = 1, 0, -1)$, and the five components of the symmetrized (algebraic) quadrupole operator,

$$Q^a_\mu = \sum_s q^a_{s\mu} = \sqrt{4\pi/5} \sum_s (\frac{r^2_s}{b^2} Y_{2\mu}(\hat{r}_s) + b^2 Y_{2\mu}(\hat{p}_s)) \quad (\mu = -2, -1, 0, 1, 2). \tag{2.1}$$

where the sums run over all particles in the valence shell and the oscillator length is given by $b = \sqrt{\hbar/m}$. Elliott was the first to realize the group theoretical as well as practical implications of introducing the algebraic quadrupole operator in place of the usual “collective” quadrupole operator,

$$Q^c_\mu = \sum_s q^c_{s\mu} = \sqrt{16\pi/5} \sum_s \frac{r^2_s}{b^2} Y_{2\mu}(\hat{r}_s). \tag{2.2}$$

Within a major oscillator shell the matrix elements of $Q^c$ and $Q^a$ are identical, however $Q^c$ couples states belonging to the $s$-th shell with those of the $s'$-th shell with $s' = s \pm 2$, whereas the matrix elements of $Q^a$ between states belonging to different shells vanish.

An obvious subgroup of SU(3) is the well-known rotational group SO(3), generated by the $L_\mu$. The reduction $U(\Omega) \supset SU(3) \supset O(3)$ yields quantum labels $(\lambda \mu)$ and $L$ with multiplicities $\alpha$ and $\kappa$, respectively. The multiplicity labels are needed to distinguish between multiple occurrences of $(\lambda \mu)$ in a given $|f|$ symmetry and multiple $L$ values in a given $(\lambda \mu)$ irrep. The unitary group $U(k)$
corresponding to the intrinsic part of the wave function - can be reduced similarly: $U(2) \supset SU(2)$ for identical particles, where the spin $S$ labels the $SU(2)$ irrep; and $U(4) \supset SU(2) \otimes SU(2)$ in the spin-isospin formalism, which yields quantum numbers $\beta(ST)$, where $S$ and $T$ denote spin and isospin and $\beta$ gives the multiplicity of $(ST)$ in the $U(4)$ irrep. Thus one can construct $m$-particle states $|\Phi\rangle$ which are labeled as

$$|\Phi\rangle = |m[f\alpha(\lambda\mu)\kappa L, S; JM]\rangle \quad (2.3)$$

for an identical-particle system, and

$$|\Phi\rangle = |m[f\alpha(\lambda\mu)\kappa L, \beta(ST); JM, M_T]\rangle \quad (2.4)$$

in the spin-isospin formalism. Here $[f]$ labels the irreducible representation (irrep) of $U(\Omega)$, $(\lambda\mu)$ refers to the irrep of $SU(3)$, $L$ and $S$ are the orbital and spin angular momenta of the system, respectively, and $J$ is the total angular momentum with projection $M$ along the $z$-axis of the laboratory frame. The quantum numbers that identify the irrep of $U(k)$ are suppressed in Equations 2.3 and 2.4 since they are fixed by the labels $[f]$ of $U(\Omega)$ and the requirement of overall antisymmetry. Basis states for light nuclei ($A \lesssim 28$) with neutrons and protons in the $\eta$-th harmonic oscillator shell are of the form shown in Equation 2.4. For heavy nuclei, where protons and neutrons occupy different major oscillator shells, basis states of each subsystem are of the form given in Equation 2.3; a basis for the combined neutron-proton system is obtained via coupling of the neutron and proton states in the $SO(3)$ (angular momentum) coupled ($SU(3)$ uncoupled) scheme or in the $SU(3)$ coupled scheme. In what follows we will consider systems of identical particles only, since the extension to coupled neutron-proton systems or to the spin-isospin case is straightforward.
2.1.2 Geometrical interpretation of the model space

The SU(3) model allows for a geometrical interpretation of the many-nucleon states via a relation between the invariants of the SU(3) group and those of the Geometric Collective Model [82, 60, 86]. The su(3) Lie algebra associated with the SU(3) group contracts to rot(3) $= [R^3] so(3)$, the algebra associated with the rotational limit of the Geometric Collective Model. The su(3) algebra is generated by the orbital angular momentum operator $\hat{L}$ and the Elliott (or algebraic) quadrupole operator $Q^a$; the generators of rot(3) are the components of $\hat{L}$ and those of the collective quadrupole operator, $Q^c$.

The commutation relations for the generators of su(3) and rot(3) are given by:

$$
\begin{align*}
[L_\mu, L_\nu] &= -\sqrt{2}(1\mu, 1\nu) L_{\mu+\nu}, \\
[L_\mu, Q_\nu] &= -\sqrt{6}(1\mu, 2\nu) Q_{\mu+\nu}, \\
[Q_\mu, Q_\nu] &= \text{sgn} 3\sqrt{10}(2\mu, 2\nu) L_{\mu+\nu}.
\end{align*}
$$

(2.5)

where sgn = 1 for $Q=Q^a$ (for the su(3) case) and sgn = 0 for $Q=Q^c$ (for rot(3)). To demonstrate the contraction su(3) $\rightarrow$ rot(3) one can introduce a rescaled quadrupole operator, $Q^a \rightarrow Q^{a'} \equiv Q^a / \sqrt{C_2}$ with $C_2(\lambda\mu) \equiv \langle \hat{C}_2 \rangle_{(\lambda\mu)} = \frac{3}{2}[\lambda^2 + \lambda\mu + \mu^2 + 3(\lambda + \mu)]$, where $\hat{C}_2$ is the second-order Casimir invariant (see Appendix E) of SU(3), which by definition commutes with the generators $L$ and $Q^a$, and $\langle O \rangle_{(\lambda\mu)}$ denotes the expectation value of an operator $O$ in a SU(3) basis state with quantum labels $(\lambda\mu)$. The first two commutation relations in Equation 2.5 remain the same for the new set of generators but in the last equation $L_{\mu+\nu}$ has to be replaced by $L_{\mu+\nu}/\hat{C}_2$. This shows that when $L$ is small compared to $C_2(\lambda\mu)$, the algebras su(3) and rot(3) obey the same commutation relations, that is, su(3) contracts to rot(3). Closely related to this is the fact that the invariants $\text{tr}[(Q^c)^2]$ and $\text{tr}[(Q^c)^3]$, with $\text{tr}[O]$ denoting the trace of the operator $O$, of ROT(3)

---

1For the sake of simplicity we will generally refrain from using a caret above a symbol to denote an operator. We will only use the caret to distinguish an operator from its associated eigenvalue in situations where the two might otherwise be confused with each other, as, for example, $\hat{L}$ and $L$.
$= [R^3]|SO(3)$, the Lie group associated with $\text{rot}(3)$, and those of $SU(3)$, namely $C_2(\lambda \mu)$ and $C_3(\lambda \mu)$. The expectation values of the second and third order Casimir operators, can be linearly related to each other. The latter results in a direct connection between the microscopic quantum numbers $\lambda$ and $\mu$ and the collective shape variables $\beta$ and $\gamma$ [110, 33, 111, 25, 24, 50, 46, 28]:

$$\langle \text{tr}[(Q^3)^2]\rangle = \frac{3}{2}k^2 \beta^2 \quad \iff \quad C_2(\lambda \mu) = \frac{2}{3}[\lambda^2 + \lambda \mu + \mu^2 + 3(\lambda + \mu)]$$

$$\langle \text{tr}[(Q^3)^3]\rangle = \frac{3}{4}k^3 \beta^3 \cos 3\gamma \quad \iff \quad C_3(\lambda \mu) = \frac{1}{9}(\lambda - \mu)(\lambda + 2\mu + 3)(2\lambda + \mu + 3) \quad (2.6)$$

where the constant $k = \sqrt{5/9\pi}AR_0^2$, with $A$ being the number of nucleons in the nucleus and $R_0 \equiv \sqrt{(r^2)}$ the mean square radius of the system. The exact relation between $(\beta \gamma)$ and $(\lambda \mu)$ is given by:

$$k \beta \cos \gamma = (2\lambda + \mu + 3)/3$$

$$k \beta \sin \gamma = (\mu + 1)/\sqrt{3}, \quad (2.7)$$

which implies that each $SU(3)$ irrep $(\lambda \mu)$ corresponds to a unique geometrical shape $(\beta \gamma)$. This correspondence can be illustrated with the help of a grid which is superposed on the well-known $(\beta \gamma)$-plane of the Geometric Collective Model (Fig. 2.1). In the oscillator picture, core configurations couple to the $SU(3)$ irrep $(00)$, and the $(\lambda \mu)$ irreps that can occur in the model basis for other cases are determined by the valence shell and the number of valence protons or neutrons under consideration.

The grid structure has its origin in the discreteness of the $\lambda$ and $\mu$ labels, a result that stands in contrast to the continuous nature of the $\beta$ and $\gamma$ variables. This is only one of several fundamental differences between the $(\lambda \mu)$ irrep labels and the $(\beta \gamma)$ variables. One also finds, for example, that the allowed $(\lambda \mu)$ irreps are bounded by statistical considerations (Pauli Exclusion Principle), while the $(\beta \gamma)$ values are not. Furthermore, the $SU(3)$ model allows for multiple occurrences of the same irrep $(\lambda \mu)$ within a given representation $[f]$ of $U(\Omega)$, which are labeled by the index $\alpha$ and
Figure 2.1: Traditional $({\beta}\gamma)$ plot. A traditional $({\beta}\gamma)$ plot, where $\beta$ is the radius vector and $\gamma$ the azimuthal angle, demonstrates the relationship between the collective shape variables $({\beta}\gamma)$ and the SU(3) irrep labels $(\lambda\mu)$. The $({\beta}\gamma)$ vary continuously ($0 \leq \beta \leq 0.6\gamma \leq 60^\circ$), while $\lambda$ and $\mu$ take on positive integer values only, as is indicated with the help of a grid, with each node corresponding to a $(\lambda\mu)$ pair.
correspond to distinct arrangements of the valence particles giving rise to the same quadrupole geometry while the collective model does not exhibit such a multiplicity. Despite these differences, the \((\beta\gamma) \leftrightarrow (\lambda\mu)\) correspondence serves as a valuable connection between the two models; in particular, it allows for a geometrical analysis of the eigenstates of a nuclear system and hence gives insight into phenomena associated with nuclear deformation.

2.1.3 SU(3) model Hamiltonians

The group theoretical approach becomes particularly convenient if the physical system under consideration possesses a *dynamical symmetry*, that is, if the Hamiltonian of the system can be expressed solely in terms of Casimir invariant operators of a chain of nested groups \(G_0 \supset G_1 \supset \ldots \supset G_i \supset \ldots \supset K\). A dynamical symmetry provides considerable insight into the physics of the system since it allows all properties of the system to be calculated in closed form. The labels of the irreducible representations (irreps) of the groups in the chain serve as quantum numbers to classify members of a complete basis in which the Hamiltonian is diagonal; eigenvalues and other observables can be obtained analytically.

A physically relevant Hamiltonian which can be expressed in terms of Casimir operators of SU(3) and SO(3) is given by [45]:

\[
H = H_0 - \frac{1}{2} \chi Q^a \cdot Q^a ,
\]

since the quadrupole-quadrupole interaction can be written as

\[
Q^a \cdot Q^a = 6 \hat{C}_2 - 3 \hat{L}^2 .
\]

where \(\hat{C}_2\) and \(\hat{L}^2\) denote the second-order Casimir invariants of SU(3) and SO(3), respectively. The harmonic oscillator term, \(H_0\), is proportional to the boson number operator \(\hat{N}\), which is a generator and invariant of U(3). This simple Hamiltonian provides an appropriate starting point.
for a description of rotational motion. It gives rise to a \( L(L + 1) \) rotational spectrum, with the various allowed SU(3) irreps corresponding to rotational bands which lie at relative excitation energies determined by the factor \( -\frac{1}{2} \chi C_2(\lambda \mu) \) in \( H \).

Not surprisingly, it turns out that the above Hamiltonian is too schematic to reproduce the details of realistic rotational spectra. In particular, states of a given SU(3) irrep \((\lambda \mu)\) which have the same angular momentum are degenerate, whereas in experimental spectra one finds individual rotational bands - corresponding to different multiplicity labels \( \kappa \) - which are shifted relatively to each other [134, 86, 122, 123]. (This phenomenon is usually referred to as "K-band splitting").

where \( K \) is a quantum label of the collective model which refers to the projection of the angular momentum on the intrinsic symmetry axes of the system. The quantum number \( \kappa \) carries the significance of \( K \) since there is a one-to-one correspondence between the two.) Including further Casimir invariants in the Hamiltonian, as, for example, the third-order Casimir operator \( \hat{C}_3 \) of SU(3), does not resolve the problem, since none of the relevant Casimir invariants distinguishes between the \( L \)-values which occur multiple times in a given SU(3) irrep.

The next logical step in generalizing the above Hamiltonian is to include more general terms which are rotationally invariant and conserve the U(3) symmetry of the system, that is, the additional terms need to be SO(3) scalars and multinomial functions of U(3) generators. (By definition, a group \( G \) is a conserved symmetry if the Hamiltonian \( H \) is expressible solely in terms of the generators of \( G \). Then \( H \) has no matrix elements connecting different irreps of \( G \) and every \( H \) eigenstate belongs to a unique \( G \) irrep.) This can be achieved most efficiently by employing the boson number operator \( \hat{N} \) plus a special minimal set of SO(3) scalars, the so-called SU(3) \( \rightarrow \) SO(3) integrity basis [107, 55, 80, 35]. Judd et al. [107] have shown that the SU(3) \( \rightarrow \) SO(3) integrity basis contains five operators that give rise to real symmetric matrix forms, two of degree two in the generators, two of degree three, and one of degree four. They show that these can be chosen to be the Casimir invariants \( \hat{L}^2, \hat{C}_2, \) and \( \hat{C}_3 \), and two non-SU(3) invariant SO(3) scalars, generically labeled \( X_3 \) and \( X_4 \), which are of degree three and four, respectively, in the generators. (Note: We reserve the
terminology "G-invariant" or "G-scalar" for operators which transform according to the scalar
irrep of the group G under consideration.) The $X_3$ and $X_4$ operators can be defined in a variety
of ways. As they are SO(3) scalars, it is most convenient to define them in terms of (contracted)
spherical tensors:

$$X_3 = (\hat{L} \times Q^a) \cdot \hat{L}$$
$$X_4 = (\hat{L} \times Q^a) \cdot (Q^a \times \hat{L}).$$

(2.10)

Of the three types of SU(3) → SO(3) integrity basis operators that can occur, invariants of
SU(3), invariants of SO(3), and non-SU(3) invariant SO(3) scalars, only the last two can spread
states within a SU(3) irrep and only the last one can couple and mix multiple occurrences of
a given SO(3) irrep in SU(3). It is the latter property that allows for a significantly improved
agreement between experimental spectra and transmission probabilities and theoretical predictions
thereof, as has been demonstrated for representative nuclei, such as $^{24}$Mg and $^{168}$Er [122, 25]. A
correspondence between the microscopic SU(3) Hamiltonian built from members of the SU(3) →
SO(3) integrity basis plus the boson number operator $\hat{N}$,

$$H_{mic} = a_1 \hat{N} + a_2 \hat{C}_2 + a_3 \hat{C}_3 + a_4 \hat{L}^2 + a_5 X_3 + a_6 X_4,$$

(2.11)

and the macroscopic Hamiltonian of a triaxial quantum rotor can be established for a particular
choice of the parameters $a_1 \ldots a_6$, thus demonstrating that a shell model realization of collective
rotational dynamics can be achieved in the framework of the SU(3) model.

For real nuclear systems SU(3) is only an approximate symmetry and therefore a Hamiltonian
has to be employed which no longer conserves SU(3) symmetry. Additional interactions like the
one-body spin-orbit and orbit-orbit forces need to be included, as well as two-body pairing correla-
tions, all of which break SU(3) symmetry (The spin-orbit term even mixes different representations
of U(Ω)). The one-body terms effect important modifications to the harmonic oscillator mean field
and the pairing interaction plays an essential role in reproducing triaxially deformed nuclear shapes [5, 162, 161, 9, 67].

The group theoretical approach facilitates the calculation of the matrix elements, eigenstates, and observables, particularly in the dynamical symmetry limit of the theory, for the Casimir operators are diagonal in the dynamical symmetry basis and can be expressed analytically. Even in the more general case, when the Hamiltonian is expressed in terms of SU(3) → SO(3) integrity basis operators (and thus preserves SU(3) symmetry), the calculations do not become very complicated since the matrix elements of the non-SU(3) invariant SO(3) scalars $X_3$ and $X_4$ can be expressed in terms of SU(3) coupling coefficients and sums over matrix elements of Casimir invariants.

Evaluating the matrix elements of a general symmetry-breaking Hamiltonian, on the other hand, becomes much more involved since the SU(3)-breaking interactions have to be expanded ("decomposed") into a basic set of operators, the set of irreducible SU(3) tensor operators (see Appendix C.3). This is achieved employing the formalism of second quantization (see Appendix B) and making use of SU(3) coupling and recoupling techniques (see Appendix C.2). Since the usefulness of this approach depends to a large extent upon the availability of the appropriate coupling coefficients and (reduced) matrix elements, much effort has been devoted to the development of fast and efficient computer algorithms for their generation, storage, and retrieval [1, 128, 127, 6, 17, 16].

The value of an approximate symmetry depends upon how badly it is broken, and this, in turn, depends on the relative strengths of the inter-representation versus intra-representation couplings. (Statistical measures for the probable goodness of an approximate symmetry have been defined and can be expressed in terms of the group's coupling coefficients and reduced matrix elements [93, 72, 71, 74, 73, 75, 32, 131].) The importance of SU(3) follows from the fact that it is the exact symmetry group of the spherical oscillator (which is a reasonable approximation for the common potential experienced by nucleons in nuclei) and, furthermore, it is the dynamical symmetry group of the deformed oscillator when, as is usually the case, the deformation is generated by quadrupole interactions. Specifically, under the influence of a residual interaction that is dominated by $Q_a$.
and heavy rare earth and actinide species ($A \geq 150$), the complete many-particle space factorizes into a collection of subspaces that are only weakly coupled to one another, yielding eigenstates of relatively pure SU(3) character. In a situation where $Q^a \cdot Q^a$ is the dominating interaction in the Hamiltonian it becomes possible to further truncate the single-major oscillator model space to one or a few energetically low-lying SU(3) irreps. In many cases, a single-irrep calculation suffices to achieve good agreement with experimental data [56, 57, 26].

2.1.4 Pseudospin and pseudo-SU(3)

The pseudo-spin concept extends the applicability of the SU(3) model to the region of heavy deformed nuclei. In this region of the nuclear chart not only do protons and neutrons occupy different major shells, but a strong spin-orbit interaction emerges which breaks the underlying harmonic oscillator symmetry [89, 83, 84, 85]. Specifically, the largest spin member, $j_{\text{max}} = \eta + \frac{1}{2}$, of the $\eta$-th shell (which consists of single-particle orbitals with $j = l \pm s$ where $s = \frac{1}{2}$ and $l = \eta - 2, \ldots, 1$ or 0) is pushed down among the levels of the next lower shell. Fortunately, it is possible to employ a transformation to a new space with good symmetry, namely pseudo-SU(3) symmetry. This procedure presupposes that the concept of pseudo-spin [3, 90, 132] is valid for heavy deformed nuclei - an assumption that numerous applications have shown to hold true [155, 43, 165, 162, 161, 163, 11, 29].

In the pseudo-spin approach the largest-$j$ orbital of the $\eta$-th major shell is considered to be part of the core ("defector level") since it drops below the Fermi level and thus it is removed from active consideration (see Figure 2.2). Pseudo-orbital and pseudo-spin angular momenta are assigned to the remaining single-particle states which, in turn, form a complete set for a pseudo oscillator shell with one less oscillator quantum, $\tilde{\eta} = \eta - 1$. (A tilde is used to denote pseudo quantities.) The single-particle total angular momenta remain good quantum numbers, $j = \tilde{j} = \tilde{l} \pm \tilde{s}$, where $\tilde{s} = \frac{1}{2}$ and $\tilde{l} = \tilde{\eta}, \tilde{\eta} - 2, \ldots, 1$ or 0. Furthermore, in analogy to the degenerate spin-orbit doublets...
\[ j = l \pm \frac{1}{2}, \]
which exist in absence of a spin-orbit interaction. pseudo spin-orbit partners \[ \tilde{j} = \tilde{l} \pm \frac{1}{2}. \]
which are nearly degenerate, can be identified for axially symmetric heavy nuclei.

The algebraic properties of the pseudo oscillator are identical with those of the usual oscillator, its abstract algebra is just \(\text{su}(3)\) and the Hamiltonian in the new coupling scheme has the same form as in the normal SU(3) scheme [30, 31. 8. 48, 12. 13. 15. 14. 81]. The advantage of the pseudo-spin realization is that the symmetry-breaking spin-orbit interaction is weak in the new scheme, so pseudo-SU(3) quantum numbers can be assigned to the resulting many-particle wave functions and the same powerful tools that work for SU(3) in light nuclei can be applied to heavy nuclei.

The challenge that remains is the question of how to incorporate the largest-\(j\) level ("intruder level"), \(j_{\text{intr}} = \eta + \frac{3}{2}\), which originates in the next higher shell \(\eta + 1\) and is pushed down into the valence space by the strong spin-orbit force. A reasonable approach for the like-particle (proton or neutron) sub-systems found in heavy nuclei might consider the valence space to consist of the normal parity pseudo orbitals of the \(\eta\)-th shell and the unique parity \(j = \eta + 3/2\) "intruder" orbital from the \((\eta + 1)\)-st shell, possibly augmented by its like-parity partners. The latter choice implies a Hilbert space that is a direct product of the "\(\eta\)-th shell space" (usually referred to as the "normal parity space") and the "\((\eta + 1)\)-st shell space" (the "unique parity space") with basis states of the form \(|\phi\rangle \equiv [|N, J^N\rangle|U, J^U\rangle]^{JM}\), where \(J^N(J^U)\) is the angular momentum of the normal (unique) parity part of the nuclear wave function and \(N\) and \(U\) denote additional quantum numbers necessary to classify the wave function.

Since for all but few-particle systems the normal-unique coupled product space is too large to be handled completely with the currently available computational tools, it becomes necessary to restrict the space. For low-energy phenomena it has been shown that in spite of deformation-driving correlations generated among particles in the unique parity sector and by the interaction of nucleons in the normal parity orbitals with those in the unique parity orbitals, it is possible to employ truncation procedures which reduce the model space to a manageable size. In the normal
parity subspace a restriction to the leading spatial irrep is known to produce good results for
strongly deformed nuclei. Reducing the unique parity subspace to the largest-j orbital and further
considering low-seniority configurations only turns out to yield a good approximation to the
unique parity part of the complete wave function [69, 68, 66]. Furthermore, for most applications
which involve collective nuclear properties it suffices to base the calculations on the normal parity
space and to rescale the resulting observables accordingly. The scaling factors can be expressed
simply in terms of the second-order Casimir invariant $C_2(\lambda \mu)$ of SU(3) and a percentage which
takes account of the SU(3) symmetry breaking interactions in the unique parity sector.

The use of scaling factors is limited to those situations where the nucleons in the unique
parity subspace follow in an adiabatic way the collective motion of their partners in the normal
parity orbitals, that is, the unique parity configurations that couple to their corresponding normal
parity structures track the behavior of these configurations as one moves up the yrast band. This
assumption obviously breaks down when backbending occurs, and a more sophisticated approach
then becomes necessary for a proper description of higher-lying states.

Furthermore, to what extent electron scattering form factors can be reproduced in the various
truncation schemes outlined above, remains to be investigated. Form factors are very sensitive
to the details of the nuclear wave functions. Therefore, a radical truncation of the Hilbert space
to its normal parity component only and a subsequent rescaling is not expected to yield good
results for the form factors. However, a truncation of the unique parity subspace to low-seniority
configurations might very well give a reasonable approximation to the exact form factors, since
wave functions truncated in this manner display a large overlap with the exact wave functions
[69, 68, 66]. The pseudo scheme has been applied with success in calculations of a variety of
physical phenomena, such as backbending [133], magnetic dipole transitions [26, 165], and in
studies of the structure of superdeformed bands [124, 156].

2 The seniority quantum label counts the number of nucleons in a given space that are not coupled pairwise to
angular momentum zero. When a seniority-zero restriction is imposed, major simplifications result: in particular,
the coupling to a seniority-zero state is trivial, as this state can only make an angular momentum independent
contribution to the dynamics of the system.
Figure 2.2: Pseudo-SU(3) scheme. Schematic plot illustrating the Pseudo-SU(3) transformation. Taken from [69].
2.1.5 Effective charges and multishell correlations - the need for an extension

The strength of the SU(3) model arises from the underlying physical symmetries of deformed nuclei which allow for a classification of nuclear states by quantum labels associated with group chains and make further truncations in the single-major shell model space possible. On the other hand, the restriction to the valence shell points immediately to the limitations of the SU(3) model: Since couplings between major shells play an important role in strongly collective phenomena, the description of those makes it necessary to introduce effective charges. The need for effective charges is a common feature in all single major shell model theories. Effective charges produce the required enhancements of collective observables like quadrupole moments and electromagnetic transition strengths, due to contributions from the core ("core polarization"). While global rescaling works for a description of transition strengths, it fails to reproduce observables that are sensitive to the details of inter-shell correlations. For example, predictions for single-particle densities and electron scattering form factors cannot be improved in a simple manner by introducing effective charges. The symplectic extension of the model, which will be described in the next section, eliminates the need for effective charges in light nuclei by allowing for inter-shell excitations. An analogous extension, the pseudo-symplectic model, can be defined for the pseudo-SU(3) scheme and employed for a study of heavy ($A \geq 150$) nuclei. Since the symplectic shell model takes into account multi-shell correlations explicitly, rather than via a renormalization procedure, it promises a better characterization of the nuclear wave function and therefore an improved description of nuclear form factors.

2.2 The Symplectic Extension

The symplectic shell model, also called the microscopic collective model, is a shell-model scheme which extends the Elliott SU(3) model to include multiple $2\hbar\omega$ excitations of the monopole and quadrupole type [144, 145, 149]. It fully accommodates the action of the real collective quadrupole operator, $Q^c$, and not only the symmetrized $0\hbar\omega$ part, $Q^s$. and is therefore able to reproduce
intra-band and inter-band E2 transition strengths between low-lying, as well as giant resonance, states without introducing proton and neutron effective charges [143, 58, 23].

2.2.1 Generators of the symplectic algebra

The symmetry algebra of the scheme is spanned by one-body operators which are bilinear products in the position and momentum observables. In order to eliminate spurious center-of-mass excitations, these bilinear products are constructed from relative position and momentum coordinates \( x_{\alpha i}, p_{\alpha i} \) which obey the standard commutation relations \( [x_{\alpha i}, p_{\beta j}] = i\hbar \delta_{\alpha \beta} \delta_{ij} \):

\[
\begin{align*}
Q_{ij} & = \sum_{\alpha} x_{\alpha i} x_{\alpha j} \\
T_{ij} & = \sum_{\alpha} p_{\alpha i} p_{\alpha j} \\
L_{ij} & = \sum_{\alpha} (x_{\alpha i} p_{\alpha j} - x_{\alpha j} p_{\alpha i}) \\
S_{ij} & = \sum_{\alpha} (x_{\alpha i} p_{\alpha j} + p_{\alpha i} x_{\alpha j}) .
\end{align*}
\]

(2.12)

where \( i, j = 1, 2, 3 \) denote the cartesian directions, and \( \alpha, \beta \) refer to the individual Jacobi particles.

The quadrupole moment operator, \( Q_{ij}^c \), the vibrational momentum operator, \( S_{ij} \), and the quadrupole flow tensor, \( T_{ij} \), contribute six components each, and the angular momentum operator, \( L_{ij} \), has three components. Together they generate the 21-dimensional symplectic algebra \( sp(3, \mathbb{R}) \), that is, the Lie algebra of linear transformations which preserve a skew-symmetric bilinear form on a six-dimensional real vector space. (While \( sp(6, \mathbb{R}) \) is the standard mathematical notation for this 21-dimensional classical Lie algebra, the symbol \( sp(3, \mathbb{R}) \) is commonly used in the context of physical systems in a three-dimensional space.) It is the smallest Lie algebra that contains both the quadrupole moments, \( Q_{ij}^c \), and the many-nucleon kinetic energy, \( \sum_{\alpha i} p_{\alpha i}^2 / (2m) \), and it has several physically relevant subalgebras. This includes the general collective motion algebra \( gcm(3) \), which is spanned by \( \{ Q_{ij}^c, L_{ij}, S_{ij} \} \), the algebra \( gl(3, \mathbb{R}) \) of the general linear motion group, which is generated by \( \{ L_{ij}, S_{ij} \} \), and the algebra \( so(3) \) of the rotation group, generated by the angular momentum components \( \{ L_{ij} \} \).
The algebra also contains Elliott’s \( su(3) \) algebra; and the harmonic oscillator Hamiltonian \( H_0 \) is an element of the Lie algebra as well. This can be seen more readily if \( sp(3, R) \) is realized in terms of bilinear products in the harmonic oscillator bosons \( \eta_{\alpha i} = \frac{1}{\sqrt{2}}(x_{\alpha i} - ip_{\alpha i}) \), \( \xi_{\alpha i} = \eta_{\alpha i}^\dagger = \frac{1}{\sqrt{2}}(x_{\alpha i} + ip_{\alpha i}) \), which satisfy the commutation relations \( [\xi_{\alpha i}, \eta_{\beta j}] = \delta_{\alpha\beta} \delta_{ij}, \ [\xi_{\alpha i}, \xi_{\beta j}] = [\eta_{\alpha i}, \eta_{\beta j}] = 0 \). The one-body operators \( \eta_{\alpha i} \) and \( \xi_{\alpha i} \) create and annihilate, respectively, one oscillator quantum in the \( i \)-th direction of the \( \alpha \)-th Jacobi particle. In the new basis the generators of the symplectic algebra take the form:

\[
B_{ij}^\dagger = \frac{1}{2} \sum_\alpha \eta_{\alpha i}\eta_{\alpha j}, \quad B_{ij} = \frac{1}{2} \sum_\alpha \xi_{\alpha i}\xi_{\alpha j}, \quad C_{ij} = \frac{1}{2} \sum_\alpha (\eta_{\alpha i}\xi_{\alpha j} + \xi_{\alpha j}\eta_{\alpha i}) .
\]

(2.13)

The \( C_{ij} \) close under commutation and generate the nine-dimensional algebra \( u(3) \), which is associated with \( U(3) \), the group of unitary transformations in three dimensions. The harmonic oscillator Hamiltonian is given by \( H_0 = \hbar \omega \hat{N} \), where \( \hat{N} = \sum_{i=1}^N C_{ii} \) is the boson number operator, which counts the total number of oscillator bosons in the system. The \( su(3) \) subalgebra of \( u(3) \) is spanned by the eight independent traceless operators \( C_{ij} - \frac{1}{3} \delta_{ij} \hat{N} \). The \( C_{ij} \), being generators of \( U(3) \), act only within a major harmonic oscillator shell, whereas the \( B_{ij}^\dagger \) and \( B_{ij} \) are \( 2\hbar \omega \) raising and lowering operators, respectively, which generate (particle-symmetric) couplings to shells that lie \( 2\hbar \omega \) above or below the \( 0\hbar \omega \) valence space. This is illustrated schematically in Figure 2.3, which shows the structure of the \( sp(3, R) \) algebra and its relation to \( su(3) \).

In order to take full advantage of the \( Sp(3, R) \subset SU(3) \) group-subgroup structure, it is necessary to view the symplectic generators as \( SU(3) \) tensor operators. The number operator, \( \hat{N} \), is a \( SU(3) \) scalar, that is, it transforms according to the scalar irrep, \( (\lambda \mu) = (0,0) \), of the group. The eight traceless operators \( C_{ij} - \frac{1}{3} \delta_{ij} \hat{N} \) form a \( SU(3) \) irreducible tensor operator, which has tensor character \( (\lambda \mu) = (1,1) \); it contains angular momentum \( l = 1 \) and \( l = 2 \) components, and will be denoted by
Figure 2.3: Symplectic extension of the Elliott SU(3) scheme. Schematic plot illustrating the symplectic extension of the Elliott SU(3) scheme. Taken from [45].

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\( C_{lm}^{(11)} \), where \( m = -l, -l + 1, \ldots, +l \). As will be discussed in more detail in Section 3.1, the \( l = 1 \) components are proportional to the standard angular momentum, \( C_{1q}^{(11)} \propto L_q \) (\( q = 0, \pm 1 \)), and the \( l = 2 \) components are proportional to the algebraic quadrupole operator, \( C_{2m}^{(11)} \propto Q_2^m \) (\( m = 0, \pm 1, \pm 2 \)). The raising and lowering operators \( B_{ij}^l \) and \( B_{ij} \) can be combined to form \( SU(3) \) tensor operators \( A_{lm}^{(20)} \) and \( B_{lm}^{(02)} \) with tensor character \( (\lambda \mu) = (2, 0) \) and conjugate \( (\lambda \mu) = (0, 2) \) symmetry, respectively; both contain angular momentum \( l = 0 \) and \( l = 2 \) components.

### 2.2.2 Symplectic model space

A basis for the Hilbert space is generated by applying symmetrically coupled products of the raising operator \( A^{(20)} \) with itself to the usual 0\( \hbar \omega \) shell-model states. The 0\( \hbar \omega \) starting configurations are labeled by the Elliott \( SU(3) \) quantum numbers \( (\lambda_\sigma \mu_\sigma) \) and by \( N_\sigma \), the eigenvalue of the oscillator boson number operator which takes the minimum value consistent with the Pauli Exclusion Principle. The product of \( N_n/2 \) raising tensors \( A^{(20)} \), each of which promotes a particle from a given shell into a higher-lying shell \( 2\hbar \omega \) above, generates \( N_n\hbar \omega \) excitations for each starting irrep \( N_\sigma(\lambda_\sigma \mu_\sigma) \). Each such product operator \( P_\alpha^{N_n(\lambda_\sigma \mu_\sigma)} \), labeled according to its \( SU(3) \) content, \( (\lambda_\sigma \mu_\sigma) \), and defined recursively:

\[
P_{\alpha_n}^{N_n(\lambda_\sigma \mu_\sigma)}(A^{(20)}) = \sum_{\beta} \langle (20) | \beta; (\lambda_\sigma \mu_\sigma) | N_n(\lambda_\sigma \mu_\sigma) \rangle X^{N_n(\lambda_\sigma \mu_\sigma)}(N'_n(\lambda'_\sigma \mu'_\sigma)) A_{\beta}^{(20)} P_{\alpha'_n}^{N'_n(\lambda'_\sigma \mu'_\sigma)}(A^{(20)}).
\]

(2.14)

where \( N'_n = N_n - 2 \), and

\[
X^{N_n(\lambda_\sigma \mu_\sigma)}(N'_n(\lambda'_\sigma \mu'_\sigma)) = \frac{1}{n_1 + n_2 + n_3} (n_1 n_2 n_3 || A^{(20)} || n'_1 n'_2 n'_3)
\]

(2.15)

is required to properly orthonormalize the polynomial, is then coupled with \( |N_\sigma(\lambda_\sigma \mu_\sigma)\rangle \) to good \( SU(3) \) symmetry \( \rho(\lambda_\omega \mu_\omega) \), with \( \rho \) denoting the multiplicity of the coupling. The \( n_i \), in the above
The operator $A^{(20)}$ is a generator of the $u(3) \otimes \text{Weyl}$ algebra; the evaluation of its matrix elements and its relations to the symplectic generator $A^{(20)}$ will be discussed in Subsection 3.1.6. (For further information on the basis state construction, see references [95, 149, 157], and for details on the SU(3) coupling scheme, refer to Appendix C.2).

For each $\omega \in \text{SU}(3)$ starting irrep $N_\sigma(\lambda_\sigma \mu_\sigma)$ one obtains a basis for a symplectic representation:

$$|\Phi\{N_\sigma(\lambda_\sigma \mu_\sigma); N_n(\lambda_n \mu_n)\rho N_\omega(\lambda_\omega \mu_\omega)\alpha_\omega\} \rangle .$$

(2.16)

where $N_\omega = 0, 1, 2, \ldots$ counts the number of boson excitations. $N_\omega = N_\sigma + N_n$, $(\lambda_n \mu_n)$ ranges over the set $\Omega = \{(n_1 - n_2, n_2 - n_3)| n_1 \geq n_2 \geq n_3 \geq 0; n_1, n_2, n_3 \text{ even integers}\}$. $\rho(\lambda_\omega \mu_\omega)$ includes all SU(3) irreps resulting from the coupling $(\lambda_n \mu_n) \times (\lambda_\sigma \mu_\sigma)$. and $\alpha_\omega = \kappa \Lambda M$ denotes quantum numbers associated with the group chain $\text{SU}(3) \supset \text{SO}(3) \supset \text{SO}(2)$. Alternatively, one can also choose subgroup labels $\alpha_\omega = \varepsilon \Lambda M_A$, which are associated with the chain $\text{SU}(3) \supset \text{SU}(2) \times \text{U}(1) \supset \text{SO}(2)$. The states of the $\text{Sp}(3,\mathbb{R}) \supset \text{SU}(3)$ basis are thus labeled by three types of U(3) quantum numbers: $N_\sigma(\lambda_\sigma \mu_\sigma)$, the symplectic bandhead or $\text{Sp}(3,\mathbb{R})$ lowest weight U(3) symmetry, which specifies the $\text{Sp}(3,\mathbb{R})$ irreducible representation; $N_n(\lambda_n \mu_n)$, the u(3) symmetry of the raising polynomial; and $N_\omega(\lambda_\omega \mu_\omega)$, the U(3) symmetry of the final state. Any given symplectic representation space $N_\sigma(\lambda_\sigma \mu_\sigma)$ is infinite dimensional, since $N_n/2$, the number of boson excitations, can take any positive integer value. In practical applications, one must therefore either truncate the symplectic Hilbert space, or restrict oneself to interactions and observables for which the matrix elements depend solely on the symplectic irrep and can be calculated analytically.

It will be convenient to use the general shorthand notation, $\Gamma$, for a U(3) or SU(3) representation label. and $\alpha$ for an appropriate set of U(3) subgroup labels. We thus introduce, following the
notation of Hecht [95]:

\[
\begin{align*}
\Gamma_\sigma & \equiv [\sigma_1 \sigma_2 \sigma_3] \equiv N_\sigma(\lambda_\sigma \mu_\sigma) = N_\sigma(\sigma_1 - \sigma_2, \sigma_2 - \sigma_3) \\
\Gamma_n & \equiv [\pi_1 \pi_2 \pi_3] \equiv N_n(\lambda_n \mu_n) = N_n(\pi_1 - \pi_2, \pi_2 - \pi_3) \\
\Gamma_\omega & \equiv [\omega_1 \omega_2 \omega_3] \equiv N_\omega(\lambda_\omega \mu_\omega) = N_\omega(\omega_1 - \omega_2, \omega_2 - \omega_3).
\end{align*}
\] (2.17)

where \((\lambda \mu)\) are Elliott SU(3) labels and the \(N_\sigma = \sigma_1 + \sigma_2 + \sigma_3\), \(N_n = \pi_1 + \pi_2 + \pi_3\), and \(N_\omega = \omega_1 + \omega_2 + \omega_3\) give the number of squares in the U(3) Young tableaux (see Appendix C.1). With this convention, the basis states of Equation 2.16 can be written as:

\[
|\Phi[\Gamma_\sigma \Gamma_n \rho \Gamma_\omega \alpha_\omega]\rangle.
\] (2.18)

We thus obtain a basis of Sp(3,R) states that reduce the subgroup chain

\[
\text{Sp}(3,R) \supset \text{U}(3) \supset \text{SO}(3) \supset \text{SO}(2)
\] (2.19)

These states are eigenstates of the harmonic oscillator Hamiltonian. \(H_0|\Phi\rangle = E_0|\Phi\rangle\), with eigenvalues \(E_0 = N_\sigma \lambda_\omega \omega\). Two such states with different U(3) content \(\Gamma_\omega = N_\omega(\lambda_\omega \mu_\omega)\) are orthogonal, whereas two states with identical U(3) symmetry \(\Gamma_\omega\), but different \(\rho \Gamma_n = \rho N_n(\lambda_n \mu_n)\) quantum numbers are generally not orthogonal. The states \(|\Phi(\Gamma_\sigma \Gamma_n \rho \Gamma_\omega \alpha_\omega)\rangle\) of Equation 2.18 can be related to the orthonormal basis states \(|\Gamma_\sigma \Gamma_n \rho \Gamma_\omega \alpha_\omega\rangle\) of the unitary irreducible representation of Sp(3,R) by

\[
|\Phi[\Gamma_\sigma \Gamma_n, \rho \Gamma_\omega \alpha_\omega]\rangle = \sum_{j} \{\mathcal{K}(\Gamma_\sigma, \Gamma_\omega)\}_{n, \rho, \pi, \rho, \rho} |\Gamma_\sigma \Gamma_n, \rho \Gamma_\omega \alpha_\omega\rangle.
\] (2.20)

Here \(|\Gamma_\sigma \Gamma_n \rho \Gamma_\omega \alpha_\omega\rangle\), without the letter \(\Phi\), stands for the orthonormal basis states, and the symbol \([\mathcal{K}(\Gamma_\sigma, \Gamma_\omega)\] denotes the matrix elements of \(\mathcal{K}\). the positive Hermitian square root of the
overlap matrix $\mathcal{K}^2$, which has matrix elements

$$[\mathcal{K}^2(\Gamma_\sigma, \Gamma_\omega)]_{\nu', \nu, \rho', \rho} \equiv \langle \Phi[\Gamma_\sigma \Gamma_\nu \rho', \Gamma_\omega \rho] \mid \Phi[\Gamma_\sigma \Gamma_\nu \rho, \Gamma_\omega \rho] \rangle .$$  \hspace{1cm} (2.21)

The matrix $\mathcal{K}^2$ is diagonal in $\Gamma_\sigma$ and $\Gamma_\omega$ and independent of $U(3)$ subgroup labels $\alpha_\omega$, and its rows and columns are labeled by $\Gamma_\nu$ and $\rho$. Due to the smallness of the off-diagonal matrix elements of $\mathcal{K}^2$ the orthonormal basis states in Equation 2.20 can also be tagged by those labels $\Gamma_\nu, \rho$, which correspond to the dominant values of $\Gamma_\nu, \rho$ in these states. The method for calculating the matrix elements of $\mathcal{K}^2$, and therefore of $\mathcal{K}$, will be outlined in Subsection 3.1.7.

The collection of all $0\hbar \omega$ configurations is referred to as the $0\hbar \omega$ horizontal shell-model space and the set of states built on each $u(3)$ irrep $N_\sigma(\lambda_\sigma \mu_\sigma)$ is called the vertical extension of that irrep. Each vertical extension can be partitioned into horizontal slices with the states within the $\frac{N_\sigma}{2}$-th slice representable as a homogeneous polynomial of degree $\frac{N_\sigma}{2}$ in the $A^{(20)}$ tensors acting on a parent $0\hbar \omega$ configuration (see also Figure 2.4). Interactions can thus be classified according to their effect on this structure; pairing, for example, causes only horizontal mixing while the quadrupole-quadrupole interaction induces vertical mixing without breaking the $SU(3)$ symmetry within the horizontal slices.

### 2.2.3 Symplectic model Hamiltonians

The goal of the symplectic shell model is to achieve a microscopic description of light and heavy deformed nuclei [149, 42, 44, 46, 45, 151, 150]. These nuclei exhibit collective behavior, that is, modes of excitation in which an appreciable fraction of the nucleons in the system participate in a coherent manner, as for example, is the case for rotations. An appropriate Hamiltonian for describing rotational phenomena within the symplectic model consists of the harmonic oscillator, which provides the background shell structure, the quadrupole-quadrupole interaction, $Q^2 \cdot Q^2$, and a residual interaction that should include, for example, the single-particle orbit-orbit term as well as pairing and other interactions involving currents and a hexadecupole-hexadecupole form as needed.
BASIS STATES
SYMPLECTIC SHELL-MODEL

\[ (\lambda_s, \mu_s) \times (2,0) \times (2,0) \]

Figure 2.4: Symplectic shell model space. Schematic plot illustrating the symplectic shell model space. Taken from [45].

to get M1 (magnetic dipole) and E4 (electric octupole) transition strengths correct. However, most applications of the theory are much less ambitious than this, restricting the interaction to terms that can be expressed solely in terms of generators of the \(sp(3, R)\) algebra [52, 143, 23, 7, 141]. Interactions of the latter form do not mix different symplectic irreps and therefore the Hamiltonian matrix for such interactions becomes block-diagonal. Furthermore, in most practical applications the Hilbert space of the system is truncated to one single symplectic representation. This is accomplished by selecting the vertical slice (symplectic irrep) constructed from the leading starting irrep of the \(0\hbar\omega\) space. This is the SU(3) representation from the lowest layer, \(\Gamma_\sigma = N_\sigma(\lambda_\sigma\mu_\sigma)\), with the most symmetric spatial permutation symmetry consistent with the Pauli principle, and the maximal possible SU(3) Casimir operator value \(C_2(\lambda_\mu)\). The single symplectic irrep approximation is a sensible choice for nuclear systems which have a dominant quadrupole-quadrupole force, since this interaction does not mix symplectic representations and favors states with large \(C_2(\lambda_\mu)\) values.
A typical Hamiltonian for a calculation in a space truncated in the described manner is given by a harmonic oscillator term $H_0$ plus a collective potential and a SU(3) residual interaction:

$$H = H_0 + V_{\text{coll}} + V_{\text{res}} .$$

(2.22)

A rotationally invariant collective potential $V_{\text{coll}}$ can be constructed from the quadrupole tensor $Q^e$. Specifically, the quadratic and cubic rotational scalars in $Q^e$ can be related to the Bohr-Mottelson shape variables $\beta$ and $\gamma$ (see also Equation 2.6):

$$a_2 \equiv \frac{1}{12} [Q^c \times Q^c] = \frac{3}{20} A^2 (\frac{R_0}{b})^4 \beta^2$$

$$a_3 \equiv \frac{1}{108} (\frac{7}{2})^\frac{3}{2} [Q^c \times Q^c \times Q^c] = \frac{1}{20 \pi \sqrt{3 \pi}} A^3 (\frac{R_0}{b})^6 \beta^3 \cos 3\gamma .$$

(2.23)

where $R_0$ is the nuclear radius and $b$ the oscillator length. By choosing the appropriate parameters the potential can be adjusted to exhibit a minimum at the experimental deformation; by varying the depth of the minimum the rotational energy spectrum is adjusted to reproduce the observed moment of inertia. The collective potential mixes states from different major shells since the collective quadrupole operator $Q^e$ has non-vanishing matrix elements between shells differing by zero or two oscillator quanta. Thus the potential generates coherent multi-shell admixtures in the wave functions of the system and so achieves the experimentally observed nuclear deformations and absolute $B(E2)$ rates.

The effective residual interaction, $V_{\text{res}}$, is usually expressed in terms of the SU(3) $\supset$ SO(3) integrity basis, which was introduced in Subsection 2.1.3. The integrity basis consists of the second and third order Casimir invariants, $\hat{C}_2$ and $\hat{C}_3$, of SU(3), which are just constants within any SU(3) representation, the square of the angular momentum operator, $\hat{L}^2$, and the three- and four-body scalars $X_3$ and $X_4$. Such a residual interaction does not couple different major oscillator shells, but it produces the observed K-band splitting, as explained in Subsection 2.1.3. A more general residual interaction can be constructed from U(3) scalar operators which belong to the
enveloping algebra of \( sp(3, R) \). It is known that any such operator must be a polynomial in the \( Sp(3,R) \supset U(3) \) integrity basis [55, 80]. To fourth degree in the symplectic generators, the \( Sp(3,R) \supset U(3) \) integrity basis is given by the following eight generators:

\[
\{ \hat{N}, \hat{C}_2, \hat{C}_3, \hat{G}_2, \hat{G}_4, Y, Z_1, Z_2 \} .
\]  

(2.24)

where \( \hat{C}_2 \) and \( \hat{C}_3 \) are the quadratic and cubic SU(3) Casimir invariants (see also Equation 2.6). \( \hat{G}_2 \) and \( \hat{G}_4 \) denote the quadratic and quartic Casimir invariants of \( Sp(3,R) \), which are constant within a given symplectic representation:

\[
\hat{G}_2 \equiv \hat{C}_2 + \frac{1}{3} \hat{N}^2 - 4\hat{N}
\]

\[
\hat{G}_4 \equiv \frac{1}{2}((\hat{C}_2)^2 - 8\hat{C}_3 + 26\hat{C}_2 + (\frac{4}{3}\hat{C}_3 - 8\hat{C}_2)\hat{N}) + \frac{2}{3}\hat{C}_2\hat{N}^2 + \frac{1}{27}\hat{N}^4 - \frac{8}{9}\hat{N}^3 + \frac{28}{3}\hat{N}^2 - 48\hat{N} .
\]

(2.25)

where \( \hat{C}_2 \) and \( \hat{C}_3 \) are evaluated for the \( (\lambda, \mu, \nu) \) starting representation. \( Y, Z_1, \) and \( Z_2 \) are \( U(3) \) scalars in the \( sp(3,R) \) enveloping algebra which are neither Casimir invariants of \( U(3) \) nor of \( Sp(3,R) \):

\[
Y \equiv \sqrt{5} \left[ A^{(20)} \times C^{(11)} \times B^{(02)} \right]^{(00)},
\]

\[
Z_1 \equiv \sqrt{6} \left[ \left[ A^{(20)} \times C^{(11)} \right]^{(20)} \times \left[ C^{(11)} \times B^{(02)} \right]^{(02)} \right]^{(00)},
\]

\[
Z_2 \equiv \sqrt{3} \left[ \left[ A^{(20)} \times C^{(11)} \right]^{(01)} \times \left[ C^{(11)} \times B^{(02)} \right]^{(10)} \right]^{(00)} .
\]

(2.26)

While elements of the \( SU(3) \supset SO(3) \) integrity basis are commonly included in symplectic calculations in order to obtain proper K-band splitting, the effects of \( Sp(3,R) \supset U(3) \) integrity basis elements remain to be explored.

Matrix elements for the \( Q^c \cdot Q^c \) term in the collective potential can be calculated analytically in the so-called U(3)-boson approximation. In this approximation, the symplectic generator \( A^{(20)} \)
and its adjoint $B^{(02)}$ are replaced by phonon operators $\sqrt{2N_e}A^{(20)}$ and $\sqrt{2N_e}B^{(02)}$, respectively, where $N_e$ counts the number of oscillator quanta up through the $0\hbar\omega$ level. The phonon operators raise and lower the number of oscillator quanta by two and have the same SU(3) tensor character as the symplectic generators. The simplifications arise from the fact that U(3)-boson operators $A^{(20)}$ and $B^{(02)}$ obey much simpler commutation relations than do their symplectic counterparts. As a result, matrix elements of the phonon operators are less complex than those of the symplectic generators. The U(3)-boson approximation becomes exact in the limit $N_e \rightarrow \infty$; and in heavy deformed nuclei it is known to yield matrix elements which deviate from the exact ones by only a few percent. While the agreement between approximate and exact matrix elements decreases for light nuclei, this approach still gives good results for the spectra and B(E2) transitions of ds-shell nuclei like $^{24}\text{Mg}$ [139]. Alternatively, matrix elements of any term in $V_{coll}$, including $Q^{\nu} \cdot Q^{\nu}$, can be obtained exactly since the potential is constructed solely from $Q^{\nu}$ which in turn can be expressed as a sum of symplectic generators:

$$Q^{\nu}_{2\mu} = \alpha C^{(11)}_{2\mu} + \beta (A^{(20)}_{2\mu} + B^{(02)}_{2\mu}) \quad (\mu = -2, -1, 0, 1, 2). \quad (2.27)$$

Several strategies for calculating matrix elements of the symplectic generators $C^{(11)}, A^{(20)}, B^{(02)}$ have been explored. A direct way is to use the Sp(3,R) commutation relations to derive recursion formulae, as shown by Rosensteel [138]. This method will be discussed in more detail in Section 3.3, since we will make use of this strategy when deriving symplectic matrix elements of arbitrary one-body operators. Another approach is to start from approximate matrix elements and to proceed by successive approximations, adjusting the matrix elements until the commutation relations are precisely satisfied [149]. The most elegant method, however, involves vector-valued coherent state representation theory (also referred to as "vector coherent state theory") and evaluates matrix elements of the symplectic raising and lowering operators by relating them to the known matrix elements of a much simpler $u(3) \otimes Weyl$ algebra. This approach will be outlined in more detail in Subsections 3.1.6 and 3.1.7.
The term $H_0$ in Equation 2.22 generates the shell structure. To preserve this structure under the addition of the quadrupole-quadrupole and rotor interactions, one needs to require that the average expected value of the Hamiltonian in the $2\hbar\omega$ major shell is approximately $2\hbar\omega$ greater than in the $0\hbar\omega$ space, etc. This can be achieved by subtracting from every term in $V_{\text{coll}}$ and $V_{\text{res}}$ its major-shell trace-equivalent or centroid (energy average). The average energy or centroid of a Hamiltonian $H$ is given by

$$
\langle H \rangle_{N, (\lambda, \mu, \omega)} = \frac{1}{\text{dim}(\lambda, \mu, \omega)} \text{tr}(H),
$$

where the trace is evaluated within the U(3) irrep $N, (\lambda, \mu, \omega)$ and $\text{dim}(\lambda, \mu, \omega) \equiv \text{dim}(\lambda, \mu, \omega)$ denotes the dimension of $(\lambda, \mu, \omega)$. In the general case of an arbitrary Hamiltonian $H$, one needs to first expand $H$ in terms of U(3) tensor operators (which can, in principle, always be accomplished). One can show that the trace of any irreducible U(3) tensor vanishes within a given U(3) irrep unless the tensor is a U(3) scalar. Thus the centroid of a given Hamiltonian $H$ is completely determined by the scalar terms in its tensor expansion. This scalar part of the expansion is referred to as the U(3) scalar core of $H$ and denoted by $H^{\text{core}}$. It is obvious that $\langle H \rangle_{N, (\lambda, \mu, \omega)} = \langle H^{\text{core}} \rangle_{N, (\lambda, \mu, \omega)}$.

Analytic expressions for the trace-equivalents (cores) of relevant operators have been obtained by Rosensteel and Draayer [53, 54, 142]; we list a few which are important for our purposes:

$$
\begin{align*}
\alpha_2^{\text{core}} &= \frac{25}{48} \hat{C}_2 + \frac{5}{72} \hat{N} - \frac{5}{24} \hat{C}_2 \\
X_3^{\text{core}} &= -\frac{9}{2} \sqrt{10} \hat{C}_3 \\
X_4^{\text{core}} &= -\frac{9}{20} \hat{C}_2(\hat{C}_2 + \frac{3}{2}) \\
\hat{L}^2^{\text{core}} &= \frac{3}{4} \hat{C}_2 \\
\hat{L}^4^{\text{core}} &= \frac{3}{4} \hat{C}_2(\hat{C}_2 - \frac{2}{3}).
\end{align*}
$$

(2.29)
where \( \mathcal{C}_2 \) and \( \mathcal{C}_3 \) are evaluated for the \( N_\sigma(\lambda_\pi\mu_\rho) \) starting irrep. The trace equivalents for other polynomials in the integrity basis can be found in [53, 54, 142].

### 2.2.4 Symmetry-breaking and truncations in the symplectic model

The Hamiltonian described above does not break symplectic symmetry, and is thus consistent with a truncation of the model space to a single symplectic representation. A more realistic calculation would allow for interactions that mix different symplectic irreps, such as spin-orbit and pairing terms.

Draayer, Weeks, and Rosensteel studied the effect of these terms for the case of \(^{20}\text{Ne} \) [58]. They performed a symplectic multi-irrep calculation, using a Hamiltonian that included a collective quadrupole potential as well as symmetry-breaking single-particle energy and monopole-pairing terms. The action of the symmetry-breaking interactions was restricted to the valence shell and thus caused "horizontal" mixing only at the \( 0 \hbar \omega \) level, and the quadrupole potential accommodated the "vertical" mixing. While the model did not describe the non-yrast states very well, it produced a good description of the energy spectrum, the intrinsic moment of inertia, and the \( B(E2) \) strengths for the yrast band. It was found that the symmetry-breaking terms are crucial for obtaining the correct moment of inertia; in their absence, the low-lying spectrum, though properly rotational, is too compressed, that is, the yrast band moment of inertia is too large.

A generalization of the symmetry-breaking interaction used by Draayer et. al. from terms which connect different symplectic irreps at the \( 0 \hbar \omega \) level to terms which connect states of arbitrary excitations \( N_n \hbar \omega \) and \( N_n' \hbar \omega \) in different symplectic representations is very difficult to implement. Suzuki and Hecht [157, 158] provide a method for evaluating matrix elements of general translationally-invariant two-body interactions in a symplectic basis. They give a reduction formula which relates a two-body matrix element between states of excitations \( N_n \hbar \omega \) and \( N_n' \hbar \omega \) in the same or in different symplectic bands to matrix elements of simple SU(3) unit tensor operators connecting the \( \text{Sp}(3,\mathbb{R}) \) bandhead states. Since the bandhead states are simple SU(3) shell model states, the problem is thus reduced to the evaluation of matrix elements of standard SU(3) shell

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model calculations (see previous section). The ingredients needed for an actual calculation are: i) SU(3) coupling and recoupling coefficients (see Appendix C.2), which are readily available through published computer codes [1, 47]; ii) the $\mathcal{K}$-matrix elements, which can be calculated by techniques outlined in Subsection 3.1.7; iii) a set of expansion coefficients, which are given in the publication of Suzuki and Hecht for excitations of up to $N_n = 10\hbar\omega$ [157]; iv) $0\hbar\omega$ matrix elements of SU(3) unit operators, which can be evaluated with the code developed by Bahri and Draayer [6, 5].

It is furthermore necessary to express the two-body interaction of interest in terms of SU(3) tensor operators. In principle, this can be done for any interaction, although the procedure may become fairly lengthy and complicated. Suzuki and Hecht give the tensor decomposition for a Gaussian interaction, as well as for the spin-orbit and tensor interactions, explicitly [157, 158]. They apply their method to a very simple system, the $^8$Be nucleus, thus demonstrating the validity and usefulness of their approach. Nevertheless, a decade later, there is still no symplectic code available which makes use of the reduction formalism and provides symplectic matrix elements for general two-body interactions, even though a user-friendly code for the calculation of the matrix elements between the bandhead states has been placed in public domain a few years ago [6]. The complexity of the recursion formula, in conjunction with the large bases that one needs, are the primary obstacles for a real symplectic shell model calculation which takes into account multi-irrep as well as multi-shell correlations. Thus, most practical applications of the theory so far had to be restricted to single major shell calculations or single symplectic irrep calculations. The former approximation, which corresponds to the SU(3) submodel of the symplectic shell model, has been discussed in many publications [61, 62, 64, 65, 88, 41, 56, 57, 26], and the latter truncation, which will be employed here, is discussed in what follows.

Each symplectic representation $\Gamma_\sigma = N_\sigma(\lambda_\sigma,\mu_\sigma)$ has associated with it an infinite number of basis states, $|\Gamma_\sigma\Gamma_n\rho\Gamma_\omega\alpha_\omega\rangle$, since $N_n/2$, the number of boson excitations, takes on all positive integer values, $N_n/2 = 0, 1, 2, \ldots$. As $N_n$ increases, the number of states in each level of excitation increases as well: the number of possible U(3) symmetries $\Gamma_\omega = N_\omega(\lambda_\omega,\mu_\omega)$ increases, and the
values of \((\lambda_\omega \mu_\omega)\) become larger, thus allowing for more possible \(\alpha_\omega\) combinations. Therefore, even a single symplectic irrep space needs to be further truncated. A very natural truncation is accomplished by restricting the number of boson excitations that are taken into account. Previous applications have shown that including up to \(\approx 10\hbar \omega\) improves significantly the results for energy spectra and electromagnetic transition rates when compared to \(0\hbar \omega\) calculations. Higher excitations are generally found to yield only small corrections to the observables. Nevertheless, convergence needs to be tested for every individual case by comparing the results obtained in the selected Hilbert space with those of slightly smaller model spaces and checking for stability of excitation spectra and transition strengths.

Despite these limitations, the theory has turned out to be appropriate for a description of the low-energy structure of deformed nuclear systems and has provided useful insights into the dynamics of collective phenomena. Applications to both light and heavy deformed nuclei [149, 23, 7, 27, 126, 42, 44] have shown that single-symplectic-irrep calculations, using non-symmetry-breaking interactions yield results that are in reasonable agreement with experimental findings. Indeed, in many cases further truncations may be acceptable, such as restrictions to the \(sp(1, R)\) or the \(sp(2, R)\) subalgebras of \(sp(3, R)\).

Calculations show that for each level of excitation, a dominant SU(3) irrep \((\lambda_\omega \mu_\omega)\) can be identified. More specifically, for each \(N_{\omega} \hbar \omega\) shell \((N_{\omega} = N_\sigma + N_n)\) the dominant state is the SU(3) state \((\lambda_\omega \mu_\omega)\) within the \(Sp(3,R)\) representation \(N_\sigma(\lambda_\omega \mu_\sigma)\) with the maximum \(\lambda_\omega\); its SU(3) symmetry is given by \((\lambda_\sigma + N_n, \mu_\sigma)\), and it is referred to as the stretched configuration. Starting from the \(0\hbar \omega\) lowest weight state \(N_\sigma(\lambda_\omega \mu_\sigma)\), the first stretched state is obtained by applying the raising operator \(A^{(20)}\) to the starting irrep \(N_\sigma(\lambda_\omega \mu_\sigma)\) and keeping only the \(N_{\omega}(\lambda_\omega \mu_\omega) = N_\sigma + 2(\lambda_\sigma + 2, \mu_\sigma)\) configuration from the resulting set

\[
\left\{ N_{\omega}(\lambda_\sigma + 2, \mu_\sigma), N_{\omega}(\lambda_\sigma, \mu_\sigma + 1), N_{\omega}(\lambda_\sigma - 2, \mu_\sigma + 2), N_{\omega}(\lambda_\sigma + 1, \mu_\sigma - 1), N_{\omega}(\lambda_\sigma - 1, \mu_\sigma), N_{\omega}(\lambda_\sigma, \mu_\sigma - 2) \mid N_{\omega} = N_\sigma + 2 \right\}
\]
Here it is understood that a SU(3) representation $(\lambda \mu)$ vanishes identically unless $\lambda \geq 0$ and $\mu \geq 0$. Constructing the stretched $N_\sigma + 2(\lambda_\sigma + 2, \mu_\sigma)$ state corresponds to adding two oscillator quanta in the $z$ direction to the starting configuration. The stretched state in any given shell is precisely the state with the largest value of the Casimir invariant $\hat{C}_2$.

The subset of stretched SU(3) states within a symplectic representation can be generated by a $Sp(1, R)$ subgroup of $Sp(3, R)$. The restriction of a symplectic calculation to the subspace of stretched states is therefore often called the $Sp(1, R)$ model. This model, introduced by Arickx in 1976 [2], preceded the development of the $Sp(3, R)$ model, and was only later recognized to be a submodel of the latter. (Arickx referred to his model as an $Sp(2, R)$ model, using the strict mathematical notation, rather than the notation which refers to the dimension of the physical space under consideration.) The $Sp(1, R)$ model is more amenable to calculations than the full $Sp(3, R)$ model: There are fewer basis states, and the basis is orthogonal by construction, that is, the $K$ matrix is trivial, since it becomes diagonal. Despite these simplifications, the model provides a good first approximation to the complete symplectic model. Among other applications, it has been used successfully for the description of $^8\text{Be}$ [149] and for the giant monopole and quadrupole excitations of $^{16}\text{O}$ and $^{40}\text{Ca}$.

The stretched states have also proven valuable for enhancing a symplectic Hilbert space which is truncated at a given level of excitation. It has become common practice to include all possible symplectic states up to a fixed level of excitation plus additional stretched states of higher shells.

The success and usefulness of the $Sp(1, R)$ submodel of $Sp(3, R)$ have lead Peterson and Hecht to propose a $Sp(2, R)$ model in which excited states are constructed from the $0\hbar \omega$ starting configuration $N_\sigma (\lambda_\sigma \mu_\sigma)$ by adding oscillator quanta in the $z$ and $x$ direction, but not in the $y$ direction [129]. Applications show that this latter approximation works very well, even for electron scattering form factor predictions [4, 170], but further comparisons between $Sp(3, R)$ and $Sp(2, R)$ results are necessary.
2.2.5 Sample application for a light nucleus

We will now discuss a typical application of the symplectic model. This serves several purposes: The example will illustrate the ideas outlined above, demonstrate the successes and limitations of a single-irrep calculation, and establish the selected Hamiltonian and parameters as appropriate. The latter point is important, since we will later on use a very similar symplectic model space and Hamiltonian to obtain wave functions for which we will evaluate electron scattering form factors. The application we selected is a symplectic shell model calculation for $^{24}\text{Mg}$ performed by Rosensteel, Draayer, and Weeks [143]. For this nucleus both a rotational ground band (with $K^*=0^+$ and $J=0, 2, 4, 6, 8, \ldots$) and an excited so-called "γ-band" ($K^*=2^+$ and $J=2, 3, 4, 5, 6, 7, \ldots$) have been identified. Both bands exhibit strong E2 intraband transition rates in the 20 Weisskopf units range, whereas interband rates are of single-particle magnitude ($\approx 5$ Weisskopf units). While single-shell calculations which use effective charges are able to reproduce the strong intraband transitions, they fail to model the interband transitions and the $2.87 \text{ MeV}$ energy gap between the two low-lying $J^*=2^+$ states.

Rosensteel et al. [143] succeeded in reproducing both these features without the use of effective charges; their transition rates (both intraband and interband) as well as their $2^+-2^+$ energy gap are in reasonable agreement with experiment. Because of the rapid proliferation of basis states for $^{24}\text{Mg}$, they had to restrict their calculation to the single Sp(3,R) representation based on the U(3) $0\hbar\omega$ lowest weight state $N_\sigma(\lambda_\sigma\mu_\sigma) = 62.5(8, 4)$ ($N_\sigma$ is obtained by adding up the oscillator quanta for the ground state of the nucleus under consideration). All SU(3) representations from the leading slice $N_\sigma(\lambda_\sigma\mu_\sigma)$ up to and including $6\hbar\omega$ of excitation were considered, plus stretched configurations for the $N_\hbar\omega$ level with $N_\hbar = 8, 10, \ldots, 20$. As a result there were 88 SU(3) representations ($\lambda_\omega\mu_\omega$) and the dimensions of the angular momentum subspaces for $J = 0, 2, 3, 4, 5, 6, 7,$ and 8 were 39, 124, 129, 192, 185, 219, 196, and 208. This basis was shown to yield convergent eigenstates. The model Hamiltonian was of the form discussed above (see Equation 2.22) with a simple $\gamma$-independent
potential

$$V_{coll} = b_2 a_2 + b_4 (a_2)^2$$  \hspace{1cm} (2.30)

and a residual interaction

$$V_{res} = c_3 X_3 + c_4 X_4 + d_2 \hat{L}^2 + d_4 \hat{L}^4.$$  \hspace{1cm} (2.31)

The six parameters in this Hamiltonian were adjusted to fit the experimental energy spectra, intraband transitions, and moments of inertia of the ground and $\gamma$ bands; and $\hbar \omega$ was fixed using the empirical rule $\hbar \omega = 45 A^{-1/3} - 25 A^{-2/3} = 12.6$ MeV [143]. In MeV, the parameters take the following best fit values: $b_2 = -0.2, b_4 = 7.2 \times 10^{-5}, c_3 = 7.1 \times 10^{-3}, c_4 = -1.45 \times 10^{-3}, d_2 = 0.194, d_4 = -4.85 \times 10^{-4}$. The results of this study are summarized in Figure 2.5, which gives the theoretical and experimental energy spectra, and Table 2.1, which compares the experimental $B(E2)$ strengths with symplectic and other model calculations. Note, in particular, that the location of the $\gamma$-band and the interband transition rates are correctly reproduced. The static quadrupole moment of the yrast $2^+$ state was found to be $-0.184 \text{ eb}$ compared to the experimental value $-0.178 \pm 0.013 \text{ eb}$.

In order to provide insight into the structure of the wave functions of $^{24}\text{Mg}$ the contributions from SU(3) irreps at different levels of excitation are listed as well. Table 2.2 gives the probabilities of the ground band states in the different SU(3) irreps. From this table one infers the amount of shell mixing in the ground band: One finds that the $0\hbar\omega$ contribution to members of this band is about 70%, the contribution from the $2\hbar\omega$ level is approximately 20%, from the $4\hbar\omega$ level roughly 6%, etc. Also note that the $0\hbar\omega$ contribution increases slightly with angular momentum. while this trend is reversed at the higher excitation levels. These results are characteristic for symplectic calculations for light deformed nuclei.
Figure 2.5: Energy spectrum of $^{24}$Mg. Comparison of the theoretical energy spectrum of $^{24}$Mg, obtained from a symplectic model calculation, with the experimental energies of $^{24}$Mg collective states. Taken from [143].
Table 2.1: B(E2) strengths of $^{24}\text{Mg}$. Comparison between experimental B(E2) strengths of $^{24}\text{Mg}$ and results of various model calculations. All $B(E2: J_i K_i \rightarrow J_f K_f)$ transition strengths are given in Weisskopf units: 1 W.u. = $4.112 \times 10^{-3} e^2 fm^4$. PHF$^{a-b,c}$ refer to various Projected Hartree Fock calculations. Note that all calculations, with the exception of the SU(3)$^a$ case [129] and the symplectic calculations, employ effective charges. Data taken from [143, 129].

<table>
<thead>
<tr>
<th>Transition</th>
<th>Model B(E2)</th>
<th>B(E2)</th>
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<td></td>
<td>PHF$^a$</td>
<td>PHF$^b$</td>
</tr>
<tr>
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<td>$K_i$</td>
<td>$J_f$</td>
</tr>
<tr>
<td>2 0 0 0</td>
<td>22.9</td>
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</tr>
<tr>
<td>4 0 2 0</td>
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<tr>
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<td>20.4</td>
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</tr>
<tr>
<td>8 0 6 0</td>
<td>16.0</td>
<td>40.2</td>
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<td>3 2 2 2</td>
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<tr>
<td>6 2 4 2</td>
<td>21.2</td>
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<td>8 2 6 2</td>
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Table 2.2: Probabilities of the $^{24}\text{Mg}$ ground band. Probabilities of the $^{24}\text{Mg}$ ground band states in SU(3) irreps at levels of excitation $n=0, 2, 4, 6,$ and $8 \hbar \omega$. Probabilities contributing less than 0.5% have been omitted and the probabilities of multiply-occurring irreps have been summed over. Results are taken from [143].

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<td>0.001</td>
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<tr>
<td></td>
<td>$\Sigma</td>
<td>(\ldots</td>
<td>J^* )</td>
<td>.</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$\Sigma |(\ldots | J^* ) |^2 | 0.997 | 0.998 | 0.998 | 0.994 | 0.996$
2.2.6 Pseudo-symplectic extension

A full pseudo-symplectic shell model calculation would consider the Hilbert space of a heavy nucleus to be a product of a neutron and a proton subspace \( \mathcal{H} = \mathcal{H}_n \otimes \mathcal{H}_p \), with each of these being comprised of a normal and a unique parity component \( \mathcal{H}_\tau = \mathcal{H}^N_\tau \otimes \mathcal{H}^U_\tau \), where \( \tau = \pi \) or \( \nu \) for protons and neutrons, respectively. An orthonormal basis for the normal parity component \( \mathcal{H}^N_\tau \) is obtained by constructing the \( 0\hbar\omega \) starting configurations \( (\lambda^N_\tau, \mu^N_\tau) \) from the single-particle pseudo orbitals of the \( \eta_\tau \)-th \( (\eta_\tau = \eta_\tau - 1) \) major oscillator shell and proceeding as outlined above.

The starting configurations for the unique parity component \( \mathcal{H}^U_\tau \) are the SU(3) many-particle wave functions of the \( (\eta_\tau + 1) \)-st major oscillator shell, that is, the \( j^m_{\text{intr}} = \eta_\tau + \frac{3}{2} \) intruder orbital as well as its like-parity partners \( (j^m = \eta_\tau + \frac{3}{2}, \eta_\tau - \frac{1}{2}, \ldots \frac{1}{2}) \) are included. The task of handling this Hilbert space, a product of four infinite-dimensional subspaces, completely, while including all possible interactions, both within each component and in-between the spaces, is not possible with currently available tools and techniques. Fortunately, a series of assumptions can be introduced which render the calculations feasible and, at the same time, yield reasonable results. Although some of the approximations might seem quite drastic they are justifiable for heavy deformed nuclei which display strong rotational features as, for example, \(^{238}\text{U}\) does [27].

In applications of the pseudo-symplectic model to heavy nuclei, the normal parity subspaces for both protons and neutrons are truncated at the \( 0\hbar\omega \) level to leading pseudo-SU(3) configurations \( (\lambda^N_\sigma, \mu^N_\sigma) \) and \( (\lambda^N_\nu, \mu^N_\nu) \) only. These are then coupled to yield the \( 0\hbar\omega \) representations \( (\lambda_\sigma, \mu_\sigma) \in \{(\lambda^N_\sigma, \mu^N_\sigma) \otimes (\lambda^N_\nu, \mu^N_\nu)\} \) for the normal parity proton-neutron space \(^a\). Although in principle it is possible to retain all resulting \( (\lambda_\sigma, \mu_\sigma) \) labels, it is common practice to use only the leading irrep \( (\lambda_\sigma, \mu_\sigma)_{\text{max}} = (\lambda^N_\sigma + \lambda^N_\nu, \mu^N_\sigma + \mu^N_\nu) \) as the starting point for the vertical extension of the space. The entire set of states (infinite in number because \( \text{Sp}(3,\mathbb{R}) \) is non-compact) can be generated from \( (\lambda_\sigma, \mu_\sigma)_{\text{max}} \) through the repeated action of the raising operator \( A^{(20)} \). Realistic pseudo-symplectic

\(^a\)Note that for a given kind of particle (proton or neutron) "normal parity" refers to states which do not belong to the "mother shell" of the intruder level. Therefore the parity of the "normal parity" proton orbitals does in general not equal the parity of the "normal parity" neutron orbitals.
calculations for heavy deformed nuclei are based on those normal parity neutron-proton states that are obtained from the $0\hbar\omega$ starting irrep $(\lambda_\sigma, \mu_\sigma)$ by applying homogenous polynomials of degree $N_\lambda \leq N_{\lambda, \text{max}} / 2$ in the $B^{(20)}$ tensors, where $N_{\lambda, \text{max}} \lesssim 10$.

A study in the framework of the pseudo-SU(3) model has shown that representing the dynamics of a deformed nuclear system by its normal parity constituents only yields a good description of the physics of the nucleus, as long as the unique parity nucleons track the behavior of the particles in the normal parity sector and an appropriate scaling procedure is employed to rescale the results [69, 68, 66]. Pseudo-symplectic calculations which are based on normal parity neutron-proton states only assume that this prescription can be extended to the pseudo-symplectic case.

So far, there have been only a few applications to heavy deformed nuclei which made use of the symplectic extension of the pseudo-SU(3) scheme [42, 44, 27, 164]. One study, carried out by Castaños, Hess, Draayer, and Rochford, focused on $^{238}$U [27]. They introduced a scaling factor, in order to account for the influence of the unique parity nucleons, based on geometric arguments. Using this scaling factor, but no effective charges, they were able to reproduce experimental energies and electric quadrupole intraband transition rates for the ground band in the single-symplectic irrep approximation. Detailed results for ground band excitation energies and transition rates are given in Table 2.3. Results for the pseudo-SU(3) scheme (using effective charges) and the collective model are included for comparison.

A careful analysis of the eigenstates of the system showed that the contribution of the $0\hbar\omega$ configuration to the ground state is about 80%, the $2\hbar\omega$ level contributes approximately 15%, and the $4\hbar\omega$ level adds roughly another 5%. It was furthermore found that the stretched irreps. $(\lambda_\sigma + N_n, \mu_\sigma)$, were dominant at each level, $N_n \lambda / 2 = 1, 2, \ldots$, with the other representations being sufficiently important that they could not be excluded from the basis without changing the results in a significant manner.

This application demonstrates the basic validity of the pseudo-symplectic approach and the adiabatic assumption for low-lying collective phenomena. It also indicates that the much simpler
Sp(1,R) scheme may be too restrictive to properly describe the dynamics of strongly deformed nuclei. As mentioned before, the assumption that the unique parity nucleons can be accounted for via a scaling procedure is expected to break down for higher-lying states. Also, in order to better evaluate the success of the pseudo-symplectic model it is necessary to consider measures which are more sensitive to the fine details of the nuclear wave functions, such as electron scattering form factors. Such a study remains to be carried out.

Table 2.3: Energies and B(E2) strengths for $^{238}$U. Comparison between experimental and calculated energies and B(E2) strengths of $^{238}$U. B(E2) values are quoted for the pseudo SU(3) and collective model (CM) theories in addition to those for the pseudo-symplectic scheme. All energies are given in MeV and the $B(E2 : J_i, K_i \rightarrow J_f, K_f)$ transition strengths are listed in units of $e^2b^2$. Note that the pseudo SU(3) results were renormalized to the adopted experimental $B(E2 : 2_1 \rightarrow 0_1)$ value, $2.42 \ e^2b^2$. Data taken from [27].

<table>
<thead>
<tr>
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<th>Transition</th>
<th>B(E2) [$e^2b^2$]</th>
</tr>
</thead>
<tbody>
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<td></td>
<td>Exp.</td>
<td>Sp(3,R)</td>
</tr>
<tr>
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<td>0.0435</td>
<td>0</td>
</tr>
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<td>0.1487</td>
<td>0.1451</td>
<td>4</td>
</tr>
<tr>
<td>0.3072</td>
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</tr>
<tr>
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<td>0.5225</td>
<td>8</td>
</tr>
<tr>
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</tr>
<tr>
<td>1.0765</td>
<td>1.1320</td>
<td>12</td>
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Chapter 3

From a Bosonic Basis to a Fermion Realization

All practical applications of the symplectic model so far have been based either on boson realizations of Sp(3,R) or made use of coherent state theory of the symplectic group [23, 36, 96, 145, 138, 137, 139, 153, 148, 149, 170, 172, 171]. A large number of publications has been devoted to the construction of symplectic representation theories and to the evaluation of matrix elements of symplectic generators. In Section 3.1 we will review the findings that are relevant for our purposes, and in Section 3.2 we will make a transition to a fermion realization of the symplectic shell model. In Section 3.3 we will employ this formalism in order to derive a recursive process in which symplectic matrix elements of arbitrary one-body operators between states of excitation $N\hbar\omega$ and $N'\hbar\omega$ in the same or in different symplectic bands are related back to valence shell matrix elements, which can be evaluated by standard shell model techniques. While the important results and definitions of Section 3.1 can be found in the literature on the subject, we give additional details which aide the understanding of the group-theoretical aspects of the model in general and of the subsequent sections in particular. The step-by-step development of a fermion realization of the symplectic model, given in Section 3.2, and the derivation of the recursion formula, presented in Section 3.3, have been the primary goals of this chapter and represent new contributions to the literature on the symplectic model.
3.1 Symplectic Model in a Bosonic Basis

For simplicity we will make use of units in which $\hbar = \omega = m = 1$, where $m$ denotes the mass of a nucleon (we assume that $m_{\text{proton}} = m_{\text{neutron}}$) and $\omega$ is the frequency that occurs in the harmonic oscillator Hamiltonian:

$$H_0 = \sum_s \left( \frac{p_s^2}{2m} + \frac{1}{2}m\omega^2 x_s^2 \right).$$

(3.1)

where $x_s$ and $p_s$ denote the relative (Jacobi) position and momentum coordinates of the $s$-th Jacobi particle, and $[p_s, x_s] = i\hbar\delta_{st} \delta_{st}$ holds. Introducing $\hbar = \omega = m = 1$, one obtains the new commutation relation $[p_s, x_{t\bar{s}}] = i\delta_{t\bar{s}} \delta_{st}$, and the harmonic oscillator Hamiltonian takes the form

$$H_0 = \frac{1}{2} \sum_s (p_s^2 + x_s^2).$$

(3.2)

Similarly, the spherical components of the (algebraic) quadrupole operator.

$$Q_{2\mu} = \sqrt{\frac{4\pi}{5}} \sum_s \left( \frac{x_s^2}{b^2} Y_{2\mu}(\hat{x}_s) + b^2 p_s^2 Y_{2\mu}(\hat{p}_s) \right).$$

(3.3)

become

$$Q_{2\mu}^\theta = \sqrt{\frac{4\pi}{5}} \sum_s \left( x_s^2 Y_{2\mu}(\hat{x}_s) + p_s^2 Y_{2\mu}(\hat{p}_s) \right).$$

(3.4)

where $b = \sqrt{\hbar/m\omega}$ denotes the oscillator length parameter and $Y_{2\mu}(\hat{\psi})$ is a shorthand notation for the spherical harmonic $Y_{2\mu}(\theta, \phi)$ with arguments $\theta$ and $\phi$ which are determined by the unit vector $\hat{\psi}$ through $v_1 = \sin \theta \cos \phi$, $v_2 = \sin \theta \sin \phi$, and $v_3 = \cos \theta$.

It is furthermore necessary to introduce a "renormalized" quadrupole operator $Q$ as follows:

$$Q = \frac{1}{\sqrt{3}} Q$$

(3.5)
for both $Q = Q^a$, the algebraic quadrupole operator, and $Q = Q^c$, the collective quadrupole operator. As will be explained in Subsection 3.1.3, this normalization is necessary in order to achieve a consistent description of the spherical components of $\tilde{L}$ and $Q^a$ as components of a SU(3) irreducible tensor operator.

### 3.1.1 Cartesian Scheme

As previously explained (see Subsection 2.2.1), the symplectic algebra $sp(3, R)$ can be realized in terms of bilinear products of harmonic oscillator bosons in a cartesian scheme. If $x_{si}$ and $p_{si}$ denote the relative position and momentum coordinates of the $s$-th Jacobi particle, one-body operators $\eta_{si}$ and $\xi_{si}$, which create and annihilate, respectively, one oscillator quantum in the $i$-th direction of the $s$-th Jacobi particle, can be defined as follows:

\[
\eta_{si} \equiv \frac{1}{\sqrt{2}} (x_{si} - i p_{si}) \\
\xi_{si} \equiv \frac{1}{\sqrt{2}} (x_{si} + i p_{si}).
\]  

(3.6)

These operators are related to each other by hermitean conjugation $\xi_{si} = \eta^\dagger_{si}$ and satisfy the commutation relations

\[
[\xi_{si}, \eta_{s'j}] = \delta_{si} \delta_{ij} \\
[\eta_{si}, \eta_{s'j}] = [\xi_{si}, \xi_{s'j}] = 0.
\]  

(3.7)

The generators of the symplectic algebra can then be written as bilinear products of the creation and annihilation operators, contracted with respect to the particle index $s$:

\[
B^i_{ij} = \frac{1}{2} \sum_s \eta_{si} \eta_{sj} \\
B_{ij} = \frac{1}{2} \sum_s \xi_{si} \xi_{sj}
\]
\[ C_{ij} = \frac{1}{2} \sum_s (\eta_s \xi_{ij} + \xi_s \eta_{si}) \quad (3.8) \]

and the commutation relations for the symplectic algebra in this basis are easily inferred from the commutation relations of its building blocks. One finds:

\[
\begin{align*}
[B_{ij}, B_{kl}] &= [B^\dagger_{ij}, B^\dagger_{kl}] = 0 \\
[C_{ij}, B^\dagger_{kl}] &= B^\dagger_{il} \delta_{jk} + B^\dagger_{ik} \delta_{jl} \\
[C_{ij}, B_{kl}] &= -B_{jl} \delta_{ik} - B_{jk} \delta_{il} \\
[B_{ij}, B^\dagger_{kl}] &= C_{ij} \delta_{ik} + C_{kj} \delta_{il} + C_{li} \delta_{jk} + C_{ki} \delta_{lj} \\
[C_{ij}, C_{kl}] &= C_{il} \delta_{jk} + C_{kj} \delta_{il} .
\end{align*}
\quad (3.9)\]

One can now express the harmonic oscillator Hamiltonian, \( H_0 \), the angular momentum operator, \( \bar{L} \), and the (renormalized) algebraic quadrupole operator, \( Q^a \), in terms of boson creation and annihilation operators \( \eta_{st} \) and \( \xi_{st} \), or, alternatively, as linear combinations of the generators \( C_{ij} \). Making use of the inverse of Equations 3.6,

\[ x_{st} = \frac{1}{\sqrt{2}} (\eta_{st} + \xi_{st}) \]
\[ p_{st} = \frac{i}{\sqrt{2}} (\eta_{st} - \xi_{st}) . \quad (3.10)\]

the definition of the spherical harmonics [169], trigonometric relations, and Equation 3.8, one obtains the following expressions:

\[ H_0 = \sum_s (\bar{\eta}_s \cdot \bar{\xi}_s + \frac{3}{2}) = C_{11} + C_{22} + C_{33} + \frac{3}{2} (A - 1) \]
\[ \bar{L} = i \sum_s (\bar{\xi}_s \times \bar{\eta}_s) = -i \sum_{jk} \xi_{ij} \xi_{jk} \]
\[ Q^a_{20} = \frac{1}{\sqrt{3}} \sum_s (2\bar{\eta}_{a3} \bar{\xi}_{a3} - \bar{\eta}_{a1} \bar{\xi}_{a1} - \bar{\eta}_{a2} \bar{\xi}_{a2}) = 2C_{33} - C_{11} - C_{22} \]
where \( A - 1 \) is the number of Jacobi particles in the system.

3.1.2 Spherical Scheme

In order to take full advantage of group theoretical methods and techniques, it is necessary to express the symplectic generators as SU(3) tensor operators. Since SO(3), the group associated with the angular momentum operator \( \bar{L} \), is a physically significant subgroup of SU(3), we choose to express the relevant operators first as irreducible SO(3) tensor operators. Later on we will show that the spherical operators constructed here satisfy a particular set of commutation relations and are thus SU(3) irreducible tensor operators.

In characterizing SO(3) irreducible tensor operators we follow the book "Quantum Theory of Angular Momentum" by Varshalovich et al. [169, p. 61]:

Definition A SO(3) irreducible tensor operator \( T_J \) of rank \( J \) (with \( J \) integer or half-integer) is a set of \( 2J + 1 \) functions (components) \( T_{JM} \) (where \( M = -J, -J + 1, \ldots, J - 1, J \)) which satisfy the following commutation rules with the spherical components \( \hat{J}_q (q = 0, \pm 1) \) of the angular momentum operator:

\[
[\hat{J}_{\pm 1}, T_{JM}] = \mp \frac{1}{\sqrt{2}} e^{\pm i \delta} \sqrt{J(J+1) - M(M \pm 1)} T_{JM \mp 1}
\]

\[
[\hat{J}_0, T_{JM}] = M T_{JM}.
\]

The quantity \( \delta \) determines the relative phases of the different \( T_{JM} \) components and is, like the sign of the square root, arbitrary.
The linear Equations 3.12 define the components $T_{JM}$ up to an arbitrary overall scale factor, which is the same for all components. This factor can be a real or complex number, function, or operator. For our purposes it is expedient to define the overall phase of the components of $T_J$ such that $(T_{JM})^* = (-1)^{J-M}T_{J-M}$ holds. Making use of this particular phase convention for tensor operators as well as for wave functions describing initial $|J_iM_i>$ and final $|J_fM_f>$ states leads to the following relation for matrix elements of Hermitean operators $(T_J)^\dagger = T_J$: $(J_iM_i|T_{JM}|J_fM_f) = (J_iM_i|(T_{JM}^*)^\dagger|J_fM_f)^*$. Another possible phase convention leads to $(T_{JM})^* = (-1)^M T_{J-M}$, which is the convention that is used in the standard definition of the spherical harmonics, $(Y_{LM})^* = (-1)^M Y_{L-M}$.

Examples of SO(3) irreducible tensor operators include the orbital angular momentum $L$, the spin $S$, and the total angular momentum $\bar{J}$, as well as the quadrupole operator $Q^a$. We verify this for the cases of the orbital angular momentum $\bar{L}$, which is Hermitean, $(\bar{L})^\dagger = \bar{L}$, purely imaginary, $(\bar{L})^* = -\bar{L}$, and has spherical components:

\begin{align*}
L_+ & \equiv -\frac{1}{\sqrt{2}}(L_1 + iL_2) = -\frac{1}{\sqrt{2}}(i(C_{23} - C_{32}) + (C_{31} - C_{13})) \\
L_0 & \equiv L_3 = -i(C_{12} - C_{21}) \\
L_- & \equiv \frac{1}{\sqrt{2}}(L_1 - iL_2) = \frac{1}{\sqrt{2}}(-i(C_{23} - C_{32}) - (C_{31} - C_{13})) ,
\end{align*}

and for the algebraic quadrupole operator $Q^a_{2\mu}$. The spherical components of the angular momentum operator commute among themselves:

\begin{align*}
[L_0, L_\pm] & = \pm L_\pm \\
[L_-, L_+] & = -L_0
\end{align*}

and the commutation relations $[L, Q^a]$ are given by:

$$[L_0, Q^a_{2\mu}] = \mu Q^a_{2\mu}$$
\[ [L_\pm, Q^\mu_{2\mu}] = \pm \frac{1}{\sqrt{2}} \sqrt{6 - \mu(\mu \pm 1)} Q^\mu_{2\mu \pm 1} \]  \hspace{1cm} (3.15) 

for \( \mu = 0, \pm 1, \pm 2 \).

A comparison of the results 3.14 and 3.15 with the commutation relations 3.12 leads to the conclusion that the three angular momentum components \( L_0, L_\pm \) form an irreducible SO(3) tensor operator of rank 1, and the five components \( Q^\mu_{2\mu}(\mu = 0, \pm 1, \pm 2) \) form an irreducible tensor of rank 2. Furthermore, we check the phase convention of these operators and find that:

\[
(L_q)^* = (-1)^{(1-q)} (L_{-q})
\]

\[
(Q^\mu_{2\mu})^* = (-1)^{(2-q)} Q^\mu_{2\mu}
\]  \hspace{1cm} (3.16) 

which is in agreement with the choice made earlier.

Analogously, we now introduce the "spherical" components of the oscillator boson creation and annihilation operators:

\[
\eta_+ \equiv -\frac{1}{\sqrt{2}} (\eta_1 + i\eta_2)
\]

\[
\eta_0 \equiv \eta_3
\]

\[
\eta_- \equiv \frac{1}{\sqrt{2}} (\eta_1 - i\eta_2)
\]  \hspace{1cm} (3.17)

and

\[
\xi_+ \equiv -\frac{1}{\sqrt{2}} (\xi_1 + i\xi_2)
\]

\[
\xi_0 \equiv \xi_3
\]

\[
\xi_- \equiv \frac{1}{\sqrt{2}} (\xi_1 - i\xi_2).
\]  \hspace{1cm} (3.18) 

respectively. Here and in what follows we have suppressed the particle index \( s \). It is to be
understood that $\eta$ and $\xi$ refer to one particle only. One can now easily verify that the relation

$$\xi_q = (-1)^q (\eta_{-q})^\dagger$$

(3.19)

holds and that the commutator of $\xi_q$ and $\eta_q$ is given by

$$[\xi_q, \eta_{q'}] = (-1)^q \delta_{q(-q')}. \quad (3.20)$$

Working out the commutation relations of the angular momentum operator with the spherical components of the oscillator creation and annihilation operators yields:

$$[L_0, \eta_q] = q \eta_q$$
$$[L_{\pm}, \eta_q] = \mp \frac{1}{\sqrt{2}} \sqrt{2 - q(q \pm 1)} \eta_{q \pm 1}$$
$$[L_0, \xi_q] = q \xi_q$$
$$[L_{\pm}, \xi_q] = \mp \frac{1}{\sqrt{2}} \sqrt{2 - q(q \pm 1)} \xi_{q \pm 1}. \quad (3.21)$$

Thus $\eta$ and $\xi$ are irreducible SO(3) tensor operators of rank 1 with components $\eta_q$ and $\xi_q$, respectively, where $q = 0, \pm 1$. In the next section we will show that the spherical components of the boson creation and annihilation operators constructed above form SU(3) irreducible tensor operators.

For future reference we list the expressions for the cartesian components of the boson operators in the spherical basis:

$$\eta_1 = -\frac{1}{\sqrt{2}} (\eta_+ - \eta_-)$$
$$\eta_2 = \frac{i}{\sqrt{2}} (\eta_+ + \eta_-)$$
$$\eta_3 = \eta_0$$
\[ \xi_1 = -\frac{1}{\sqrt{2}}(\xi_+ - \xi_-) \]
\[ \xi_2 = \frac{i}{\sqrt{2}}(\xi_+ + \xi_-) \]
\[ \xi_3 = \xi_0, \]
\[ (3.22) \]

and express the angular momentum and quadrupole operators, as well as the harmonic oscillator Hamiltonian, in terms of the spherical components of the boson creation and annihilation operators:

\[ H_0 = \sum_s \left( \eta_0 \xi_0 + \eta_+ \xi_+ + \eta_- \xi_- + \frac{3}{2} \right) \]
\[ L_0 = \sum_s (\eta_- \xi_+ - \eta_+ \xi_-) \]
\[ L_\pm = \pm \sum_s (\eta_\pm \xi_0 - \eta_0 \xi_\pm) \]
\[ Q^0_{2\pm} = \frac{1}{\sqrt{3}} \sum_s \left( 2 \eta_0 \xi_0 + \eta_- \xi_+ + \eta_+ \xi_- \right) \]
\[ Q^q_{2\pm 1} = \sum_s \left( \eta_\pm \xi_0 + \eta_0 \xi_\pm \right) \]
\[ Q^q_{2\pm 2} = \sqrt{2} \sum_s (\eta_\pm \xi_\pm) \]
\[ (3.23) \]

3.1.3 SU(3) Tensor Operators

Irreducible tensor operators acting on the Hilbert space of a physical system behave in a well-defined manner under the transformations of one or several symmetry groups and are thus analogously to basis states - naturally classified according to the irreps of the relevant groups. In the previous sections spherical operators \( L_0, Q^0_{2M}, \eta_q, \) and \( \hat{\xi}_q \) were constructed from cartesian position and momentum coordinates \( x_i \) and \( p_i \). They were shown to transform as the components of SO(3) irreducible tensor operators and angular momentum labels \( jm \) were assigned accordingly. These labels take the values \( jm = 2M \) with \( M = 0, \pm 1, \pm 2 \) for \( Q^q \), and \( jm = 1q \) with \( q = 0, \pm 1 \) for \( L, \eta, \) and \( \hat{\xi} \).

A physically significant subgroup of Sp(3,R) is given by SU(3), which in turn has SO(3) as a subgroup. Because of this, and since we view the symplectic shell model as an extension of the
SU(3) shell model, it is natural to generalize the concept of a SO(3) irreducible tensor operator and establish a definition of a SU(3) irreducible tensor operator:

**Definition** A SU(3) irreducible tensor operator $T^\Gamma$ is a set of $r \equiv \text{dim}(\Gamma)$ components $T^\Gamma_\alpha$ which satisfy the following commutation rules with the generators $X$ of the group SU(3):

$$[X, T^\Gamma_\alpha] = \sum_{\Gamma'\alpha'} \langle \Gamma'\alpha' | X | \Gamma\alpha \rangle T^\Gamma_{\alpha'}. \quad (3.24)$$

Here $\Gamma$ labels an irreducible representation of SU(3) and $\alpha$ specifies a set of subgroup labels.

The operator $T^\Gamma_\alpha$ is well-defined once all matrix elements of the generators $X$ are determined.

As in the definition for the SO(3) irreducible tensor operator, Equation 3.24 determines the components $T^\Gamma_\alpha$ up to an arbitrary overall scale factor. This factor has to be the same for all components of a given tensor operator.

An example for a SU(3) irreducible tensor operator is given by the three spherical components $L_q$ of the orbital angular momentum plus the five spherical components $Q_{2\mathcal{M}}$ of the (renormalized) algebraic quadrupole operator. This statement is only true if the rescaled quadrupole operator $Q^a = \frac{1}{\sqrt{3}} Q_a$ is used. The necessity for this normalization can be traced back to the requirement that all components of a given SU(3) irreducible tensor operator have by definition the same scale factor. Since these components transform according to the SU(3) irrep $(\lambda\mu) = (11)$, additional SU(3) quantum labels can be assigned which explicitly state the tensor character of the SU(3) operator: $L_{1q} \rightarrow L_{1q}^{(11)}$ and $Q_{2\mathcal{M}} \rightarrow Q_{2\mathcal{M}}^{(11)}$. Using the SU(3) ⊂ SO(3) labeling scheme for the basis states, $|\Gamma\alpha\rangle = |(\lambda\mu)\kappa\mu\rangle$, and the fact that the set $\{L_q, Q_{2\mathcal{M}}^a | q = 0, \pm 1; \mathcal{M} = 0, \pm 1, \pm 2\}$ generates the group SU(3), condition 3.24 can be rewritten as:

$$[L_q, T^\Gamma_{\kappa\mu\lambda\mu}] = \sum_{(\lambda'\mu')\kappa'\mu'} \langle L_q | (\lambda'\mu')\kappa'\mu'\rangle T^\Gamma_{\kappa'\mu'\lambda\mu}, \quad (3.25)$$

$$[Q_{2\mathcal{M}}^a, T^\Gamma_{\kappa\mu\lambda\mu}] = \sum_{(\lambda'\mu')\kappa'\mu'} \langle Q_{2\mathcal{M}}^a | (\lambda'\mu')\kappa'\mu'\rangle T^\Gamma_{\kappa'\mu'\lambda\mu}. \quad (3.26)$$
The matrix element \( \langle (\lambda'\mu')\kappa'\ell'm'|L_q(\lambda\mu)\kappa l m \rangle \) can be determined with the help of the relations \( L_0 = L_3 \) and \( L_3(\lambda\mu)\kappa l m = mL(\lambda\mu)\kappa l m \) and the use of the Wigner-Eckart theorem (see Appendix C.3 for the definition and use of the double-barred matrix elements):

\[
\langle (\lambda'\mu')\kappa'\ell'm'|L_q(\lambda\mu)\kappa l m \rangle = \langle (\lambda'\mu')\kappa'\ell'||L||(\lambda\mu)\kappa l m \rangle \langle lmq|\ell'm' \rangle
\]

\[
\langle (\lambda'\mu')\kappa'\ell'm'|L_q=0(\lambda\mu)\kappa l m \rangle = m \delta_{(\lambda'\mu')(\lambda\mu)} \delta_{\kappa'\kappa} \delta_{\ell_1'\ell_1} \delta_{m'm} .
\] (3.27)

The relevant Clebsch-Gordan coefficient is given by \( \langle lm = 0|lm \rangle = \frac{m}{\sqrt{l(l + 1)}} \) [169]. Thus we determine:

\[
\langle (\lambda'\mu')\kappa'\ell'||L||(\lambda\mu)\kappa l m \rangle = \sqrt{l(l + 1)} \delta_{(\lambda'\mu')(\lambda\mu)} \delta_{\kappa'\kappa} \delta_{\ell_1'\ell_1}
\] (3.28)

and the commutation rule 3.25 becomes:

\[
[L_0, T^{(\lambda\mu)}] = \langle lm 1q|l(m + q)\rangle \sqrt{l(l + 1)} T^{(\lambda\mu)}_{m+q} .
\] (3.29)

Since \( \langle lm 10|lm \rangle \sqrt{l(l + 1)} = m \) and \( \langle lm 1 \pm 1|l(m \pm q)\rangle \sqrt{l(l + 1)} = \mp \frac{1}{2} \sqrt{l(l + 1) - m(m \pm 1)} \)
hold [169], we find that condition 3.25 is equivalent to requiring that \( T^{(\lambda\mu)}_{m+q} \) is a SO(3) irreducible tensor operator of rank \( l \).

The matrix element \( \langle (\lambda'\mu')\kappa'\ell'm'|Q^a_M(\lambda\mu)\kappa l m \rangle \) can be evaluated in a similar fashion. Making use of the Wigner-Eckart theorem for SU(3) (see Appendix C.3 for details), one finds:

\[
\langle (\lambda'\mu')\kappa'\ell'm'|Q^a_M(\lambda\mu)\kappa l m \rangle = \langle (\lambda\mu)\kappa l m; (11)12M|(\lambda'\mu')\kappa'\ell'm' \rangle \langle (\lambda'\mu')||Q^a||\rangle (\lambda\mu) \] (3.30)

where the triple-reduced matrix element is given by [91, 55]:

\[
\langle (\lambda'\mu')||Q^a||\rangle (\lambda\mu) = (-1)^{a} \sqrt{2C_2(\lambda\mu)} \delta_{(\lambda'\mu')(\lambda\mu)}
\]
\[ \varphi = \begin{cases} 
1 & \text{for } \mu \neq 0 \\
0 & \text{for } \mu = 0
\end{cases} \]

\[ C_2(\lambda \mu) = \frac{2}{3} (\lambda^2 + \lambda \mu + \mu^2 + 3(\lambda + \mu)) \quad (3.31) \]

Here \( C_2(\lambda \mu) \) is the second-order Casimir invariant of SU(3), which was introduced earlier, and the choice of the phase is consistent with that of reference [55]. Therefore the commutation rule 3.26 becomes:

\[ [Q_{\lambda \mu}^a, T_{\kappa \lambda }^{(\lambda \mu)}] = \sum_{\kappa' \mu'} \left( (\lambda \mu)_{\kappa \lambda}; (11)_{\frac{1}{2} \frac{1}{2}} \right) (-1)^{\sigma} \sqrt{2C_2(\lambda \mu)} T_{\kappa' \mu'}^{(\lambda \mu)} \quad (3.32) \]

We can now verify that \( \vec{L} \) and \( Q^a \) are SU(3) irreducible tensor operators of the form \( T_{\lambda \mu}^{(11)} \). Since both operators are SO(3) irreducible tensor operators (see the previous section), they automatically satisfy condition 3.25. It thus remains to be shown that they also obey the commutation relation 3.32. Since \( (\lambda \mu) = (11) \) we have \((-1)^{\sigma} = -1\) and \( C_2(11) = 6 \). The SU(3) Wigner coefficient \( ((\lambda \mu)_{\kappa \lambda}; (11)_{\frac{1}{2} \frac{1}{2}}) = (\lambda \mu)_{\kappa \lambda}; (11)_{\frac{1}{2} \frac{1}{2}} = 1 \) \( (\lambda \mu)_{\kappa \lambda}; (11)_{\frac{1}{2} \frac{1}{2}} = 2 \) needs to be evaluated for only a few cases, namely for \( (\lambda \mu) = (11); l, l' \in \{1, 2\} \). Analytic expressions for these cases are given in Vergados [173]; we obtain the following values:

\[
\begin{align*}
\langle (11) \kappa = 1 l = 1; (11) \kappa_0 = 1 l_0 = 2 || (11) \kappa' = 1 l' = 1 \rangle &= 0 \\
\langle (11) \kappa = 1 l = 1; (11) \kappa_0 = 1 l_0 = 2 || (11) \kappa' = 1 l' = 2 \rangle &= -\frac{1}{\sqrt{2}} \\
\langle (11) \kappa = 1 l = 2; (11) \kappa_0 = 1 l_0 = 2 || (11) \kappa' = 1 l' = 1 \rangle &= \frac{\sqrt{5}}{6} \\
\langle (11) \kappa = 1 l = 2; (11) \kappa_0 = 1 l_0 = 2 || (11) \kappa' = 1 l' = 2 \rangle &= 0 .
\end{align*}
\]

Thus \( L_q \) and \( Q^a_{\lambda \mu} \) must satisfy the following commutation rules in order to be considered proper
SU(3) irreducible tensors:

\[
[Q^{a}_{M}, L_{q}] = \sqrt{18} \langle 1q2M|2(q + M) \rangle Q^{a}_{M+q}
\]

\[
[Q^{a}_{M}, Q^{a'}_{M'}] = -\sqrt{30} \langle 2M'2M|1(M + M') \rangle L_{M+M'}.
\]  \hspace{1cm} (3.34)

It is now somewhat tedious, but straightforward, to show that \(L_q\) and \(Q^{a}_{M}\) are indeed the eight components of a SU(3) irreducible tensor operator of tensor character \((\lambda \mu) = (11)\).

Since we will make extensive use of the transformation properties of the spherical components \(R_{iq}\) and \(\xi_{iq}\) of the boson creation and annihilation operators, it is necessary to show that each set comprises a SU(3) irreducible tensor operator. We have already shown that both sets form SO(3) irreducible tensor operators of rank 1 (see Equation 3.21), thus condition 3.25 is satisfied. We will now verify that \(\eta\) is a SU(3) irreducible tensor operator, which transforms according to \((\lambda \mu) = (10)\) and that \(\xi\) is a \((\lambda \mu) = (01)\) tensor operator. It thus needs to be shown that the commutation relations 3.32 hold. We find that both the \((\lambda \mu) = (10)\) and \((\lambda \mu) = (01)\) SU(3) irreps contain \(l = 1\) as the only possible angular momentum value, and that \(l = 1\) occurs with multiplicity \(\kappa = 1\) (see Appendix C.1). Furthermore, \(C_2[(10)] = C_2[(01)] = \frac{3}{3}\) and thus Equation 3.32 becomes:

\[
[Q^{a}_{M}, T^{(\lambda \mu)}_{11q}] = (-1)^{\phi} \frac{4}{\sqrt{3}} \langle (\lambda \mu)11q; (11)12M|(\lambda \mu)11(M + q) \rangle T^{(\lambda \mu)}_{11(M+q)}
\]  \hspace{1cm} (3.35)

for \((\lambda \mu) = (10)\) or \((01)\) and \(\phi\) is 0 for \(\mu = 0\) and 1 for \(\mu \neq 0\).

The SU(3) Wigner coefficients used here, \(\langle (\lambda \mu)11q; (11)12M|(\lambda \mu)11(M + q) \rangle = \langle 1q2M|1(M + q) \rangle \langle (\lambda \mu)1; (11)2|(\lambda \mu)1 \rangle\), can be evaluated using the analytic expressions given by Vergados [173]. We find:

\[
\langle (\lambda \mu)\kappa = 1 \ l = 1; (11)\kappa_{\sigma} = 1 \ l_{\sigma} = 2||(\lambda \mu)\kappa' = 1 \ l' = 1 \rangle = -\frac{1}{2} \sqrt{\frac{5}{2}}
\]  \hspace{1cm} (3.36)
for both \((\lambda\mu) = (10)\) and \((\lambda\mu) = (01)\), and thus Equation 3.35 becomes:

\[
\mathcal{Q}_{\lambda\mu} = \left\{ \begin{array}{ll}
\frac{10}{2} M \mathcal{M} + q) & \text{for} (\lambda\mu) = (10) \\
\frac{10}{3} (1q 2M) & \text{for} (\lambda\mu) = (01)
\end{array} \right.
\]

with the positive sign for \((\lambda\mu) = (10)\) and the negative one for \((\lambda\mu) = (01)\).

Using the expressions for \(\mathcal{Q}_{\lambda\mu}^2\) in terms of the boson creation and annihilation operators (see Equation 3.23), and the commutator of \(\xi_q\) and \(\eta_q\), \([\xi_q, \eta_q] = (-1)^q \xi_q (-q')\), it is straightforward to verify that relation 3.35 is satisfied for both \(\eta\) and \(\xi\) and for all components \(\mathcal{Q}_{\lambda\mu}^2\). We therefore conclude that \(\eta\) and \(\xi\) are irreducible tensor operators with respect to \(\text{SO}(3)\) and \(\text{SU}(3)\) and assign the appropriate quantum labels: \(\eta_q \rightarrow T^{(\lambda\mu)}_{\alpha\beta} = \eta_{1q10}\) and \(\xi_q \rightarrow T^{(\lambda\mu)}_{\alpha\beta} = \xi_{1q01}\). For the sake of clarity and brevity, however, we will drop redundant labels, such as the multiplicity index \(\kappa\), and write \(\eta_{1q}^{(10)}\) and \(\xi_{1q}^{(01)}\) or, even simpler, \(\eta_q\) and \(\xi_q\).

### 3.1.4 SU(3) Tensor Products

The transformation properties of the oscillator boson creation and annihilation operators, \(\eta_q\) and \(\xi_q\), allow us to construct combinations which form new tensor operators. Of particular interest are the tensor products that are obtained by coupling two irreducible tensors \(T^{\Gamma_1}_{\alpha_1}\) and \(T^{\Gamma_2}_{\alpha_2}\) with respect to \(\text{SO}(3)\) and \(\text{SU}(3)\) (see Appendix A.3):

\[
T^{\Gamma}_{\alpha} = \sum_{\alpha_1\alpha_2} (\Gamma_1 \alpha_1; \Gamma_2 \alpha_2 | \Gamma \alpha) \ T^{\Gamma_1}_{\alpha_1} T^{\Gamma_2}_{\alpha_2}.
\]

Here \(\Gamma\) specifies a \(\text{SU}(3)\) irreducible representation \((\lambda_i\mu_i)\) and \(\alpha_i\) denotes a set of labels which are associated with an appropriate subgroup chain. We will focus here on the chain \(\text{SU}(3) \supset \text{SO}(3) \supset \text{SO}(2)\); and therefore we have \(\alpha_i = \kappa_i l_i m_i\).

The possible labels \(\Gamma\alpha\) of the product operator depend of course on the irrep labels of the original operators \(T^{\Gamma_1}_{\alpha_1}\) and \(T^{\Gamma_2}_{\alpha_2}\), as well as on the non-vanishing of the coupling coefficient \(\left\{ \Gamma_1 \alpha_1; \Gamma_2 \alpha_2 | \Gamma \alpha \right\}\)

\[
= \langle \langle \lambda_1 m_1 | \lambda_2 m_2 \rangle \rangle \langle \langle \mu_1 | \mu_2 \rangle \rangle \langle \langle l_1 m_1 | l_2 m_2 \rangle \rangle.
\]

Angular momentum coupling rules, for exam-
ple, dictate that the Clebsch-Gordan coefficient \( \langle l_1 m_1 l_2 m_2 | l m \rangle \) is nonzero only if \( l_1, l_2 \) and \( l \) satisfy the triangular inequality \( |l_1 - l_2| \leq l \leq l_1 + l_2 \) and if \( m = m_1 + m_2 \) holds. For the case \( l_1 = l_2 = 1 \), for example, only product tensors with \( l = 0, 1, 2 \) may occur.

Analogously, there are \( SU(3) \) coupling rules which determine the possible \( SU(3) \) irreps \( \lambda \mu \) that can be obtained by coupling \( \lambda_1 \mu_1 \) with \( \lambda_2 \mu_2 \) (see Appendix C.2). For the cases that are of interest here, these rules allow the following couplings:

\[
\begin{align*}
(10) \times (10) & \rightarrow (\lambda \mu) \in \{(20), (01)\} \\
(01) \times (01) & \rightarrow (\lambda \mu) \in \{(02), (10)\} \\
(10) \times (01) & \rightarrow (\lambda \mu) \in \{(00), (11)\} \\
(01) \times (10) & \rightarrow (\lambda \mu) \in \{(00), (11)\}.
\end{align*}
\] (3.39)

We may furthermore use the Elliott rule [61] and the multiplicity formulae from Appendix C.1 to determine the possible \( l \)-values that are contained in the resulting irreps and their respective multiplicities \( \kappa \). We find that \((20)\) and \((02)\) contain \( l=0 \) and \(2\), \((10)\) and \((01)\) allow for \( l=1\), \((11)\) permits \( l=0 \) and \( 1\), and \((00)\) contains only \( l=0 \). The multiplicity index \( \kappa \) is 1 for all these cases.

We are specifically interested in the tensor products

\[
\begin{align*}
\{\eta^{(10)} \times \eta^{(10)}\}_{{\lambda \mu}}^{(\lambda \mu)}_{\kappa l(q_1 + q_2)} &= \sum_{q_1 q_2} \langle (10)1q_1; (10)1q_2 | (\lambda \mu)_{\kappa l} | (q_1 + q_2) \rangle \eta_{q_1}^{(10)} \eta_{q_2}^{(10)} \\
&= \langle (10)1; (10)1 | (\lambda \mu)_{\kappa l} \rangle \sum_{q_1 q_2} \langle 1q_1, 1q_2 | (q_1 + q_2) \rangle \eta_{q_1}^{(10)} \eta_{q_2}^{(10)} \\
&= \{\xi^{(01)} \times \xi^{(01)}\}_{{\lambda \mu}}^{(\lambda \mu)}_{\kappa l(q_1 + q_2)} \\
&= \{\eta^{(10)} \times \xi^{(01)}\}_{{\lambda \mu}}^{(\lambda \mu)}_{\kappa l(q_1 + q_2)} \\
&= \{\xi^{(01)} \times \eta^{(10)}\}_{{\lambda \mu}}^{(\lambda \mu)}_{\kappa l(q_1 + q_2)}.
\end{align*}
\] (3.40)

Here we have dropped the multiplicity index \( \kappa \) for all cases where it is clearly equal to 1. For example, the Wigner coupling coefficient \( \langle (10) | \kappa = 1 l = 1 q_1; (10) | \kappa = 1 l = 1 q_2 | (\lambda \mu)_{\kappa l} | (q_1 + q_2) \rangle \) has
been written as \((\langle 10 \rangle_{1q}; \langle 10 \rangle_{1q_2}(\lambda \mu)_{\sigma}(q_1 + q_2))\) and similarly for the reduced coupling coefficient. We will continue to use this abbreviated notation wherever the meaning is clear.

The double-barred coefficients can be evaluated with the help of Vergados' tables in [173]; all turn out to be either +1 or -1. If we furthermore make use of the analytic expressions for the ordinary \(SO(3)\) Clebsch-Gordan coefficients [169], we obtain the following (explicit) expressions for \(\{\eta \times \xi\}_{\lambda \mu \nu}^{(o)}\):
\[ Q_{2M}^a = \frac{1}{\sqrt{3}} Q_{2M}^a \] of SU(3):

\[ C_{im}^{(11)} = \sqrt{2} \sum_s \{ \eta^{(10)} \times \xi^{(01)} \}_{lIm}^{(11)} . \]  

Similarly one can list explicit expressions for the tensor products \( \{ \eta \times \eta \}^{(\lambda \mu)} \) and \( \{ \xi \times \xi \}^{(\lambda \mu)} \).

We do not need to consider the case \( \{ \xi \times \eta \}^{(\lambda \mu)} \) separately, since one can show that

\[ \{ \xi \times \eta \}^{(\lambda \mu)}_{\alpha \beta \phi \sigma} = (-1)^{\lambda + \mu} \{ \eta \times \xi \}^{(\lambda \mu)}_{\alpha \beta \phi \sigma} \]  

holds. One also finds that coupling \( \eta^{(10)} \) with \( \eta^{(10)} \) can only yield \( \{ \eta^{(10)} \times \eta^{(10)} \}^{(20)} \) and the tensor product of \( \xi^{(01)} \) with \( \xi^{(01)} \) has to be of the form \( \{ \xi^{(01)} \times \xi^{(01)} \}^{(02)} \):

\[ \{ \eta^{(10)} \times \eta^{(10)} \}^{(20)}_{00} = \frac{1}{\sqrt{3}}(\eta_0 \eta_0 - 2\eta_+ \eta_-) \]

\[ \{ \eta^{(10)} \times \eta^{(10)} \}^{(20)}_{2(q_1 + q_2)} = \sum_{q_1, q_2} (1 + 1, 1 + 2q_1 + q_2) \eta_0 \eta_0 \]

\[ \{ \xi^{(01)} \times \xi^{(01)} \}^{(02)}_{00} = \frac{1}{\sqrt{3}}(\xi_0 \xi_0 - 2\xi_+ \xi_-) \]

\[ \{ \xi^{(01)} \times \xi^{(01)} \}^{(02)}_{2(q_1 + q_2)} = -\sum_{q_1, q_2} (1 + 1, 1 + 2q_1 + q_2) \xi_0 \xi_0 \]  

(3.45)

3.1.5 Symplectic raising and lowering operators \( B^\dagger \) and \( B \)

In order to achieve a consistent notation and the ability to employ SO(3) and SU(3) coupling techniques as well as the Wigner-Eckart theorem throughout our calculations, we need to express the symplectic raising and lowering operators \( B_{\perp}^{\dagger} = \frac{1}{2} \sum_s \eta_s \eta_s \) and \( B_{\perp} = \frac{1}{2} \sum_s \xi_s \xi_s \) (see Equation 3.8) as proper SU(3) irreducible tensor operators. It is obvious that such tensor operators \( B_{\perp}^{(\lambda \mu)} \) and \( B_{\perp}^{(\lambda \mu)} \) can be written as linear combinations of \( \eta^{(10)} \eta^{(10)} \) and \( \xi^{(01)} \xi^{(01)} \), respectively.

The considerations of the previous section show that the only proper SU(3) tensors that can be constructed as such linear combinations are \( \{ \eta^{(10)} \times \eta^{(10)} \}_{lIm}^{(20)} \) and \( \{ \xi^{(01)} \times \xi^{(01)} \}_{lIm}^{(02)} \) with \( l=0 \) or
2. Thus the proper irreducible raising and lowering operators will necessarily be of the form:

\[
A_{lm}^{(20)} = \text{const} \sum_s \{ \eta^{(10)} \times \eta^{(10)} \}^{(20)}_{lm}
\]

\[
B_{lm}^{(02)} = \text{const} \sum_s \{ \xi^{(01)} \times \xi^{(01)} \}^{(02)}_{lm}.
\] (3.46)

(The motivation for using the letter \( A \) for the symplectic raising operator will become clear shortly.)

The overall scale factors \( \text{const} \) and \( \text{const}' \) are arbitrary. We follow the convention of G. Rosensteel [138] and set \( \text{const} = \text{const}' = \frac{1}{\sqrt{2}} \). This normalization leads to the following relations between the spherical components \( A_{l_0}^{(20)} \) and \( B_{l_0}^{(02)} \) and the cartesian components \( B_{ll}^{l_0} \) and \( B_{ll}^{l_0} \):

\[
A_{00}^{(20)} = \sqrt{\frac{2}{3}} (B_{11}^1 + B_{22}^1 + B_{33}^1)
\]

\[
A_{20}^{(20)} = \frac{1}{\sqrt{3}} (2B_{33}^1 - B_{11}^1 - B_{22}^1)
\]

\[
B_{00}^{(02)} = \sqrt{\frac{2}{3}} (B_{11}^{1*} + B_{22}^{1*} + B_{33}^{1*})
\]

\[
B_{20}^{(02)} = \frac{1}{\sqrt{3}} (2B_{33}^{1*} - B_{11}^{1*} - B_{22}^{1*})
\] (3.47)

and insures that

\[
(A_{lm}^{(20)})^* = (-1)^{l-m} A_{l-m}^{(20)}
\]

\[
(B_{lm}^{(02)})^* = (-1)^{l-m} B_{l-m}^{(02)}
\] (3.48)

holds. Furthermore, \( A_{lm}^{(20)} \) and \( B_{lm}^{(02)} \) are related to each other via Hermitean conjugation:

\[
B_{lm}^{(02)} = (-1)^{l-m} (A_{l-m}^{(20)})^\dagger.
\] (3.49)

The fact that the above relation holds, while \( B_{ij} = (B_{ij}^l)^l \), explains the use of the notation \( A \) for the symplectic raising operator in the spherical scheme.
We can now use Equations 3.42 and 3.46 to express the collective quadrupole operator

\[ Q_{2,M} = \sqrt{\frac{16\pi}{5}} \sum_s r_s^2 Y_{2M}(\vec{r}_s), \]  

(3.50)

(here given in units of \( \hbar = \omega = m = 1 \)) as a linear combination of SU(3) irreducible tensor operators. For the renormalized operator \( Q^c = \frac{1}{\sqrt{2}} Q^c \) this yields:

\[ Q_{2,M}^c = Q_{2,M}^a + \sqrt{2}(A_{2,M}^{(20)} + B_{2,M}^{(02)}). \]  

(3.51)

It is also straightforward, but tedious, to work out the commutation relations between the spherical components of the symplectic raising and lowering operators. One obtains the following results:

\[
\begin{align*}
[A_{i_1 m_1}^{(20)}, A_{i_2 m_2}^{(20)}] = [B_{i_1 m_1}^{(02)}, B_{i_2 m_2}^{(02)}] &= 0 \\
[B_{i_1 m_1}^{(02)}, A_{i_2 m_2}^{(20)}] &= 2\sqrt{10} \sum_{l,m} \langle (02) l_1 m_1; (20) l_2 m_2 | \{11\} l m \rangle C_{lm}^{(11)} \\
&+ \frac{8}{3} (-1)^{l_1 + m_2} \delta_{l_1 l_2} \delta_{m_1(-m_2)} H_0 .
\end{align*}
\]  

(3.52)

3.1.6 Matrix Elements of the \( u(3) \otimes Weyl \) Algebra

Matrix elements of the generators \( A^{(20)}, B^{(02)}, \) and \( C^{(11)} \) of the symplectic algebra can be calculated in several ways. We will outline a strategy forwarded by Rowe, Rosentsteel and others in [147, 153, 148, 149], which makes use of vector coherent states in order to relate the \( sp(3, R) \) algebra to a simpler boson algebra. This particular approach is not only very elegant, it also reveals the connection between the symplectic algebra \( sp(3, R) \) and the simpler \( u(3) \) boson algebra, which has been used as an approximation to the full symplectic algebra in a variety of applications [146, 147, 139, 20, 23, 136]. In addition, the vector coherent state approach produces matrix elements of the \( \mathcal{K} \) matrix, which in turn are required to achieve a proper orthonormalization of the
symplectic basis state (see Equation 2.21). In this and the following sections we will summarize Rosensteel and Rowe's prescription for evaluating matrix elements of generators of the $u(3) \otimes \text{Weyl}$ algebra, of the $\mathcal{K}$-matrix, and of the symplectic generators. For a comprehensive account of the vector coherent state method the reader is referred to the book “The Vector Coherent State Method and Its Application to Problems of Higher Symmetry” by K.T Hecht [96], the review by Zhang, Feng and Gilmore [176], and to various additional publications by K. T. Hecht, as well as by G. Rosensteel and D. Rowe.

Rosensteel and Rowe have shown [146, 152] that, with $N_\sigma \to \infty$, the $sp(3, R)$ algebra contracts to a $u(3) \otimes \text{Weyl}$ boson algebra in which the raising and lowering operators behave like single boson creation and annihilation operators, respectively:

\[
B^\dagger_{ij} - \sqrt{\frac{2N_\sigma}{3}} B_{ij}
\]
\[
B_{ij} - \sqrt{\frac{2N_\sigma}{3}} B_{ij}
\]
\[
C_{ij} - \sqrt{\frac{2N_\sigma}{3}} C_{ij} + (B^\dagger B)_{ij} .
\] (3.53)

Here $B^\dagger_{ij}$ and $B_{ij}$ are generators of the $u(3) \otimes \text{Weyl}$ boson algebra satisfying the commutation relations

\[
[B_{ij}, B_{kl}] = [B^\dagger_{ij}, B^\dagger_{kl}] = 0
\]
\[
[B_{ij}, B^\dagger_{kl}] = \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}
\]
\[
[C_{ij}, B^\dagger_{kl}] = [C_{ij}, B_{kl}] = 0
\]
\[
[C_{ij}, C_{kl}] = \delta_{jk} C_{il} - \delta_{il} C_{kj} .
\] (3.54)

and $N_\sigma$ counts the number of oscillator quanta up through the $0\hbar\omega$ level. That is, $N_\sigma$ is the expectation value of $\hat{N} = \sum_i C_{ii}$ for states of $0\hbar\omega$ excitation. Rowe [148] has shown that the expressions on the right-hand side of Equation 3.53 are the leading terms in a unitary realization
of \textit{sp}(3, R) in terms of the \textit{u}(3)-boson algebra. Higher order corrections are obtained via a so-called Holstein-Primakoff expansion.

In direct analogy to the construction of the spherical symplectic generators \( A^{(20)}, B^{(02)}, \) and \( C^{(11)} \) (see Subsections 3.1.4 and 3.1.5), one can introduce spherical components \( A^{(20)}_{lm}, B^{(02)}_{lm}, \) with \( l=0 \) or \( 2, \) and \( C^{(11)}_{lm}, \) with \( l=1 \) or \( 2, \) for the generators, which form proper \textit{SU}(3) irreducible tensor operators. The tensor operators are normalized such that:

\[
\begin{align*}
A^{(20)}_{00} &= \sqrt{\frac{2}{3}} \sum_i A_{i1}, \\
A^{(20)}_{20} &= \frac{1}{\sqrt{3}} (2A_{33} - A_{11} - A_{22}), \\
B^{(02)}_{00} &= \sqrt{\frac{2}{3}} \sum_i B_{i1}, \\
B^{(02)}_{20} &= \frac{1}{\sqrt{3}} (2B_{33} - B_{11} - B_{22})
\end{align*}
\] (3.55)

An irrep of the \( \textit{u}(3) \otimes \textit{Weyl} \) algebra is characterized by the \textit{U}(3) quantum numbers \( \Gamma_\sigma = N_\sigma(\lambda_\sigma \mu_\sigma) \) of its lowest-weight state which corresponds to an Elliott \textit{SU}(3) shell model state (compare also the construction of the symplectic basis states in Subsection 2.2.2). The complete basis for this irrep is then generated by applying symmetrically coupled products of the \textit{U}(3) raising operator \( A^{(20)} \) with itself to the lowest weight state \( |\Gamma_\sigma \alpha\rangle \), where \( \alpha \) denotes a set of appropriate subgroup labels, here taken to be \( \alpha = \kappa lm. \) and rounded brackets are used to distinguish \( \textit{u}(3) \otimes \textit{Weyl} \) states from symplectic basis states.

As in the symplectic case, we can define \textit{U}(3)-coupled raising polynomials:

\[
\mathcal{P}^n(A^{(20)}) = N_n\{A^{(20)} \times A^{(20)} \times \ldots \times A^{(20)}\}_{n \text{ times}}^{n(\lambda_\mu)}
\] (3.56)

and thus define basis states for an \( \textit{u}(3) \otimes \textit{Weyl} \) irrep \( \Gamma_\sigma \):

\[
|\Gamma_\sigma \Gamma_n \rho \Gamma_\omega \rangle = \{\mathcal{P}^n(A^{(20)}) \times |\Gamma_\sigma\rangle\}_{\rho,\omega}^{\alpha,\sigma}. \] (3.57)

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where \( \Gamma_\omega = N_\omega (\lambda_\omega \mu_\omega) \) labels the U(3) irrep contained in the product \( \Gamma_n \times \Gamma_\sigma \), \( \rho \) indexes the multiplicity, and \( \alpha_\omega = \kappa l m \) denotes a set of subgroup labels. By appropriate choice of the normalization factor \( N_n \), this basis is made orthonormal. U(3)-reduced matrix elements of the boson operators in this basis are given by Rosenteel and Rowe \[147\]:

\[
(\Gamma_\sigma \Gamma_{n'} \rho' \Gamma_{\omega'} || |A^{(20)}|| | \Gamma_\sigma \Gamma_n \rho \Gamma_\omega ) = (-1)^{\Gamma_\omega - \Gamma_{n'} \rho' \Gamma_{\omega'}} U(\Gamma_\sigma \Gamma_n \Gamma_{(20)}; \Gamma_\omega \rho \Gamma_{n'} \rho') (\Gamma_{n'} || |A^{(20)}|| | \Gamma_n ) .
\]

(3.58)

where \((-1)^{\Gamma_{n'}} = (-1)^{\lambda_{n'} + \mu_{n'}}\) and \(U[...]\) is a SU(3) Racah coefficient (for details on the definition and use of Racah coefficients see Appendix C.2.2). The boson SU(3) reduced matrix element,

\[
(\Gamma_{n'} || |A^{(20)}|| | \Gamma_n ) = (n'_1 n'_2 n'_3 || |A^{(20)}|| |n_1 n_2 n_3 ),
\]

is given by:

\[
(n'_1 n'_2 n'_3 || |A^{(20)}|| |n_1 n_2 n_3 ) = \sqrt{\frac{(n_1 + 4)(n_1 - n_2 + 2)(n_1 - n_3 + 3)}{(n_1 - n_2 + 3)(n_1 - n_3 + 4)}} \delta_{n'_1,n_1+2} \delta_{n'_2,n_2} \delta_{n'_3,n_3} \\
+ \sqrt{\frac{(n_2 + 3)(n_1 - n_2)(n_2 - n_3 + 2)}{(n_1 - n_2 - 1)(n_2 - n_3 + 3)}} \delta_{n'_1,n_1} \delta_{n'_2,n_2+2} \delta_{n'_3,n_3} \\
+ \sqrt{\frac{(n_3 + 2)(n_2 - n_3)(n_1 - n_3 + 1)}{(n_1 - n_3)(n_2 - n_3 - 1)}} \delta_{n'_1,n_1} \delta_{n'_2,n_2} \delta_{n'_3,n_3+2} .
\]

(3.59)

Note that \( A^{(20)} \) does not connect different \( u(3) \otimes Weyl \) irreps \( \Gamma_\sigma \neq \Gamma_{\sigma'} \), and that \( N_{n'} = N_n + 2 \) must hold, where \( N_{n'} = n'_1 + n'_2 + n'_3 \) and \( N_n = n_1 + n_2 + n_3 \). One can furthermore show that the boson matrix elements have the property \( \sum_{\Gamma_n} \mid (\Gamma_{n'} || |A^{(20)}|| | \Gamma_n ) \mid^2 = 1 \).

Matrix elements of the Weyl boson lowering operator \( B^{(02)} \) can easily be obtained from the reduced matrix elements of the raising operator \( A^{(20)} \) via the relation:

\[
(\Gamma_\sigma \Gamma_n \rho \Gamma_\omega || |B^{(02)}|| | \Gamma_\sigma \Gamma_{n'} \rho \Gamma_{\omega'} ) = (-1)^{\Gamma_\omega - \Gamma_{n'} \rho' \Gamma_{\omega'}} \sqrt{\frac{\dim(\lambda' \mu')}{\dim(\lambda \mu)}} \sqrt{\frac{\dim(\lambda' \mu')}{\dim(\lambda \mu)}} (\Gamma_\sigma \Gamma_{n'} \rho' \Gamma_{\omega'} || |A^{(20)}|| | \Gamma_\sigma \Gamma_n \rho \Gamma_\omega ) \gamma (3.60)
\]

where \((-1)^{\Gamma_{n'}}\) is a short-hand notation for \((-1)^{\lambda_{n'} + \mu_{n'}}\).
3.1.7 Matrix Elements of the \( sp(3, R) \) Algebra and the \( K \)-matrix

In [148] Rowe constructs a coherent state realization of the symplectic group \( Sp(3,R) \) and uses it to obtain the matrix elements of the \( sp(3, R) \) Lie algebra for all lowest weight representations, that is, for all representations that are relevant in applications of the symplectic model to nuclear collective states. He finds a non-unitary generalized Dyson expansion of the symplectic algebra \( sp(3, R) \) in terms of the \( u(3) \otimes \text{Weyl} \) algebra. Upon invoking a similarity transform from the Dyson boson expansion to an (equivalent) unitary representation, he obtains the following realization \( \gamma \) of the symplectic algebra:

\[
\begin{align*}
\gamma(B_{ij}^1) &= \mathcal{K}B_{ij}\mathcal{K}^{-1} \\
\gamma(B_{ij}) &= \mathcal{K}B_{ij}\mathcal{K}^{-1} \\
\gamma(C_{ij}) &= C_{ij} + (B^1B)_{ij}
\end{align*}
\]

(3.61)

which can directly be employed to relate the \( sp(3, R) \) matrix elements to those of the much simpler \( u(3) \otimes \text{Weyl} \) algebra. Here \( \mathcal{K} \) is the Hermitean square root of the positive definite overlap operator \( \mathcal{K}^2 \) defined in Subsection 2.2.2 (see Equation 2.21). The above realization \( \gamma \) (see Equation 3.61) is consistent with a mapping which associates with every symplectic state \( |\Psi(\Gamma_\sigma \Gamma_n \rho \Gamma_\omega \alpha)\rangle = \mathcal{K}(\Gamma_\sigma, \Gamma_\omega)(|\Gamma_\sigma \Gamma_n \rho \Gamma_\omega \alpha\rangle) \) a state \( |\Psi(\Gamma_\sigma \Gamma_n \rho \Gamma_\omega \alpha)\rangle = \mathcal{K}(\Gamma_\sigma, \Gamma_\omega)(|\Gamma_\sigma \Gamma_n \rho \Gamma_\omega \alpha\rangle) \) in the \( U(3) \times \text{Weyl} \) space:

\[
|\Psi(\Gamma_\sigma \Gamma_n \rho \Gamma_\omega \alpha\rangle) \rightarrow |\Psi(\Gamma_\sigma \Gamma_n \rho \Gamma_\omega \alpha)\rangle
\]

(3.62)

From these considerations it follows that the \( sp(3, R) \)-reduced matrix elements for the irreducible tensor operator \( A^{(20)} \) are given by:

\[
\langle \Gamma_\sigma \Gamma_n \rho_1 \Gamma_\omega_1 | A^{(20)} | \Gamma_\sigma \Gamma_n \rho_2 \Gamma_\omega_2 \rangle = \langle \Gamma_\sigma \Gamma_n \rho_1 \Gamma_\omega_1 | \gamma(A^{(20)}) | \Gamma_\sigma \Gamma_n \rho_2 \Gamma_\omega_2 \rangle
\]
Making use of vector coherent state techniques, Rowe shows [148] that

\[
(\Gamma_{\sigma_1, \Gamma_{\omega_1} \Gamma_{\omega_2} \Gamma_{\omega_3}} ||| \mathcal{K}(A^{(20)}) \mathcal{K}^{-1} ||| \Gamma_{\sigma_2, \Gamma_{n_2} \Gamma_{\omega_2}} = \\
\sqrt{\Delta \Omega(\Gamma_{n_1, \Gamma_{\omega_1} \Gamma_{n_2} \Gamma_{\omega_2}})} (\Gamma_{\sigma_1, \Gamma_{n_1} \Gamma_{\omega_1}} ||| A^{(20)} ||| \Gamma_{\sigma_2, \Gamma_{n_2} \Gamma_{\omega_2}})
\]

holds, and thus

\[
(\Gamma_{\sigma_1, \Gamma_{n_1} \Gamma_{\omega_1}} ||| A^{(20)} ||| \Gamma_{\sigma_2, \Gamma_{n_2} \Gamma_{\omega_2}} = \\
\sqrt{\Delta \Omega(\Gamma_{n_1, \Gamma_{\omega_1} \Gamma_{n_2} \Gamma_{\omega_2}})} (\Gamma_{\sigma_1, \Gamma_{n_1} \Gamma_{\omega_1}} ||| A^{(20)} ||| \Gamma_{\sigma_2, \Gamma_{n_2} \Gamma_{\omega_2}})
\]

allows one to obtain matrix elements for the symplectic raising operator \(A^{(20)}\). The value of \(\Delta \Omega(\Gamma_{n_1, \Gamma_{\omega_1} \Gamma_{n_2} \Gamma_{\omega_2}}) = \Omega(\Gamma_{n_1, \Gamma_{\omega_1}}) - \Omega(\Gamma_{n_2, \Gamma_{\omega_2}})\) is determined using the expression:

\[
\Omega(\Gamma_{n, \Gamma_{\omega}}) = \frac{1}{4} \sum_{k=1}^{3} (2\omega_k^2 - n_k^2 + 8(\omega_k - n_k) - 2k(2\omega_k - n_k)) .
\]

Matrix elements of the symplectic lowering operator \(B^{(02)}\) can then be obtained from the reduced matrix elements of the raising operator \(A^{(20)}\) via the relation:

\[
(\Gamma_{\sigma_1, \Gamma_{n_1} \Gamma_{\omega_1}} ||| B^{(02)} ||| \Gamma_{\sigma_2, \Gamma_{n_2} \Gamma_{\omega_2}} = \\
(-1)^{\Gamma_{\omega_1} - \Gamma_{\omega_2}} \sqrt{\frac{\dim(\lambda_2 \mu_2)}{\dim(\lambda_1 \mu_1)}} (\Gamma_{\sigma_2, \Gamma_{n_2} \Gamma_{\omega_2}} ||| A^{(20)} ||| \Gamma_{\sigma_1, \Gamma_{n_1} \Gamma_{\omega_1}})^* .
\]

Note that the matrix elements that are evaluated in this manner are exact matrix elements. Although the method outlined above makes use of the close connection between the \(sp(3, R)\) and
$u(3) \otimes Weyl$ algebras and (explicitly) employs the matrix elements of the $U(3)$-boson raising and lowering operators, it yields the proper matrix elements of the symplectic generators $A^{(20)}$ and $B^{(02)}$. Throughout this dissertation we will consider the exact operators and matrix elements only, and all calculations are performed in the same spirit, unless noted otherwise. Our approach is thus different from the so-called $U(3)$-boson approximation, which replaces the symplectic generators and matrix elements by their $U(3)$-boson analogs [20, 23].

Using the vector coherent state method Rowe [148] also derives a simple recursion formula for the matrix elements of $K^2$, which utilizes the matrix elements of $A^{(20)}$. Note that $K$ is a $U(3)$-invariant operator and thus cannot connect states with $\Gamma_{\sigma_1} \neq \Gamma_{\sigma_2}$, $\Gamma_{\omega_1} \neq \Gamma_{\omega_2}$, $\alpha_1 \neq \alpha_2$:

\begin{equation}
(\Gamma_{\sigma_1} \Gamma_{n_1} \rho_1 \Gamma_{\omega_1} \alpha_1 | K | \Gamma_{\sigma_2} \Gamma_{n_2} \rho_2 \Gamma_{\omega_2} \alpha_2) = \\
\delta_{\sigma_1, \sigma_2} \delta_{\omega_1, \omega_2} \delta_{\alpha_1, \alpha_2} (\Gamma_{\sigma_1} \Gamma_{n_1} \rho_1 \Gamma_{\omega_1} \alpha_1 | K | \Gamma_{\sigma_2} \Gamma_{n_2} \rho_2 \Gamma_{\omega_2} \alpha_1).
\end{equation}

Rowe thus finds:

\begin{equation}
(\Gamma_{\sigma} \Gamma_{n_1} \rho_1 \Gamma_{\omega} | | K^2 | | \Gamma_{\sigma} \Gamma_{n_2} \rho_2 \Gamma_{\omega}) = \frac{2}{N(\Gamma_{\sigma} \Gamma_{n_2} \rho_2 \Gamma_{\omega})} \\
\times \sum_{\Gamma_{n_1} \rho_1 \Gamma_{\omega}} \Delta\Omega(\Gamma_{n_1} \Gamma_{\omega}, \Gamma_{n_2} \Gamma_{\omega}) (\Gamma_{n_1} \rho_1 \Gamma_{\omega} | | K^2 | | \Gamma_{n_2} \rho_2 \Gamma_{\omega}) \\
\times (\Gamma_{\sigma} \Gamma_{n_1} \rho_1 \Gamma_{\omega} | | A^{(20)} | | \Gamma_{\sigma} \Gamma_{n_2} \rho_2 \Gamma_{\omega}) (\Gamma_{\sigma} \Gamma_{n_2} \rho_2 \Gamma_{\omega} | | A^{(20)} | | \Gamma_{\sigma} \Gamma_{n_2} \rho_2 \Gamma_{\omega})^*.
\end{equation}

where

\begin{equation}
N(\Gamma_{\sigma} \Gamma_{n_2} \rho_2 \Gamma_{\omega}) = \sum_{ik} (\Gamma_{\sigma} \Gamma_{n} \rho_1 \Gamma_{\omega} \alpha | B_{ik}^a B_{kl}^a | \Gamma_{\sigma} \Gamma_{n} \rho_1 \Gamma_{\omega} \alpha) \\
= n_1 + n_2 + n_3
\end{equation}

with $(n_1 n_2 n_3)$ given by $\Gamma_n = (n_1 n_2 n_3)$ and $\Delta\Omega(\Gamma_{n_1} \Gamma_{\omega}, \Gamma_{n_2} \Gamma_{\omega})$ as defined in Equation 3.66. For
multiplicity-free states $\rho_{\text{max}} = 1$ the recursion relations of Equation 3.69 simplify to:

$$
\frac{(r_{n_1} r_{\omega_1} || | K || | r_{n_1} r_{\omega_1})}{(r_{n_2} r_{\omega_2} || | K || | r_{n_2} r_{\omega_2})} = \frac{(r_{\sigma_1} r_{n_1} 1 r_{\omega_1} || | K || | r_{\sigma_1} r_{n_1} 1 r_{\omega_1})}{(r_{\sigma_1} r_{n_2} 1 r_{\omega_2} || | K || | r_{\sigma_1} r_{n_2} 1 r_{\omega_2})} = \sqrt{\Delta \Omega (r_{n_1} r_{\omega_1}, r_{n_2} r_{\omega_2})}.
$$

(3.71)

The recursion relations given in Equations 3.69 and 3.71 are easily solved starting from the $0 \hbar \omega$ states, for which $r_{\omega} = r_{\sigma}$ holds, with the normalization

$$
(r_{\sigma} || | K^2 || | r_{\sigma}) = 1.
$$

(3.72)

The $2 \hbar \omega$ state is multiplicity-free, thus the matrix elements of $K^2$ for this level can be evaluated using Equation 3.71. For the $4 \hbar \omega$ and subsequent levels, however, $\rho > 1$ may occur, and then it becomes necessary to employ Equation 3.69 to find the $K^2$ matrix elements and hence those for $K$. Numerical calculations for $K^2$ show that for representations with large values of $N_\sigma$ the off-diagonal matrix elements of $K^2$ are very small compared to the diagonal matrix elements, thus implying that for such representation the symplectic basis states $|\Phi r_{\sigma} r_n r_{\omega} \rangle$ are almost orthogonal. (This fact has also been used to justify the use of an approximation in which the non-diagonal matrix elements of $K^2$ are set to zero.)

### 3.2 Symplectic Model in a Fermionic Basis

In the previous section we have employed the cartesian components of the generators of $sp(3, R)$ to construct a set of tensor operators which transform irreducibly under SO(3) and SU(3) symmetry group operations. A method has been outlined for evaluating exact matrix elements of these tensor operators by making use of the close connection between the symplectic algebra and a much simpler $u(3)$-boson algebra. This method has also been shown to yield matrix elements of a Hermitean operator $K$ which is required to orthonormalize the symplectic basis. We have furthermore shown
how the generators of the symplectic algebra \( \mathfrak{sp}(3, R) \) can be realized in terms of harmonic oscillator creation and annihilation operators \( \eta \) and \( \xi \).

In this section we will make a transition from the boson basis that has previously been employed to a fermionic description of the symplectic shell model. The new realization turns out to be very valuable. For example, in the new scheme it becomes possible to relate symplectic matrix elements of arbitrary one-body operators between states of excitation \( N_n \hbar \omega \) and \( N'_n \hbar \omega \) back to valence shell matrix elements which can be evaluated using standard shell model techniques. Thus a variety of new applications of the symplectic model become feasible, such as form factor predictions for deformed nuclei.

We will first express the symplectic generators in terms of oscillator creation and annihilation operators \( b^\dagger \) and \( b \). The operators \( b^\dagger \) and \( b \) are defined in direct analogy to the previously introduced boson operators \( \eta \) and \( \xi \); the only difference being that \( b^\dagger \) and \( b \) are constructed from the actual particle coordinates, whereas \( \eta \) and \( \xi \) are linear combinations of relative (Jacobi) coordinates. As a consequence, in the new formalism it becomes necessary to explicitly remove the center-of-mass contribution from all operators that act on the A-particle system. The advantage of employing the boson operators \( b^\dagger \) and \( b \) lies in the fact that their (single-particle) matrix elements can easily be evaluated. These matrix elements, in conjunction with second quantization techniques, will allow us to express the symplectic generators in terms of fermion creation and annihilation operators, which are proper SU(3) tensors. Using a series of commutation relations which will be deduced for SU(3) tensor products of the fermion operators, we will derive a recursion formula that allows us to evaluate symplectic matrix elements of arbitrary one-body operators.

### 3.2.1 Symplectic generators in terms of \( b^\dagger \) and \( b \)

In direct analogy to the definition of the boson operators \( \eta \) and \( \xi \) (see Equation 3.6), we introduce the harmonic oscillator boson creation and annihilation operators \( b^\dagger \) and \( b \):
Unlike $\eta$ and $\xi$, which were constructed from relative (Jacobi) position and momentum coordinates, $x_{st}$ and $p_{st}$, respectively, the operators $b^\dagger_{st}$ and $b_{st}$ are linear combinations of the actual particle coordinates $x_{st}$ and $p_{st}$. Like $\eta_{st}$ and $\xi_{st}$, the operators $b^\dagger_{st}$ and $b_{st}$ create and annihilate, respectively, one oscillator quantum in the $i$-th direction of the $s$-th particle (Jacobi “particle” for $x_{st}$ and $p_{st}$), are related to each other by hermitean conjugation $b_{st} = (b^\dagger_{st})^\dagger$, and satisfy the standard boson commutation rules:

$$[b^\dagger_{st}, b_{tj}] = \delta_{st} \delta_{ij}$$

$$[b^\dagger_{st}, b^\dagger_{tj}] = [b_{st}, b_{tj}] = 0 .$$  (3.74)

The new boson operators can also be employed to realize the symplectic algebra [137]:

$$C_{ij} = \sum_s (b^\dagger_{st} b_{sj} + \frac{1}{2} \delta_{ij}) - \frac{1}{A} \left( \sum_s b^\dagger_{st} \right) \left( \sum_t b_{tj} \right) - \frac{1}{2} \delta_{ij} = \sum_{st} (b^\dagger_{st} b_{tj} + \frac{1}{2} \delta_{ij}) (\delta_{st} - \frac{1}{A})$$

$$B^\dagger_{ij} = \frac{1}{2} \sum_s (b^\dagger_{st} b^\dagger_{tj}) - \frac{1}{2A} \left( \sum_s b^\dagger_{st} \right) \left( \sum_t b_{tj} \right) = \frac{1}{2} \sum_{st} b^\dagger_{st} b^\dagger_{tj} (\delta_{st} - \frac{1}{A})$$

$$B_{ij} = \frac{1}{2} \sum_s (b_{st} b_{tj}) - \frac{1}{2A} \left( \sum_s b_{st} \right) \left( \sum_t b_{tj} \right) = \frac{1}{2} \sum_{st} b_{st} b_{tj} (\delta_{st} - \frac{1}{A}) .$$  (3.75)

where the sums run over all $A$ particles in the system (instead of over $A-1$ Jacobi particles, as in Equation 3.8), and the two-body $\frac{1}{A}$ terms effect the removal of spurious center-of-mass excitations from the $A$-particle system.

Note that Equation 3.75 yields a realization of the symplectic algebra that is slightly different from the one given in Equation 3.8. Nevertheless, results like the commutation relations of Equation 3.9 or the expansion of $H_0$, $\vec{L}$, and $Q^2_{2A}$ in terms of the SU(3) generators $C_{ij}$, which were derived...
in Subsection 3.1.1, are independent of the realization and can therefore be used here without further proof.

As was done in Subsection 3.1.2 for the operators $\eta$ and $\xi$, we will now introduce spherical components for the oscillator boson creation and annihilation operators:

$$b^\dagger_+ \equiv -\frac{1}{\sqrt{2}} (b^\dagger_1 + ib^\dagger_2)$$

$$b^\dagger_0 \equiv b^\dagger_3$$

$$b^\dagger_- \equiv \frac{1}{\sqrt{2}} (b^\dagger_1 - ib^\dagger_2)$$

(3.76)

and

$$\tilde{b}^\dagger_+ \equiv -\frac{1}{\sqrt{2}} (b_1 + ib_2)$$

$$\tilde{b}_0 \equiv b_3$$

$$\tilde{b}^-_\equiv \frac{1}{\sqrt{2}} (b_1 - ib_2) .$$

(3.77)

These satisfy the relation

$$\tilde{b}^\dagger_q = (-1)^q (b^\dagger_{-q})^\dagger$$

(3.78)

and the commutator of $\tilde{b}_q$ and $\tilde{b}^\dagger_q$ is given by

$$[\tilde{b}_q, \tilde{b}^\dagger_q] = (-1)^q \delta_q(\nu^\dagger) .$$

(3.79)

The operators $b^\dagger_q$ and $\tilde{b}_q$ form SU(3) irreducible tensor operators of the type $b^\dagger_{1q}$ and $\tilde{b}^\dagger_{1q}$, respectively, and, consequently, two or more of these operators may be coupled to form SU(3) irreducible tensor products. In particular, the symplectic generators $C^{(11)}$, $A^{(20)}$, and $B^{(02)}$ can
be written as linear combinations of such products:

\[ C^{(11)}_{LM} = \sqrt{2} \sum_s \{ b_s^1 \times b_s^1 \}_{LM}^{(11)} - \frac{\sqrt{2}}{\Lambda} \sum_{st} \{ b_s^1 \times b_t^1 \}_{LM}^{(11)}, \]

\[ A^{(20)}_{LM} = \frac{1}{\sqrt{2}} \sum_s \{ b_s^1 \times b_s^1 \}_{LM}^{(20)} - \frac{1}{\sqrt{2} \Lambda} \sum_{st} \{ b_s^1 \times b_t^1 \}_{LM}^{(20)}, \]

\[ B^{(02)}_{LM} = \frac{1}{\sqrt{2}} \sum_s \{ \tilde{b}_s^1 \times \tilde{b}_s^1 \}_{LM}^{(20)} - \frac{1}{\sqrt{2} \Lambda} \sum_{st} \{ \tilde{b}_s^1 \times \tilde{b}_t^1 \}_{LM}^{(20)}. \] (3.80)

As before, the two-body $\frac{1}{\Lambda}$ terms removes the spurious center-of-mass excitations from the A-particle system. Note that the center-of-mass correction vanishes as $A$ approaches infinity. Therefore, in a system with many particles, such as a heavy nucleus, the two-body term can be neglected - to a high degree of accuracy. Nevertheless, since we are interested in describing both light and heavy nuclei, we will treat the center-of-mass corrections explicitly in what follows.

### 3.2.2 Matrix Elements of $b^\dagger$ and $b$

The single-particle matrix elements of the harmonic oscillator creation and annihilation operators $b^\dagger$ and $\tilde{b}$ are important ingredients for establishing a fermion realization of the symplectic model.

We are in a position to evaluate matrix elements of $b^\dagger$ and $\tilde{b}$ by making use of the transformation properties of these operators and their tensor products and by invoking SU(3) coupling rules. Starting with the number operator $\tilde{N} = \sqrt{3} \sum_s \{ b_s^{(10)} \times b_s^{(01)} \}_{00}^{(00)}$, where $\hat{n}_s = \{ b_s^{(10)} \times b_s^{(01)} \}_{00}^{(00)}$ counts the number of oscillator bosons associated with particle $s$, we have:

\[ \frac{\tilde{N}}{\sqrt{3}} = \sum_s \langle (\lambda \mu) | \{ b_s^{(10)} \times b_s^{(01)} \}_{00}^{(00)} | (\lambda \mu) \rangle | \chi \rangle | m \rangle \]

\[ = \frac{1}{\sqrt{3}} \sum_s \sum_q (-1)^q \langle (\lambda \mu) | \chi \rangle \langle b_q^{(10)} \tilde{b}_q^{(01)} | (\lambda \mu) \rangle | m \rangle \] (3.81)

where $\tilde{N}$ denotes the number of quanta in the system. Inserting a complete set of states

\[ 1 = \sum_{\lambda'' \mu'' \eta'' m''} \langle (\lambda'' \mu'') | \kappa'' l'' m'' | (\lambda' \mu') \rangle \kappa' l' m' \]

(3.82)
between $b_{1q}^{(10)}$ and $\tilde{b}_{1q}^{(01)}$ of Equation 3.81, and using the relation $\langle (\lambda'' \mu'' \kappa'' l'' m'') | b_{1q}^{(10)} | (\lambda \mu \kappa l m) \rangle = \langle (\lambda \mu \kappa l m) | b_{1q}^{(10)} | (\lambda'' \mu'' \kappa'' l'' m'') \rangle^*$. we find:

$$N = \sum_{s} \sum_{q} \sum_{(\lambda'' \mu'' \kappa')} \left| \langle (\lambda \mu \kappa l m) | b_{1q}^{(10)} | (\lambda'' \mu'' \kappa'' l'' m'') \rangle \right|^2$$

$$= \sum_{s} \sum_{(\lambda'' \mu'' \kappa')} \left| \langle (\lambda \mu) || \langle \lambda'' \mu'' || (\lambda'' \mu'' \kappa'' l'' m'') \rangle \right|^2. \tag{3.83}$$

where the latter follows from the orthonormality of the SU(3) Wigner coefficients (see Appendix C.2.1): $\sum_{\kappa'' l'' m''} \left| \langle (\lambda'' \mu'' \kappa'') | (\lambda'' \mu'' \kappa'' l'' m'') \rangle \right|^2 (10)_{1q}(\lambda \mu \kappa l m) = 1$. Invoking the appropriate coupling rule for $(\lambda'' \mu'') \times (10)$ (see Appendix C.2) we find:

$$(\lambda'' \mu'') \times (10) = (\lambda'' - 1, \mu'' + 1) \oplus (\lambda'' + 1, \mu'') \oplus (\lambda'', \mu'' - 1). \tag{3.84}$$

Thus the sum on the right-hand side of 3.83 reduces to three terms:

$$N = \sum_{s} \left( \left| \langle (\lambda \mu) || \langle \lambda + 1, \mu - 1) \rangle \right|^2 + \left| \langle (\lambda \mu) || \langle \lambda, \mu + 1 \rangle \rangle \right|^2 + \left| \langle (\lambda \mu) || \langle \lambda, \mu + 1 \rangle \rangle \right|^2. \tag{3.85}$$

Since we only need single-particle matrix elements, we can consider the special case of one particle in a harmonic oscillator potential. The single-particle wave function can be classified by $(\lambda \mu) = (\eta \mu)$. where $\eta$ labels the major oscillator shell in which the particle under consideration resides. Then $N$, the number of oscillator quanta in the system, equals $\eta$, and the first term in Equation 3.85 vanishes, since a negative value for $\mu''$ is not allowed. The last term, $|\langle (\eta \mu) || \langle (\lambda + 1, \mu - 1) \rangle \rangle |^2$, is zero since the boson creation and annihilation operators $b_{1q}^{(10)}$ and $\tilde{b}_{1q}^{(01)}$ can only connect SU(3) irreps $(\lambda \mu)$ and $(\lambda'' \mu'')$ which have the same $U(\Omega)$ symmetry, and it can be shown that $(\eta \mu)$ and $(\eta 1)$ belong to different $U(\Omega)$ irreps. Chosing the positive value of the square root, we thus obtain:

$$\langle (\eta \mu) || \langle (\lambda + 1, \mu - 1) \rangle \rangle = \sqrt{\eta} \delta_{\lambda \mu 1}(\eta - 1, 0). \tag{3.86}$$
Using the relation between a triple-reduced matrix element of a SU(3) tensor $T^{(\lambda \mu \nu)}$ and the equivalently reduced matrix element of its Hermitean adjoint $(T^{(\lambda \mu \nu)})^\dagger$ (see Appendix C.3) for the case of $\delta_{q_1 q_2}^{(01)} = (-1)^q(b_{1-q_1}^{(10)})^\dagger$ leads to the following result:

$$
\langle (\lambda \mu) || |\tilde{b}^{(01)}|| |(\eta 0)\rangle = \langle (\eta - 1, 0) || |\tilde{b}^{(01)}|| |(\lambda + 1, \mu)\rangle = \sqrt{\eta + 2} \delta_{(\lambda \mu)(\eta - 1, 0)} \quad (3.87)
$$

### 3.2.3 Fermion creation and annihilation operators $a^\dagger$ and $a$

A general one-body operator that acts symmetrically on a system of $A$ identical particles is given by

$$
\mathcal{F} = \sum_s f(\vec{r}_s, \vec{\sigma}_s) . \quad (3.88)
$$

where $\vec{r}_s$ and $\vec{\sigma}_s$ represent the position and spin (or spin-isospin) coordinates, respectively, of the $s$-th particle. In a fermion second quantization formulation this one-body operator takes the form:

$$
\mathcal{F} = \sum_{\rho, \rho'} \langle \rho | f(\vec{r}, \vec{\sigma}) | \rho \rangle \ a_{\rho'}^\dagger \ a_{\rho} \quad (3.89)
$$

(for details see Appendix B). In Equation 3.89 the symbol $\rho$ labels the available single-particle states and $a_{\rho}^\dagger$ and $a_{\rho}$ are single-particle creation and annihilation operators that satisfy the usual fermion anti-commutation relations:

$$
\{a_{\rho}, a_{\rho'}^\dagger\} = \delta_{\rho, \rho'}
$$

$$
\{a_{\rho}, a_{\rho'}\} = \{a_{\rho'}^\dagger, a_{\rho}^\dagger\} = 0 . \quad (3.90)
$$

For fermions in a harmonic oscillator potential, $\rho$ stands for a set of quantum numbers $\rho = \eta m_{1/2} \sigma$ or $\rho = \eta l_{1/2} j m_j$, depending on whether the states are characterized by an LS- or $jj$-coupling scheme, respectively. Here $\eta$ is the principal quantum number (major oscillator shell) of the single-
particle level; \( l, \frac{1}{2}, \) and \( j \) label the orbital, spin, and total angular momenta with projections \( m, \sigma, \) and \( m_j, \) respectively. (In a spin-isospin formalism, one has \( \rho = \eta(lm \frac{1}{2} \sigma \frac{1}{2} \tau) \) or \( \rho = \eta(lj m_j \frac{1}{2} \tau) \), respectively, where the additional \( \frac{1}{2} \) denotes the isospin quantum number with projection \( \tau \).) For our purposes it is most convenient to use the LS-coupling scheme, and this is what we will focus on from here on.

Since the single-particle harmonic oscillator wave functions, \( |\eta(lm \frac{1}{2} \sigma)\rangle = a_{\eta l m \frac{1}{2} \sigma}^\dagger |\psi\rangle \), where \( |\psi\rangle \) denotes the particle vacuum, transform irreducibly under a set of physically relevant SU(3) and SU(2) symmetry group operations, the fermion creation operator \( a_{\eta l m \frac{1}{2} \sigma}^\dagger \) is a double irreducible tensor operator of rank \((\lambda \mu) = (\eta 0)\) in SU(3), which labels its orbital character (with subgroup labels \( l \) and \( m \)), and of rank \( s = \frac{1}{2} \) in SU(2) for the spin part (with subgroup label \( \sigma \)):

\[
a_{\eta l m \frac{1}{2} \sigma}^\dagger = a_{(\eta 0)l m \frac{1}{2} \sigma}^\dagger .
\] (3.91)

It turns out that \( a_\mu = (a_\mu^\dagger)^\dagger \) is not a proper irreducible tensor operator with respect to the above group transformations. One can, however, show that

\[
a_{(\eta 0)l m \frac{1}{2} \sigma} = (-1)^{m+l+m+\frac{1}{2}+\sigma} a_{(\eta 0)l -m \frac{1}{2} -\sigma}
\] (3.92)

is a proper irreducible tensor operator of rank \((\lambda \mu) = (0 \eta)\) in SU(3) and rank \( s = \frac{1}{2} \) in (spin-)SU(2) (see also Appendix C.3).

Hence it becomes possible to construct tensor products from \( a^\dagger \) and \( \tilde{a} \), such as

\[
\{a_{(\eta 0)l \frac{1}{2} \sigma}^\dagger \times \tilde{a}_{(\eta' 0')l' \frac{1}{2} \sigma'}\}_{\lambda \mu \Sigma \Sigma'} = \sum_{\alpha_1, \alpha_2 = \pm \frac{1}{2}} ((\eta_1 0) \alpha_1; (0 \eta_2) \alpha_2 |(\lambda \mu) \kappa \Sigma \Sigma) \frac{1}{2} \sigma_1 \frac{1}{2} \sigma_2 |\Sigma \Sigma \rangle a_{(\eta_1 0)l_1 \frac{1}{2} \sigma_1}^\dagger \tilde{a}_{(\eta_2 0)l_2 \frac{1}{2} \sigma_2} .
\] (3.93)

which moves a particle from the \( \eta_2 \)-th major oscillator shell to the \( \eta_1 \)-th shell. The possible \((\lambda \mu)\) values are given by the coupling rule \((\eta_1 0) \times (0 \eta_2) = \bigoplus_{k=0}^{\min(\eta_1, \eta_2)} (\eta_1 - k, \eta_2 - k)\) and \( \alpha \), is an
abbreviation for the set of possible subgroup labels \( a_j = \kappa_j m_\alpha \), where \( \kappa_j = 1 \) must hold here. The total intrinsic spin \( S \) can take the values 0 or 1 with projection \( \Sigma = 0 \) or \( \Sigma = 0, \pm 1 \), respectively. The product

\[
\{ a^\dagger_{\eta_0 \frac{1}{2}} \times a^\dagger_{\eta_2 \frac{1}{2}} \}^{(\lambda \mu) S} = \\
\sum_{\alpha_1 \alpha_2 \sigma_1 \sigma_2} \langle (\eta_0) \alpha_1; (\eta_2) \alpha_2 | (\lambda \mu) \kappa LM \rangle \langle \frac{1}{2} \sigma_1 \frac{1}{2} \sigma_2 | S \Sigma \rangle a^\dagger_{(\eta_0) \alpha_1 \frac{1}{2} \sigma_1} a^\dagger_{(\eta_2) \alpha_2 \frac{3}{2} \sigma_2} \ . (3.94)
\]

on the other hand, creates a pair of fermions with one particle in the \( \eta_1 \)-th shell and one in the \( \eta_2 \)-th shell, and the pair is coupled to \( (\lambda \mu) \in \{ (\eta_0) \times (\eta_2) \} = \left\{ \bigoplus_{k=0}^{\min(\eta_1, \eta_2)} (\eta_1 + \eta_2 - 2k, k) \right\} \) and \( S=0 \) or 1. Similarly, the product

\[
\{ \bar{a}^\dagger_{0 \eta_1 \frac{1}{2}} \times \bar{a}^\dagger_{0 \eta_2 \frac{1}{2}} \}^{(\lambda \mu) S} = \\
\sum_{\alpha_1 \alpha_2 \sigma_1 \sigma_2} \langle (0 \eta_1) \alpha_1; (0 \eta_2) \alpha_2 | (\lambda \mu) \kappa LM \rangle \langle \frac{1}{2} \sigma_1 \frac{1}{2} \sigma_2 | S \Sigma \rangle \bar{a}^\dagger_{0 \eta_1 \alpha_1 \frac{1}{2} \sigma_1} \bar{a}^\dagger_{0 \eta_2 \alpha_2 \frac{3}{2} \sigma_2} \ . (3.95)
\]

annihilates a SU(3)-coupled pair of fermions with one particle in the \( \eta_1 \)-th shell, one in the \( \eta_2 \)-th shell, \( (\lambda \mu) \in \{ (0 \eta_1) \times (0 \eta_2) \} = \left\{ \bigoplus_{k=0}^{\min(\eta_1, \eta_2)} (k, \eta_1 + \eta_2 - 2k) \right\} \), and \( S=0 \) or 1.

One can furthermore construct a SU(3) irreducible tensor which destroys a pair of fermions in a given SU(3)-coupled configuration, and creates a new pair configuration:

\[
\left\{ \{ a^\dagger_{\eta_0 \frac{1}{2}} \times a^\dagger_{\eta_2 \frac{1}{2}} \}^{(\lambda_1 \mu_1) S_1} \times \{ \bar{a}^\dagger_{0 \nu_1 \frac{1}{2}} \times \bar{a}^\dagger_{0 \nu_2 \frac{1}{2}} \}^{(\lambda_2 \mu_2) S_2} \right\}^{(\lambda \mu) S} = \\
\sum_{\alpha_1 \alpha_2 \Sigma_1 \Sigma_2} \langle (\lambda_1 \mu_1) \alpha_1; (\lambda_2 \mu_2) \alpha_2 | (\lambda \mu) \rangle \rho \langle S_1 \Sigma_1 S_2 \Sigma_2 | S \Sigma \rangle \\
\times \{ a^\dagger_{\eta_0 \frac{1}{2}} \times a^\dagger_{\eta_2 \frac{1}{2}} \}^{(\lambda_1 \mu_1) S_1} \alpha_1 \Sigma_1 \{ \bar{a}^\dagger_{0 \nu_1 \frac{1}{2}} \times \bar{a}^\dagger_{0 \nu_2 \frac{1}{2}} \}^{(\lambda_2 \mu_2) S_2} \alpha_2 \Sigma_2 \ . (3.96)
\]

where \( \rho \) denotes the multiplicity of \( (\lambda \mu) \) in the coupling \( (\lambda_1 \mu_1) \times (\lambda_2 \mu_2) \rightarrow (\lambda \mu) \).

The coupled tensor operators introduced here are important for constructing one- and two-body operators which are irreducible tensor operators and for decomposing arbitrary one-body and two-body operators into their irreducible tensor components. In the next section, for example.
we will express the symplectic raising and lowering operators $A^{(02)}$ and $B^{(02)}$ in terms of the above SU(3)-coupled tensor products.

For future use and reference we will list the Hermitean adjoint of the above products here:

\[
\begin{align*}
\left\{ a^\dagger_{(\eta_1,0)_\frac{1}{2}} \times a_{(n_2,0)_\frac{1}{2}} \right\}_{\lambda_L \lambda_M \Sigma} & = (-1)^{n_2 - n_1 + L + M + \Sigma} \left\{ a^\dagger_{(\eta_2,0)_\frac{1}{2}} \times a_{(n_1,0)_\frac{1}{2}} \right\}_{\lambda_L \lambda_M \Sigma} \\
\left\{ a^\dagger_{(\eta_1,0)_\frac{1}{2}} \times a^\dagger_{(n_2,0)_\frac{1}{2}} \right\}_{\lambda_L \lambda_M \Sigma} & = (-1)^{-n_1 - n_2 - L + M - i + \Sigma} \left\{ a_{(n_2,0)_\frac{1}{2}} \times a_{(n_1,0)_\frac{1}{2}} \right\}_{\lambda_L \lambda_M \Sigma} \\
\left\{ a_{(n_1,0)_\frac{1}{2}} \times a_{(n_2,0)_\frac{1}{2}} \right\}_{\lambda_L \lambda_M \Sigma} & = (-1)^{-n_1 - n_2 + L + M + \Sigma} \left\{ a^\dagger_{(\eta_1,0)_\frac{1}{2}} \times a^\dagger_{(n_2,0)_\frac{1}{2}} \right\}_{\lambda_L \lambda_M \Sigma}
\end{align*}
\]

and

\[
\begin{align*}
\left\{ \{ a^\dagger_{(\eta_1,0)_\frac{1}{2}} \times a^\dagger_{(n_2,0)_\frac{1}{2}} \right\}_{\lambda_L \lambda_M \Sigma} & = (-1)^{\nu_1 + \nu_2 - n_1 - n_2 + (\lambda_1 + \mu_1 + \lambda_2 + \mu_2) + \lambda_3 + \mu_3 - L + M + \Sigma} \sum_{\rho'} (-1)^{\rho_{\max} - \rho'} \Phi_{\rho \rho'} \left\{ (\lambda_2 \mu_2)(\lambda_1 \mu_1); (\lambda \mu) \right\} \\
& \times \left\{ \{ a^\dagger_{(\nu_1,0)_\frac{1}{2}} \times a^\dagger_{(\nu_2,0)_\frac{1}{2}} \right\}_{\lambda_L \lambda_M \Sigma} \times \{ a_{(n_2,0)_\frac{1}{2}} \times a_{(n_1,0)_\frac{1}{2}} \right\}_{\lambda_L \lambda_M \Sigma} \right. \\
& \left. \left\{ (\lambda_2 \mu_2)(\lambda_1 \mu_1); (\lambda \mu) \right\} \right. \right.
\end{align*}
\]

where the phase matrix $\Phi$ is a special case of the recoupling coefficient $Z. \Phi_{\rho \rho'} \left\{ (\lambda_1 \mu_1)(\lambda_2 \mu_2); (\lambda \mu) \right\} = Z(\lambda_1 \mu_1)(00)(\lambda \mu)(\lambda_2 \mu_2); (\lambda_1 \mu_1) \rho(\lambda_2 \mu_2) \rho'$ (see also Appendix C.2.2). $\rho_{\max}$ denotes the maximum multiplicity in the coupling $(\mu_2 \lambda_2) \times (\mu_1 \lambda_1) \rightarrow (\lambda \mu)$, and $\rho'$ takes on values $1, 2, \ldots, \rho'_{\max}$.

It will also become necessary to employ the following computation relations, which can be derived by making use of the commutation rules of the uncoupled components (see Equation 3.90) and SU(3) coupling and recoupling techniques (which are explained in detail in Appendix C.2):

\[
\begin{align*}
\left\{ \{ a_{\eta,0} \times a_{\eta,0} \right\}_{\lambda_1 \mu_1, \Sigma_1} \times \{ a_{\eta,0} \times a_{\eta,0} \right\}_{\lambda_2 \mu_2, \Sigma_2} & = \\
(-1)^{\eta + \nu} & \sum_{s \sigma} \sqrt{(2S_1 + 1)(2S_2 + 1)} (S_1 S_2 S_1 S_2 | s \sigma) \left\{ \frac{1}{2} \frac{1}{2} S_1 \right\} \\
& \times \left\{ -\delta_{\eta',\nu} (-1)^{s - (\lambda_1 + \mu_1)} \sqrt{(d(\lambda_1 \mu_1)) \sum_{(\lambda \mu) a} a_{\eta,0} \times a_{\eta,0} \right\}_{\lambda \mu, s \sigma}
\end{align*}
\]
\[
x \times \sum_{\rho} \{(\lambda_1 \mu_1)_{\alpha_1}; (\lambda_2 \mu_2)_{\alpha_2}((\lambda \mu)_{\alpha})_{\rho} U[(\lambda_1 \mu_1)(\nu_0)(\lambda \mu)(\eta_0); (\eta \rho; \lambda_2 \mu_2)_{-\rho}]
\]
\[+ \tilde{\delta}_{\eta \nu}(-1)^{S_1 + S_2 - (\lambda_2 \mu_2)_{\alpha_2}} \sqrt{\frac{d(\lambda_2 \mu_2)}{d(\nu_0)}} \sum_{(\lambda \mu)_{\alpha}} \{\tilde{a}_{\eta}^{\alpha} \times \tilde{a}_{\nu}^{\sigma}\}^{(\lambda \mu)_{\alpha}}
\]
\[\times \sum_{\rho} \{(\lambda_2 \mu_2)_{\alpha_2}; (\lambda_1 \mu_1)_{\alpha_1}((\lambda \mu)_{\alpha})_{\rho} U[(\lambda_2 \mu_2)(\eta_0)(\lambda \mu)(\eta_0); (\nu_0; -(\lambda_1 \mu_1)_{-\rho})]\} (3.99)
\]
and
\[
\left\{\{a_{\eta}^{\alpha} \times a_{\nu}^{\sigma}\}^{(\lambda_1 \mu_1)_{\alpha_1}}_{\Sigma_1} \{a_{\eta}^{\alpha} \times a_{\nu}^{\sigma}\}^{(\lambda_2 \mu_2)_{\alpha_2}}_{\Sigma_2}\right\} =
\]
\[(-1)^{\eta + \nu - (\lambda_2 \mu_2)_{\alpha}} \sqrt{\frac{d(\lambda_2 \mu_2)}{d(\nu_0)}} \sum_{(\lambda \mu)_{\alpha}} \sqrt{(2S_1 + 1)(2S_2 + 1)} \left\{\frac{1}{2} \frac{1}{2} S_2 \right\}
\]
\[\times \left\{\delta_{\nu \eta}(-1)^{s + S_1 - (\lambda_1 \mu_1)_{\alpha}} \sum_{(\lambda \mu)_{\alpha}} \{a_{\eta}^{\alpha} \times a_{\nu}^{\sigma}\}^{(\lambda \mu)_{\alpha}}_{\alpha \sigma}
\]
\[\times \sum_{\rho} \{(\lambda_2 \mu_2)_{\alpha_2}; (\lambda_1 \mu_1)_{\alpha_1}((\lambda \mu)_{\alpha})_{\rho} U[(\lambda_2 \mu_2)(\eta_0)(\lambda \mu)(\eta_0); (\nu_0; -(\lambda_1 \mu_1)_{-\rho})]\}
\]
\[\times \sum_{\rho} \{(\lambda_2 \mu_2)_{\alpha_2}; (\lambda_1 \mu_1)_{\alpha_1}((\lambda \mu)_{\alpha})_{\rho} U[(\lambda_2 \mu_2)(\eta_0)(\lambda \mu)(\eta_0); (\nu_0; -(\lambda_1 \mu_1)_{-\rho})]\} (3.100)
\]
and
\[
\left\{\{\tilde{a}_{\eta} \times \tilde{a}_{\nu}\}^{(\lambda_1 \mu_1)_{\alpha_1}}_{\Sigma_1} \{\tilde{a}_{\eta} \times \tilde{a}_{\nu}\}^{(\lambda_2 \mu_2)_{\alpha_2}}_{\Sigma_2}\right\} =
\]
\[- \sum_{\sigma} \sqrt{(2S_1 + 1)(2S_2 + 1)} \left\{\frac{1}{2} \frac{1}{2} S_1 \right\}
\]
\[\times \left\{\tilde{\delta}_{\eta \nu}(-1)^{\eta + \nu - (\lambda_1 \mu_1)_{\alpha}} \sqrt{\frac{d(\lambda_1 \mu_1)}{d(\eta_0)}} \sum_{(\lambda \mu)_{\alpha}} \{\tilde{a}_{\eta}^{\alpha} \times \tilde{a}_{\nu}^{\sigma}\}^{(\lambda \mu)_{\alpha}}_{\alpha \sigma}
\]
\[\times \sum_{\rho} \{(\lambda_1 \mu_1)_{\alpha_1}; (\lambda_2 \mu_2)_{\alpha_2}((\lambda \mu)_{\alpha})_{\rho} U[(\lambda_1 \mu_1)(\eta_0)(\lambda \mu)(\eta_0); (\nu_0; -(\lambda_2 \mu_2)_{-\rho})]\}
\]
\[\times \sum_{\rho} \{(\lambda_1 \mu_1)_{\alpha_1}; (\lambda_2 \mu_2)_{\alpha_2}((\lambda \mu)_{\alpha})_{\rho} U[(\lambda_1 \mu_1)(\eta_0)(\lambda \mu)(\eta_0); (\nu_0; -(\lambda_2 \mu_2)_{-\rho})]\} (3.101)
\]
\[
\times \sum_{\rho} \left( (\lambda_1 \mu_1) \alpha_1; (\lambda_2 \mu_2) \alpha_2 | (\lambda \mu) \alpha_\rho \right) U |(\lambda_1 \mu_1)(\eta_0)(\lambda \mu)(0 \nu') \rangle \langle 0 \eta' \rangle |(\lambda_2 \mu_2) \alpha \rangle \right) .
\]

(3.101)

Here we have introduced the abbreviation \( d(\lambda \mu) \) for \( \dim(\lambda \mu) = \frac{1}{2} (\lambda + 1)(\mu + 1)(\lambda + \mu + 1) \).

### 3.2.4 Fermion realization of the symplectic algebra

We can now combine the findings from the previous sections to express the symplectic generators \( C^{(11)} \), \( A^{(20)} \), and \( B^{(02)} \) in terms of fermion creation and annihilation operators. As has been shown in Subsection 3.2.1, \( C^{(11)} \), \( A^{(20)} \), and \( B^{(02)} \) are one-plus-two body operators which can be written as linear combinations of SU(3) tensor products of boson creation and annihilation operators:

\[
\begin{align*}
C_{LM}^{(11)} &= \sqrt{2} \sum_s \{ \tilde{b}_s \times \tilde{b}_s \}_{LM}^{(11)} - \frac{\sqrt{2}}{A} \sum_{st} \{ \tilde{b}_s \times \tilde{b}_t \}_{LM}^{(11)}, \\
A_{LM}^{(20)} &= \frac{1}{\sqrt{2}} \sum_s \{ \tilde{b}_s \times \tilde{b}_s \}_{LM}^{(20)} - \frac{1}{2A} \sum_{st} \{ \tilde{b}_s \times \tilde{b}_t \}_{LM}^{(20)}, \\
B_{LM}^{(02)} &= \frac{1}{\sqrt{2}} \sum_s \{ \tilde{b}_s \times \tilde{b}_s \}_{LM}^{(02)} - \frac{1}{2A} \sum_{st} \{ \tilde{b}_s \times \tilde{b}_t \}_{LM}^{(02)}.
\end{align*}
\]

(3.102)

The two-body terms in the above expressions effect the removal of spurious center-of-mass excitations and vanish as \( A \), the number of particles in the system, goes to infinity.

In a fermion second quantization formulation, the one-body part of \( C^{(11)} \) takes the form:

\[
\mathcal{F}(C_{LM}^{(11)S=0}) = \sqrt{2} \sum_{\nu \nu'} \left( \langle (\nu \nu') | \frac{1}{2} \sum_{\rho} \left( b_\rho^+ \times \tilde{b}_\rho \right)^{(11)S=0}_{LM} \right) (\nu \nu')(\nu \nu') \frac{1}{2} \right)
\]

\[
= \sqrt{2} \sum_{\nu \nu'} \left( \langle (\nu \nu') | \frac{1}{2} \sum_{\rho} \left( b_\rho^+ \times \tilde{b}_\rho \right)^{(11)S=0}_{LM} \right) \langle \nu \nu' | \frac{1}{2} \right)
\]

\[
\times \sum_{\nu \nu', \nu' \nu'} \left( \langle (\nu \nu') | (\nu \nu') \frac{1}{2} \sum_{\rho} \left( b_\rho^+ \times \tilde{b}_\rho \right)^{(11)S=0}_{LM} \right) \langle \nu \nu' | \frac{1}{2} \right)
\]

(3.103)
Note that \( b^\dagger \), \( \tilde{b} \), and \( C^{(11)}_{LM} \) do not act on the spin part of the wave functions; thus we need to treat these operators as \( S = \Sigma = 0 \) objects, as has been explicitly expressed in the above equation.

Making use of the symmetry properties of the Clebsch-Gordan and SU(3) Wigner coefficients, more specifically \( \langle \frac{1}{2} \sigma 0 0 | \frac{1}{2} \sigma' \rangle = (-1)^{1-\sigma} \sqrt{2 \delta_{\sigma \sigma'}} \langle \frac{1}{2} \sigma \frac{1}{2} - \sigma'(00) \rangle \) and \( \langle (\nu'0)l'm'; (11)LM|(\nu0)lm \rangle = (-1)^{\nu' + l' - m'} \sqrt{\frac{d(l0)}{8}} \langle (\nu'0)l'm'; (11)LM|(\nu0)lm \rangle \), and the definition of the proper SU(3) irreducible tensor operator \( \delta_{0(\nu')l'-m', 1-\sigma'} = (-1)^{\nu' + l' - m' + \frac{1}{2} - \sigma'} \alpha_{(\nu0)l'm' \frac{1}{2} \sigma'} \), we obtain

\[
\mathcal{F}(C^{(11)}_{LM} = 0) = \sqrt{2} \sum_{\nu' \sigma'} \langle (\nu0) \frac{1}{2} || (b^\dagger \times \tilde{b})^{(11)}_{LM} = 0 || (\nu'0) \frac{1}{2} \rangle \sqrt{d(\nu0)} \frac{1}{2} \langle \alpha_{(\nu0)\frac{1}{2}} \rangle \times \tilde{\alpha}_{(\nu')\frac{1}{2}}\rangle||LM = 0 \rangle . \tag{3.104}
\]

In order to evaluate the triple-reduced matrix elements, we need to employ relations which express the (reduced) matrix element of a product of two irreducible tensor operators in terms of the (reduced) matrix elements of the individual operators. Varshalovich [169, p. 476] gives the appropriate relations for SO(3)-coupled products (here needed to treat the spin correctly), and Appendix C.3.2 gives the relevant relation for the SU(3)-coupled tensors. We find:

\[
\langle (\nu0) \frac{1}{2} || (b^\dagger (10)_{s=0} \times \tilde{b} (01)_{s=0})^{(11)}_{LM = 0} || (\nu'0) \frac{1}{2} \rangle = \sum_{(\lambda'' \mu'')} \left\{ \begin{array}{ccc}
(00) & (10) & (10) \\
(01) & (00) & (01) \\
(01) & (10) & (11) \\
- & - & -
\end{array} \right\} U[(\nu'0)(01)(\nu0)(10); (\lambda'' \mu'')(11)]
\times \langle (\nu0) \frac{1}{2} || b^\dagger (10)_{s=0} || (\lambda'' \mu'')^{1/2} \frac{1}{2} \rangle \langle (\lambda'' \mu'')^{1/2} \frac{1}{2} || \tilde{b} (01)_{s=0} || (\nu0) \frac{1}{2} \rangle \tag{3.105}
\]

Here \( U[(\nu'0)(01)(\nu0)(10); (\lambda'' \mu'')(11)] = 1 \) when \( \rho_{\text{max}} = 1 \). The nine-\( (\lambda \mu) \) coefficient turns out to be +1 [98], and the triple-reduced matrix elements of \( b^\dagger \) and \( \tilde{b} \) are given in Subsection 3.2.2:

\[
\langle (\nu0) \frac{1}{2} || b^\dagger (10)_{s=0} || (\lambda'' \mu'')^{1/2} \frac{1}{2} \rangle = \sqrt{\nu} \delta_{(\lambda'' \mu'')(\nu - 1.0)} .
\]
\[ \langle \lambda'' \mu'' \rangle_{\frac{1}{2}}^{1} \langle | \tilde{\xi}^{(10)}_{\nu=0} \rangle | \langle \nu' \rangle_{\frac{1}{2}}^{1} = \sqrt{\nu' + 1} \delta(\lambda'' \mu'' (\nu' - 1.0)) \] 

(3.106)

As a consequence of the delta functions, the sum \( \sum_{(\lambda'' \mu'')} \) in Equation 3.104 reduces to a single term, and the relevant Racah coefficient becomes \( U((\nu\lambda\lambda')(01)(\nu0)(10); (\nu - 1.0)(11)) \), which is determined with the help of Vergados' tables [173] as \( \sqrt{2(\nu+1)} \). One thus finds:

\[ \langle \nu 0 \rangle_{\frac{1}{2}}^{1} \langle | b_1 \times \delta^{(11)}_{\nu=0} \rangle | \langle \nu' 0 \rangle_{\frac{1}{2}}^{1} = \frac{2}{3} \nu(\nu + 3) \delta_{\nu'}. \] 

(3.107)

and therefore the one-body term 3.104 reduces to

\[ \mathcal{F}(C^{(11)S=0}_{LM\Sigma=0}) = \sum_{\nu} \sqrt{\nu(\nu + 1)(\nu + 2)(\nu + 3)} \{ a_{(\nu 0)\frac{1}{2}}^{\dagger} \times a_{(0\nu')\frac{1}{2}} \}^{(11)S=0}_{LM\Sigma=0}. \] 

(3.108)

Analogously one derives the fermion realization for the one-body part of the symplectic raising operator:

\[ \mathcal{F}(A^{(20)S=0}_{LM\Sigma=0}) = \frac{1}{\sqrt{2}} \sum_{\nu \nu'} \langle \nu 0 \rangle^{1} \langle | b_1 \times \delta^{(20)}_{Lm\Sigma=0} \rangle \langle \nu' 0 \rangle_{\frac{1}{2}}^{1} \{ a_{(\nu 0)\frac{1}{2}}^{\dagger} \times a_{(0\nu')\frac{1}{2}} \}^{(20)S=0}_{LM\Sigma=0}, \] 

(3.109)

where the triple-reduced matrix element is found to be

\[ \langle \nu 0 \rangle_{\frac{1}{2}}^{1} \langle | b_1 \times \delta^{(20)}_{Lm\Sigma=0} \rangle \langle \nu' 0 \rangle_{\frac{1}{2}}^{1} = \sqrt{\nu(\nu - 1)} \delta_{\nu'2}. \] 

(3.110)

and thus the one-body part of the symplectic raising operator becomes:

\[ \mathcal{F}(A^{(20)S=0}_{LM\Sigma=0}) = \sum_{\nu} \sqrt{\frac{1(\nu + 1)(\nu + 2)(\nu + 3)(\nu + 4)}{12}} \{ a_{(\nu 2)\frac{1}{2}}^{\dagger} \times a_{(0\nu')\frac{1}{2}} \}^{(20)S=0}_{LM\Sigma=0}, \] 

(3.111)
Similarly, for the symplectic lowering operator, one finds the following one-body part:

\[ \mathcal{F}(B^{(02)S=0}_{LM\Sigma=0}) = \frac{1}{\sqrt{2}} \sum_{\nu \nu'} \frac{1}{2} \langle (\nu 0)| \hat{b} \hat{b} |(\nu' 0) \rangle_{LM\Sigma=0} |(\nu 0)| \hat{b} \hat{b} |(\nu' 0) \rangle_{LM\Sigma=0} \]  

\[ = \frac{1}{\sqrt{12}} \sum_{\nu \nu'} \sqrt{(\nu + 1)\nu + 2} \langle (\nu 0)| \hat{b} \hat{b} |(\nu' 0) \rangle_{LM\Sigma=0} |(\nu 0)| \hat{b} \hat{b} |(\nu' 0) \rangle_{LM\Sigma=0} \]  

with the triple-reduced matrix element given by:

\[ \langle (\nu 0)| \hat{b} \hat{b} |(\nu' 0) \rangle_{LM\Sigma=0} = \sqrt{(\nu + 3)(\nu + 4)} \delta_{\nu' \nu + 2} \]  

Thus the one-body part of the symplectic lowering operator becomes:

\[ \mathcal{F}(A^{(20)S=0}_{LM\Sigma=0}) = \sum_{\nu} \sqrt{\frac{1}{12} \nu + 1(\nu + 2)(\nu + 3)(\nu + 4)} \langle (\nu 0)| \hat{b} \hat{b} |(\nu' 0) \rangle_{LM\Sigma=0} \]  

The two-body parts of the symplectic generators can be obtained in the same manner. As shown in Appendix B, a general symmetric two-body operator for \( A \) identical particles, \( g(\sigma_1, \sigma_2, \ldots, \sigma_A) \), takes the following form in a fermion second quantized formulation:

\[ \mathcal{G} = \sum_{s < t = 1}^{A} g(\sigma_s, \sigma_t, \ldots, \sigma_s) \]  

where \( s \) and \( t \) refer to the \( s \)-th and \( t \)-th particles, respectively, takes the following form in a fermion second quantized formulation:

\[ \mathcal{G} = \frac{1}{4} \sum_{s_1, s_2, \ldots, s_A} \langle \rho_1 \rho_2 | (\mathcal{G}^{(1)}_{s_1, s_2, \ldots, s_A}) | \rho_1' \rho_2' \rangle \]  

where \( |\rho_1, \rho_2 \rangle \) denotes the direct product of the single-particle wave functions \( |\rho_1 \rangle \) and \( |\rho_2 \rangle \). For the cases that are of interest here, the function \( g(\sigma_1, \sigma_1, \sigma_2, \sigma_2) \) can be written as a product \( g(1)g(2) \)
where we have made use of the symmetry properties of the Clebsch-Gordan and Wigner coefficients and of the Wigner-Eckart theorem for both SU(2) and SU(3).

Similarly, the two-body part of the symplectic lowering operator can be written as:

\[
\mathcal{G}(B_{L,0}^{(02),\Sigma=0})
= \frac{1}{2} \sum_{(\lambda\mu)S} \left\langle (\lambda\mu)S || \{\tilde{b}(1) \times \tilde{b}(2)\}^{(02),\Sigma=0} \right| || (\lambda'\mu')S' \rangle \sqrt{\frac{1}{6}d(\lambda\mu) \sqrt{2S+1}}
\times \sum_{\nu_1\nu_2} \{a^\dagger_{\nu_10} \times a^\dagger_{\nu_20}\}^{(\lambda\mu)S} \times \{\tilde{a}_{0\nu_1} \times \tilde{a}_{0\nu_2}\}^{(\mu'\lambda')S'}_{L',M'_0,\Sigma=0}
\times (-1)^{\nu_1^1+\nu_2^1+(\lambda'+\mu')} .
\]
In order to evaluate the triple-reduced matrix elements of $\{b^\dagger(1) \times b^\dagger(2)\}^{(20)}$ and $\{\hat{b}(1) \times \hat{b}(2)\}^{(02)}$, we make use of a relation given by J. Millener [119, Equation 4b] (see also Appendix C.3):

$$
\langle \{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}||\langle\{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}||\langle\{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}
\rangle
\langle \{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}||\langle\{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}||\langle\{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}
\rangle
$$

The reduced matrix elements of $b^\dagger$ are given in Subsection 3.2.2, and the 9-j symbol reduces to $\frac{1}{2\sqrt{S+1}} \delta_{SS'}$. Thus we obtain:

$$
\langle \{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}||\langle\{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}||\langle\{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}
\rangle
\langle \{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}||\langle\{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}||\langle\{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}
\rangle
$$

Analogously we determine the triple-reduced matrix elements relevant for the symplectic lowering operator:

$$
\langle \{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}||\langle\{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}||\langle\{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}
\rangle
\langle \{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}||\langle\{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}||\langle\{v'0\} \times \{v''0\}\rangle(b^\dagger(1) \times b^\dagger(2))^{(20)}
\rangle
$$
We thus find the following fermionic expressions for the symplectic raising and lowering operators $A^{(20)}$ and $B^{(02)}$, respectively:

\[
A^{(20)}_{LM} = \frac{1}{\sqrt{2}} \sum_s \{ b_s^\dagger \times b_s^\dagger \}_{LM\Sigma=0}^{(20)S=0} - \frac{1}{\sqrt{2}A} \sum_{at} \{ b_t^\dagger \times b_t^\dagger \}_{LM\Sigma=0}^{(20)S=0}
\]

\[
= (1 - \frac{1}{A}) \sum_{\nu} \sqrt{\frac{1}{12} \frac{1}{\nu + 1} (\nu + 2)(\nu + 3)(\nu + 4)} \{ a_{\nu+2,0}^\dagger \times \tilde{a}_{\nu+2,0} \}_{LM\Sigma=0}^{(20)S=0}
\]

\[
- \frac{1}{4A} \sum_{\nu' \mu' \equiv \nu \mu} \sqrt{\frac{1}{12} d(\lambda \mu) \nu \nu'} (2S + 1) \left\{ \begin{array}{cccc}
(\nu - 1, 0) & (10) & (\nu 0) & - \\
(\nu' - 1, 0) & (10) & (\nu' 0) & - \\
(\lambda' \mu') & (20) & (\lambda \mu) & - \\
- & - & - & -
\end{array} \right\}
\]

\[
\times \left\{ \begin{array}{c}
a_{(\nu+2,0)}^\dagger \times a_{(\nu+2,0)}^\dagger \\
(\lambda \mu) S \times \{ \tilde{a}_{(0,0'-1)} \times \tilde{a}_{(0,0'-1)} \}_{LM\Sigma=0}^{(20)S=0} (-1)^{\nu+\nu' + (\lambda' + \mu')}
\end{array} \right\}
\]

(3.122)

and

\[
B^{(02)}_{LM} = \frac{1}{\sqrt{2}} \sum_s \{ b_s \times b_s \}_{LM\Sigma=0}^{(02)S=0} - \frac{1}{\sqrt{2}A} \sum_{at} \{ b_t \times b_t \}_{LM\Sigma=0}^{(02)S=0}
\]

\[
= (1 - \frac{1}{A}) \sum_{\nu} \sqrt{\frac{1}{12} \frac{1}{\nu + 1} (\nu + 2)(\nu + 3)(\nu + 4)} \{ a_{\nu+2,0}^\dagger \times \tilde{a}_{(0,0+2)} \}_{LM\Sigma=0}^{(02)S=0}
\]

(3.123)
Making use of the properties of the coupling coefficients and of the Hermitean conjugation properties given in Subsection 3.2.3, one can now verify that

\[ B^{(02)}_{L,M} = (-1)^{L-M} \langle A^{(20)}_{L-M} \rangle \]

holds, as expected. This relation is non-trivial to verify and thus serves as a stringent test for the above expressions.

### 3.3 Recursion Relation

In this section we will derive a recursion formula in which symplectic matrix elements of arbitrary one-body operators between states of excitation \( N_n \hbar \omega \) and \( N'_n \hbar \omega \) in the same or in different symplectic bands are related back to valence shell matrix elements, which can be evaluated by standard shell model techniques.

#### 3.3.1 Derivation

The derivation of the desired recursion formula makes use of the fact that the symplectic basis states

\[ |\Phi[\Gamma_\sigma \Gamma_\rho \Gamma_\omega \alpha] \rangle \equiv \sum_{\alpha_n \alpha_\sigma} \langle \Gamma_n \alpha_n; \Gamma_\sigma \alpha_\sigma | \Gamma_\omega \alpha_\omega \rangle \rho \mathcal{P}^{(20)}_{\alpha} (A^{(20)}) | \Gamma_\sigma \alpha_\sigma \rangle \]  

(3.125)
are constructed by applying polynomials $P_{\alpha_n}^{\Gamma_n}(A^{(20)})$ of symmetrically coupled products of the symplectic raising operator $A^{(20)}$ with itself to $0\hbar\omega$ shell model configurations $|\Gamma_\sigma\alpha_\sigma\rangle$. The raising polynomials are defined recursively:

$$P_{\alpha_n}^{\Gamma_n}(A^{(20)}) = \sum_{\Gamma_n^0,\beta\alpha_n^0} \langle(20)|\beta;\Gamma_n^0\alpha_n^0|\Gamma_n\alpha_n\rangle X^{\Gamma_n}(\Gamma_n') A^{(20)}_{\beta} P_{\alpha_n^0}^{\Gamma_n^0}(A^{(20)})$$

with $P_{\alpha_n}^{\Gamma_n}(A^{(20)})$ adding a $2\hbar\omega$ excitation to the $N_n'$ excitation ($N_n' = n_1' + n_2' + n_3'$ and $\Gamma_n' = (n_1'n_2'n_3')$) that is created by acting with the operator $P_{\alpha_n}^{\Gamma_n}(A^{(20)})$ on the $0\hbar\omega$ configuration $|\Gamma_\sigma\alpha_\sigma\rangle$:

and the factor

$$X^{\Gamma_n}(\Gamma_n') = \frac{1}{n_1 + n_2 + n_3} (n_1n_2n_3||A^{(20)}||n_1'n_2'n_3')$$

is required to properly normalize the raising polynomials (for details see Subsection 2.2.2 and reference [95]). As discussed in Subsection 2.2.2, the basis states so constructed for each symplectic irrep $\Gamma_\sigma$, $|\Phi[\Gamma_\sigma\Gamma_n\rho\Gamma_\omega\alpha_\omega]\rangle$, need to be orthonormalized at each level of excitation $N_n$. This is achieved with the help of the $K$-matrix, which was introduced in Subsection 2.2.2:

$$|\Phi[\Gamma_\sigma\Gamma_n\rho\Gamma_\omega\alpha_\omega]\rangle = \sum_j \langle K(\Gamma_\sigma, \Gamma_\omega)|_{n, \rho, n, \rho} |\Gamma_\sigma\Gamma_n, \rho_j \Gamma_\omega\alpha_\omega\rangle . \quad (3.128)$$

As before, we will denote the orthonormal basis states by $|\Gamma_\sigma\Gamma_n\rho\Gamma_\omega\alpha_\omega\rangle$, without the letter $\Phi$. Using Equations 3.125 and 3.126 and the definition of the SU(3) Racah coefficients $U$ (see Appendix C.2), we can now express a symplectic basis state $|\Phi[\Gamma_\sigma\Gamma_n\rho\Gamma_\omega\alpha_\omega]\rangle$ of excitation $N_n\hbar\omega$ in terms of basis states $|\Phi[\Gamma_\sigma\Gamma_n'\rho'\Gamma_\omega'\alpha_\omega']\rangle$ of excitation $N_n'\hbar\omega$ with $N_n' = N_n - 2$:

$$|\Phi[\Gamma_\sigma\Gamma_n\rho\Gamma_\omega\alpha_\omega]\rangle = \sum_{\Gamma_n',\rho',\Gamma_\omega'} U[(20)|\Gamma_n'\Gamma_\omega\Gamma_\sigma;\Gamma_n-\rho\Gamma_\omega'\rho'|\langle(20)|\beta;\Gamma_\omega'\alpha_\omega'|\Gamma_\omega\alpha_\omega\rangle X^{\Gamma_n}(\Gamma_n') A^{(20)}_{\beta} |\Phi[\Gamma_\sigma\Gamma_n'\rho'\Gamma_\omega'\alpha_\omega']\rangle . \quad (3.129)$$
(This can be proved by decoupling the raising polynomial $P_{\Gamma_n}(A^{(20)})$ from the lowest weight state $|\Gamma_0, \alpha_0\rangle$, inserting the definition of $P_{\Gamma_n}(A^{(20)})$ given in Equation 3.126, coupling the raising polynomial $P_{\Gamma_n}(A^{(20)})$ to $|\Gamma_0, \alpha_0\rangle$, and making use of the property C.35 (see Appendix C.2) of the SU(3) Racah coefficient $U$.) An analogous expression can be obtained for the bra state $\langle \Phi|\Gamma_0, \Gamma_n, \rho, \Gamma_0, \alpha_0\rangle$.

The task at hand is to evaluate matrix elements of arbitrary one-body operators. Since any one-body operator can be expanded in terms of the fermion unit operators $\{a^\dagger_{(\gamma_0)\frac{1}{2}} \times \hat{a}_{(\gamma_0)\frac{1}{2}}\}$ by employing the formalism of second quantization (see Appendix B) and SU(3) coupling and recoupling techniques (see Appendix C) it suffices to evaluate the following matrix element:

$$\langle \Gamma_0, \Gamma_n, \rho, \Gamma_0, \alpha_0 \rangle \langle S_1 \Sigma_1 | \Gamma_0, \rho, \Gamma_0, \alpha_0 \rangle = \sum_{\Gamma, \rho, \omega_1} [\mathcal{K}^{-1}(\Gamma, \omega_1)]_{\Gamma_0, \rho, \Gamma_0, \rho_1} \times (\Gamma_0, \rho, \Gamma_0, \alpha_0 \rangle \langle S_2 \Sigma_2 | \Gamma_0, \rho, \Gamma_0, \alpha_0 \rangle = \sum_{\Gamma, \rho, \omega_1} [\mathcal{K}^{-1}(\Gamma, \omega_1)]_{\Gamma_0, \rho, \Gamma_0, \rho_1} \times (\Gamma_0, \rho, \Gamma_0, \alpha_0 \rangle \langle S_2 \Sigma_2 | \Gamma_0, \rho, \Gamma_0, \alpha_0 \rangle$$

(3.130)

Here we have introduced a simplified, but unambiguous, notation for the fermion creation and annihilation operators:

$$a^\dagger_{(\gamma_0)\frac{1}{2}} = a_{(\gamma_0)\frac{1}{2}}$$

$$\hat{a}_{(\gamma_0)\frac{1}{2}} = \hat{a}_{(\gamma_0)\frac{1}{2}}$$

(3.131)

and $S_1 \Sigma_1$ and $S_2 \Sigma_2$ denote the spin and spin projection of the ket and bra states, respectively.

Using the $\mathcal{K}$-matrix (see Equation 3.128) and applying the step-down procedure outlined above to the ket state $|\Phi|\Gamma_0, \Gamma_n, \rho, \Gamma_0, \alpha_0\rangle$, the matrix element can be written as:

$$(\Gamma_0, \Gamma_n, \rho, \Gamma_0, \alpha_0 \rangle \langle S_1 \Sigma_1 | \Gamma_0, \Gamma_n, \rho, \Gamma_0, \alpha_0 \rangle = \sum_{\Gamma, \rho, \omega_1} [\mathcal{K}^{-1}(\Gamma, \omega_1)]_{\Gamma_0, \rho, \Gamma_0, \rho_1} \times (\Gamma_0, \rho, \Gamma_0, \alpha_0 \rangle \langle S_2 \Sigma_2 | \Gamma_0, \rho, \Gamma_0, \alpha_0 \rangle = \sum_{\Gamma, \rho, \omega_1} [\mathcal{K}^{-1}(\Gamma, \omega_1)]_{\Gamma_0, \rho, \Gamma_0, \rho_1} \times (\Gamma_0, \rho, \Gamma_0, \alpha_0 \rangle \langle S_2 \Sigma_2 | \Gamma_0, \rho, \Gamma_0, \alpha_0 \rangle$$

(3.131)

and $S_1 \Sigma_1$ and $S_2 \Sigma_2$ denote the spin and spin projection of the ket and bra states, respectively.

Using the $\mathcal{K}$-matrix (see Equation 3.128) and applying the step-down procedure outlined above to the ket state $|\Phi|\Gamma_0, \Gamma_n, \rho, \Gamma_0, \alpha_0\rangle$, the matrix element can be written as:
\[ \times \left\{ \sum_{\alpha_{\uparrow \downarrow}} \langle \langle 20 \rangle \beta_1; \Gamma_{\omega_1} \alpha_{\omega_1} | \Gamma_{\omega_1} \alpha_{\omega_2} \rangle \langle \langle 20 \rangle \beta_1; \Gamma_{\omega_1} \alpha_{\omega_1} | \Gamma_{\omega_1} \alpha_{\omega_2} \rangle \right\}, \tag{3.132} \]

Note that the symplectic raising and lowering operators do not act on the spin part of the wave functions.

We now consider the term in parentheses and express the operator \( \{ a_\eta \times \tilde{a}_{\eta'} \}_{\alpha \Sigma} A_{\beta_1}^{(20)} \) as:

\[ \{ a_\eta \times \tilde{a}_{\eta'} \}_{\alpha \Sigma} A_{\beta_1}^{(20)} = A_{\beta_1}^{(20)} \{ a_\eta \times \tilde{a}_{\eta'} \}_{\alpha \Sigma} + \left[ \{ a_\eta \times \tilde{a}_{\eta'} \}_{\alpha \Sigma}, A_{\beta_1}^{(20)} \right]. \tag{3.133} \]

Recalling that the fermion realization of \( A^{(20)} \) is given by Equation 3.122, we obtain:

\[ \{ a_\eta \times \tilde{a}_{\eta'} \}_{\alpha \Sigma} A_{\beta_1}^{(20)} = A_{\beta_1}^{(20)} \{ a_\eta \times \tilde{a}_{\eta'} \}_{\alpha \Sigma} + \left( \frac{1}{4A} \sum_{\nu} \sqrt{\frac{1}{12}(\nu + 1)(\nu + 2)(\nu + 3)(\nu + 4)} \times \{ \{ a_{\nu + 2} \times \tilde{a}_{\nu} \}_{i_{11}m_{11}=0}, \{ a_\eta \times \tilde{a}_{\eta'} \}_{\alpha \Sigma} \right) \]

\[ \times \left[ \left\{ \{ a_\eta \times a_{\eta'} \}_{\Gamma_\nu s_{\nu}}, \{ \tilde{a}_{\nu} S_{\nu}, \tilde{a}_{\nu-1} \tilde{a}_{\nu-1} \}_{\Gamma_\nu s_{\nu} s_{\nu}}, \{ a_\eta \times a_{\eta'} \}_{\alpha \Sigma} \right\} \right] \times \left[ \left\{ \{ a_\eta \times a_{\eta'} \}_{\Gamma_\nu s_{\nu} s_{\nu}}, \{ \tilde{a}_{\nu} S_{\nu}, \tilde{a}_{\nu-1} \tilde{a}_{\nu-1} \}_{\Gamma_\nu s_{\nu} s_{\nu}}, \{ a_\eta \times a_{\eta'} \}_{\alpha \Sigma} \right\} \right]. \tag{3.134} \]

From Equation 3.134 it follows that the expression in parentheses in Equation 3.132 is comprised of three terms: \( \ldots = C_1 + (1 - \frac{1}{A}) C_2 + \frac{1}{4A} C_3 \), where \( A \) denotes the number of nucleons in the
system. The first of these is given by:

\[ C_1 \equiv \sum_{\alpha_1} \langle (20) \beta_1; \Gamma_{\omega_1} \alpha_1' | \Gamma_{\omega_1} \alpha_1 \rangle \times \langle \Gamma_{\alpha_1} \Gamma_n \rho_2 \Gamma_{\omega_2} \alpha_{\omega_2}; S_2 \Sigma_2 | A_{\beta_1}^{(20)} \{ a_1^+ \times \tilde{a}_{\gamma'} \} \Gamma_{\alpha_1} \Gamma_{\gamma'} \rho_1 \Gamma_{\omega_1} \alpha_1'; S_1 \Sigma_1 \rangle . \]  

(3.135)

To evaluate \( C_1 \), we insert a complete set of states:

\[ 1 = \sum_{\Gamma'' \Gamma'''} | \Gamma''_{\sigma'} \Gamma''_{\rho''} \Gamma''_{\omega''} | \langle \Gamma''_{\sigma''} \Gamma''_{\rho''} \Gamma''_{\omega''} ; S'' \Sigma'' \rangle \]  

between \( A_{\beta_1}^{(20)} \) and \( \{ a_1^+ \times \tilde{a}_{\gamma'} \} \Gamma_{\alpha_1} \Gamma_{\gamma'} \) and make use of the following relation:

\[ \langle \Gamma_{\sigma_2} \Gamma_n \rho_2 \Gamma_{\omega_2} \alpha_{\omega_2}; S_2 \Sigma_2 | A_{\beta_1}^{(20)} \{ a_1^+ \times \tilde{a}_{\gamma'} \} \Gamma_{\alpha_1} \Gamma_{\gamma'} \rho_1 \Gamma_{\omega_1} \alpha_1'; S_1 \Sigma_1 \rangle = \delta_{\Gamma_{\sigma_1} = \Gamma_{\sigma_2}} \delta_{N''_{\omega} N_{\omega} - 2 \delta_{S'' \Sigma''}} . \]  

(3.136)

between \( A_{\beta_1}^{(20)} \) and \( \{ a_1^+ \times \tilde{a}_{\gamma'} \} \Gamma_{\alpha_1} \Gamma_{\gamma'} \) and make use of the following relation:

\[ \langle \Gamma_{\sigma_2} \Gamma_n \rho_2 \Gamma_{\omega_2} \alpha_{\omega_2}; S_2 \Sigma_2 | A_{\beta_1}^{(20)} \{ a_1^+ \times \tilde{a}_{\gamma'} \} \Gamma_{\alpha_1} \Gamma_{\gamma'} \rho_1 \Gamma_{\omega_1} \alpha_1'; S_1 \Sigma_1 \rangle = \delta_{\Gamma_{\sigma_1} = \Gamma_{\sigma_2}} \delta_{N''_{\omega} N_{\omega} - 2 \delta_{S'' \Sigma''}} . \]  

(3.137)

The delta functions in this expression reflect the fact that the symplectic generator \( A^{(20)} \) only connects states within a symplectic irrep which have the same spin and differ by \( 2 \hbar \omega \) in their excitation. Note that these delta functions significantly restrict the sum over \( \Gamma''_{\sigma''} \Gamma''_{\rho''} \Gamma''_{\omega''} ; S'' \Sigma'' \) of the complete set of states. Only states which are constructed from the lowest weight irrep \( \Gamma''_{\sigma''} = \Gamma_{\sigma_1} \), by applying a raising polynomial \( \rho''_{\alpha''} (A^{(20)}) \) which is characterized by \( \Gamma_n'' = (n''_{1'}, n''_{2'}, n''_{3'}) \) with \( N''_{\omega} = n''_{1'} + n''_{2'} + n''_{3'} = n''_{1} + n''_{2} + n''_{3} - 2 \) (where \( \Gamma_{n_2} = (n_{1'}, n_{2'}, n_{3'}) \)) can yield non-vanishing contributions.

Employing the (generalized) Wigner-Eckart theorem (see Appendix C.3), and making use of the symmetry properties of the SU(3) coupling and recoupling coefficients (see Appendix C.2), we obtain the following expression for \( C_1 \):

[Insert equation here]
\[ C_1 = (-1)^{F + \Gamma_{\omega_1} + \Gamma_{\omega_2}} \sqrt{\frac{d(\Gamma_{\omega_1})}{d(20)}} \sum_{\Gamma_{\omega''}} \sqrt{d(\Gamma_{\omega''})} \langle \Gamma_{\sigma_3} \Gamma_{n_2} \rho_2 \Gamma_{\omega_2}; S_2 || \lambda^{(20)} || \Gamma_{\omega''} \Gamma_{\omega''}; S_2 \rangle \]

\[ \times \sum_{\rho_2} \langle \Gamma_{\omega_2} \Gamma_{n_2} \rho' \Gamma_{\omega''}; S_2 || \{ a_q \times \bar{a}_{\eta'} \}^{\Gamma_{\omega''}} || \Gamma_{\sigma_1} \Gamma_{\eta_1} \rho_1 \Gamma_{\omega_1}; S_1 \rangle_{\rho_2} \]

\[ \times \sum_{\rho_4} \Phi_{\rho_3 \rho_4} \langle \Gamma_{\omega_2} \Gamma_{\omega''}; \Gamma_{\omega_1} \Gamma_{\omega''}; \Gamma \rangle \sum_{\rho_6} U[\Gamma_{\omega_2} \Gamma_{\omega''}; \Gamma_{\omega_1} \Gamma_{\omega''}; (20) \Gamma_{\rho_5 \rho_6}] \]

\[ \times \langle \Gamma_{\omega_1} \alpha_{\omega_1}; \Gamma_{\alpha} | \Gamma_{\omega_2} \alpha_{\omega_2}; \rho_3 \rangle_{\rho_6} \langle S_1 \Sigma_1 \Sigma_2 | S_2 \Sigma_2 \rangle . \] (3.138)

The second term in Equation 3.134 takes the form:

\[ C_2 = (1 - \frac{1}{A}) \sum_{\nu} \sqrt{\frac{1}{12} (\nu + 1)(\nu + 2)(\nu + 3)(\nu + 4)} \]

\[ \times \sum_{\alpha \omega_1 \beta_1} \langle (20\beta_1; \Gamma_{\omega_1} \alpha_{\omega_1} | \Gamma_{\omega_1} \alpha_{\omega_1} \rangle \]

\[ \times \langle \Gamma_{\sigma_2} \Gamma_{n_2} \rho_2 \Gamma_{\omega_2}; S_2 \Sigma_2 || \{ a^t_{\nu+2} \times \bar{a}_{\nu} \}^{(20)\lambda=0} \rangle \langle \Gamma_{\sigma_1} \Gamma_{n_1} \rho_1 \Gamma_{\omega_1}; S_1 \Sigma_1 \rangle \] (3.139)

and can be evaluated by using the commutator of Equation 3.99. The delta functions in Equation 3.99 restrict the sum over \( \nu \) to two terms only, one term with \( \nu = \eta \) and one with \( \nu = \eta' - 2 \).

Again making use of the Wigner-Eckart theorem and the symmetry properties of the coupling coefficients, we obtain:

\[ C_2 = -(-1)^F \sqrt{\frac{1}{2} (\eta + 1)(\eta + 2)} \sqrt{\frac{d(\Gamma_{\omega_1})}{d(\Gamma)}} \]

\[ \times \sum_{\Gamma''_{\omega_1}} (-1)^{\Gamma''} \sqrt{d(\Gamma'')} U[(20)(\eta 0) \Gamma'' || (\eta'0); (\eta - 2, 0) \Gamma] \]

\[ \times \sum_{\rho_2} \langle \Gamma_{\sigma_2} \Gamma_{n_2} \rho_2 \Gamma_{\omega_2}; S_2 || \{ a^t_{\nu+2} \times \bar{a}_{\nu} \}^{\Gamma''} || \Gamma_{\sigma_1} \Gamma_{\eta_1} \rho_1 \Gamma_{\omega_1}; S_1 \rangle_{\rho_2} \]

\[ \times \sum_{\rho_4} U[\Gamma_{\omega_2} \Gamma''_{\omega_1}; (20); \Gamma_{\omega_1} \rho_3 \Gamma_{\omega_2}; \Gamma \Gamma_{\omega_2} \alpha_{\omega_2}; \Gamma \alpha | \Gamma_{\omega_2} \alpha_{\omega_2}; \rho_4 \]

\[ \times \langle S_1 \Sigma_1 \Sigma_2 | S_2 \Sigma_2 \rangle . \]
Note that the sum over $\Gamma''$ is restricted by coupling rules $(\eta - 2, 0) \times (0, \eta') \rightarrow \Gamma''$, $(20) \times \Gamma \rightarrow \Gamma''$, and $\Gamma_{\omega_1} \times \Gamma'' \rightarrow \Gamma_{\omega_2}$ in the first term and $(\eta 0) \times (0, \eta' - 2) \rightarrow \Gamma''$, $(\eta 0) \times (20) \rightarrow \Gamma''$, and $\Gamma_{\omega_1} \times \Gamma'' \rightarrow \Gamma_{\omega_2}$ in the second term.

The third term in Equation 3.134 originates from the two-body center-of-mass correction in the fermion realization of $A^{(20)}$ (Equation 3.123) and can be evaluated once the commutator

$$\left\{ \{a_{\eta} \times \tilde{a}_{\eta'}\}_{\alpha_2}^{\Gamma_{\omega_2}} \times \{a_{\eta} \times \tilde{a}_{\eta'}\}_{\alpha_2}^{\Gamma_{\omega_2}} \times \{a_{\eta'} \times \tilde{a}_{\eta'}\}_{\alpha_2}^{\Gamma_{\omega_2}} \times \{a_{\eta'} \times \tilde{a}_{\eta'}\}_{\alpha_2}^{\Gamma_{\omega_2}} \right\} \right|_{t=0, m=0} \}$$

is worked out. Upon doing so and employing the Wigner-Eckart theorem and coupling and re-coupling coefficients and their various symmetry and orthogonalization properties, it turns out that (while the commutator is nonzero) the contribution to the matrix element of Equation 3.130 vanishes identically: $C_3 = 0$.

We can now combine Equations 3.132, 3.138, 3.140, apply the Wigner-Eckart theorem to the matrix element under consideration:

$$(\Gamma_{\sigma_1} \Gamma_{n_2} \Gamma_{\omega_2} \Gamma_{\omega_2} \alpha_{\omega_2} \{a_{\eta} \times \tilde{a}_{\eta'}\}_{\alpha_2}^{\Gamma_{\omega_2}} \{a_{\eta} \times \tilde{a}_{\eta'}\}_{\alpha_2}^{\Gamma_{\omega_2}} \{a_{\eta'} \times \tilde{a}_{\eta'}\}_{\alpha_2}^{\Gamma_{\omega_2}} \{a_{\eta'} \times \tilde{a}_{\eta'}\}_{\alpha_2}^{\Gamma_{\omega_2}} \right| S_1 S_2 S_1 S_2 \}$$

$$\times \sum_{\rho_{12}} (\Gamma_{\sigma_1} \Gamma_{n_2} \Gamma_{\omega_2} \Gamma_{\omega_2} \{a_{\eta} \times \tilde{a}_{\eta'}\}_{\alpha_2}^{\Gamma_{\omega_2}} \{a_{\eta} \times \tilde{a}_{\eta'}\}_{\alpha_2}^{\Gamma_{\omega_2}} \{a_{\eta'} \times \tilde{a}_{\eta'}\}_{\alpha_2}^{\Gamma_{\omega_2}} \{a_{\eta'} \times \tilde{a}_{\eta'}\}_{\alpha_2}^{\Gamma_{\omega_2}} \right|_{\rho_{12}} \} (\Gamma_{\omega_1} \alpha_{\omega_1} ; \Gamma \alpha_{\omega_2} \alpha_{\omega_2} \right|_{\rho_{12}} \}$$

(3.142)
and utilize the orthonormality of the Clebsch-Gordan and Wigner coupling coefficients:

\[ \sum_{\omega_{1},\omega_{2}} \langle \Gamma_{\omega_{1}}\alpha_{\omega_{1}};\Gamma_{\omega_{2}}\alpha_{\omega_{2}} \rangle_{\rho_{12}} \langle \Gamma_{\omega_{1}}\alpha_{\omega_{1}};\Gamma_{\omega_{2}}'\alpha_{\omega_{2}}' \rangle_{\rho} = \delta_{\Gamma_{\omega_{1}}'\Gamma_{\omega_{2}}}\delta_{\rho_{12},\rho} \]  

(3.143)

to obtain the final expression, a recursion formula for triple-reduced matrix elements of the one-body unit operator \( \{ a_{\eta}^* \times \tilde{a}_{\eta'} \}^{PS} \):

\[ (\Gamma_{\alpha_1}\Gamma_{\alpha_2}\Gamma_{\omega_3}; S_2)\{ a_{\eta}^* \times \tilde{a}_{\eta'} \}^{PS} \{ a_{\eta_2} \times \tilde{a}_{\eta_2'} \}^{PS} \{ a_{\eta_3} \times \tilde{a}_{\eta_3'} \}^{PS} \]  

(3.144)
3.3.2 Testing the recursion relation

A stringent test of Equation 3.144 is given by the following: One can evaluate the matrix element

$$\langle \Gamma_3 \Gamma_3 \rho_2 \Gamma_\omega_2 ; S_2 \rangle \{ a_\eta^I \times \bar{a}_\eta \}^{F_S} \{ \Gamma_2 \Gamma_1 \rho_1 \Gamma_\omega_1 ; S_1 \} \rho$$  \hspace{1cm} (3.145)

by stepping down on the bra-side, and proceeding analogously to the derivation given above. The result is a recursion formula analogous to Equation 3.144. Alternatively, using the following relation in conjunction with Equation 3.144 yields an expression for the matrix element of Equation 3.145 which exactly equals the formula that is obtained by stepping down on the ket-side:

$$\langle \Gamma_3 \Gamma_3 \rho_2 \Gamma_\omega_2 ; S_2 \rangle \{ a_\eta^I \times \bar{a}_\eta \}^{F_S} \{ \Gamma_2 \Gamma_1 \rho_1 \Gamma_\omega_1 ; S_1 \} \rho$$

$$= (-1)^{\eta + \eta'} - \gamma_{\omega_1 + \omega_2 + S_1 + S_2} \frac{d(\Gamma_{\omega_1})}{d(\Gamma_{\omega_2})} \sqrt{\frac{2S_1 + 1}{2S_2 + 1}}$$

$$\times \langle \Gamma_2 \Gamma_1 \rho_1 \Gamma_\omega_1 ; S_1 \rangle \{ a_\eta^I \times \bar{a}_\eta \}^{F_S} \{ \Gamma_3 \Gamma_3 \rho_2 \Gamma_\omega_2 ; S_2 \} \rho \hspace{1cm} (3.146)$$

Another very reliable test is given by encoding the recursion formula and using the one-body matrix elements so obtained to calculate expectation values of the particle number operator \( \hat{N} \) and the symplectic raising and lowering operators \( A^{(20)} \) and \( B^{(02)} \), as well as the expectation values of \( C^{(11)} \) for the valence shell. For \( A \rightarrow \infty \) we find perfect agreement with the matrix elements of \( A^{(20)} \) and \( B^{(02)} \) as evaluated by means of a code that is based on the vector coherent state method outlined in Subsections 3.1.6 and 3.1.7, and also with the matrix elements of \( \hat{N} \) and \( C^{(11)} \) which can be evaluated analytically.

3.3.3 Some special relations for the SU(3) Racah coupling coefficients

We can now employ the recursion formula of Equation 3.144 to derive a recursion relation for \( A^{(20)} \) for the special case of a large number of nucleons in the system (\( A \rightarrow \infty \)). Upon doing so and comparing the result to the formula that was derived by G. Rosensteel [138] using a step-down procedure analogous to the one outlined above, we find exact agreement provided the following
relations hold:

\[(\eta + 3)(\eta + 4) \ U[[02](\eta + 2, 0)(22)(0\eta); (\eta\theta)(20)] \]
\[= (\eta - 1)\eta \ U[[20](\eta - 2, 0)(22)(0\eta); (\eta\theta)(02)]. \quad (3.147)\]

\[(\eta + 3)(\eta + 4) \ U[[02](\eta + 2, 0)(11)(0\eta); (\eta\theta)(20)] \]
\[\ - (\eta - 1)\eta \ U[[20](\eta - 2, 0)(11)(0\eta); (\eta\theta)(02)] \]
\[= \sqrt{10\eta(\eta + 3)} . \quad (3.148)\]

\[U[[02](\eta + 2, 0)(00)(0\eta); (\eta\theta)(20)] \]
\[= \ U[[20](\eta - 2, 0)(00)(0\eta); (\eta\theta)(02)] = 1 . \quad (3.149)\]

While Equation 3.149 is given in [98], the other two relations. Equation 3.147 and Equation 3.148 are new and may prove valuable for analytic work that involves SU(3) Racah coefficients.

Although the outlined deduction of these relations provides a complete proof (and a numeric check of the above relations for \( \eta = 0.1 \ldots .25 \) has shown that they hold), it would be desirable to find an alternative, simpler proof, such as an inductive derivation. This remains to be done.
Chapter 4

Electron Scattering

In this chapter we will summarize the formalism that is usually employed to extract nuclear structure information from electron scattering experiments. We will discuss previous efforts to describe electron scattering results in the framework of the symplectic model and its various submodels. In particular, the generator function method, the boson second quantization formalism, and the fermion second quantization approach will be considered. We then employ the fermion second quantization formalism in conjunction with our findings from Section 3.3 to evaluate electron scattering form factors for $^{24}\text{Mg}$ and discuss the results.

4.1 Electron scattering as a probe of nuclear structure

The electron is a probe which is uniquely well suited to reveal many aspects of nuclear structure [37, 167, 39, 40, 100, 38, 120, 78, 174]. Its interaction with the electromagnetic charge and current density of the target nucleus via the electromagnetic field is well understood and described by an exact theory, quantum electrodynamics. Moreover, the electromagnetic force is relatively weak: the coupling constant of $\alpha = \frac{1}{137}$ is much smaller than the characteristic strength of the nuclear force which is responsible for most of the properties of the nucleus. Therefore, the electron hardly perturbs the structure of the nucleus under investigation. (As a consequence, the scattering cross
section can be immediately related to the structure of the target itself, and nuclear properties can be extracted from scattering data in a quantitative way.) The relative weakness of the electromagnetic interaction makes it furthermore possible safely to ignore most complications associated with multiple-step terms in a transition between the target and a final nuclear state and to describe electron scattering with sufficient accuracy in the first Born or one-photon exchange approximation, which is expected to be a good approximation for small $Z\alpha$. The only terms not known a priori in this description are the matrix elements of the nuclear charge and current operators between the initial and final nuclear wave functions, the so-called transition charge and current densities.

A second significant advantage of using electrons as a probe of nuclear structure is the opportunity to vary independently the momentum and energy transferred to the target: For fixed nuclear excitation energy $\omega$, one can vary the three-momentum $q = |\mathbf{q}|$ transferred by the scattered electron and thus map out the Fourier transforms of the transition charge and current densities. The larger the momentum transfer, the finer the details of the densities that can be probed. Upon inverting the transforms, the microscopic spatial distributions of the charge densities as well as the nuclear convection and magnetization current densities are obtained. This is certainly a source of tremendously rich and unique information on the structure of nuclei. Our best knowledge of the sizes and shapes of nuclear charge distributions comes from electron scattering. By varying $\omega$, the energy transferred to the target (at fixed momentum transfer), one obtains an excitation profile of the nucleus. Varying $\omega$ at low momentum transfer, one gains information similar to that obtained in photonuclear reactions, and at high values of $q$, it becomes possible to study new phenomena, such as high spin states and states of magnetic character.

Since electrons are point particles, they offer superb spatial resolution that can be adjusted to the scale of the process under investigation. This scale is related to the momentum transfer $q$. Incident electron energies of 500 MeV, for example, result in spatial resolutions of the order of 0.5 fm, and are thus ideally suited for the study of nuclear charge and current distributions in nuclei. Higher energies, such as those currently available at the Thomas Jefferson Lab (formerly CEBAF
for Continuous Electron Beam Accelerator Facility) in Newport News, Virginia, have a spatial resolution sufficient to probe the quark structure of the nucleons.

Many experimental difficulties associated with electron scattering had to be overcome in order to exploit the potential of this probe of nuclear structure. In particular, accelerators that provide electrons of several hundred MeV to a few GeV are required in order to achieve a short wavelength for the electron despite its small mass. High intensity beams (of order 50mA and more) are imperative to overcome small cross sections (form factors of heavy nuclei decrease rapidly as a function of momentum transfer), and excellent energy resolution (\( \frac{\Delta E}{E} \leq 10^{-4} \)) is needed to obtain the absolute energy resolution \( \Delta E \) imposed by nuclear level spacings. Despite the difficulties, many experiments on the scattering of electrons off nuclei have been carried out, yielding rich information on nuclear structure, ranging from collective features to single-particle properties and subnuclear aspects.

Electron scattering experiments do not only provide insight into the effects of the strong interaction. The information obtained from electron scattering can be used to eliminate many of the uncertainties associated with the nuclear many-body problem and provide a relatively reliable nuclear laboratory in which to study the less well known weak interaction.

In order to achieve a coherent theoretical description of electron scattering, it is necessary to employ a microscopic theory which successfully accounts for a variety of aspects of nuclear structure, such as static electromagnetic moments, collective excitations, beta decay, etc. In a complementary sense, electron scattering experiments provide crucial tests for the applicability and limitations of modern nuclear models. The capability of explaining such unambiguous and fundamental results as those embodied in electron scattering data are an excellent criterion by which to evaluate the success of a microscopic theory of nuclear structure.
4.2 Quantities measured in electron scattering studies

Electron scattering is most conveniently approached within the framework of the “plane-wave” first Born approximation (PWBA). In this description a plane-wave electron is scattered through an angle $\Theta$ from an initial state of four-momentum $k_\mu = (k, \epsilon)$ to a final state $k'_\mu = (k', \epsilon')$ \(^1\). In this process, a single virtual photon with four-momentum $q_\mu = (q, \omega)$ is exchanged with the nuclear target. Conservation of four-momentum implies that $q_\mu = k_\mu - k'_\mu$ holds, that is, there is energy transfer $\omega = \epsilon - \epsilon'$, and three-momentum transfer $q = |\vec{q}| = \sqrt{k^2 + k'^2 - 2k \cdot k' \cos \Theta}$.

In a general scattering process, the target nucleus may absorb the energy $\omega$ and momentum $q$ transferred from the electron and make a transition from the initial ground state $|i\rangle$ to some (in general excited) final state $|f\rangle$. If $\omega = 0$, that is, when $|f\rangle$ as well as $|i\rangle$ refers to the nucleus in the ground state (recoiling with momentum $\vec{q}$), one calls the process elastic electron scattering. If $\omega \neq 0$, that is, when $|f\rangle$ denotes some excited nuclear state, one speaks about inelastic electron scattering. At the energies of interest (hundreds of MeV) the electron mass can be neglected, and one can write:

\begin{align*}
q &= \sqrt{\omega^2 + 4\epsilon\epsilon' \sin^2 \left(\frac{\Theta}{2}\right)}, \\
q'^2 &= q^2 - \omega^2 = 4\epsilon\epsilon' \sin^2 \left(\frac{\Theta}{2}\right). \quad (4.1)
\end{align*}

Invoking Lorentz invariance, parity conservation, and current conservation, deForest and Walecka [37] show that the differential cross section for electron scattering from an unpolarized target (in the one-photon exchange approximation) takes the following (simple) form:

\begin{equation}
\frac{d\sigma}{d\Omega} = \frac{4\pi}{M_T} \sigma_M \left| f_{\text{rec}}^{-1} F^2(q, \Theta) \right|. \quad (4.2)
\end{equation}

\(^1\) We use four-vectors $a_\mu = (a, a_0)$ with a metric $ab = a \cdot \vec{b} - a_0 b_0$. 

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where $\sigma_M$ is the Mott cross section

$$\sigma_M = \left( \frac{\alpha \cos\left(\frac{\Theta}{2}\right)}{2\sin^2\left(\frac{\Theta}{2}\right)} \right)^2 \tag{4.3}$$

for scattering an electron from a point charge. The recoil correction is given by

$$f_{rec} = 1 + \frac{2e}{M_T \sin^2\left(\frac{\Theta}{2}\right)} \tag{4.4}$$

and $M_T$ is the initial target mass. For all but the lightest targets at high momentum transfer $q$ the recoil factor becomes $f_{rec} \approx 1$.

The electron scattering form factor has a longitudinal component, $F_L^2(q)$, and a transverse component, $F_T^2(q)$:

$$F^2(q, \Theta) = \left( \frac{q \mu}{q} \right)^4 F_L^2(q) + \left[ \frac{1}{2} \left( \frac{q \mu}{q} \right)^2 + \tan^2\left(\frac{\Theta}{2}\right) \right] F_T^2(q) \tag{4.5}$$

The longitudinal and transverse form factors $F_L^2(q)$ and $F_T^2(q)$ (which are sometimes referred to as dynamic structure functions or nuclear response surfaces) contain all the information on the electromagnetic charge and current density distribution of the target nucleus. They depend only on $q$ and $\omega$, but not on $\Theta$, and may thus be separated by fixing $q$ and $\omega$ and varying $\Theta$ (Rosenbluth separation) \(^2\), or by working at $\Theta = 180^\circ$ where only the transverse form factor contributes.

In [37] deForest and Walecka derive the multipole expansion of the cross section for electron scattering to discrete nuclear levels. Assuming that the electron is scattered in the electromagnetic potential of the nucleus, they show how the form factors are related to the matrix elements of the nuclear (electromagnetic) four-current density operator

$$J_\mu(\vec{r}) = (\vec{j}(\vec{r}), \rho(\vec{r})) \tag{4.6}$$

\(^2\)A Rosenbluth plot of $F^2(q, \Theta)$ versus the factor in square brackets in Equation 4.5 yields a straight line with intercept $F_L^2(q)$ and slope $F_T^2(q)$. 

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where $\rho(\vec{r})$ is the charge-density operator and $\vec{J}(\vec{r})$ denotes the three-current density operator

$$\vec{J}(\vec{r}) = \vec{J}^c(\vec{r}) + \vec{J}^m(\vec{r}), \quad (4.7)$$

which is comprised of a convection current $\vec{J}^c(\vec{r})$ and a magnetization current $\vec{J}^m(\vec{r}) = \nabla \times \vec{\mu}(\vec{r})$ with $\vec{\mu}(\vec{r})$ denoting the nuclear magnetization density.

It is furthermore assumed that in the scattering process the nucleus makes a transition from one state of definite angular momentum to another. It then becomes expedient to expand the Fourier transforms of the components of the current-density operator.

$$J_\mu(\vec{q}) = \int e^{i\vec{q}\cdot\vec{r}} J_\mu(\vec{r}) d\vec{r}, \quad (4.8)$$

in a multipole series. The Fourier transform of the charge-density operator, $\rho(\vec{q})$, for example, can be expressed in terms of Coulomb multipole operators.

$$\hat{M}_{LM}^C(q) \equiv \int j_L(\vec{q}r) Y_{LM}(\hat{r}) \rho(\vec{r}) d\vec{r}, \quad (4.9)$$

where $j_L$ is a spherical Bessel function and the $Y_{LM}$ denote spherical harmonics.

The three-vector current density operator may be written in terms of two "tranverse" components, which are orthogonal to the momentum transfer $\vec{q}$, and one "longitudinal" component along the direction of $\vec{q}$. Using current conservation, the latter can be shown to be proportional to the charge-density operator, and can thus be eliminated. The two transverse components may be expressed in terms of the electric and magnetic multipole operators,

$$\hat{T}^E_{LM}(q) \equiv \int \frac{1}{q} [\nabla \times \{j_L(\vec{q}r) Y_{LM}^{L1}(\hat{r})\}] \cdot \vec{J}(\vec{r}) d^3r$$

$$\hat{T}^{mag}_{LM}(q) \equiv \int \{j_L(\vec{q}r) Y_{LM}^{L1}(\hat{r})\} \cdot \vec{J}(\vec{r}) d^3r \quad (4.10)$$

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where the symbols $Y^{LSJ}_M$ denote vector spherical harmonics (for details about the definition and properties of the vector spherical harmonics, see [169]). Note that in general both electric and magnetic transverse multipoles have convection and magnetization current contributions.

Making use of the multipole analysis of the electromagnetic current operator $J_μ$ and of the Wigner-Eckart theorem (see Appendix C.3.2), deForest and Walecka show that the differential cross section can be written in terms of these multipole operators [37]: the terms $F^2_\ell(q)$ and $F^2_T(q)$ in Equation 4.5 are simply given by:

$$
F^2_\ell(q) = \frac{4\pi}{2^2} \frac{2J_\ell + 1}{2J_\ell + 1} \sum_{J=0}^{\infty} |\langle J_\ell | M^{Coul}(q) | J_I \rangle|^2,
$$

$$
F^2_T(q) = \frac{4\pi}{2^2} \frac{2J_\ell + 1}{2J_\ell + 1} \sum_{J=1}^{\infty} \left\{ |\langle J_\ell | \tilde{M}^{el}(q) | J_I \rangle|^2 + |\langle J_\ell | \tilde{M}^{mag}(q) | J_I \rangle|^2 \right\}. \quad (4.11)
$$

Therefore the cross section may be expressed directly in terms of Coulomb, electric, and magnetic multipole moments. Time reversal invariance and parity conservation imply that Coulomb and electric multipoles have parity $(-1)^L$ and magnetic multipoles have parity $(-1)^{L+1}$.

**4.3 Electron scattering and the symplectic shell model**

A microscopic theory for deformed nuclei, which takes proper account of the exclusion principle as well as of intershell couplings, has been described in Chapter 2: the symplectic shell model for light nuclei, developed by Rosensteel and Rowe [144, 145, 149], and its pseudo-symplectic extension for heavy nuclei, put forward by Castanos et al. [27]. In the context of electron scattering, these models provide a multi-shell realization of the nuclear shell model which then allows for a careful study of the relevance of multi-shell correlations. Once the influence of these correlations is elucidated, limits can be placed on the importance of other contributions, as, for example, meson exchange currents, and the need for additional corrections, such as relativistic effects, Coulomb and dispersive corrections, can be investigated.
Furthermore, the symplectic model takes into account irrotational as well as vorticity degrees of freedom [149] and therefore has the potential to describe a range of possible current flows, including rigid-rotational and irrotational flows. Hence it is of interest to see whether the symplectic model yields form factors that are in better agreement with the data than those predicted by alternative models.

Of course, it is not possible to address all these points in a satisfactory manner within the limitations of a dissertation. Our goal here is to demonstrate the validity of our approach and its value for addressing these questions. We hope that the formalism and tools developed here will pave the way for further and more detailed study of the above-mentioned questions and many other related problems.

Most of the work in the area of applying the symplectic model to electron scattering has been done by David Rowe and his group in Toronto. There are mainly two strategies that are followed by the Toronto group: The development of a generator function method and the implementation of boson second quantization techniques. An alternative approach, which makes use of a fermion second quantization formalism, has been developed by Rochford and Draayer. All three of these approaches fit in the framework of the symplectic model, although none so far has resulted in a full symplectic multi-$\hbar\omega$ calculation. In what follows, we will briefly summarize their findings.

### 4.3.1 Generator function method

In reference [170], Vassanji and Rowe lay down the formalism for applying a previously initiated method, the generator function method, to the Sp(3,R) model. They employ this formalism to evaluate Coulomb form factors for $^{20}$Ne in the SU(3), Sp(1,R), and SO(3)×D approximations of the full symplectic model (see Section 2.2). Their results show that for the $0^+_1 \rightarrow 0^+_1$ transition all three submodels of Sp(3,R) yield good agreement with the data up to the first minimum, but fall short thereafter. The $0^+_1 \rightarrow 2^+_1$ inelastic form factor turns out to be too small in the SU(3) model, but reaches close to the experimentally observed maximum value in the Sp(1,R) and SO(3)×D models.
In reference [22], the same formalism is used to evaluate the transverse form factor for the $0_1^+ \rightarrow 2_1^+$ and $0_1^+ \rightarrow 2_2^+$ transitions in $^{24}\text{Mg}$. The calculations are performed in the $\text{SO}(3) \times D$ submodel of $\text{Sp}(3,\mathbb{R})$ and results for the $0_1^+ \rightarrow 2_1^+$ transition show improvements over predictions obtained in $\text{SU}(3)$ calculations which were restricted to the valence shell. The authors find that the inclusion of higher shells does not simply renormalize the valence shell results, but rather displaces the peak of the transverse form factor to smaller momentum transfer values, in better agreement with the available experimental data. Comparison of their calculated $0_1^+ \rightarrow 2_2^+$ transverse form factor with experiment (which is difficult, since the data do not resolve the $2_2^+$ and $4_1^+$ states) is reasonable, but inconclusive with respect to a possible improvement over $\text{SU}(3)$ valence shell calculations.

In [4] Avancini and de Passos employ the generator function method developed by Rowe and Vassanji to evaluate the longitudinal form factors for the states of the ground band in $^{12}\text{C}$. They restrict their calculations to the $\text{Sp}(1,\mathbb{R})$ submodel of $\text{Sp}(3,\mathbb{R})$ and find that the deformation-driving multi-shell correlations incorporated in the $\text{Sp}(1,\mathbb{R})$ model are essential for reproducing the scattering data at low momentum transfer $q$. Their model, however, gives a poor description of the high-$q$ data.

### 4.3.2 Boson second quantization formalism

In references [36, 172, 171], Vassanji and Rowe develop boson second quantization techniques for the calculation of electron scattering form factors. They show that the charge and current density multipole operators, when restricted to a harmonic-oscillator shell-model space, can be written as squared matrix elements of simple operators involving a few one-body operators, multiplied by fixed functions of the momentum transfer $q$. In [170] they employ their formalism to evaluate longitudinal form factors for $^{20}\text{Ne}$. Both the elastic $0_1^+ \rightarrow 0_1^+$ and the inelastic $0_1^+ \rightarrow 2_1^+$ form factors are in reasonable agreement with experiment, but they fall short in describing the second and first experimental maximum, respectively.
In [172] Vassanji and Rowe conclude that dominant corrections to a single-irrep SU(3) calculation will come from admixtures of higher shell configurations, rather than from other valence shell irreps, and in [171] the same authors outline a method for extending the boson second quantization formalism to include higher shells in order to account for core polarization effects. It would be of great interest to see the results of such an extension.

4.3.3 Fermion second quantization approach

An alternative approach, followed by Rochford and Draayer [135], expresses both the states and the operators in fermion second quantized form. Starting from the fermion second quantized expressions for the charge and current density multipole operators, the authors derive the general SU(3) tensorial expansion of these one-body multipole operators. This procedure is necessary, since practical symplectic shell model calculations are usually carried out in a SU(3) symmetry basis.

They obtain expressions for the longitudinal form factor, $F^L_{i\rightarrow f}(q)$, which involves the charge density multipole operator, $\hat{M}^{C\mu}_{LM}(q)$, and for the transverse form factor $F^T_{i\rightarrow f}(q)$, which involves the transverse electric and magnetic multipoles of the three-current density $\vec{j}(\vec{r})$, where the latter can be decomposed into a convection current density, $\vec{j}^c(\vec{r})$, and a magnetization current density, $\vec{j}^m(\vec{r})$. The final expressions are exact representations of the density multipoles, extend over all shells, and are tailored for symplectic shell model applications. In order to obtain matrix elements of these operators, one has to evaluate a set of coefficients, for which analytical formulae exist, as well as matrix elements of arbitrary one-body operators of the form $\{a^\dagger_{\eta_1} \times a_{\eta_2}\}^{(1\mu)S/J:T}_{\lambda\nu L M_L M_J M_T}$.  

At the time when Rochford and Draayer developed the above formalism, matrix elements of arbitrary one-body operators were only available for the special case $\eta_1 = \eta_2$, that is, for a single-major oscillator shell calculation. In that case, the symplectic model reduces to the Elliott SU(3) submodel. In [135] Rochford and Draayer perform such SU(3) shell model calculations and formulate form factor predictions for $^{20}$Ne, $^{22}$Ne, and $^{24}$Mg using both single-irrep and multi-irrep Hilbert spaces. They find that valence shell irreps mixing influences Elliott SU(3) model...
predictions only moderately for all the elastic and most of the inelastic longitudinal form factors of ds-shell nuclei. They thus predict that single-irrep symplectic model calculations should give a good approximation to complete mixed-irrep calculations for the longitudinal form factors. A tensor analysis of the multipole operators leads them to expect that multi-shell correlations up to about $6\hbar\omega$ will provide significant contributions to longitudinal and transverse form factors. In order to demonstrate the effects of including multi-$\hbar\omega$ excited states in the symplectic model space, we will compare our results for $^{24}\text{Mg}$ with the form factors obtained by Rochford and Draayer.

4.4 Electron scattering predictions in the symplectic model

The work of Rochford and Draayer [135] demonstrates the basic validity of the fermion second quantization approach to electron scattering and, at the same time, underscores the need for an extension to the full symplectic model which includes multi-shell correlations.

Given the formalism developed in this dissertation, in particular the recursion formula of Section 3.3, we are now in a position to calculate the required symplectic matrix elements and thus evaluate form factors in the full $N\hbar\omega$ symplectic space. We will do this for the case of $^{24}\text{Mg}$, a well-deformed nucleus with a distinctly rotational spectrum and well-determined static properties. As has been shown previously (see reference [143] and our discussion in Subsection 2.2.5) the symplectic model is able to reproduce both the energy spectrum and the reduced transition probabilities of $^{24}\text{Mg}$ very well.

For our purposes it is more convenient to perform the calculations in a proton-neutron formalism, rather than in the isospin formalism employed by Rochford and Draayer. Hence we need to recast the expressions given in [135]. The derivations involved are basically the same as Rochford and Draayer's. Therefore, details will be omitted here. We will restrict ourselves to summarizing our assumptions and giving the final results.
4.4.1 Longitudinal and transverse form factors

The longitudinal and transverse electron scattering form factors for nuclear transitions from an initial state of angular momentum $J_i$ to a final state of angular momentum $J_f$ are given in the first-order plane-wave Born approximation by (see also Section 4.2):

\[
\begin{align*}
F_{i \rightarrow f}^L(q) &= \frac{4\pi(2J_f + 1)}{2^2(2J_i + 1)} \sum_{L=0}^{\infty} \left| \langle J_f | \hat{M}_L(q) | J_i \rangle \right|^2, \\
F_{i \rightarrow f}^T(q) &= \frac{4\pi(2J_f + 1)}{2^2(2J_i + 1)} \sum_{L=0}^{\infty} \left\{ \left| \langle J_f | \hat{T}_L^d(q) | J_i \rangle \right|^2 + \left| \langle J_f | \hat{T}_L^{mag}(q) | J_i \rangle \right|^2 \right\}. \quad (4.12)
\end{align*}
\]

Note that the reduced matrix element convention differs from that of reference [135] by a factor of $\sqrt{2J_f + 1}$ (for details refer to the Appendix C.2), and the overall factor $\frac{4\pi}{2^2}$ ensures that $F_{i \rightarrow f}^L(q) \rightarrow 1$ as the momentum transfer $q$ approaches zero.

The charge density multipole operator $\hat{M}_{LM}(q)$ has been defined in Equation 4.9 as:

\[
\hat{M}_{LM}(q) = \int j_L(qr) \gamma^L_M(\hat{r}) \rho(\hat{r}) d^3 r, \quad (4.13)
\]

and the electric and magnetic transverse multipole operators are given by Equation 4.10:

\[
\begin{align*}
\hat{T}_L^d(q) &= \int \frac{1}{q} \{ \nabla \times [j_L(qr) \gamma^L_{LM}(\hat{r})] \} \cdot \vec{j}(\hat{r}) d^3 r, \\
\hat{T}_L^{mag}(q) &= \int [j_L(qr) \gamma^L_{LM}(\hat{r})] \cdot \vec{j}(\hat{r}) d^3 r. \quad (4.14)
\end{align*}
\]

In the standard shell-model picture, the nucleons are taken to be point particles. The charge density is thus given by

\[
\rho(\hat{r}) = \sum_{s=1}^{A} \frac{1 - \frac{1}{2}}{2} \delta(\hat{r} - \hat{r}_s). \quad (4.15)
\]

and the convection $\vec{j}^c$ and magnetization $\vec{j}^m = \nabla \times \vec{\mu}$ contributions to the current density $\vec{j}$ are
given via:

\[
\begin{align*}
\mathbf{j}^e(\mathbf{r}) &= \frac{1}{2mc} \sum_{s=1}^{A} \left( \frac{1 - \hat{t}_3(s)}{2} \right) (\mathbf{p}_s \delta(\mathbf{r} - \mathbf{r}_s) + \delta(\mathbf{r} - \mathbf{r}_s) \mathbf{p}_s) \\
\hat{\mu}(\mathbf{r}) &= \frac{\hbar}{2mc} \sum_{s=1}^{A} \hat{\mu}(s) \delta(\mathbf{r} - \mathbf{r}_s) \hat{\sigma}_s = \frac{\hbar}{4mc} \sum_{s=1}^{A} (\mu_+ + \mu_- \hat{t}_3(s)) \delta(\mathbf{r} - \mathbf{r}_s) \hat{\sigma}_s .
\end{align*}
\]  

(4.16)

where \( \hat{t}_3(s) \) refers to the isospin-projection of the \( s \)-th particle and \( c(s) = \frac{1}{2}(1 - \hat{t}_3(s)) = 1(0) \) for protons (neutrons); \( m \) is the nucleon mass, \( \hat{\sigma} \) denotes the Pauli spin operator, and \( \mu_{\pm} = \frac{1}{2}(\mu_{\pi} \mp \mu_{\nu}) \), where \( \mu_{\pi} = 2.79 \) (\( \mu_{\nu} = -1.91 \)) is the magnetic moment of the proton (neutron) in nuclear magnetons.

With the assumption that the charge density distribution follows the mass density distribution, we can write:

\[
\hat{\rho}(\mathbf{r}) = \frac{Z}{A} \sum_{s=1}^{A} \delta(\mathbf{r} - \mathbf{r}_s) .
\]  

(4.17)

and analogously for the convection and magnetization contributions to the current density:

\[
\begin{align*}
\mathbf{j}^c(\mathbf{r}) &= \frac{1}{2mc} \frac{Z}{A} \sum_{s=1}^{A} (\mathbf{p}_s \delta(\mathbf{r} - \mathbf{r}_s) + \delta(\mathbf{r} - \mathbf{r}_s) \mathbf{p}_s) , \\
\hat{\mu}(\mathbf{r}) &= \frac{\hbar}{4mc} \sum_{s=1}^{A} \frac{1}{A} (Z \mu_+ + N \mu_-) \delta(\mathbf{r} - \mathbf{r}_s) \hat{\sigma}_s .
\end{align*}
\]  

(4.18)

Using the formalism of second quantization (see Appendix B) one can express the electron scattering multipole operators in terms of fermion creation and annihilation operators. Following the steps given in [135], one arrives at the SU(3) tensorial expansion for the Coulomb multipole:

\[
\tilde{M}_{LM}(q) = \frac{Z}{A} \sum_{n_1 n_2} C_{(\lambda \mu)\lambda L \eta_1 \eta_2} (b q) \{ a_{n_1}^i \times \tilde{a}_{n_2}^j \}^{(\lambda \mu)S=0}_{\xi LM \Sigma=0} .
\]  

(4.19)

The SU(3) tensorial expansions for the convection and magnetization contributions to the electric

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current multipole operator are given by:

\[
\hat{T}_{LM}^{el,c}(q) = \frac{\hbar Z}{mcA} \sum_{\ell \mu \lambda} C_{(\ell \mu \lambda) \subseteq L} \{ a_{\ell \mu}^\dagger \times \bar{a}_{\mu} \}^{(\lambda \mu) S=0},
\]

\[
\hat{T}_{LM}^{el,m}(q) = \frac{\hbar}{2mcA} (Z\mu_+ + N\mu_-) \sum_{\ell \mu \lambda} C_{(\ell \mu \lambda) \subseteq L} \{ a_{\ell \mu}^\dagger \times \bar{a}_{\mu} \}^{(\lambda \mu) S=1},
\]

and the corresponding contributions to the magnetic current multipole operator can be expressed as:

\[
\hat{T}_{LM}^{imag,c}(q) = -\frac{i\hbar Z}{mcA} \sum_{\ell \mu \lambda} C_{(\ell \mu \lambda) \subseteq L} \{ a_{\ell \mu}^\dagger \times \bar{a}_{\mu} \}^{(\lambda \mu) S=0},
\]

\[
\hat{T}_{LM}^{imag,m}(q) = -\frac{i\hbar}{2mcA} (Z\mu_+ + N\mu_-) \sum_{\ell \mu \lambda} \left\{ \sqrt{\frac{L+1}{L+1}} C_{(\ell \mu \lambda) \subseteq L-1} \{ a_{\ell \mu}^\dagger \times \bar{a}_{\mu} \}^{(\lambda \mu) S=1}

- \sqrt{\frac{L}{L+1}} C_{(\ell \mu \lambda) \subseteq L+1} \{ a_{\ell \mu}^\dagger \times \bar{a}_{\mu} \}^{(\lambda \mu) S=1} \right\}.
\]

The coefficients \( C_{(\ell \mu \lambda) \subseteq L} \{ a_{\ell \mu}^\dagger \times \bar{a}_{\mu} \}^{(\lambda \mu) S=0} \) involve the oscillator size parameter \( b \) since the shell model wave functions are used in dimensionless units. The coefficients are given by:

\[
C_{(\ell \mu \lambda) \subseteq L} \{ a_{\ell \mu}^\dagger \times \bar{a}_{\mu} \}^{(\lambda \mu) S=0} = \sqrt{\frac{2d(\eta_0)}{d(\lambda \mu)}} \Theta((\lambda \mu) \subseteq L \eta_1; b q),
\]

\[
C_{(\ell \mu \lambda) \subseteq L} \{ a_{\ell \mu}^\dagger \times \bar{a}_{\mu} \}^{(\lambda \mu) S=1} = \frac{1}{b} \sqrt{\frac{d(\eta_0)}{d(\lambda \mu)}} \sum_{(\lambda' \mu')} (-1)^{\lambda'+\lambda'\mu'-\lambda}\mu

\times \left\{ \Theta((\lambda' \mu') \kappa' L \eta_1 \eta_2 + 1; b q)((\lambda' \mu') \kappa' L; (10)1 || (\lambda \mu) \kappa J)

- \Theta((\lambda' \mu') \kappa' L \eta_1 \eta_2 - 1; b q)((\lambda' \mu') \kappa' L; (01)1 || (\lambda \mu) \kappa J)

- \Theta((\lambda' \mu') \kappa' L \eta_1 \eta_2; b q)((\lambda' \mu') \kappa' L; (\eta_2 - 1)0 || (\lambda \mu) \kappa J)

\right\}.
\]
\[
C_{(\lambda \mu) \kappa LL_{1}l_{2}}^{vw}(bq) = \sqrt{\frac{L+1}{2L+1}} C_{(\lambda \mu) \kappa LL_{1}l_{2}}^{vw}(bq) - \sqrt{\frac{L}{2L+1}} C_{(\lambda \mu) \kappa LL_{1}l_{2}}^{vw}(bq).
\]

(4.22)

where \(\langle ;|;\rangle\) is a reduced SU(3) Wigner coefficient (see Appendix C.2.1), \(U[\ldots]\) denotes a SU(3) Racah recoupling coefficient (see Appendix C.2.2), and the \(\Theta\)-coefficient is given by:

\[
\Theta((\lambda \mu) \kappa L \eta_{1} \eta_{2}; bq) = \exp \left( -\frac{1}{4}(bq)^{2} \right) \left[ \frac{d(\lambda \mu)}{4\pi(2L+1)d(\eta_{1}0)} \right]^{1/2} \times \sum_{n=0}^{\eta_{1}-\lambda} \frac{(bq)^{2}}{2}^{(n_{1}+n_{2}-2n)/2} (-1)^{(n_{1}+n_{2}-2n-L)/2} \left[ \frac{(n_{1}-\lambda)!}{n!(n_{1}-\lambda-n)!} \cdot \frac{(\eta_{2}+\lambda+2)!}{\eta_{2}!(\eta_{2}+\lambda+2-n)!} \right]^{1/2} \times \sum_{\ell_{1}=0}^{n_{1}-n} \sum_{\ell_{2}=0}^{n_{2}-n} \left[ \frac{(2\ell_{1}+1)(2\ell_{2}+1)2\ell_{1}+\ell_{2}}{(n_{1}^{2}-\ell_{1}^{2})/2!(n_{2}^{2}-\ell_{2}^{2})/2!(n_{1}-n+\ell_{1}+1)!} \cdot \frac{(\eta_{2}-n+\ell_{2}+1)!}{(\eta_{2}+\lambda+2-n)!} \right]^{1/2} \times \langle \ell_{1}0\ell_{2}0|L0 \rangle \langle \eta_{1}-n,0|l_{1};(0,\eta_{2}-n)l_{2}||(\lambda \mu) \kappa L \rangle.
\]

(4.23)

Note that the \(\eta\)-summations, while in principle extending over all possible major shells, are restricted since parity and the number of oscillator quanta must be conserved. Parity conservation implies that \(L + \eta_{1} + \eta_{2}\) must be even for the Coulomb and electric multipoles and odd for the magnetic multipoles.

### 4.5 Application to \(^{24}\text{Mg}\)

In this section we will present symplectic shell model predictions for the light, well-deformed nucleus \(^{24}\text{Mg}\). We will first determine the parameters of the selected Hamiltonian by fitting calculated energies and electromagnetic transition strengths to experimental data. We will then use the eigenfunctions of the "best-fit" Hamiltonian to evaluate electron scattering form factors.
4.5.1 The calculation

In Subsection 2.2.5 we discussed a symplectic shell model calculation for $^{24}$Mg, performed by Rosensteel, Draayer, and Weeks [143]. We saw that Rosensteel et al. succeeded in reproducing the energies as well as the reduced quadrupole intraband and interband transition rates without the use of effective charges. An analysis of the structure of the ground band wave functions revealed the amount of shell mixing: the $0\hbar\omega$ contributions add up to about 70%, the contributions from the $2\hbar\omega$ level is approximately 20%, from the $4\hbar\omega$ level roughly 6%, etc. From this we conclude that a $4\hbar\omega$-calculation should suffice to obtain representative symplectic form factor predictions.

Since we are interested in studying the effects of intershell correlations, we will carry out both $2\hbar\omega$ and $4\hbar\omega$ symplectic calculations and compare the resulting form factors with each other as well as with the SU(3) ($0\hbar\omega$) predictions of Rochford and Draayer [135]. We select a Hamiltonian that is slightly simpler in structure than that of Rosensteel et al. (since it does not contain a $(Q \cdot Q)^2$ interaction):

$$H = b_2a_2 + c_3X_3 + c_4X_4 + d_2L^2 + d_4L^4.$$  \hspace{2cm} (4.24)

where $a_2 = \frac{1}{12}Q^c \cdot Q^c$, $L$ denotes the angular momentum operator, and the integrity basis operators $X_3$ and $X_4$, are included to produce the correct K-band splitting.

A least squares fit to the experimentally observed energies and B(E2) values yields the parameters listed in Table 4.1; for reference purposes we are including the parameter set of a $6\hbar\omega$ calculation as well as that of the Rosensteel et al. calculation. The oscillator size parameter was taken to be $b = 1.813$ fm [19] and $\hbar\omega$ was fixed at 12.6 MeV.

In Figure 4.1, the calculated energy spectra for the $2\hbar\omega$, $4\hbar\omega$, and $6\hbar\omega$ cases are compared to the experimental energies, and Table 4.2 shows the B(E2) values we obtained. We observe that the calculated energies are in good agreement with the experimental values. Note in particular that the $\gamma$-band is correctly located in all three calculations. It can be seen that the inclusion
Table 4.1: Hamiltonian parameters of symplectic calculations for $^{24}$Mg. Listed are the best fit parameters of the Hamiltonian 4.24 for various symplectic calculations for $^{24}$Mg. Parameters for the symplectic model calculations of Rosensteel et al., shown in the column denoted by $(6+)$ $\hbar \omega$, are taken from [143].

<table>
<thead>
<tr>
<th>Parameter (in MeV)</th>
<th>Model Space</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$2\hbar \omega$</td>
</tr>
<tr>
<td>$b_2$</td>
<td>-0.677</td>
</tr>
<tr>
<td>$b_4^4$</td>
<td>0.0</td>
</tr>
<tr>
<td>$c_3$</td>
<td>0.0232</td>
</tr>
<tr>
<td>$c_4$</td>
<td>-0.00127</td>
</tr>
<tr>
<td>$d_2$</td>
<td>0.0287</td>
</tr>
<tr>
<td>$d_4$</td>
<td>0.0</td>
</tr>
</tbody>
</table>

of higher shells yields an improved fit to the $\gamma$-band, although at the cost of slightly worsening the fit to the higher ground band states. Both intraband and interband $B(E2)$ transition strength are well reproduced in all three symplectic calculations (for reference purposes we list the SU(3) results from reference [129] and the values from the $(6+)$ $\hbar \omega$ calculation of Rosensteel et al. [143]. We find that the $4\hbar \omega$ results are better than those of the $2\hbar \omega$ calculation. Since the $6\hbar \omega$ case does not yield significant additional improvements, we will evaluate form factors for this nucleus in the $2\hbar \omega$ and $4\hbar \omega$ symplectic spaces only. Unless the resulting form factors of these calculations differ drastically from each other, we would not expect significant improvements in the form factors by including additional excitations.

Using the symplectic wave functions generated as described above and the expansions given in the previous section, longitudinal and transverse form factors are calculated in the plane-wave Born approximation (PWBA) for the elastic and inelastic scattering transitions to the low-lying $0^+$, $2^+$, $3^+$, and $4^+$ states of $^{24}$Mg. The required triple-bar matrix elements are obtained using the recursion formula of Section 3.3, valence shell matrix elements are computed with the code of Bahri and Draayer [6], and a special-purpose computer program provides the requisite SU(3) coupling and recoupling coefficients [1].

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Figure 4.1: Calculated energy spectra of $^{24}\text{Mg}$. Comparison of the theoretical energy spectra of $^{24}\text{Mg}$, obtained from $2\hbar\omega$, $4\hbar\omega$, and $6\hbar\omega$ symplectic model calculations, with the experimental energies of $^{24}\text{Mg}$ collective states.
Table 4.2: B(E2) strengths of $^{24}$Mg. Comparison between experimental B(E2) strengths of $^{24}$Mg and results of $2\hbar \omega$, $4\hbar \omega$, and $6\hbar \omega$ symplectic model calculations. The results of Rosensteel et al. [143] are listed in the column denoted by (6+)h$\omega$. and the SU(3) results are taken from [129]. All $B(E2: J_iK_i \rightarrow J_fK_f)$ transition strengths are given in Weisskopf units: 1 W.u. = 4.112 $e^2 f m^4$. The static quadrupole moment of the $2^+_1$ state is given in the last row in units of eb. Note that the calculations do not employ effective charges.

<table>
<thead>
<tr>
<th>Transition</th>
<th>Model B(E2)</th>
<th>Exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$J_i$ $K_i$ $J_f$ $K_f$</td>
<td>SU(3) $2\hbar \omega$ $4\hbar \omega$ $6\hbar \omega$ (6+)h$\omega$</td>
<td></td>
</tr>
<tr>
<td>2 0 0 0</td>
<td>6.9 17.7 20.2 20.5 20.3</td>
<td>20.5±0.6</td>
</tr>
<tr>
<td>4 0 2 0</td>
<td>9.5 24.5 27.1 27.1 26.9</td>
<td>23±4</td>
</tr>
<tr>
<td>6 0 4 0</td>
<td>9.7 25.3 26.2 25.2 25.6</td>
<td>34±6</td>
</tr>
<tr>
<td>8 0 6 0</td>
<td>9.0 24.5 21.8 18.8 20.5</td>
<td>16±2</td>
</tr>
<tr>
<td>3 2 2 2</td>
<td>31.6 35.4 35.5 34.7</td>
<td>34±6</td>
</tr>
<tr>
<td>4 2 2 2</td>
<td>3.6 9.6 11.0 11.1 10.8</td>
<td>16±3</td>
</tr>
<tr>
<td>5 2 3 2</td>
<td>5.7 15.3 16.8 16.7 16.3</td>
<td>28±5</td>
</tr>
<tr>
<td>5 2 4 2</td>
<td>17.3 18.2 17.7 17.5</td>
<td>14±6</td>
</tr>
<tr>
<td>6 2 4 2</td>
<td>5.6 15.2 18.5 18.5 17.7</td>
<td>23±23</td>
</tr>
<tr>
<td>8 2 6 2</td>
<td>4.3 12.5 15.5 16.3 14.8</td>
<td>≥3</td>
</tr>
<tr>
<td>2 2 0 0</td>
<td>2.5 1.0 1.3 1.3 1.3</td>
<td>1.4±0.3</td>
</tr>
<tr>
<td>2 2 2 0</td>
<td>2.3 2.0 1.8 2.0</td>
<td>2.7±0.4</td>
</tr>
<tr>
<td>3 2 2 0</td>
<td>1.8 2.2 2.3 2.2</td>
<td>2.1±0.3</td>
</tr>
<tr>
<td>4 2 2 0</td>
<td>1.3 0.2 0.7 0.9 0.8</td>
<td>1.0±0.2</td>
</tr>
<tr>
<td>4 2 4 0</td>
<td>3.0 2.4 2.2 2.4</td>
<td>1.0±1.0</td>
</tr>
<tr>
<td>5 2 4 0</td>
<td>1.0 1.9 2.1 1.9</td>
<td>3.4±0.8</td>
</tr>
<tr>
<td>6 2 4 0</td>
<td>0.8 0.2 0.7 1.1 0.8</td>
<td>0.8±0.8</td>
</tr>
</tbody>
</table>

$2^+_1$ quad. moment: -0.171 -0.184 -0.186 -0.184 -0.178±0.013
The calculated form factors include corrections for center-of-mass motion (following the prescriptions outlined in [37] and [135]) and for the finite-size effect of the nucleons following the method of [40]). Note that no effective charges were introduced, since the effect of multishell correlations is taken into account explicitly in the symplectic shell model.

Note also that all experimental results are plotted at the effective momentum transfer

$$q_{\text{eff}} = q \left(1 + 1.5 \frac{Z \alpha h c}{E R_0}\right).$$

where $E$ is the energy of the incoming electron and $R_0$ is the nuclear rms charge radius: in practice one uses $R_0 = 1.12 \times A^{1/3}$. The effective momentum transfer is introduced as a zeroth order correction for distortion effects due to the Coulomb field of the nucleus [100, 19]. These distortion effects are taken into account explicitly in the distorted wave Born approximation (DWBA). The changes introduced by calculating the cross section in DWBA can be understood in a qualitative way: through the Coulomb attraction the electrons are accelerated upon approaching the nucleus and the electron wave is focused onto the nucleus. This increases the cross section and causes a smearing of the form factor, which primarily results in a filling in of the minima that a plane wave prediction yields. In addition, an experiment actually samples the form factor at a larger momentum transfer than given by the asymptotic values of the kinematic variables. Thus, data measured at a certain $q$ value are usually plotted at the slightly larger $q_{\text{eff}}$ in order to allow for a comparison between experimental results and theoretical form factors calculated in the plane wave Born approximation (PWBA). In accordance with this we plot all experimental form factors at $q_{\text{eff}}$. The theoretical prediction, on the other hand, are plotted as a function of $q$.

### 4.5.2 Longitudinal form factors

The longitudinal form factors for $^{24}$Mg are shown in Figures 4.2 to 4.6. For the elastic case (see Figure 4.2a), the predictions from both the $2\hbar \omega$ and $4\hbar \omega$ calculations are found to be in very good agreement with experiment for momentum transfer values up to the first minimum. The calculated
minimum is located at about $q = 1.4 - 1.5 \text{ fm}^{-1}$ and the data support this result. The value of the form factor at the minimum, however, is not reproduced correctly since the symplectic calculation predicts $F_{0^-}^C(q) \rightarrow 0$, whereas the experiment yields finite values. It is known, however, that calculations performed in the distorted wave Born approximation (DWBA) yield a non-zero first minimum at finite $q$-values. Hence we may attribute the discrepancy at the minimum to distortion effects due to the Coulomb field of the nucleus. The location of the second maximum is correctly predicted at about $q = 1.6 - 1.7 \text{ fm}^{-1}$. The shape of the second peak follows the data and the strength at the maximum, $F_{0^+}^C \approx 3 \times 10^{-4}$, lies between the values experimentally obtained with 250 MeV electrons ($1.5 \times 10^{-4}$) and 500 MeV electrons ($5 \times 10^{-4}$), respectively.

For comparison we show the results of the $0\hbar\omega$ SU(3) calculation by Rochford and Draayer [135] in Figure 4.2b. We find that the SU(3) and symplectic results agree up to the minimum, but differ for the second maximum: while the locations of the predicted maxima are approximately the same, we observe that the symplectic form factor is quenched by a factor of about four with respect to the SU(3) prediction, and is in better agreement with the data. Note that Rochford and Draayer obtain nearly indistinguishable results from single-SU(3) irrep (not shown) and mixed-irrep calculations. Thus we may conclude that the observed quenching is not related to mixing within a major oscillator shell, but is a true multi-$\hbar\omega$ effect. We furthermore see that the $2\hbar\omega$ and the $4\hbar\omega$ cases yield nearly identical results. Hence we do not expect further changes from the inclusion of higher-$\hbar\omega$ excitations.

The inelastic form factor for the transition to the first excited $2^+$ state is shown in Figure 4.3a. The agreement with experiment is fair, with the predicted first maximum located at about $q = 0.8 \text{ fm}^{-1}$ and the second maximum located at about $q = 2.0 \text{ fm}^{-1}$. The experiment yields maxima at $q \approx 0.9 - 1.0 \text{ fm}^{-1}$ and $q \approx 2.2 \text{ fm}^{-1}$. The predicted minimum lies at $q = 1.6 - 1.7 \text{ fm}^{-1}$, and the data gives $q = 1.8 - 1.9 \text{ fm}^{-1}$. Overall, the predicted form factor seems to be shifted with respect to the data by about $0.1 \text{ fm}^{-1}$ towards lower values of the momentum transfer. The first
Figure 4.2: Elastic form factor for $^{24}$Mg. Results of our calculations are shown in Part a. The solid and dashed lines correspond to the $4\hbar\omega$ and the $2\hbar\omega$ calculations, respectively. The data has been extracted from the $^{24}$Mg cross section listed in [112], with the dots referring to an incident electron energy of 250 MeV, and the inverted triangles referring to an energy of 500 MeV. Part b shows the results of the $0\hbar\omega$ SU(3) calculation of Rochford and Draayer [135] with the solid curve representing both the mixed-irrep and the single-SU(3) irrep calculation.
maximum is slightly underpredicted (a factor of about 2/3) and the second maximum is slightly overpredicted by the same amount.

Upon comparing these results with the $0h\omega$ calculation of Rochford and Draayer (see Part b of Figure 4.3), we find that the location of the first maximum is barely changed, but its magnitude is increased by a factor of $2-3$ in the symplectic calculation and is in much better agreement with the data. The maximum of the $4h\omega$ calculation is slightly stronger than that of the $2h\omega$ calculation: thus the inclusion of higher-$h\omega$ excitations might yield slight, but insignificant, improvements. The second maximum is slightly overpredicted in the symplectic model as well as in the SU(3) model, but the latter is in better agreement with the data. In-shell irrep mixing cannot account for this since the single-irrep and mixed-irrep calculations of Rochford and Draayer yield identical results for the second maximum.

In order to illustrate the effects of multi-shell correlations, we also show the results of a calculation by Karataglidis et al. [109] (see Part c of Figure 4.3). The solid line is the result of an sd-shell model calculation and the dotted line corresponds to a calculation using projected-Hartree Fock wave functions. The latter incorporates some multi-shell correlations and is clearly in better agreement with the data. The observed enhancement of the form factor in the first maximum is in accord with our findings. There is also a shift in the location of the second maximum, to larger values of $q$, however. The physical origin of this shift thus requires further study.

The inelastic form factor for the $0_1^+ \rightarrow 2_2^+$ transition is shown in Figure 4.4a. Both the $2h\omega$ and the $4h\omega$ calculations predict the strength and shape of the first maximum perfectly, although the peak is shifted slightly with respect to the data to too large a $q$ value. Comparison with the $0h\omega$ calculations [135] (see Part b in Figure 4.4) shows that the latter overpredicts the first maximum by a factor two. Thus, the inclusion of multi-shell correlations improves the agreement with experiment. Part c shows the results of a relativistic (solid curve) and a nonrelativistic (dashed curve) calculation by Hotta et al.[103]. We observe that relativistic effects might be responsible

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3The relative lack of data points (compared to the $F^5(0_1^+ \rightarrow 0_1^+)$ and $F^5(0_1^+ \rightarrow 2_2^+)$ cases) originates from the difficulty to experimentally separate the energetically very similar $2_2^+$ and $4_1^+$ states.
Figure 4.3: Inelastic form factor for the $0^+_1 \rightarrow 2^+_1$ transition. The solid and dashed curves in Part a correspond to $4\hbar\omega$ and $2\hbar\omega$ symplectic calculations, respectively. The data is from [160] (open squares), [108] (open circles), as quoted in [103], and [112] (open triangles). Part b shows the results of the $0\hbar\omega$ calculations of [135] with the solid and dashed lines referring to the mixed and single-irrep calculations, respectively. Part c illustrates the findings of Karataglidis et al.[109]. The solid and dotted lines correspond to single-shell and multi-shell (projected-Hartree Fock) calculations, respectively.
for improving the location of the maximum. Nevertheless, none of the theoretical curves yields perfect agreement with the data. Note also that Hotta et al. employ an effective charge \( e^* = 1.58 \) in order to properly reproduce the strength of the first peak.

Figure 4.5a, which shows the longitudinal form factor for the \( 0^+_1 \rightarrow 4^+_1 \) transition, illustrates very nicely how the inclusion of multishell correlations improves the description of nuclear structure. The symplectic extension does not simply renormalize the magnitude of the calculated maxima in the form factor curves, but leads to a significant shift in the position of the peak, as can be seen when comparing the current \( 2\hbar \omega \) and \( 4\hbar \omega \) calculations with each other and with the \( 0\hbar \omega \) results of Rochford and Draayer [135] (see Part b of the figure) and of Hotta et al. [103] (see Part c): the single-major shell descriptions are not able to reproduce the proper location of the \( F_{0^+_1}^{L+} \rightarrow 4^+_1 \) peak. The symplectic \( 2\hbar \omega \) calculation allows for a better description of the scattering data, with the \( 4\hbar \omega \) extension yielding additional improvements in both location and magnitude of the two peaks and the minimum. It would be interesting to see whether a \( 6\hbar \omega \) calculation can further improve the results.

Figure 4.6a shows the longitudinal form factor for the \( 0^+_1 \rightarrow 4^+_2 \) transition. We observe that the location as well as the strength of the calculated peak fit the data fairly well. Upon comparing the \( 2\hbar \omega \) and \( 4\hbar \omega \) results with each other as well as with the \( 0\hbar \omega \) results of Rochford and Draayer [135] (see Figure 4.6b), we find that the agreement with experiment improves when multi-shell correlations are taken into account. Note also that irrep-mixing in the \( SU(3) \) case improves the predicted magnitude of the peak but not its location. For comparison, we also show the results of Hotta et al.[103] (see Part c). Note that the latter calculations overpredict the data at high-\( q \) values (less for the relativistic [solid] curve than for the nonrelativistic [dashed] curve); the near-perfect agreement between the magnitude of the peak and the data can be related to the use of an effective charge \( e^* = 1.67 \).
Figure 4.4: Inelastic form factor for the $0_1^+ \rightarrow 2_2^+$ transition. The solid and dashed curves in Part a give the results of the $4\hbar\omega$ and $2\hbar\omega$ calculations. The data is taken from Zarek et al [175]. Part b illustrates the predictions of the $0\hbar\omega$ calculation by Rochford and Draayer [135], with the solid (dashed) curve denoting a mixed-irrep (single-irrep) Hilbert space. Part c shows the results of a relativistic (solid curve) and a non-relativistic (dashed curve) calculation by Hotta et al. [103]. Note that Hotta et al. employ an effective charge of $e^* = 1.58$. 

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Figure 4.5: Inelastic form factor for the $0^+_1 \rightarrow 4^+_1$ transition. Shown are symplectic $2\hbar\omega$ (dashed curve) and $4\hbar\omega$ (solid curve) predictions for the inelastic longitudinal $0^+_1 \rightarrow 4^+_1$ form factor (see Part a). Parts b and c show $0\hbar\omega$ calculations by Rochford and Draayer [135] (Part b) and by Hotta et al. [103] (Part c). The former gives the results of a single-irrep (dashed) and a mixed irrep (solid curve) calculation, and the latter compares a relativistic (solid curve) with a nonrelativistic (dashed curve) treatment. Note that Hotta et al. employ an effective charge of $e' = 3.84$. 

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Figure 4.6: Longitudinal form factor for the inelastic $0^+_1 \rightarrow 4^+_2$ transition. The $4\hbar\omega$ (solid curve) and $2\hbar\omega$ (dashed curve) symplectic predictions of Part a are compared with $0\hbar\omega$ SU(3) calculations from [135] (see Part b) and from [103] (Part c). Data are taken from [108] (as quoted in [103]) (solid circles) and from [112] (open circles).
4.5.3 Transverse form factors

Transverse form factors contain valuable information on nuclear current flows. In the case of $^{24}\text{Mg}$, an even-even rotational nucleus, the transverse form factor for inelastic scattering from the ground state to an excited state of angular momentum $J$ measures directly the electric $EJ$ multipole of the nuclear current and thus yields information on the current flows associated with collective motion. Since the currents associated with different models of collective rotations are qualitatively different, experimental form factors may provide us with a means to distinguish models that describe equally well the static electromagnetic properties of rotational nuclei. This topic has been of particular interest to various authors, such as Carvalho and Rowe [22, 21] and Rosensteel [140]. Recent results of Carvalho and Rowe [21], for example, show that the irrotational-flow model, the rigid rotor model, and the Riemann flow model yield clearly distinguishable predictions for the transverse $F_{0^+}^{T}$ form factor.

Transverse form factors may also reveal valuable information on violation of current conservation by shell model wave functions. Current conservation follows from the gauge invariance of the electromagnetic field. However, there is still some uncertainty with regard to the appropriate form of the nuclear currents that are required in the analysis of form factors. In principle, the charge and current density contain one-, two-, up to A-body components, corresponding to the exchange of charged bosons responsible for the nuclear interaction. In some calculations, two-body meson exchange contributions are considered, but most practical applications employ the usual free-nucleon one-body operator. In addition, by using a truncated Hilbert space, as is the case in most nuclear models, the resulting wave functions may not satisfy charge-current conservation themselves. This problem is considerably more severe for the three-current than for the charge density [100] and thus affects transverse form factors more than longitudinal ones. To partially circumvent this problem, alternative forms for the transverse electric operators have been derived by invoking current conservation, either in the long-wavelength limit [77], or for arbitrary wavelength [76]. Electric transverse form factors obtained with the various operators are equivalent for...
a conserved current and differ significantly when model wave functions are used which violate current conservation. This fact has been employed to show that conventional $0\hbar\omega$ shell model wave functions violate current conservation, whereas wave functions obtained from multi-shell models of nuclear structure are significantly closer to being current conserving [109]. It is thus worthwhile to carefully study theoretical predictions of transverse form factors.

Measurements of transverse form factors are difficult since the large longitudinal transitions dominate the cross sections; for the transitions of interest here, the longitudinal form factors exceed their transverse counterparts by as much as a factor of $10^4$. Experiments designed to measure transverse form factors usually observe electrons scattered at 180° in order to minimize longitudinal contributions.

In what follows, we show symplectic shell model predictions for the transverse form factors associated with transitions to low-lying energy levels in $^{24}\text{Mg}$. Since we perform a single-symplectic irrep calculation, all calculated eigenstates have spin zero, and thus the magnetization current contributions to the transverse form factors vanish. As a result of parity constraints, the transverse form factor associated with transitions to the $2^+$ and $4^+$ states is pure electrical in character, and the form factor for the $3^+_1$ transition is purely magnetic. The data has been taken from Hotta et al. [103], who measured transitions to the first $2^+$ (1.37 MeV) and $3^+$ (5.24 MeV) states, the second $4^+$ (6.01 MeV) state and for unresolved doublet at 4.12 MeV ($4^+_2$) and 4.24 MeV ($2^+_2$).

Figure 4.7 shows the symplectic $2\hbar\omega$ (dashed curve) and $4\hbar\omega$ (solid curve) predictions for the transverse $F^{T}_{01^+\rightarrow2^+_1}$ form factor, compared with experimental results. For comparison, we also show the results of the $0\hbar\omega$ calculations of Rochford and Draayer [135] (see Figure 4.8a). We find that both the SU(3) and symplectic calculations overpredict the strength of the maximum. Furthermore, the maximum is located at too large a $q$ value in the SU(3) case and too small a $q$ value in the symplectic case. Upon closer inspection, we observe that the mixed-irrep prediction (solid curve) is better than the single-irrep prediction (dashed curve) (see Figure 4.8a), and that

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4 Magnetic transitions are unconstrained by current conservation.
taking into account $4\hbar\omega$ excitations yields improvements over the $2\hbar\omega$ calculation (see Figure 4.7). The changes associated with going from the $2\hbar\omega$ to the $4\hbar\omega$ case seem to indicate that further improvements are possible by including higher excitations.

The effects of multishell correlations can also be studied by investigating Figure 4.8b and 4.8c. Figure 4.8b shows the results of a single major shell calculation by Hotta et al. [103]. The solid and dashed curves are the relativistic and nonrelativistic results, absolutely normalized, without an effective charge. We observe that the strength of the maximum is underpredicted and that an effective charge ($e^* = 2.03$) is required to achieve better agreement with the data. (For details about the procedure for employing an effective charge in conjunction with transverse form factors, see [103].) Figure 4.8c is taken from a publication by Carvalho and Rowe [22]. Here the shift from larger to smaller values of momentum transfer $q$ associated with the inclusion of multishell correlations can be observed, in agreement with what has been found above. The symplectic results are too high at smaller $q$ values and fit the data better at larger $q$ values.

Experimentally, the transverse form factors for the transitions to the $2^+_2$ (4.24 MeV) and $4^+_1$ (4.12 MeV) states have not been resolved yet. We therefore combine the theoretical predictions for these two transitions in Figure 4.9. The calculated contribution from the $0^+_1 \rightarrow 4^+_1$ transition to the total transition strength is about an order of magnitude smaller than that originating from the $0^+_1 \rightarrow 2^+_2$ transition. We see that the agreement with the data is not good: the strength of the predicted form factor is not too bad, but the location of the minimum is not properly reproduced. For comparison, we also show the SU(3) results of Rochford and Draayer [135] in Figure 4.10 (Parts a and b), as well as $0\hbar\omega$ results from Hotta et al. [103] in Figure 4.10c. A comparison of SU(3) and Sp(3R) calculations, as performed by Carvalho and Rowe [22] is shown in Figure 4.10d.

Figure 4.11a shows the predicted transverse form factor for the $0^+_1 \rightarrow 4^+_2$ transition. As in the previous case, the agreement with experiment is not good. Neither the magnitude nor the position of the peak is properly represented. The $0\hbar\omega$ calculations of Rochford and Draayer [135] (see Part b) and of Hotta et al. [103] (see Part c) reproduce the shape of the form factor better, although
Figure 4.7: Transverse form factor for the $0^+_1 \rightarrow 2^+_1$ transition. The solid curve shows the result of the $4\hbar \omega$ calculation, the dashed curve that of the $2\hbar \omega$ calculation.
Figure 4.8: Transverse form factor predictions from various models for the $0^+_1 \rightarrow 2^+_1$ transition. Part a gives the $0\hbar\omega$ SU(3) shell model results of Rochford and Draayer [135], with the solid (dashed) curve corresponding to a mixed-irrep (single-irrep) calculation. Part b gives the results of the relativistic (solid curve) and nonrelativistic (dashed) curve predictions (without effective charge) by Hotta et al. [103]; the dot-dashed (relativistic) and double-dot-dashed (non-relativistic) curves are the results obtained by using an effective charge of $e^*=2.03$. Part c gives the symplectic (solid curve) and SU(3) (dot-dashed curve) results of Carvalho and Rowe [22].
Transverse form factor for transition to the unresolved $2_{2}^{+}$ and $4_{1}^{+}$ states

Figure 4.9: Transverse form factor for the transition to $2_{2}^{+}$ and $4_{1}^{+}$. Shown are symplectic $2\hbar\omega$ (dashed curve) and $4\hbar\omega$ (solid curve) predictions for the transition to the unresolved $2_{2}^{+}$ (4.24 MeV) and $4_{1}^{+}$ (4.12 MeV) states.

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Figure 4.10: Predicted transverse form factor for the transition to $2^+_2$ and $4^+_1$. Given are various predictions for the transition to the unresolved $2^+_2$ (4.24 MeV) - $4^+_1$ (4.12 MeV) doublet. Parts a and b show separate results for the two transitions as obtained by Rochford and Draayer [135], the solid (dashed) curves correspond to mixed-irrep (single-irrep) calculations. Part c gives the relativistic (solid curve) and non-relativistic (dashed) results of Hotta et al. [103], and Part d shows Carvalho et al.'s comparison between a SU(3) (dot-dashed) and a symplectic (solid curve) calculation [22].

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the former overpredicts the strength of the maximum by an order of magnitude, and the latter underpredicts it by a factor of 5 in the nonrelativistic calculation (dashed curve) and a factor 2 in the relativistic calculation (solid curve).

One might be tempted to relate the discrepancy between our results and experiment (for both this and the previous form factor) to an improper amount of K-band mixing. Zarek et al. [175], for example, found that by varying the amount of mixing between the $4^+_1$ and $4^+_2$ states, the predictions within the framework of the projected-Hartree Fock approach for the longitudinal $F_{0^+_1-4^+_1}^L$ form factor can be improved. A look at our calculated (excellent) interband transition probabilities (see Table 4.2), however, makes this explanation unlikely. It is more likely that in-shell mixing and the inclusion of states with non-zero spin in the calculation will improve the predictions. Another possible explanation for the observed discrepancies is that our assumption that the nuclear current distributions, analogously to the charge distribution, scale as $Z/A$ breaks down. This would imply that an explicit treatment of both proton and neutron degrees of freedom would better represent the structure of the nucleus. This point remains to be investigated further.

Figure 4.12a shows the symplectic prediction for the purely magnetic $0^+_1 \rightarrow 3^+_1$ transition. We find fair agreement with experiment, but also observe that the $4h\omega$ result does not give any improvement over the $2h\omega$ calculation. To achieve better agreement it might be necessary to allow for mixing between different symplectic irreps. For comparison, we also show the predictions of Hotta et al.[103] (see Part b).

4.5.4 Conclusions

We have implemented $2h\omega$ and $4h\omega$ symplectic calculations for $^{24}$Mg. We obtain energies and reduced quadrupole transition probabilities that are in good agreement with experimental findings. The wave functions of these calculations have been used to formulate form factor predictions for the low-lying $2^+$, $3^+$, and $4^+$ states of the ground and $\gamma$ bands of $^{24}$Mg. The calculated longitudinal form factors are in good agreement with experiment and exhibit improvements over $0h\omega$ single-major shell predictions. We have shown that multi-shell correlations may enhance or quench the
Figure 4.11: Transverse form factor for the $0^+_1 \rightarrow 4^+_2$ transition. Shown are symplectic $2\hbar\omega$ (dashed) and $4\hbar\omega$ (solid) predictions for the transverse $0^+_1 \rightarrow 4^+_2$ form factor (Part a). Parts b and c give the results of the $0\hbar\omega$ calculations by Rochford and Draayer (Part b) [135] and by Hotta et al. [103] (see Part c). The latter shows both relativistic (solid curve) and non-relativistic (dashed) results and illustrates the consequences of including an effective charge of $e^*=1.67$ (dot-dashed and double-dot-dashed curves).
Figure 4.12: Transverse form factor for the $0_1^+ \rightarrow 3_1^+$ transition. Symplectic $4\hbar\omega$ (solid curve) and $2\hbar\omega$ (dashed curve) predictions for the inelastic magnetic transition to the $3_1^+$ state are shown in Part a. Part b gives the relativistic and nonrelativistic results of Hotta et al. [103] as solid and dashed curves, respectively.
maxima that are predicted by $0\hbar \omega$ calculations and, in addition, displace the peaks to smaller or higher momentum transfer. We have found similar patterns for the transverse form factors, but overall the agreement between the calculated and measured results is much worse than for the longitudinal cases. This reflects the fact that nuclear current density distributions are much more complex in nature than the nuclear charge density. We may thus agree with Carvalho and Rowe [22] in the assessment that correlations to higher shells contribute in a much more complex way to nuclear current and charge densities than anticipated by the shell model.
Chapter 5

Summary and Conclusion

The Elliot SU(3) shell model and its multi-shell extension, the symplectic shell model, have been reviewed. We have established their usefulness for obtaining a microscopic description of nuclear structure. The focus has particularly been on the symplectic model which provides a multi-shell realization of the nuclear shell model and has proven to be very successful in describing nuclear collective properties such as deformations and electromagnetic transition strengths, without the use of effective charges.

We have recast the relevant symplectic algebra $sp(3, R)$, which is usually expressed in a boson basis, in terms of fermion creation and annihilation operators. This formulation enabled us to derive a recursion formula in which symplectic matrix elements of arbitrary one-body fermion operators between states of excitation $N\hbar\omega$ and $N'\hbar\omega$ in the same or in different symplectic bands are related back to valence shell matrix elements, which can be evaluated by standard shell model techniques. Since this formula is generic, valid for arbitrary one-body operators, it has the potential to lead to a variety of new applications within the framework of the symplectic model.

We have applied the formalism developed in this dissertation to evaluate electron scattering form factors in the symplectic model. To this end we adopted the approach of Rochford and Draayer [135], who derived expressions for the nuclear charge and current density multipole operators in a
SU(3) tensorial basis. Their expressions are given explicitly in fermion second quantized form, are exact shell-model representations of the multipole operators, and extend over all possible oscillator shells. We have used these expressions in conjunction with the recursion relation presented here to compute nuclear structure form factors with symplectic wave functions.

Results for the deformed light nucleus \( ^{24}\text{Mg} \) have shown improvements over earlier, single-shell calculations, in particular for the longitudinal form factors. We found that multi-shell correlations do not simply renormalize the single-shell results, but contribute in a much more complex way to nuclear dynamics. Transverse form factors have proven to be particularly difficult to reproduce, which reflects the fact that nuclear current density distributions are more complex in nature than the nuclear charge density.

Transverse form factors certainly merit additional attention. It would be of interest to extend the current study to include nuclear states of nonzero spin, since in that case the magnetization current density contributes to the transverse form factor. Since both protons and neutrons contribute to the magnetization current through their intrinsic spin magnetization, it becomes possible to examine the distribution of neutrons through magnetic scattering. It would furthermore be worthwhile to address the question about the nature of collective rotational flows. This topic has been explored by Carvalho and Rowe [22, 21] as well as Rosensteel [140], but a full symplectic treatment of rotational nuclei might give additional insight.

Further extensions include an examination of current conservation in nuclear shell model approaches, an investigation of the effects of non-collective degrees of freedom (such as pairing and spin-orbit forces [9, 67]) on nuclear form factors, and a study of heavy deformed nuclei in the rare earth and actinide regions.
Bibliography


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142


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Appendix A

Basic Elements of the Theory of Groups and Their Representations

In this appendix we introduce some key elements of group and representation theory which form the basis of the formalism utilized in this dissertation. We restrict ourselves to defining concepts which are frequently used in the text or which place the formalism into a broader mathematical context. The purpose of this appendix is to help the reader follow the standard notation and language employed by theorists who rely heavily on group theoretical concepts in their description of physical phenomena. We also hope that the reader will gain some appreciation for the beauty of symmetry-based approaches to physical systems and for the simplifications that can be achieved by employing the powerful tools of group theory. In this compilation we have made use of the following textbooks and articles: Morton Hamermesh: *Group Theory and its Applications to Physical Problems* [87]; J. P. Elliott and P. G. Dawber: *Symmetry in Physics* [63]; Barut and Raczkowski: *Theory of Group Representations and Applications* [10]; Wu-Ki Tung: *Group Theory in Physics* [166]; J. F. Cornwell: *Group Theory in Physics* [34]; Loeb: *Group Theory and Its Applications* [116]; J. E. Humphreys: *Introduction to Lie Algebras and Representation Theory* [104]; Robert Gilmore: *Lie Groups, Lie Algebras, and Some of Their Applications* [79]; Sigurdur Helgason: *Differential Geometry, Lie Groups, and Symmetric Spaces* [101]; V. S. Varadarajan: *Lie Groups, Lie Algebras, and Their Representations* [168]; James R. Munkres: *Topology - A First Course* [121]; N. Jacobson: *Lie Algebras* [105]; A. Sagle and R. Walde: *Introduction to Lie Groups and Lie Algebras* [154];
etc. For a more in-depth and complete treatment of the subject the reader may refer to these publications and other standard literature.

A.1 Groups and Their Representations

Whenever a quantum mechanical system possesses a symmetry the basis states are naturally labeled according to their behavior under symmetry transformations. Similarly, one can classify physical observables, such as position, momentum, angular momentum, electromagnetic field, ... etc. by their invariance properties with respect to these transformations. Basis states and observables are then characterized by the irreducible representations of the symmetry groups associated with the system. In what follows we introduce the notions of groups and irreducible representations.

Definition Group. A group consists of the following.

1. A set $G$;
2. An operation which associates each pair of elements $g_1, g_2$ in $G$ with an element $g_1 g_2$ in $G$ such that
   - (a) $g_1 (g_2 g_3) = (g_1 g_2) g_3$, for all $g_1, g_2, g_3$ in $G$ (associativity);
   - (b) there exists an element $e$ in $G$ such that $eg = ge = g$ for every $g$ in $G$ (existence of an identity element);
   - (c) to each element $g$ in $G$ corresponds an elements $g^{-1}$ in $G$ such that $gg^{-1} = g^{-1}g = e$ (existence of inverse elements).

Definition Group Representation. Let $G$ be a locally compact, separable, unimodular topological group and let $\mathcal{H}$ be a separable complex Hilbert space. A map $g \rightarrow T_g$ of $G$ into the set $\mathcal{L}(\mathcal{H})$ of linear bounded operators in $\mathcal{H}$ is said to be a representation of $G$ in $\mathcal{H}$ if the following conditions hold:
1. $T_{g_1 g_2} = T_{g_1} T_{g_2}$;
2. $T_e = I$, where $I$ denotes the Identity operator.

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The first condition is equivalent to the statement that the map \( g \mapsto T_g \) is a homomorphism of \( G \) into the set of linear operators on \( G \), and the second condition then guarantees the existence of invertible operators.

**Definition Invariant Subspace.** Let \( g \mapsto T_g \) be a representation of a topological group \( G \) in a Hilbert space \( \mathcal{H} \). A subspace or subset \( \mathcal{H}_1 \) of \( \mathcal{H} \) is said to be invariant (with respect to \( T \)) if \( u \in \mathcal{H} \) implies \( T_g u \in \mathcal{H}_1 \) for every \( g \in G \).

Every representation has at least two invariant subspaces, the null space and the whole space \( \mathcal{H} \), both of which are said to be trivial. The nontrivial invariant subspaces or subsets are called *proper*.

**Definition Irreducible Representation.** A representation \( g \mapsto T_g \) of a group \( G \) in \( \mathcal{H} \) is called *irreducible*, if it has no proper invariant subsets in \( \mathcal{H} \).

The expression *irreducible representation* is commonly abbreviated as *irrep.*

In order to gain an appreciation for the usefulness of the above concepts let us examine how wave functions associated with a physical system that exhibits symmetries can be labeled according to their transformation properties. Specifically, we will consider unitary representations (that is, representations where the map \( g \mapsto T_g \) is unitary for all \( g \in G \)), since physical symmetry transformations are naturally associated with unitary operators which preserve lengths, angles, and scalar products. Unitary transformations acquire additional relevance since one can show that every representation of a finite group is equivalent to a unitary representation. Furthermore, if a unitary representation is reducible, then it is *fully reducible* (or *decomposable*), that is, the orthogonal complement of the invariant subspace is also invariant with respect to the representation. If \( g \mapsto U_g \) is a unitary representation of the group \( G \) in a vector space \( V \), and \( V_\mu \) is an invariant subspace with respect to \( U_g \) with an orthonormal basis \( \{e_1^\mu, e_2^\mu, \ldots, e_n^\mu\} \), then \( U_g |e_i^\mu\rangle = |e_i^\mu\rangle (D_g^\mu)^i_j \) holds for \( g \in G \), where \( D_g^\mu \) is an irreducible matrix representation of \( G \). Any such set of vectors \( \{e_1^\mu, e_2^\mu, \ldots, e_n^\mu\} \) which transforms under \( U_g \) as shown in the above equation is referred to as an *irreducible set* transforming according to the \( \mu \)-representation.
If one considers two irreducible sets of vectors which transform according to the $\mu$ and $\nu$ representations of a group $G$ in a vector space $V$, then one can show that the two invariant subspaces $V_\mu$ and $V_\nu$ spanned by these bases are orthogonal to each other if the representations are not equivalent. For cases where the representations are equivalent, there are two possibilities: 

i) The subspaces $V_\mu$ and $V_\nu$ do not overlap, and they may be distinguished by the eigenvalues of some other operator which lies outside the group; or ii) The two subspaces coincide with each other: $V_\mu = V_\nu$.

These findings have useful implications for physical systems which exhibit symmetries: For the Hilbert space of a given system one can now find a set of basis functions such that this set can be partitioned into subsets each of which transforms according to a particular irreducible representation of the relevant symmetry group. The subsets can then be labeled by their associated irrep.

Further partitioning the subsets into subsubsets which transform according to the irreps of a subgroup of the original symmetry group then yields additional state labels. The challenge in approaching real physical systems thus lies in finding a chain of groups and subgroups $G_0 \supset G_1 \supset \ldots \supset G_n$, such that the irreducible representation labels associated with each group $G_i$ in the chain combine to uniquely specify each basis state. A physically relevant example is given by the chain $SU(2) \supset U(1)$. Basis functions can be uniquely determined by the irrep label $L$ of the group $SU(2)$ and the label $M$ of the subgroup $U(1)$. $SU(2)$ is associated with rotations in the three-dimensional space and $L$ gives the angular momentum of the basis function with projection $M$ on the $z$-axis of the system.

A.2 Lie Groups and Lie Algebras

In physical applications both discrete and continuous groups are of interest. In the present context we are particularly interested in a special class of continuous groups, the class of linear Lie groups or classical Lie groups. Roughly speaking, a Lie group is an infinite group the elements of which
can be parametrized smoothly and analytically. A Lie group displays three different kinds of mathematical structure: it has a group structure, its elements form a topological space, and its elements constitute an analytic manifold. Therefore, a Lie group can be defined in several different, but equivalent, ways. The following defines a Lie group as a topological group with certain additional analytic properties.

**Definition** An abstract group G is called a Lie group if the following conditions hold:

1. G is an analytic manifold.
2. The mapping \((g_1, g_2) \mapsto g_1 g_2^{-1}\) of the product manifold \(G \times G\) into G is analytic.

Since a Lie group is a manifold, its identity element has a neighborhood which is homeomorphic to a subset of an \(r\)-dimensional Euclidean space, where \(r\) is then called the order of the Lie group.

One of the implications of the topological properties of the Lie group is that a Lie group is homogeneous, that is, for any given pair of points \(g_1, g_2\) in the group manifold \(G\) there exists a homeomorphism \(f: G \rightarrow G\) such that \(f(g_1) = g_2\). As a consequence, local properties of a Lie group need be stated and examined only in the neighborhood of a single point, for example, in the neighborhood of the identity element; the homogeneity of the manifold allows one to deduce the same properties at any other point of the manifold.

If one examines an analytic function, defined over the group manifold, in a small neighborhood of the group identity element, one finds that the function can be expressed in terms of its value at the identity plus \(r\) differential operators \(d_1, d_2, \ldots, d_r\) acting on the function, evaluated at the identity. These differential operators act as the generators of the infinitesimal group transformations and obey the commutation relations

\[
[d_i, d_j] = \sum_{k=1}^{r} c_{ij}^k d_k .
\]  

(A.1)

which serve to define the so-called structure constants \(c_{ij}^k\). This set of generators is closed under commutation, and the set of all their linear combinations is called the Lie algebra of the group.
Alternatively, but equivalently, one can define a Lie algebra abstractly as follows:

**Definition Lie Algebra.** A vector space $\ell$ over a field $F$ with an operation $\ell \times \ell \rightarrow \ell : (u, v) \mapsto [u, v]$, called the commutator of $u$ and $v$, is called a Lie Algebra over $F$ if the following conditions are satisfied:

1. **Bilinearity:** $[\alpha u + \beta v, w] = \alpha [u, w] + \beta [v, w]$ and $[w, \alpha u + \beta v] = \alpha [w, u] + \beta [w, v]$ for all $u, v, w$ in $\ell$ and all $\alpha, \beta$ in $F$.
2. **Antisymmetry:** $[u, v] = -[v, u]$ for all $u, v$ in $\ell$.
3. **Jacobi Identity:** $[u, [v, w]] + [v, [w, u]] + [w, [u, v]] = 0$ for all $u, v, w$ in $\ell$.

The operation $(u, v) \mapsto [u, v]$ is called Lie multiplication.

Since the generators $d_1, d_2, \ldots, d_r$ of the Lie Group $G$ span a Lie algebra, they must satisfy the three conditions above. These identities then lead to the following relations:

1. $c^k_{ij} = -c^k_{ji}$ for $1 \leq i, j, k \leq r$;
2. $\sum_{1 \leq p \leq r} (c^k_{ij} c^p_{il} + c^k_{ji} c^p_{li} + c^k_{lj} c^p_{ki}) = 0$ for $1 \leq i, j, l, m \leq r$ (Jacobi condition).

In fact, one can show that there exists a Lie algebra for every set of structure constants which satisfies these conditions. Lie's theorems provide a mechanism for constructing a Lie algebra for any Lie group and characterize the properties of the resulting algebra. The Lie algebra associated with the Lie group $G$ is determined up to isomorphisms and is usually denoted by the symbol $\mathcal{G}$.

Lie further proved that for a given (real) Lie algebra $\mathcal{G}$ with preassigned structure constants $c^k_{ij}$ which satisfy the above relations, one can construct the Lie group $G$ which has this algebra $\mathcal{G}$ as its Lie algebra. The finite group transformations of $G$ are obtained by integrating the infinitesimal generators; the structure constants determine the Lie group $G$ locally, that is, in the neighborhood of the identity element. There is, however, a whole class of Lie groups that have isomorphic Lie algebras; these Lie groups are locally isomorphic, but they may be totally different globally. Among the Lie groups that can be associated with a given Lie algebra, there is only one that is simply
connected (A topological space is said to be connected if any two points in the space can be joined by a curve and all the points of the curve lie in the space. A connected space is simply connected if a curve connecting any two points in the space can be continuously deformed into every other curve connecting the same two points.) This simply connected group is called the universal covering group; other Lie groups with isomorphic Lie algebras can be obtained from the universal covering group.

The equivalence between Lie groups and Lie algebras is very important since a Lie algebra is a linear vector space with an additional structure, the commutator. As such, the algebra is more amenable to detailed study than the group. Often Lie algebras and their representations are used to obtain information about Lie groups and their representations. The Lie algebra, because of its integrability, determines all the structures that have the desired properties of transformation under the finite elements of the group. This has turned out to be particular useful for the construction of irreducible representations. Since we are not interested in presenting the process of constructing irreducible representations, we will only list a few more frequently used terms and then return to representations of Lie groups and their use in quantum mechanics.

**Definition** Ideal. A subspace \( \ell_1 \) of a Lie algebra \( \ell \) is an ideal in \( \ell \) if \( [\ell, \ell_1] \subset \ell_1 \).

**Definition** Semisimple Lie Algebra. A Lie algebra \( \ell \) is semisimple if it contains no non-zero commutative ideal.

Every generator of a semisimple algebra has a nonzero commutator with some other generator: therefore the structure constants carry much information about the structure of the algebra and its representations.

**Definition** Simple Lie Algebra. A Lie algebra \( \ell \) is simple if it contains no ideals other than \( \{0\} \) and \( \ell \), and if \( [\ell, \ell] \neq 0 \).

A semisimple algebra can be reduced to a direct sum of simple algebras: every element in one simple subalgebra commutes with every other element in any other simple subalgebra.
A.3 Tensor Operators and the Wigner-Eckart Theorem

Operators acting on the Hilbert space of a physical system behave in definite ways under symmetry group transformations and are therefore - analogously to basis states - naturally classified according to the irreps of the relevant symmetry groups. The systematic exploitation of the transformation properties of the basis states and the operators leads to significant simplifications for the calculation of physical observables.

Definition Tensor Operator. Let \( g \rightarrow D_g \) be a finite-dimensional representation of a group \( G \) in a vector space \( V \) and let \( \{ D^*_g \} \) be its matrix form in a basis \( e_1, e_2, \ldots, e_r \) of \( V \). Let \( g \rightarrow U_g \) be a unitary representation of \( G \) in a Hilbert space \( \mathcal{H} \).

- A set \( \{ T^s \}, s = 1, 2, \ldots, d(D) \), of operators is said to be a contravariant tensor operator if
  \[
  U^{-1}_g T^s U_g = (D_g)^s T^t.
  \]
  This definition is given for finite transformations: it can also be stated in infinitesimal form, on the level of the Lie algebra, as
  \[
  [U x, T^s] = i (D_x)^s T^t
  \]
  for \( x \in \mathfrak{g} \).

- A set \( \{ T_s \}, s = 1, 2, \ldots, d(D) \), of operators is said to be a covariant tensor operator if
  \[
  U^{-1}_g T_s U_g = (D_{g^{-1}})^s T^t \equiv (D_{g^{-1}})^s T^t.
  \]
  On the level of the Lie algebra this definition corresponds to the requirement
  \[
  [U x, T_s] = -i (D_x)^s T^t
  \]
  for \( x \in \mathfrak{g} \).

Definition Irreducible Tensor Operator. The tensor operator \( \{ T^s \} \) is said to be irreducible if the representation \( g \rightarrow D_g \) is irreducible.

Definition Tensor Operator of rank \( k \). A set \( \{ T^{s_1, s_2, \ldots, s_k} \} \) is said to be a contravariant tensor of rank \( k \) if
  \[
  U^{-1}_g T^{s_1, s_2, \ldots, s_k} U_g = (D_g)^{s_1}_{t_1}(D_g)^{s_2}_{t_2} \cdots (D_g)^{s_k}_{t_k} T_{t_1, t_2, \ldots, t_k}.
  \]
  The covariant tensor operator \( \{ T_{s_1, s_2, \ldots, s_k} \} \) and the mixed tensor operator \( \{ T^{s_1, s_2, \ldots, s_k}_{t_1, t_2, \ldots, t_k} \} \) are defined analogously.

Definition Invariant Tensor Operator. A covariant tensor \( \{ T_{s_1, s_2, \ldots, s_k} \} \) of rank \( k \) is called invariant if it satisfies the condition
  \[
  (D_g)^{s_1}_{t_1}(D_g)^{s_2}_{t_2} \cdots (D_g)^{s_k}_{t_k} T_{t_1, t_2, \ldots, t_k} = T_{t_1, t_2, \ldots, t_k}.
  \]
  Analogously for contravariant tensors.
The simplest example of an irreducible tensor operator is given by any invariant operator $C$ of the group, since $U_g^{-1}CU_g = C$, which implies $g \rightarrow D_g \equiv 1$.

Tensor operators can be combined to form new tensor operators; for example, one can show that the sum of two contravariant tensor operators is a tensor operator of the same kind, and the contraction $\{T_{u_1u_2...u_n}^1212...l_k\}$ of a tensor operator $\{T_{u_1u_2...u_n}^{1212}...l_k\}$ is again a tensor operator. One can furthermore form a tensor product of two tensor operators:

**Definition Tensor Product.** Let $\{T^s\}$ and $\{T'^s\}$ be two contravariant tensor operators which transform according to representations $D$ and $D'$, respectively. Then the set $\{T'^s = T^sT'^s\}$ is a contravariant tensor, which transforms according to $U_g^{-1}T'^sU_g = (D_g)^s_{t'}(T'^sT'^t')$, where $(D_g)^s_{t'} = (D_g)^s_{t'}(D_g)^t_{t'}$. The tensor operator is referred to as the tensor product of the operators $\{T^s\}$ and $\{T'^s\}$.

The above tensor product forms (in general) a reducible tensor, which can, however, be used to construct a new irreducible tensor operator (Here, and in what follows we will consider unitary representations $g \rightarrow D_g$ only, since in that case the space $V$ has the metric $g^{st} = \delta^{st}$ and one may set $D'_g = D_{st}$): If $\{\Gamma_1\alpha_1\}$ is a basis for the irreducible space $\mathcal{H}^{\Gamma_1}$, $\{\Gamma_2\alpha_2\}$ a basis for the irreducible space $\mathcal{H}^{\Gamma_2}$, and $\{\Gamma\alpha\}$ an orthonormal basis for the irreducible subspace $\mathcal{H}^{\Gamma}$ of $\mathcal{H}^{\Gamma_1} \otimes \mathcal{H}^{\Gamma_2}$, then

$$T_\alpha^{\Gamma} \equiv \sum_{\alpha_1\alpha_2} (\Gamma_1\alpha_1;\Gamma_2\alpha_2|\Gamma\alpha) T^{\Gamma_1}_{\alpha_1} T^{\Gamma_2}_{\alpha_2}$$

(A.2)

is an irreducible tensor operator.

Irreducible tensor operators play an important role in physics, in particular since the Wigner-Eckart theorem greatly simplifies and economizes the calculation of matrix elements of irreducible tensor operators by allowing for a separation of a given matrix element into a geometric part, which carries the labels of the group-subgroup chain under consideration, and a subgroup-independent part, which reflects the specific properties if the states and the operators, the so-called reduced matrix element:
**Wigner-Eckart Theorem** Let $g \rightarrow U_g^\Gamma_1$ and $g \rightarrow U_g^\Gamma_2$ be irreducible unitary representations of a simple reducible compact group $G$ in the Hilbert spaces $\mathcal{H}_1^\Gamma$ and $\mathcal{H}_2^\Gamma$, respectively. Let $\{|\Gamma_1\alpha_1\rangle\}$ and $\{|\Gamma_2\alpha_2\rangle\}$ be orthogonal sets of basis states in $\mathcal{H}_1^\Gamma$ and $\mathcal{H}_2^\Gamma$. Let $\{T_{\alpha}^\Gamma\}$ be an irreducible tensor operator. Then

\[
\langle \Gamma_2\alpha_2|T_{\alpha}^\Gamma|\Gamma_1\alpha_1\rangle = \sum_\rho \langle \Gamma_1\alpha_1;\Gamma_2\alpha_2|\Gamma\rangle_\rho \langle \Gamma_2||T^\Gamma||\Gamma_1\rangle_\rho . \tag{A.3}
\]

where $\langle \Gamma_1\alpha_1;\Gamma_2\alpha_2|\Gamma\rangle$ is a (Clebsch-Gordan) coupling coefficient and $\rho$ is a running index which labels multiple occurrences of the irrep $\Gamma$ in the direct product $\Gamma_1 \times \Gamma_2$. $\langle \Gamma_2||T^\Gamma||\Gamma_1\rangle$ is the *reduced matrix element* of the tensor operator $T_{\alpha}^\Gamma$. It is defined by the above relation.

While in many important applications, such as those involving three-dimensional rotational symmetry, each irrep occurs only once in the reduction of the product, for the group SU(3) the multiplicity label $\rho$ is required.

The usefulness of the Wigner-Eckart theorem derives from the fact that matrix elements of a general operator can be evaluated if the operator is expanded in irreducible tensor operators and the matrix elements of the irreducible tensor operators and the appropriate coupling coefficients are known. In most physical applications there are only a few relevant reduced matrix elements, and the coupling coefficients, which are determined by group representation theory, can be obtained from published tables. In order to expand a general operator into irreducible tensors, one needs to make use of the formalism of second quantization and tensor decomposition techniques which will be discussed in the next few sections.
Appendix B

The Formalism of Second Quantization

The physical world consists of interacting many-particle systems. An accurate description of such systems necessarily requires the inclusion of not only one-body, but also two, three, four ..., $N$-body interactions in the many-particle Schrödinger equation. We will consider some of the problems that arise when writing the wave functions and Schrödinger equation for identical particle systems in the usual first quantized form. We then introduce the formalism of second quantization (also called occupation number formalism) and reformulate the Schrödinger equation. Some of the advantages of the new formalism will be immediate: The second-quantized many-particle wave functions and operators incorporate the statistics (Bose or Fermi) at each step, which contrasts with the more cumbersome approach of using symmetrized or antisymmetrized products of single-particle wave functions. This approach not only simplifies the discussion of many interacting particles considerably, it also allows for the symmetries of the quantum mechanical Hamiltonian to be taken into account and to be exploited. Using symmetry considerations is essential for solving problems involving complex many-body systems such as for example the collection of more than one hundred nucleons in a heavy nucleus. The applications of second quantization in relativistic quantum mechanics will not be discussed here, but it is worthwhile to note that the formalism plays a central role in describing the creation and annihilation of particles. (For further reading on this subject, refer to Alexander L. Fetter and John Dirk Walecka, Quantum Theory of Many-Particle Systems.)
Many-particle states and many-particle Schrödinger equation

For almost all cases of interest, the Hamiltonian takes the form

\[ H = \sum_{i=1}^{N} T(x_i) + \frac{1}{2} \sum_{i \neq j=1}^{N} V(x_i, x_j), \]  

(B.1)

where \( T(x_i) \) denotes the kinetic energy of the \( i \)-th particle, \( V(x_i, x_j) \) is the potential energy of the interaction between the \( i \)-th and \( j \)-th particles, and \( x_k \) is a short-hand notation specifying all degrees of freedom of the \( k \)-th particle. For most applications we can restrict our considerations to one and two-body interactions of the above form only. The time-dependent Schrödinger equation then becomes

\[ i\hbar \frac{\partial}{\partial t} \Psi_N(x_1, x_2, ..., x_N, t) = H \Psi_N(x_1, x_2, ..., x_N, t), \]  

(B.2)

where \( \Psi_N \) denotes a time-dependent \( N \)-particle wave function. In order to completely determine the dynamics of the physical system it is necessary to specify boundary conditions and symmetry requirements along with the Schrödinger equation.

It is useful to expand the many-particle function in a complete set of states, usually taken to be a collection of ordered single-particle wave functions (e.g. the eigenstates of a harmonic oscillator or plane wave functions). The time-dependent \( N \)-particle wave function is then written as

\[ \Psi_N(x_1, x_2, ..., x_N, t) = \sum_{\alpha_1, \alpha_2, ..., \alpha_N} C(\alpha_1, \alpha_2, ..., \alpha_N, t) \psi_{\alpha_1}(x_1) \psi_{\alpha_2}(x_2) \cdots \psi_{\alpha_N}(x_N). \]  

(B.3)
where $\psi_{\alpha_k}(x_k)$ is the single-particle wave function occupied by the $k$-th particle, $x_k$ stands for the coordinates (space, spin, etc.) of that particle, $\alpha_k$ denotes the set of quantum labels necessary to determine this single-particle state, and the sum goes over all possible combinations of $N$ single-particle states.

Note that the coefficients $C(\alpha_1, \alpha_2, \ldots, \alpha_N, t)$ now contain all the complications of the $N$-particle wave function $\Psi_N$, like boundary conditions, symmetry requirements, time dependence, etc. This becomes strikingly clear when inserting the expansion B.3 into the Schrödinger equation. For each set $\alpha_1, \alpha_2, \ldots, \alpha_N$, one obtains a differential equation which involves single-particle and two-particle matrix elements of the operators $T$ and $V$, respectively, thus leading to an infinite set of coupled differential equations for the time-dependent coefficients $C(\alpha_1, \alpha_2, \ldots, \alpha_N, t)$. Imposing additional conditions like boundary and symmetry requirements on the coefficients makes the problem of solving the Schrödinger equation extremely complex. Hence one is forced to be creative and to use a different approach.

### B.2 Symmetry requirements

The procedure outlined above attempts to solve the Schrödinger equation by expanding the $N$-particle wave function in a complete set of single-particle basis functions, thus obtaining a set of coupled differential equations along with additional requirements for the expansion coefficients. Alternatively, one can construct $N$-particle basis functions which possess certain desired symmetries ab initio. An arbitrary $N$-particle state $\Psi_N$ can then be expanded in terms of this symmetry-adapted basis. Inserting $\Psi_N$ into the Schrödinger Equation B.2 will still lead to a system of coupled equations but the resulting relations for the expansion coefficients are much easier to handle since some of the symmetries are already built-in in the basis functions. It is instructive to consider two of the more important symmetries in physics that have been incorporated in the construction of certain $N$-particle basis functions in the past: particle permutation and rotational symmetries. The latter symmetry plays an important role in most physical applications since the
majority of all physical systems display some rotational invariance. The first issue, however, is at least as important, since all quantum systems deal with bosons or fermions, that is, with particles which are symmetric or antisymmetric with respect to particle exchanges. Other symmetries that are relevant for many applications, which cannot be discussed in detail here, are time inversion, parity, charge conjugation, translational invariance, etc.

B.2.1 Particle permutation symmetry

It is worthwhile to display the explicit form of $N$-particle basis functions with given particle permutation symmetry since those expressions are frequently found in the literature on many-body problems. Furthermore, the structure of the basis functions and matrix elements of physically relevant interactions, when written in ordinary quantized form, using symmetrized (antisymmetrized) products of single-particle states, suggest a different, more practical formalism for dealing with systems of many identical particles.

Let us consider a system of identical fermions (bosons). The many-particle wave functions have to be totally antisymmetric (symmetric), that is they have to obey the following relation:

$$
\Psi_N(..., x_1, ..., x_j, ..., t) = \pm \Psi_N(..., x_j, ..., x_1, ..., t). \quad (B.4)
$$

where the upper sign applies for bosons, the lower for fermions. We now wish to expand $\Psi_N$ in a basis of completely antisymmetric states $\Phi^F_N$ for a fermion system or in a basis of completely symmetric states $\Phi^S_N$ for bosons. This can be done by introducing two new operators, the symmetrization operator $S$ and the antisymmetrization operator $A$. Both act on a product of single-particle states by building linear combinations of all possible permutations of the particles coordinates $x_1, x_2, ..., x_N$.

Fermions

Let there be $\Omega$ different single-particle states $\psi_\alpha$ and let $N$ be the number of particles to be distributed among those $\Omega$ states. If we are dealing with fermions each state can be occupied by
zero or one particle only, hence \( \Omega \geq N \) must hold. If the states \( \alpha_1, \alpha_2, \ldots, \alpha_N \) are occupied by one fermion, the appropriate totally antisymmetric wave function is given as:

\[
\Phi^F_{\alpha_1, \alpha_2, \ldots, \alpha_N}(x_1, x_2, \ldots, x_N) = \sqrt{\frac{1}{N!}} A \psi_{\alpha_1}(x_1) \psi_{\alpha_2}(x_2) \cdots \psi_{\alpha_N}(x_N). \tag{B.5}
\]

where the antisymmetrization operator \( A \) is defined as

\[
A \equiv \frac{1}{N!} \sum_P (-1)^{\sigma_P} P. \tag{B.6}
\]

Here the sum runs over all permutations of the particles in the occupied single-particle states \( \alpha_1, \alpha_2, \ldots, \alpha_N \), the phase factor \( (-1)^{\sigma_P} \) is +1 for an even or -1 for an odd permutation, and \( \frac{1}{\sqrt{N!}} \) is a normalization factor which ensures that \( A^2 = A \) holds. The above basis function can also be written as a Slater determinant:

\[
\Phi^F_{\alpha_1, \alpha_2, \ldots, \alpha_N}(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix}
\psi_{\alpha_1}(x_1) & \psi_{\alpha_1}(x_2) & \cdots & \psi_{\alpha_1}(x_N) \\
\psi_{\alpha_2}(x_1) & \psi_{\alpha_2}(x_2) & \cdots & \psi_{\alpha_2}(x_N) \\
\vdots & \vdots & \ddots & \vdots \\
\psi_{\alpha_N}(x_1) & \psi_{\alpha_N}(x_2) & \cdots & \psi_{\alpha_N}(x_N)
\end{vmatrix}. \tag{B.7}
\]

Note that the subscripts of the basis function \( \Phi^F_{\alpha_1, \alpha_2, \ldots, \alpha_N} \) are necessary in order to specify which of the \( \Omega \) available states are occupied. One can use a notation slightly different from but completely equivalent to the one used in Equations B.5–B.7 by employing occupation numbers \( n_1, n_2, \ldots, n_\Omega \), where \( n_i \) denotes the number of fermions in the \( i \)-th state of our ordered sequence of single-particle states, that is \( n_i = 0 \) or 1, and \( \sum_{i=1}^\Omega n_i = N \). Thus, \( \Phi^F_{\alpha_1, \alpha_2, \ldots, \alpha_N}(x_1, x_2, \ldots, x_N) \) can be specified completely by the sequence \( n_1, n_2, \ldots, n_\Omega \), hence we write \( \Phi^F_{n_1, n_2, \ldots, n_\Omega}(x_1, x_2, \ldots, x_N) \). Obviously, the permutations \( P \) in Equation B.6 have to be understood as permutations among particles in the occupied states only. An arbitrary antisymmetric \( N \)-particle wave function can then be expressed
where the sum goes over all allowed choices of occupation numbers $n_1, n_2, \ldots, n_\Omega$.

**Bosons**

When dealing with $N$ bosons and $\Omega$ available single-particle states $\psi_1, \psi_2, \ldots, \psi_\Omega$, it is possible to have zero, one, two, or more particles in the same state. Suppose there are $n_i$ bosons on the state $\psi_i$, with $n_i = 0, 1, 2, \ldots$. The corresponding totally symmetric $N$-particle wave function is then given by

$$
\psi^B_{n_1, n_2, \ldots, n_\Omega}(x_1, x_2, \ldots, x_N) = \sqrt{N!} \mathcal{S} \psi_1(x_1) \psi_2(x_2) \cdots \psi_{n_1}(x_{n_1}) \psi_{n_1+1}(x_{n_1+1}) \cdots \psi_\Omega(x_N),
$$

where the symmetrization operator is defined as

$$
\mathcal{S} \equiv N! \sum_P P,
$$

and $P$ permutes the $N$ particles between the occupied states of the collection $\psi_1, \psi_2, \ldots, \psi_\Omega$. The normalization factor is given by $N = n_1! n_2! \cdots n_\Omega! / \Omega!$ (The number of possible distributions of $N$ objects in $\Omega$ boxes with $n_1$ in the first, $n_2$ in the second, $\ldots$, $n_\Omega$ in the $\Omega$-th is given by $n_1! n_2! \cdots n_\Omega! / \Omega!$.)

Note that it is necessary to label $\Phi^B$ with subscripts $n_1, n_2, \ldots, n_\Omega$ in order to indicate how many particles occupy the states $\psi_1, \psi_2, \ldots, \psi_\Omega$. An arbitrary $N$-boson state can then be expressed as

$$
\psi^B_N(x_1, x_2, \ldots, x_N, t) = \sum_{n_1, n_2, \ldots, n_\Omega} f(n_1, n_2, \ldots, n_\Omega, t) \phi^B_{n_1, n_2, \ldots, n_\Omega}(x_1, x_2, \ldots, x_N).
$$

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where the sum runs over all possible partitions \( n_1, n_2, ..., n_\Omega \) such that \( n_i = 0, 1, 2, ... \) and \( \sum_{i=1}^\Omega n_i = N \).

The above considerations indicate that, due to the symmetry requirements, the \( N \)-particle basis functions defined in B.5 and B.9 are completely determined by the information of which single-particle states are occupied. This suggests that one should deal with many-particle states by using a representation in which the occupied single-particle states, rather than the particle coordinates, are specified. (Clearly, this depends on the existence of a complete, ordered set of single-particle states.)

**B.2.2 Rotational invariance**

Most physically relevant systems are rotationally invariant, that is \([\mathcal{H}, \vec{J}] = 0\), where \( \mathcal{H} \) is the Hamiltonian of the system and \( \vec{J} \equiv (J_z, J_y, J_x) \) denotes the angular momentum operator. The above basis functions, defined in Equations B.5–B.7 and B.9–B.10, however, are, in general, not rotationally invariant. In order to obtain eigenstates of \( I_z \), one has to construct linear combinations of the \( \Phi_{(n_i)}^F \) or \( \Phi_{(n_i)}^R \). Alternatively, one can construct multi-particle eigenfunctions of \( \vec{J}^2 \) and subsequently symmetrize or anti-symmetrize those. For the sake of brevity the construction of these states will not be shown here. However, it is worthwhile to note that even for the example of only a few nucleons in a single \( j \)-shell one has to introduce so-called coefficients of fractional parentage. These are very important for the description of nuclear systems, but they turn out to be sophisticated enough to occupy whole chapters of textbooks.

**B.2.3 Other symmetries**

Symmetries other than particle permutation symmetries and rotational invariance play an important role in physical many-body systems. In order to be able to incorporate these symmetries in the choice of the basis functions, one has to resort to new techniques. In the next section such a technique, the formalism of second quantization, will be introduced.
B.3 Occupation number formalism - Many-particle wave functions in second quantization

We start by defining a fixed orthonormal and complete set of single-particle states. We then introduce the formalism of second quantization:

Let \( |0\rangle \) denote the vacuum (or reference state) of the system, that is, the state with no particles present or, for the example of the nuclear or atomic shell model, the closed-major-shell state.

We define a time-independent operator \( a_\alpha^\dagger (b_\alpha^\dagger) \), which creates a fermion (boson) in the abstract time-independent state \( \alpha \), as well as its Hermitean adjoint \( a_\alpha (b_\alpha) \):

\[
\begin{align*}
a_\alpha^\dagger |0\rangle &= |\alpha\rangle & b_\alpha^\dagger |0\rangle &= |\alpha\rangle \\
\langle 0|a_\alpha &= \langle \alpha| & \langle 0|b_\alpha &= \langle \alpha| \\
[a_\alpha^\dagger]^\dagger &= a_\alpha & [b_\alpha^\dagger]^\dagger &= b_\alpha .
\end{align*}
\] (B.12)

The Hermitean adjoint \( a_\alpha, (b_\alpha) \) can be interpreted as an operator which destroys a particle in the state \( \alpha \).

\[
\begin{align*}
a_\alpha |\alpha\rangle &= |0\rangle & b_\alpha |\alpha\rangle &= |0\rangle \\
\langle \alpha|a_\alpha^\dagger &= \langle 0| & \langle \alpha|b_\alpha^\dagger &= \langle 0| .
\end{align*}
\] (B.13)

Given a coordinate representation \( \langle x_k | \), the above states corresponds to single-particle wave functions:

\[
\begin{align*}
|\alpha\rangle &\longrightarrow \psi_\alpha(x_k) = \langle x_k |\alpha\rangle \\
\langle \alpha| &\longrightarrow \psi_\alpha^*(x_k) = \langle \alpha|x_k\rangle .
\end{align*}
\] (B.14)
One can show that for the time-independent abstract state vectors defined above to satisfy the symmetry requirements (only one fermion per state allowed / an arbitrary number of bosons possible), it is sufficient and necessary to impose the following conditions on the operators:

- **Anti-commutation (commutation) relations**

Fermions

\[ \{a_\alpha, a_\alpha'\} = \{a_\alpha^\dagger, a_\alpha'^\dagger\} = 0 \]

Bosons

\[ [b_\alpha, b_\alpha'] = [b_\alpha^\dagger, b_\alpha'^\dagger] = 0 \]

\[ \{a_\alpha^\dagger, a_\alpha'\} = \delta_{\alpha\alpha'} \]

\[ [b_\alpha, b_\alpha'] = \delta_{\alpha\alpha'} \]

where \{X, Y\} \equiv XY + YX and \[X, Y\] \equiv XY - YX. The anti-commutation/commutation relations are equivalent to the following relations:

- **Action of the creation and annihilation operators:**

Fermions

\[ a_\alpha^\dagger a_\alpha |n_\alpha\rangle = |n_\alpha + 1\rangle \]

\[ a_\alpha |n_\alpha = 1\rangle = |n_\alpha = 0\rangle \]

\[ a_\alpha |n_\alpha = 0\rangle = 0 \]

Bosons

\[ b_\alpha^\dagger b_\alpha |n_\alpha\rangle = |n_\alpha + 1\rangle \]

\[ b_\alpha |n_\alpha = 0\rangle = |n_\alpha = 1\rangle \]

\[ b_\alpha |n_\alpha = 1\rangle = 0 \]

\[ b_\alpha^\dagger b_\alpha |n_\alpha = 0\rangle = |n_\alpha = 1\rangle \]

where we have \( n_i = 1 \) or 0 for fermions, and for bosons the \( n_i \) are simply nonnegative integers.

We immediately see that we can define a number operator \( N_\alpha = a_\alpha^\dagger a_\alpha (N_\alpha = b_\alpha^\dagger b_\alpha) \) which counts the number of fermions (bosons) in the state \( \alpha \).

- **Many-particle states:** The generalization to many-particle states with proper symmetry (totally antisymmetric / totally symmetric) is straightforward. For fermions we obtain:

\[ |n_1 n_2 \ldots n_\Omega\rangle = \frac{\Omega!}{\prod_{i=1}^{\Omega} n_i!} \frac{(a_\alpha^\dagger)^{n_\alpha}}{\sqrt{n_\alpha!}} |0\rangle \]
where $n_i = 0$ or $1$ corresponds to the number of fermions in the $i$-th state. The action of the creation and annihilation operators on the many-fermion states is given by:

$$a_i^+ |n_1, \ldots, n_i, \ldots, n_\Omega\rangle = \begin{cases} (-1)^{n_i} |n_1, \ldots, n_i + 1, \ldots, n_\Omega\rangle & \text{if } n_i = 0 \\ 0 & \text{otherwise} \end{cases}$$ \hspace{1cm} (B.18)

$$a_i |n_1, \ldots, n_i, \ldots, n_\Omega\rangle = \begin{cases} (-1)^{n_i} |n_1, \ldots, n_i - 1, \ldots, n_\Omega\rangle & \text{if } n_i = 1 \\ 0 & \text{otherwise} \end{cases}$$ \hspace{1cm} (B.19)

$$\sigma_i = n_1 + n_2 + \ldots + n_{i-1}$$ \hspace{1cm} (B.20)

Analogously, one has the following expressions for bosons:

$$|n_1 n_2 \ldots n_\Omega\rangle = \prod_{i=1}^{\Omega} \frac{(b_i^+)^{n_i}}{\sqrt{n_i!}} |0\rangle ,$$ \hspace{1cm} (B.21)

where $n_i$ corresponds to the number of bosons in the $i$-th state. The action of the creation and annihilation operators is given by:

$$b_i^+ |n_1, \ldots, n_i, \ldots, n_\Omega\rangle = \sqrt{n_i + 1} |n_1, \ldots, n_i + 1, \ldots, n_\Omega\rangle$$ \hspace{1cm} (B.22)

$$b_i |n_1, \ldots, n_i, \ldots, n_\Omega\rangle = \sqrt{n_i} |n_1, \ldots, n_i - 1, \ldots, n_\Omega\rangle .$$ \hspace{1cm} (B.23)

The many-particle states defined above are totally anti-symmetric (totally symmetric) if and only if the fermion (boson) creation and annihilation operators obey the anti-commutation (commutation) relations of Equation B.15. With the above conventions the states are also orthonormal.

### B.4 Operators in second quantization

In order for the occupation number formalism to be useful for a description of the dynamics of a many-particle system, one has to recast not only the wave functions of the system in second
quantized form, but also the operators that occur in the Hamiltonian. Before proceeding to the explicit forms of the physically relevant operators, we will review some important definitions. We will also take a look at the ordinary first quantized forms of one and two body operators which act on \( N \)-fermion systems in order to motivate the corresponding expressions in second quantized form. In Subsection B.4.3 we will then give the appropriate second quantized operators and verify their forms.

**B.4.1 Definitions**

The following definitions play an important role in the context of second quantization:

**Definition** A symmetric operator \( O \) is an operator which acts in the same way on each particle in a given many-body wave function. That is, \( O \) commutes with \( P \), \( OP=PO \), where \( P \) denotes an arbitrary particle permutation. [The operators that act on many-particle states with given symmetry have to be symmetric in order to preserve the symmetry of the function.]

**Definition** A general symmetric one-body operator for a system of \( N \) identical particles is given by

\[
\mathcal{F} = \sum_{i=1}^{N} f(x_i),
\]  

(B.24)

where \( f(x_i) \) only acts on the particle with the coordinates \( x_i \).

**Definition** A general symmetric two-body operator for a system of \( N \) identical particles is given by

\[
\mathcal{G} = \sum_{i<j=1}^{N} g(x_i, x_j),
\]  

(B.25)

where \( g(x_i, x_j) \) is the interaction between particles \( i \) and \( j \) with coordinates \( x_i \) and \( x_j \).

**Definition** A general symmetric \( M \)-body operator for a system of \( N \) identical particles (with \( M \leq N \)) is given by

\[
\mathcal{K} = \sum_{i_1<i_2<...<i_M=1}^{N} k(x_{i_1}, x_{i_2}, ..., x_{i_M}).
\]  

(B.26)
where \( k(x_1, x_2, \ldots, x_{1M}) \) is the interaction between the \( M \) particles with the coordinates \( x_1, x_2, \ldots, x_{1M} \).

### B.4.2 Matrix elements of one and two body fermion operators in first quantized form

We now evaluate the one-body operator \( \mathcal{F} \) and the two-body operator \( \mathcal{G} \) between two \( N \)-fermion states, expressed in ordinary first quantized form, in order to determine the matrix elements of these operators. This will help us to verify the corresponding expressions in second quantized form in the next subsection since the matrix elements should not depend on whether we employ the first or second quantization formalism.

**One-body operators**

Let \( \Phi_N \) and \( \Phi'_N \) denote two totally antisymmetric normalized \( N \)-particle basis functions. Here we choose to represent \( \Phi_N \) and \( \Phi'_N \) in terms of Slater determinants since this choice turns out to yield the clearest and most compact derivation of the relevant matrix elements. The results that are obtained are of course independent of how one writes down the basis functions. We thus write:

\[
\langle \Phi_{\alpha_1, \alpha_2, \ldots, \alpha_N}^F(x_1, x_2, \ldots, x_N) | \mathcal{F} | \Phi_{\alpha_1, \alpha_2, \ldots, \alpha_N}^F(x_1, x_2, \ldots, x_N) \rangle
\]

\[
= \sum_{i=1}^{N} \int dx_1 dx_2 \ldots dx_N \Phi_{\alpha_i', \alpha_{i+1}, \ldots, \alpha_N}^F(x_1, x_2, \ldots, x_N) f(x_i) \Phi_{\alpha_1, \alpha_2, \ldots, \alpha_N}^F(x_1, x_2, \ldots, x_N)
\]

\[
= \sum_{i=1}^{N} \sum_{l,k=1}^{N} \int dx_i \psi_{\alpha_i}^*(x_i) f(x_i) \psi_{\alpha_k}(x_i) \times
\]

\[
\times \frac{(-1)^{l+k}}{N} \int dx_1 \ldots dx_l \ldots dx_i \ldots dx_k \ldots dx_N \Phi_{\alpha_i', \ldots, \alpha_{i+k}, \ldots, \alpha_N}^F(x_1, \ldots, \tilde{x}_l, \ldots, \tilde{x}_k, \ldots, x_N) \Phi_{\alpha_1, \ldots, \alpha_{i+k}, \ldots, \alpha_N}^F(x_1, \ldots, \tilde{x}_l, \ldots, x_N)
\]

\[
= \sum_{i=1}^{N} \sum_{l,k=1}^{N} \frac{(-1)^{l+k}}{N} \langle \psi_{\alpha_i}(x_i) | f(x_i) | \psi_{\alpha_k}(x_i) \rangle \delta_{\alpha_i' \ldots \alpha_{i+k} \ldots \alpha_N}(\alpha_1 \ldots \alpha_{i+k} \ldots \alpha_N).
\]

(A caret above a symbol indicates that the particular quantity is omitted, for example the expression \( \Phi_{\alpha_1 \ldots \alpha_{i+k} \ldots \alpha_N}^F(x_1, \ldots, \tilde{x}_l, \ldots, \tilde{x}_k, \ldots, x_N) \) denotes the \((N-1)\)-fermion wave function that one obtains from the \( N \)-fermion function \( \Phi_{\alpha_1, \alpha_2, \ldots, \alpha_N}^F(x_1, x_2, \ldots, x_N) \) by deleting the \( k \)-th row and \( i \)-th column in the Slater determinant B.7.)
There are three distinct cases that we have to consider:

- **Case 1**: The collections \( \{ \alpha' \} \equiv \{ \alpha'_1, \alpha'_2, ..., \alpha'_N \} \) and \( \{ \alpha \} \equiv \{ \alpha_1, \alpha_2, ..., \alpha_N \} \) differ by more than one pair of quantum labels. It immediately follows that:

\[
\langle \Phi_{\{ \alpha' \}}^F | \mathcal{F} | \Phi_{\{ \alpha \}}^F \rangle = 0 .
\] (B.28)

- **Case 2**: The collections \( \{ \alpha' \} \) and \( \{ \alpha \} \) differ by exactly one pair of quantum labels, say \( \alpha'_\lambda \neq \alpha_\kappa \). Then the sum over \( l, k \) collapses to one term only, namely the one with \( k = \kappa, l = \lambda \), and it follows that:

\[
\langle \Phi_{\{ \alpha' \}}^F | \mathcal{F} | \Phi_{\{ \alpha \}}^F \rangle = \frac{1}{N} \sum_{i=1}^{N} (-1)^{\kappa+\lambda} \psi_{\alpha'_\lambda}(x_i) f(x_i) | \psi_{\alpha_\kappa}(x_i) \rangle
\] (independent of index \( i \))

\[
(\psi_{\alpha'_\lambda}(x_i) f(x_i) | \psi_{\alpha_\kappa}(x_i) \rangle = (-1)^{\kappa+\lambda} \psi_{\alpha'_\lambda}(x_i) f | \psi_{\alpha_\kappa}(x_i) \rangle .\] (B.29)

- **Case 3**: We have \( \{ \alpha' \} = \{ \alpha \} \). The double sum collapses into a simple sum and we obtain:

\[
\langle \Phi_{\{ \alpha' \}}^F | \mathcal{F} | \Phi_{\{ \alpha \}}^F \rangle = \frac{1}{N} \sum_{i=1}^{N} \sum_{k=1}^{N} \langle \psi_{\alpha_k}(x_i) f(x_i) | \psi_{\alpha_k}(x_i) \rangle
\]

\[
\sum_{k=1}^{N} \langle \psi_{\alpha_k} | f \psi_{\alpha_k} \rangle .\] (B.30)

**Two-body operators**

Similarly, one can calculate the matrix elements of a two-body operator by proceeding as before. We consider matrix elements of \( \mathcal{G} \) between two \( N \)-fermion basis functions, written as Slater determinants:

\[
\langle \Phi_{\alpha_1, \alpha_2, ..., \alpha_N}^F (x_1, x_2, ..., x_N) | \mathcal{G} | \Phi_{\alpha_1, \alpha_2, ..., \alpha_N}^F (x_1, x_2, ..., x_N) \rangle
\]

\[
= \sum_{i<j} \int dx_1 dx_2 \cdot \cdot \cdot dx_N \Phi_{\alpha_1, \alpha_2, ..., \alpha_N}^{F,*} (x_1, x_2, ..., x_N) g(x_i, x_j) \Phi_{\alpha_1, \alpha_2, ..., \alpha_N}^{F} (x_1, x_2, ..., x_N)
\]

\[
= \frac{2}{N(N-1)} \sum_{i<j} \sum_{\sum_i^N} (-1)^{k+i+m+n} \int dx_1 dx_2 \{ \psi_{\alpha_m}^{*} (x_i) \psi_{\alpha_n}^{*} (x_j) - \psi_{\alpha_m}^{*} (x_i) \psi_{\alpha_n}^{*} (x_j) \}
\]

\[
\times g(x_i, x_j) \psi_{\alpha_k} (x_i) \psi_{\alpha_k} (x_j) .
\]
Here we have to distinguish between four different cases:

- **Case 1:** The collections \( \{ \alpha' \} \) and \( \{ \alpha \} \) differ by more than two pairs of quantum labels. It immediately follows that:

\[
\langle \Phi^{F}_{\{\alpha'\}} | \Phi^{F}_{\{\alpha\}} \rangle = 0 . \tag{B.32}
\]

- **Case 2:** The collections \( \{ \alpha' \} \) and \( \{ \alpha \} \) differ by exactly two pairs of quantum labels, say \( \alpha'_\kappa \neq \alpha_\mu, \alpha_\nu \) and \( \alpha'_\lambda \neq \alpha_\mu, \alpha_\nu \). Then the fourfold sum (over \( k, l, m, \) and \( n \)) collapses to one term only, namely the one with \( k = \kappa, l = \lambda, m = \mu, n = \nu \). From this it now follows that:

\[
\langle \Phi^{F}_{\{\alpha'\}} | \Phi^{F}_{\{\alpha\}} \rangle = \frac{2}{N(N-1)} \sum_{i<j}^{N} (-1)^{k+l+m+n} \left( \langle \psi_{\alpha'_\kappa}(x_i) \psi_{\alpha'_\lambda}(x_j) | g(x_i, x_j) | \psi_{\alpha_\kappa}(x_i) \psi_{\alpha_\lambda}(x_j) \rangle - \langle \psi_{\alpha_\kappa}(x_i) \psi_{\alpha_\lambda}(x_j) | g(x_i, x_j) | \psi_{\alpha'_\kappa}(x_i) \psi_{\alpha'_\lambda}(x_j) \rangle \right) \delta_{\{\alpha'_1 \ldots \hat{\alpha'_\kappa} \ldots \alpha'_\lambda \ldots \alpha_N\}} \delta_{\{\alpha_1 \ldots \hat{\alpha_\kappa} \ldots \alpha_\lambda \ldots \alpha_N\}} . \tag{B.33}
\]

since the expression in the curly brackets in the second line is independent of the indices \( i \) and \( j \) and since there are \( \frac{N(N-1)}{2} \) different possibilities to pick two numbers \( i, j \) which satisfy \( i < j \) from a total of \( N \) distinct numbers.

- **Case 3:** The collections \( \{ \alpha' \} \) and \( \{ \alpha \} \) differ by exactly one pair of quantum labels, say \( \alpha'_\kappa \neq \alpha_\lambda \). Then the fourfold sum collapses to a simple sum, since \( m = \mu, k = \kappa, l = n \) must hold and hence it follows that:

\[
\langle \Phi^{F}_{\{\alpha'\}} | \Phi^{F}_{\{\alpha\}} \rangle
\]
\[
\left(\Phi_{\alpha'}^{F} | \mathcal{G} | \Phi_{\alpha}^{F}\right) = \sum_{k<l}^{N} \left\{ \langle \psi_{\alpha'}^{n} | \psi_{\alpha}^{l} | \psi_{\alpha}^{k} \psi_{\alpha} \rangle - \langle \psi_{\alpha'}^{n} | \psi_{\alpha}^{l} | \psi_{\alpha} \psi_{\alpha} \rangle \right\}.
\]

(B.35)

**B.4.3 One and two body operators in second quantized form**

If one carefully considers the expressions for the matrix elements of \( F \) and \( G \) in Subsection B.4.2, one can deduce the form of those operators in second quantization. Here, however, we will proceed as follows: We will "guess" the correct form and then verify that the second quantized operator "sandwiched" between two \( N \)-particle wave functions will yield the same results as the corresponding first quantized operators. First, however, we will give the matrix elements of some special fermion operators, namely \( a_{\alpha}^{\dagger} \), \( a_{\alpha} \), and \( a_{\alpha}^{\dagger}, a_{\alpha} \).

**Matrix elements of simple fermion operators**

It is very easy to see that the following relationships for the matrix elements of the fermion creation and annihilation operators hold:

\[
\begin{align*}
(n_{1} \ldots n_{i} = 0 \ldots n_{\Omega} | a_{i} | n_{1} \ldots n_{i} = 1 \ldots n_{\Omega}) &= (-1)^{\sigma}, \\
(n_{1} \ldots n_{i} = 1 \ldots n_{\Omega} | a_{i}^{\dagger} | n_{1} \ldots n_{i} = 0 \ldots n_{\Omega}) &= (-1)^{\sigma}.
\end{align*}
\]

(B.36)  

(B.37)
Here we have used the following abbreviation:

$$\sigma_i = n_1 + n_2 + \ldots + n_{i-1}.$$  

(B.39)

The above results were obtained by using the anti-commutation relations of the fermion creation and annihilation operators (see Equation B.15).

Matrix elements of a one body fermion operator in second quantization

We claim that a one-body operator $F$ can be expressed in second quantized form as follows:

$$F = \sum_{\beta, \gamma} \langle \beta|f|\gamma \rangle a_\beta^\dagger a_\gamma.$$  

(B.40)

Note that $\langle \beta|f|\gamma \rangle$ is the matrix element of $f$ between the single-particle states $\beta$ and $\gamma$. We verify the above claim by insertion:

$$F \equiv \langle \Phi_{\{\alpha\}'}|F|\Phi_{\{\alpha\}} \rangle$$

$$= \langle 0|a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \ldots a_{\alpha_N}^\dagger \rangle \sum_{\beta, \gamma} \langle \beta|f|\gamma \rangle a_\beta^\dagger a_\gamma (a_{\alpha_1}^\dagger a_{\alpha_N}^\dagger \ldots a_{\alpha_1}^\dagger 0)$$

$$= \sum_{\beta, \gamma} \langle \beta|f|\gamma \rangle \langle 0|a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \ldots a_{\alpha_N}^\dagger a_\beta^\dagger a_\gamma a_{\alpha_1}^\dagger a_{\alpha_N}^\dagger \ldots a_{\alpha_1}^\dagger 0 \rangle.$$  

(B.41)

If we now use the anti-commutation relations for the fermion creation and annihilation operators, we obtain the following:

- Case 1: $F = 0$ if $\{\alpha\}'$ and $\{\alpha\}$ differ by more than one set of quantum numbers.
- Case 2: If the collections $\{\alpha\}'$ and $\{\alpha\}$ differ by exactly one pair of quantum labels, say $\alpha_{\lambda}' \neq \alpha_{\kappa}$, we have:

$$F = (-1)^{\kappa + \lambda} \langle \alpha_{\lambda}'|f|\alpha_{\kappa} \rangle.$$  

(B.42)
• Case 3: If we have \( \{\alpha'\} = \{\alpha\} \), we find that the sum over \( \beta \) and \( \gamma \) reduces to a simple sum since for \( \langle 0|a_{\alpha_1}a_{\alpha_2} \ldots a_{\alpha_N} a^\dagger_{\alpha_N} a^\dagger_{\alpha_{N-1}} \ldots a_{\alpha_0}|0 \rangle \neq 0 \) to hold we must have \( \beta = \gamma \). The sum runs over all \( \alpha_k \), for \( k = 1, \ldots, N \) and we thus obtain:

\[
F = \sum_{k=1}^N \langle \alpha_k|f|\alpha_k \rangle .
\] (B.43)

We obtained exactly what we expected, hence we conclude that \( F \) has the form stated in Equation B.40.

Matrix elements of a two-body fermion operator in second quantization

Similarly we claim that a two-body operator can be expressed in the second quantized form as follows:

\[
G = \frac{1}{4} \sum_{\beta,\gamma,\delta,\epsilon} \langle \beta\gamma|g|\delta\epsilon \rangle a^\dagger_{\beta} a^\dagger_{\gamma} a_{\delta} a_{\epsilon} .
\] (B.44)

(Note the order of the indices in the two-particle matrix element.) We verify the claim by insertion:

\[
G = \langle \Phi^F_{\{\alpha'\}|G|\Phi^F_{\{\alpha\}} \rangle = \frac{1}{4} \sum_{\beta,\gamma,\delta,\epsilon} \langle \beta\gamma|g|\delta\epsilon \rangle a^\dagger_{\beta} a^\dagger_{\gamma} a_{\delta} a_{\epsilon} (a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \ldots a^\dagger_{\alpha_N} a_{\alpha_{N-1}} \ldots a_{\alpha_0}|0 \rangle .
\] (B.45)

Here we have to distinguish between four different cases:

• Case 1: \( G = 0 \) if the collections \( \{\alpha'\} \) and \( \{\alpha\} \) differ by more than two pairs of quantum labels.

• Case 2: If the collections \( \{\alpha'\} \) and \( \{\alpha\} \) differ by exactly two pairs of quantum labels, say \( \alpha_\kappa \neq \alpha'_\mu, \alpha'_\nu \) and \( \alpha_\lambda \neq \alpha'_\mu, \alpha'_\nu \). Then the sum over \( \beta, \gamma, \delta, \) and \( \epsilon \) reduces to those terms only for which we have \( \{\beta, \gamma\} = \{\alpha'_\mu, \alpha'_\nu\} \) and \( \{\delta, \epsilon\} = \{\alpha_\kappa, \alpha_\lambda\} \). Applying the relations (15), we

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obtain:

\[ G = (-1)^{λ+κ+μ+ν}\{\langle α'_μα'_ν|g|α_κα_λ\rangle - \langle α'_μα'_ν|g|α_λα_κ\rangle \}. \]  

(B.46)

• Case 3: The collections \{α'\} and \{α\} differ by exactly one pair of quantum labels, say \(α_κ \neq α'_κ\). Then the fourfold sum collapses to a simple sum only, since α'_μ = β or γ, and α_κ = δ or ε must hold and hence it follows that:

\[ G = \sum_γ (-1)^{μ+κ}\{\langle α'_μγ|g|α_κγ\rangle - \langle α'_μγ|g|γα_κ\rangle \}. \]  

(B.47)

• Case 4: If \{α'\} = \{α\} the fourfold sum reduces to a double sum, namely:

\[ G = \sum_β\sum_γ \{\langle βγ|g|β_γ\rangle - \langle βγ|g|γβ_γ\rangle \}. \]  

(B.48)

Matrix elements of a general many-body fermion operator in second quantization

By induction one can show that the above expressions generalize as follows:

\[ \mathcal{O} = \frac{1}{M!N!} \sum_{\{α_1,\ldots,α_M\},\{β_1,\ldots,β_N\}} \langle α_1α_2\ldotsα_M|β_1β_2\ldotsβ_N \rangle a_{α_1}^{\dagger}a_{α_2}^{\dagger}\ldots a_{α_M}^{\dagger}a_{β_N}a_{β_{N-1}}\ldots a_{β_2}a_{β_1}. \]  

(B.49)

Note that this operator transforms a \(N\)-particle state into a \(M\)-particle state.

Matrix elements of boson operators

We would like to note that the derivation of expressions for many-body boson operators follow through analogously to the above derivations. In general, the expressions for the boson operators look like the ones for the fermion operators, with the fermion operators \(a_{α_i}^{\dagger}, a_{α_i}\) replaced by boson operators \(b_{α_i}^{\dagger}, b_{α_i}\).
B.5 Applications of the second quantization formalism to nuclear physics

The formalism of second quantization is used very frequently in modern physics. Here we list only a few applications from the field of nuclear physics:

- The use of angular momentum coupling and recoupling techniques as well as various extensions of these techniques to other symmetry groups, e.g. SU(3), Sp(2j+1), Sp(3,R), etc., allow one to construct many-particle basis states and operators with well-defined transformation properties. This, in conjunction with the generalized Wigner-Eckart theorem, simplifies the calculation of matrix elements between the many-particle basis states tremendously.

- Hole creation and annihilation operators can be introduced. These play an important role in nuclear physics applications, which include particle-hole excitations.

- Pair creation and annihilation operators can be introduced. These are useful in nuclear physics applications, where pairing correlations play a major role.

- The $N$-particle Hilbert space can be extended to include $M$-particle states ($M \neq N$) of the same symmetry. Thus it becomes possible to formulate the transformation of a $N$-particle state into a $M$-particle state and vice versa, as is necessary, for example, in a description of $\beta$-decay.

- Relations between the coefficients of fractional parentage (c.f.p.) and the single-particle matrix elements of $a_n^\dagger$, $a_n$, exists, which can be used to determine the numerical values of the c.f.p.s.

B.6 Miscellaneous

Here we list a few definitions which the reader may encounter when dealing with problems in the second quantization formalism.
Normal ordered product of operators A product of operators is in "normal" order relative to a given reference state \(|0\rangle\) when all creation operators are at the left of the annihilation operators. In bringing a product of operators to the normal order, a number of permutations has to be carried out. When interchanging the creation and annihilation operators, one has to keep track of the sign of the permutation. Possible Kronecker \(\delta\)-symbols, however, are not considered. Notation: \(N(ABC\ldots)\) or \(\langle ABC\ldots\rangle\) (Note that the results depend on the choice of the reference state.) An example is given by:

\[
N(a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta) \equiv a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta = -a^\dagger_\alpha a_\gamma a^\dagger_\beta a_\delta = a^\dagger_\alpha a_\gamma a^\dagger_\beta a_\delta.
\] (B.50)

Time-ordered product of operators A product of operators is in "time-ordered" form if the operators with the latest time occur on the left, and operators with earlier times show up on the right. Logically, the time-ordered product is only defined for the case of time-dependent operators.

Contraction of two operators The contraction of two operators is the expectation value of the operator product with respect to the reference state. The result is simply a number which is denoted as \(\hat{A}\hat{B}\). An example for this contraction is given by:

\[
N(a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta) = -\langle0|a^\dagger_\alpha a_\gamma\langle0| a^\dagger_\beta a_\delta\rangle.
\] (B.51)

Wick's Theorem A product of a number of operators can be written as the sum of all contracted normal ordered products of the operators (considering partially and fully contracted terms, as well as the uncontracted):

\[
A_1 A_2 \ldots A_n \equiv N(A_1, A_2, \ldots, A_n) = \sum_{\alpha<\beta} N(A_1, A_2, \ldots, \hat{A}_\alpha \hat{A}_\beta, \ldots, A_n)
\]
\[
+ \sum_{\alpha < \beta, \gamma < \delta} N(A_1, A_2, \ldots, \underbrace{A_\alpha \ldots A_\beta}_{\text{left}}, \underbrace{A_\gamma \ldots A_\delta}_{\text{middle}}, \ldots, A_n)
+ \ldots
+ \ldots
+ \text{fully contracted terms}.
\] (B.52)

An example for the application of Wick's theorem is given by:

\[
A_\alpha A_\beta = N(A_\alpha A_\beta) + \underbrace{A_\alpha A_\beta}_{\text{right}}.
\] (B.53)
Appendix C

The SU(3) Scheme

This appendix is a compilation of definitions and relations that are essential for analytic work in the SU(3) and symplectic schemes. The results listed here are frequently used throughout this dissertation.

C.1 Basis States in the SU(3) Scheme

Many-particle shell-model schemes start with a single-particle picture and distribute nucleons among the lowest available single-particle levels subject to the constraint of the Pauli Exclusion Principle. The constructed $m$-particle wave functions must be totally anti-symmetric under particle interchange, that is, they must belong to the anti-symmetric irrep of the permutation group $S_m$. For the example of a space-spin product function $\Phi = \phi\chi$ this means that a symmetric spatial part $\phi$ requires an anti-symmetric spin part $\chi$ and vice versa. Since the particle permutation symmetry of a wave function and its transformation properties under a basis change are directly related, a classification of a $m$-particle wave function according to irreps of $U(n)$, the unitary group in $n$ dimensions, simultaneously specifies the irrep of $S_m$, the permutation group of $m$ objects, to which each $m$-particle wave function belongs. Thus, in order to satisfy the Pauli Principle, it suffices to consider only one of these groups: most schemes focus on $U(n)$, since it is simpler to deal with.
The irreducible representations of the group $U(n)$ can be labeled by a set of non-negative integers $[f] \equiv [f_1 f_2 \ldots f_n]$, such that $f_1 \geq f_2 \geq \ldots \geq f_n$. Since this set of numbers may be considered a partition of the sum $\sum_{i=1}^{n} f_i$, it can be represented by a so-called Young tableaux, which has $f_i$ blocks in the $i$-th row:

\[
\begin{array}{cccc}
& & & f_1 \\
& & f_2 \\
& \vdots \\
& & & f_n
\end{array}
\]

In the Elliott scheme many-particle wave functions are labeled by the irreps of $U(k\Omega)$, where $\Omega = (\eta + 1)(\eta + 2)/2$ is the spatial degeneracy of the $\eta$-th oscillator shell and $k$ denotes the intrinsic degrees of freedom ($k = 2$ for an identical particle system and $k = 4$ in a spin-isospin formalism), and the irreps of an appropriate chain of subgroups. Separation of the full $k\Omega$ dimensional space into its space and spin (or spin-isospin) parts corresponds to the reduction of $U(k\Omega)$ to its subgroup $U(\Omega) \otimes U(k)$. The Pauli Principle requires that the $U(k\Omega)$ irreps associated with nuclear many-particle wave functions belong to the totally anti-symmetric representation $[1^m] \equiv [1 \ldots 1]$, $m$ being the number of particles in the shell. It then follows that the irreps $[f] = [f_1 f_2 \ldots f_n]$ of $U(\Omega)$, specifying the spatial symmetry, and the irreps $[f^c] = [f_1 f_2]$ of $U(2)$, labeling the complementary spin symmetry, must be related by row-column interchange for the associated Young shapes. For the spin-isospin formalism $[f^c]$ is given by $[f_1 f_2 f_3 f_4]$. Further classification of the basis states can be obtained through the irreducible representations of subgroups of $U(\Omega)$ and $U(k)$. For applications to nuclear spectroscopy it is important that the $U(n)$ chain contain $SO(3)$, the rotational group in three dimensions, so that the relevant angular momentum is a good quantum number. Ideally, there would be a chain of subgroups which includes $U(\Omega)$ and $SO(3)$ such that the irreducible representation labels associated with $U(\Omega)$, $SO(3)$, and every intermediate group in the chain combine to uniquely specify each basis state. In practice, this is possible only for very special particle configurations. For the collection of states of a major harmonic oscillator shell, however, Elliott’s $SU(3)$ furnishes a relevant subgroup of
U(Ω) which contains SO(3). The unimodular group SU(3) is obtained from U(3) by removing those transformations which simply introduce an overall change of phase. As a consequence, those representations of SU(3) which correspond to tableaux differing only in the number of complete columns become equivalent:

\[ [g + f_1, g + f_2, g + f_3] \cong [f_1, f_2, f_3] \]

\[
\begin{array}{c|c}
 g & f_1 \\
\hline
 g & f_2 \\
\hline
 g & f_3 \\
\end{array}
\cong
\begin{array}{c|c}
 f_1 \\
\hline
 f_2 \\
\hline
 f_3 \\
\end{array}
\]

Hence two labels are sufficient to specify the irreps of SU(3): traditionally the symbol \((\lambda\mu)\), with \(\lambda = f_1 - f_2, \mu = f_2 - f_3\), is used to label the irreducible representations of SU(3).

The reduction \(U(\Omega) \supset SU(3) \supset O(3)\) yields quantum labels \((\lambda\mu)\) and \(L\) with multiplicities \(\alpha\) and \(\kappa\), respectively. The multiplicity labels are needed to distinguish between multiple occurrences of \((\lambda\mu)\) in a given \([\ell]\) symmetry and multiple \(L\) values in a given \((\lambda\mu)\) irrep. For fixed \((\lambda\mu)\) the multiplicity index \(\kappa\) runs from 1 to \(\kappa_{\text{max}}\), where \(\kappa_{\text{max}}\) is given by

\[
\kappa_{\text{max}} = \max \left( 0, \left\lfloor \frac{\lambda + \mu + 2 - L}{2} \right\rfloor \right) - \max \left( 0, \left\lfloor \frac{\lambda + 1 - L}{2} \right\rfloor \right) - \max \left( 0, \left\lfloor \frac{\mu + 1 - L}{2} \right\rfloor \right)
\]

(C.1)

with \([\ldots]\) denoting the largest integer or Gauss function.

The unitary group U(k) - corresponding to the intrinsic part of the wave function - can be reduced similarly: \(U(2) \supset SU_S(2)\) for identical particles, where the spin \(S\), which labels the SU(2) irrep, is fixed once \([\ell]\) is specified, since \(S = (f_1^2 - f_2^2)/2\). In the spin-isospin formalism, one has the reduction \(U(4) \supset SU_S(2) \otimes SU_T(2)\), which yields quantum numbers \(\beta(ST)\), where \(S\) and \(T\) denote spin and isospin and \(\beta\) gives the multiplicity of \((ST)\) in the \(U(4)\) irrep \([\ell]\). In Figure C.2 we show schematically the breakup of the full model space into irreps of \(U(\Omega) \otimes U(4)\) and subgroups of these symmetries.
Figure C.1: Breakup of the $U(4\Omega)$ model space. Shown is the direct product $U(4\Omega) \supset U(\Omega) \supset U(4)$ and further reductions of $U(\Omega)$ and $U(4)$. The associated irrep labels for the spatial symmetries are given on the left, and those for the intrinsic symmetries are shown on the right.

Thus one can construct $m$-particle states $|\Phi\rangle$ which are labeled as

$$|\Phi\rangle = |m[f]_{\alpha(\lambda\mu)\kappa L, S; JM}\rangle$$

for an identical-particle system, and

$$|\Phi\rangle = |m[f]_{\alpha(\lambda\mu)\kappa L, \beta(ST); JM, M_T}\rangle$$

in the spin-isospin formalism. Here $[f]$ labels the irreducible representation (irrep) of $U(\Omega)$, $(\lambda\mu)$ refers to the irrep of $SU(3)$, $L$ and $S$ are the orbital and spin angular momenta of the system, respectively, and $J$ is the total angular momentum with projection $M$ along the $z$-axis of the laboratory frame. The quantum numbers that identify the irreps of $U(k\Omega)$ and $U(k)$ are suppressed in C.2 and C.3 since they are fixed by the number of nucleons in the valence shell, the labels $[f]$ of $U(\Omega)$ and the requirement of overall anti-symmetry. Actually, the particle number $m$ is also redundant since $\sum_{i=1}^{\Omega} f_i = m$, but it is normally listed for the sake of clarity. Basis states for light nuclei ($A \approx 28$) with neutrons and protons in the $\eta$-th harmonic oscillator shell are of the form C.3. For heavy nuclei, where protons and neutrons occupy different major oscillator shells, basis states of each subsystem are of the form given in C.2: a basis for the combined neutron-proton
system is obtained via coupling of the neutron and proton states in the well-known SO(3) (angular momentum) coupled (SU(3) uncoupled) scheme or in the SU(3) coupled scheme. The techniques for coupling and re-coupling states in the SU(3) scheme will be discussed in the next section of this appendix.

C.2 Coupling and Recoupling Coefficients in the SU(3) Scheme

This part of the Appendix summarizes the results of a series of important articles on the topic, such as articles by H. A. Jahn and J. Hope [106], G. Racah [130], K. T. Hecht et al. [91, 92, 93, 97, 18, 129, 98, 99, 94], J. P. Draayer et al. [51, 59, 1, 47, 26, 117], M. F. O'Reilly [125], D. J. Millener [119], J. D. Vergados [173] etc.

C.2.1 SU(3) Wigner coefficients: Coupling of two SU(3) irreps

If \( \alpha \) represents a set of labels used to distinguish orthonormal basis states within a given SU(3) representation, the Wigner coefficients \( \langle (\lambda_1\mu_1)\alpha_1; (\lambda_2\mu_2)\alpha_2 \mid (\lambda\mu)\alpha \rangle_\rho \) are defined as the elements of a unitary transformation between coupled and uncoupled orthonormal irreps of SU(3) in the \( \alpha \)-scheme [91, 47]:

\[
|{(\lambda\mu)\alpha}_\rho = \sum_{\alpha_1, \alpha_2} \langle (\lambda_1\mu_1)\alpha_1; (\lambda_2\mu_2)\alpha_2 \mid (\lambda\mu)\alpha \rangle_\rho \langle (\lambda_1\mu_1)\alpha_1 | (\lambda_2\mu_2)\alpha_2 \rangle,
\]

(C.4)

and the inverse transformation is given by:

\[
|{(\lambda_1\mu_1)\alpha_1} \rangle \langle (\lambda_2\mu_2)\alpha_2 \rangle = \sum_{\alpha} \langle (\lambda_1\mu_1)\alpha_1; (\lambda_2\mu_2)\alpha_2 \mid (\lambda\mu)\alpha \rangle_\rho \langle (\lambda\mu)\alpha \rangle_\rho .
\]

(C.5)

Here \( \alpha = \epsilon \Lambda M_A \) for the SU(3) \( \supset \) SU(2) \( \otimes \) U(1) (canonical) group chain and \( \alpha = \kappa \ell m \) for the SU(3) \( \supset \) SO(3) reduction, and the conjugates of the relevant SU(3) basis states are given by [91, 47]:

\[
|{(\mu\lambda)\epsilon \Lambda M_A}^* = (-1)^{\frac{1}{2}(\lambda - \mu) - \frac{1}{2} \epsilon - M_A} |(\mu\lambda) - \epsilon \Lambda - M_A \rangle \text{ for } \alpha = \epsilon \Lambda M_A
\]
\[(\lambda \mu)_{\kappa \ell m}^{*} = (-1)^{\lambda + \mu + l - m} (\mu \lambda)_{\kappa \ell - m} \text{ for } \alpha = \kappa \ell m. \]  

(C.6)

The subgroup chains impose certain restrictions on the above couplings, for example \( \epsilon = \epsilon_1 + \epsilon_2 \), \( M_\Lambda = M_{\Lambda_1} + M_{\Lambda_2} \), and \( \Lambda = \Lambda_1 + \Lambda_2, \ldots, |\Lambda_1 - \Lambda_2| \) must hold for the canonical group chain, and the usual angular momentum coupling rules, \( l = l_1 + l_2, \ldots, |l_1 - l_2| \), apply for the chain containing \( \text{SO}(3) \).

The outer multiplicity label \( r = 1, 2, \ldots, r_{\text{max}} \) is used to distinguish multiple occurrences of a given \( (\lambda \mu) \) in the direct product \( (\lambda_1 \mu_1) \times (\lambda_2 \mu_2) : r = 1, 2, \ldots, r_{\text{max}} \), where \( r_{\text{max}} \) denotes the number of possible couplings \( (\lambda_1 \mu_1) \times (\lambda_2 \mu_2) \), and the possible \( (\lambda \mu) \) irreps in the product can be obtained by coupling the appropriate Young diagrams [87, 63]. O’Reilly [125] gives an analytical formula for the possible products that result from the coupling of two \( \text{SU}(3) \) irreps:

**Product of two \( \text{SU}(3) \) irreps**

Since their introduction by Littlewood [113, 114, 115], Young diagrams have served as a valuable tool for the characterization of group representations. For example, through their use with Littlewood rules the reduction of Kronecker (outer) products can be determined [18]. This method, however, turns out to be too cumbersome for all but the simplest cases. Thus efforts have been expended into finding practical alternatives [49, 117]. An important simplification is given in [125], where O’Reilly determines a closed formula in terms of \( p, q, r, \) and \( s \) for the decomposition of the outer product \( (p,q) \times (r,s) \) of finite-dimensional irreps of \( \text{SU}(3) \). He finds the following formula for arbitrary positive integers \( p, q, r, \) and \( s \):

\[(r, s) \times (p, q) = \bigoplus_{k=0}^{\min(q,r+s)} \bigoplus_{j=0}^{\min(s, q, r + s - k)} \bigoplus_{i=\max(0, j - s + k)}^{\min(p-j+k, r)} (r + p - j - 2i + k, s + q + i - j - 2k).\]  

(C.7)
For \( q = 0 \) the formula reduces to:

\[
(r, s) \times (p, 0) = \bigoplus_{j=0}^{\min(s,p)} \bigoplus_{i=0}^{\min(p-j,r)} (r + p - j - 2i, s - j + i).
\]  
(C.8)

and for \( s = q = 0 \), O’Reilly obtains:

\[
(r, 0) \times (p, 0) = \bigoplus_{i=0}^{\min(r,p)} (r + p - 2i, i).
\]  
(C.9)

For the special case \( p = 1, q = 0 \) (\( r, s \neq 0 \)) the formula becomes:

\[
(r, s) \times (1, 0) = (r + 1, s) \oplus (r - 1, s + 1) \oplus (r, s - 1).
\]  
(C.10)

and for \( p = 0, q = 1 \) (\( r, s \neq 0 \)):

\[
(r, s) \times (0, 1) = (r, s + 1) \oplus (r + 1, s - 1) \oplus (r - 1, s).
\]  
(C.11)

O’Reilly furthermore derives necessary and sufficient conditions for a SU(3) irrep \((m, n)\) to appear as summand in the products \((r, s) \times (p, q)\) (see [125, Proposition 7]).

Reduced coupling coefficients

It is possible to factor out the dependence of the above SU(3) \( \supset \) SO(3) and SU(3) \( \supset \) SU(2) \( \otimes \) U(1) Wigner coupling coefficients on the \( M\) or \( M_A\) subgroup labels, respectively, by defining so-called double-barred or “reduced” SU(3) coupling coefficients:

\[
\langle (\lambda_1 \mu_1) \kappa_1 \ell_1 m_1; (\lambda_2 \mu_2) \kappa_2 \ell_2 m_2 | (\lambda \mu) \kappa \ell m \rangle_p
\]

\[
= \left( \frac{\langle (\lambda_1 \mu_1) \kappa_1 \ell_1; (\lambda_2 \mu_2) \kappa_2 \ell_2 | (\lambda \mu) \kappa \ell \rangle_p}{\text{reduced Wigner coefficient}} \right) \left( \ell_1 m_1, \ell_2 m_2 | \ell m \right)_{\text{geometric part}}.
\]  
(C.12)
for $\alpha = \kappa M$, and

$$
\left( \begin{array}{c}
\langle \lambda_1 \mu_1 \rangle \varepsilon_1 \Lambda_1 \Lambda_1; \langle \lambda_2 \mu_2 \rangle \varepsilon_2 \Lambda_2 \Lambda_2 | \langle \lambda \mu \rangle \varepsilon \Lambda \Lambda \rangle \\
\end{array} \right)_\rho
$$

reduced Wigner coefficient

$$
\left( \begin{array}{c}
\langle \lambda_1 \mu_1 \rangle \varepsilon_1 \Lambda_1; \langle \lambda_2 \mu_2 \rangle \varepsilon_2 \Lambda_2 || \langle \lambda_3 \mu_3 \rangle \varepsilon \Lambda \rangle \\
\end{array} \right)_\rho
$$

geometric part

\[(C.13)\]

for $\alpha = \epsilon \Lambda \Lambda$. The "geometric" part $\langle \ldots \rangle$ is simply a SU(2) Clebsch-Gordan coefficient. From the unitarity of the full SU(3) Wigner and the ordinary SU(2) Clebsch-Gordan coefficients it follows that the double-bar coefficients are also unitary. With the phase convention introduced by Draayer and Akiyama [47] they become real, and therefore orthogonal.

**Symmetry relations**

Draayer and Akiyama [47] give a prescription for a unique determination, including the phases, of all SU(3) $\supset$ SU(2) $\otimes$ U(1) Wigner coefficients and derive their relevant conjugation and symmetry properties. Since the SU(3) $\supset$ SO(3) reduction is linked to the SU(3) $\supset$ SU(2) $\otimes$ U(1) reduction via the coefficients of the transformation between the $\alpha = \kappa M$ and the $\alpha = \epsilon \Lambda \Lambda$ schemes [59], it suffices to determine the conjugation relationship and symmetry properties for the SU(3) $\supset$ SU(2) $\otimes$ U(1) chain only. The corresponding SU(3) $\supset$ SO(3) results follow then from the known relationships among the transformation brackets between the two schemes. These relations are given in [47] and a computer code which allows for a numerical determination of SU(3) $\supset$ SU(2) $\otimes$ U(1) and SU(3) $\supset$ SO(3) Wigner coefficients, as well as SU(3) Racah coefficients, is published in [1].

Explicit algebraic expressions for Wigner coefficients which are of particular interest in p-shell and ds-shell nuclear shell-model calculations are tabulated in [91] for the canonical subgroup chain and in [173, 99] for the SU(3) $\supset$ SO(3) chain. Given these conjugation relation and symmetry properties for the full SU(3) Wigner coefficient, equivalent relations for reduced SU(3) coupling coefficients can then be derived by making use of the proper symmetry relations for Clebsch-Gordan coefficients [169].
The most important of the symmetry relations of the SU(3) Wigner coefficients is the one that involves a $1 \leftrightarrow 3$ interchange of the quantum labels:

\[
\langle (\lambda_1 \mu_1) \alpha_1; (\lambda_2 \mu_2) \alpha_2 \mid (\lambda_3 \mu_3) \alpha_3 \rangle \rho = (-1)^{\varphi + \chi_2} \sqrt{\frac{\dim(\lambda_3 \mu_3)}{\dim(\lambda_1 \mu_1)}} \langle (\lambda_3 \mu_3) \alpha_3; (\mu_2 \lambda_2) \alpha_2 \mid (\lambda_1 \mu_1) \alpha_1 \rangle \rho .
\]  
(C.14)

where

\[
\varphi = (\lambda_1 + \mu_1) + (\lambda_2 + \mu_2) - (\lambda_3 + \mu_3) .
\]  
(C.15)

The dimension of the SU(3) irrep $(\lambda \mu)$ is given by:

\[
dim(\lambda \mu) = \frac{1}{2}(\lambda + 1)(\mu + 1)(\lambda + \mu + 2) ,
\]  
(C.16)

and $\bar{\alpha}$ and $\chi_i$ are defined as follows:

- For $\alpha = \epsilon \Lambda M_\lambda$, we have $\bar{\alpha} = -\epsilon \Lambda - M_\lambda$ and $\chi_i = \frac{1}{3}(\lambda_i - \mu_i) - \frac{1}{6} \epsilon_i - M_\lambda$.
- For $\alpha = \kappa l m$, we have $\bar{\alpha} = \kappa l - m$ and $\chi_i = (\lambda_i - \mu_i) + l_i - m_i$.

(C.17)

The $1 \leftrightarrow 2$ interchange is more complicated since it requires a "geometrical" phase matrix $\Phi$:

\[
\langle (\lambda_1 \mu_1) \alpha_1; (\lambda_2 \mu_2) \alpha_2 \mid (\lambda_3 \mu_3) \alpha_3 \rangle \rho
\]

\[
= \sum_{\rho'} \Phi_{\rho' r'}[(\lambda_1 \mu_1), (\lambda_2 \mu_2); (\lambda_3 \mu_3)]; \langle (\lambda_3 \mu_3) \alpha_3; (\lambda_1 \mu_1) \alpha_1 \mid (\lambda_3 \mu_3) \alpha_3 \rangle \rho' .
\]  
(C.18)

where the phase matrix $\Phi$ is a special case of the recoupling coefficient $Z$ (which will be introduced in Appendix C.2.2):

\[
\Phi_{\rho' r'}[(\lambda_1 \mu_1), (\lambda_2 \mu_2); (\lambda_3 \mu_3)] = Z[(\lambda_1 \mu_1)(00)(\lambda_3 \mu_3)(\lambda_2 \mu_2); (\lambda_1 \mu_1)\rho(\lambda_2 \mu_2)\rho'] .
\]  
(C.19)

For the special case where the SU(3) coupling $\{(\lambda_1 \mu_1) \times (\lambda_2 \mu_2)\} \rightarrow (\lambda_3 \mu_3)$ is unique, that is, when
\[ \rho_{\text{max}} = 1, \text{the phase matrix reduces to a simple phase factor:} \]

\[ \Phi_{11}[(\lambda_1 \mu_1), (\lambda_2 \mu_2); (\lambda_3 \mu_3)] = (-1)^\rho = (-1)^{(\lambda_1 + \mu_1) + (\lambda_2 + \mu_2) - (\lambda_3 + \mu_3)}. \tag{C.20} \]

Furthermore, for the special case \( \lambda_i = \mu_i \) with \( i = 1, 2, 3 \) we have

\[ \Phi_{\rho \rho'}[(\lambda_1 \lambda_1), (\lambda_2 \lambda_2); (\lambda_3 \lambda_3)] = (-1)^{\rho + \rho' - \rho} \delta_{\rho \rho'}. \tag{C.21} \]

Another set of useful relations involve the conjugate irreps \((\lambda \mu) = (\mu \lambda)\) of \((\lambda \mu)\); for the canonical group chain we have the equation:

\[ \langle (\lambda_1 \mu_1)\epsilon_1 \Lambda_1 M_{\lambda_1}; (\lambda_2 \mu_2)\epsilon_2 \Lambda_2 M_{\lambda_2} | (\lambda_3 \mu_3)\epsilon_3 \Lambda_3 M_{\lambda_3} \rangle_{\rho} \]

\[ = (-1)^{\rho + \rho' - \rho} \langle (\mu_1 \lambda_1) - \epsilon_1 \Lambda_1 - M_{\lambda_1}; (\mu_2 \lambda_2) - \epsilon_2 \Lambda_2 - M_{\lambda_2} | (\mu_3 \lambda_3) - \epsilon_3 \Lambda_3 - M_{\lambda_3} \rangle_{\rho}. \tag{C.22} \]

and for \( \alpha = klm \) we have:

\[ \langle (\lambda_1 \mu_1)\kappa_1 l_1 m_1; (\lambda_2 \mu_2)\kappa_2 l_2 m_2 | (\lambda_3 \mu_3)\kappa_3 l_3 m_3 \rangle_{\rho} \]

\[ = (-1)^{\rho + \rho' - \rho + l_1 + l_2 - l_3} \langle (\mu_1 \lambda_1)\kappa_1 l_1 - m_1; (\mu_2 \lambda_2)\kappa_2 l_2 - m_2 | (\mu_3 \lambda_3)\kappa_3 l_3 - m_3 \rangle_{\rho}. \tag{C.23} \]

Employing the above relations and making use of the symmetry properties of the Clebsch-Gordan coefficients, one obtains the 1 \( \leftrightarrow \) 3 interchange relations for the double-barred SU(3) coupling coefficients; for \( \alpha = \epsilon \Lambda M \) we have:

\[ \langle (\lambda_1 \mu_1)\epsilon_1 \Lambda_1; (\lambda_1 \mu_1)\epsilon_2 \Lambda_2 | (\lambda_1 \mu_1)\epsilon_3 \Lambda_3 \rangle_{\rho} \]

\[ = (-1)^{\rho + \frac{1}{2}(\lambda_2 - \mu_2) - \frac{1}{2} \epsilon_2 + \Lambda_3 - \Lambda_1} \sqrt{\frac{\dim(\lambda_3 \mu_3)}{\dim(\lambda_1 \mu_1)}} \sqrt{\frac{2\Lambda_1 + 1}{2\Lambda_3 + 1}} \]
\[ x((\lambda_1 \mu_1)\epsilon_3 \Lambda_3; (\mu_2)\lambda_2 \epsilon_2 \Lambda_2 || (\lambda_1 \mu_1)\epsilon_1 \Lambda_1)_{\rho} \]  

(C.24)

and for \( \alpha = \kappa \lambda m \) we find:

\[ \langle (\lambda_1 \mu_1)\kappa_1 \lambda_1; (\lambda_2 \mu_2)\kappa_2 \lambda_2 || (\lambda_3 \mu_3)\kappa_3 \lambda_3 \rangle_{\rho} = (-1)^{\rho+\lambda_1+\mu_1+\lambda_2+\mu_2} \sqrt{\frac{\dim(\lambda_3 \mu_3)}{\dim(\lambda_1 \mu_1)}} \sqrt{\frac{2l_1 + 1}{2l_3 + 1}} \times \langle (\lambda_3 \mu_3)\kappa_3 \lambda_3; (\mu_2 \lambda_2)\kappa_2 \lambda_2 || (\lambda_1 \mu_1)\kappa_1 \lambda_1 \rangle_{\rho}. \]  

(C.25)

Under conjugation the reduced coupling coefficients behave as follows:

\[ \langle (\lambda_1 \mu_1)\epsilon_1 \Lambda_1; (\lambda_2 \mu_2)\epsilon_2 \Lambda_2 || (\lambda_3 \mu_3)\epsilon_3 \Lambda_3 \rangle_{\rho} = (-1)^{\rho+\mu_3-\rho+\lambda_1+\lambda_2-\lambda_3} \langle (\mu_1 \lambda_1) - \epsilon_1 \Lambda_1; (\mu_2 \lambda_2) - \epsilon_2 \Lambda_2 || (\mu_3 \lambda_3) - \epsilon_3 \Lambda_3 \rangle_{\rho}. \]  

(C.26)

for \( \alpha = \epsilon \Lambda M \), and

\[ \langle (\lambda_1 \mu_1)\kappa_1 \lambda_1; (\lambda_2 \mu_2)\kappa_2 \lambda_2 || (\lambda_3 \mu_3)\kappa_3 \lambda_3 \rangle_{\rho} = (-1)^{\rho+\mu_3-\rho} \langle (\mu_1 \lambda_1)\kappa_1 \lambda_1; (\mu_2 \lambda_2)\kappa_2 \lambda_2 || (\mu_3 \lambda_3)\kappa_3 \lambda_3 \rangle_{\rho} \]  

(C.27)

for \( \alpha = \kappa \lambda m \).

Orthonormality relations

There are several orthonormality relations for the Wigner SU(3) coupling coefficients that are frequently used [47]. The first of these is given by:

\[ \sum_{\alpha_1 \alpha_2} \langle (\lambda_1 \mu_1)\alpha_1; (\lambda_2 \mu_2)\alpha_2 || (\lambda \mu)\alpha \rangle_{\rho} \langle (\lambda_1 \mu_1)\alpha_1; (\lambda_2 \mu_2)\alpha_2 || (\lambda' \mu')\alpha \rangle_{\rho'} = \delta_{\lambda \lambda'} \delta_{\mu \mu'} \delta_{\rho \rho'}. \]  

(C.28)
For the canonical group chain, we also have

\[ \sum_{\rho} ((\lambda_1 \mu_1) \epsilon_1 \lambda_1 M_{\lambda_1}; (\lambda_2 \mu_2) \epsilon_2 \lambda_2 M_{\lambda_2}; (\lambda \mu) \epsilon \lambda M_{\lambda})_\rho \]
\[ \times ((\lambda_1 \mu_1) \epsilon_1' \lambda_1' M_{\lambda_1'}; (\lambda_2 \mu_2) \epsilon_2' \lambda_2' M_{\lambda_2'}; (\lambda \mu) \epsilon \lambda M_{\lambda})_\rho \]
\[ = \delta_{\epsilon_1} \delta_{\epsilon_2} \delta_{\lambda_1} \delta_{\lambda_2} \delta_{M_{\lambda_1}} \delta_{M_{\lambda_2}} \] (C.29)

with the summation running over all possible \{ - \} = \{ \rho, \lambda, \mu, \epsilon, \lambda, M_{\lambda} \} combinations. The analogous relation for the SU(3) ⊃ SO(3) group chain is given by

\[ \sum_{\rho} ((\lambda_1 \mu_1) \kappa_1 l_1 m_1; (\lambda_2 \mu_2) \kappa_2 l_2 m_2; (\lambda \mu) \kappa l m)_\rho \]
\[ \times ((\lambda_1 \mu_1) \kappa_1' l_1' m_1'; (\lambda_2 \mu_2) \kappa_2' l_2' m_2'; (\lambda \mu) \kappa l m)_\rho \]
\[ = \delta_{\kappa_1} \delta_{\kappa_2} \delta_{l_1} \delta_{l_2} \delta_{m_1} \delta_{m_2} \delta_{\kappa_1} \delta_{\kappa_2} \] (C.30)

with the summation running over all possible \{ - \} = \{ \rho, \lambda, \mu, \kappa, l, m \} combinations.

C.2.2 SU(3) Racah Coefficients: Coupling of three SU(3) irreps

If three SU(3) irreps \((\lambda_1 \mu_1), (\lambda_2 \mu_2), \text{ and } (\lambda_3 \mu_3)\) need to be coupled, the resulting SU(3) irrep \((\lambda \mu)\)

can be constructed in three different ways, depending on the order of the coupling:

i) \(\{(\lambda_1 \mu_1) \otimes (\lambda_2 \mu_2)\} \otimes (\lambda_3 \mu_3) \rightarrow (\lambda \mu)\), or

ii) \((\lambda_1 \mu_1) \otimes \{(\lambda_2 \mu_2) \otimes (\lambda_3 \mu_3)\} \rightarrow (\lambda \mu)\), or

iii) \(\{(\lambda_1 \mu_1) \otimes (\lambda_3 \mu_3)\} \otimes (\lambda_2 \mu_2) \rightarrow (\lambda \mu)\).

The transformation from one coupling order to another requires the introduction of a so-called

SU(3)-Racah or 6-(\lambda \mu) coefficient. More specifically, recoupling from scheme i) to ii) involves a unitary transformation with coefficients \(U[\{(\lambda_1 \mu_1)(\lambda_2 \mu_2)(\lambda \mu)(\lambda_3 \mu_3); (\lambda_1 \mu_1)(\lambda_2 \mu_2)(\lambda_3 \mu_3); (\lambda_1 \mu_1)(\lambda_2 \mu_2)(\lambda_3 \mu_3); (\lambda_1 \mu_1)(\lambda_2 \mu_2)(\lambda_3 \mu_3)]\)
[91]:

\begin{align*}
\left\{ \left[ (\lambda_1 \mu_1) \times (\lambda_2 \mu_2) \right]^{\rho_{12}} \left( \lambda_{12} \mu_{12} \right) \times (\lambda_3 \mu_3) \right\}^{\rho_{12,3} (\lambda_\mu) \alpha} \\
= \sum_{\{(\lambda_{12} \mu_{23}) p_{12} p_{32}\}} U[(\lambda_1 \mu_1) (\lambda_2 \mu_2) (\lambda_3 \mu_3); (\lambda_{12} \mu_{12}) \rho_{12} (\lambda_{23} \mu_{23}) \rho_{23} \rho_{1,23}] \\
\times \left\{ \left( \lambda_1 \mu_1 \right) \times \{ (\lambda_2 \mu_2) \times (\lambda_3 \mu_3) \}^{\rho_{23} (\lambda_{23} \mu_{23})} \right\}^{\rho_{12,23} (\lambda_\mu) \alpha}.
\end{align*}

(C.31)

where, as in the previous section, \( \alpha \) denotes a convenient set of subgroup labels for the irrep \( (\lambda \mu) \) and the outer multiplicity labels \( \rho_{12}, \rho_{12,3}, \rho_{23}, \) and \( \rho_{1,23} \) are needed to distinguish multiple occurrences of a given representation in the Kronecker product of the coupling. Whenever couplings are multiplicity-free, the \( \rho \)-labels may be omitted, as long as the meaning of the notation is unambiguous. Making use of the unitary property and reality of the transformation coefficients, one obtains the inverse transformation [98]:

\begin{align*}
\left\{ \left( \lambda_1 \mu_1 \right) \times \{ (\lambda_2 \mu_2) \times (\lambda_3 \mu_3) \}^{\rho_{23} (\lambda_{23} \mu_{23})} \right\}^{\rho_{1,23} (\lambda \mu) \alpha} \\
= \sum_{\{(\lambda_{12} \mu_{13}) p_{12} p_{13}\}} U[(\lambda_1 \mu_1) (\lambda_2 \mu_2) (\lambda_3 \mu_3); (\lambda_{12} \mu_{12}) \rho_{12} (\lambda_{23} \mu_{23}) \rho_{23} \rho_{1,23}] \\
\times \left\{ \left( \lambda_1 \mu_1 \right) \times \{ (\lambda_2 \mu_2) \times (\lambda_3 \mu_3) \}^{\rho_{12} (\lambda_{12} \mu_{12})} \right\}^{\rho_{1,23} (\lambda_\mu) \alpha}.
\end{align*}

(C.32)

The notation is a straightforward generalization of that introduced by Racah [169] for the 6-j symbols of SU(2).

Similarly, the transformation from scheme i) to scheme iii) requires a transformation coefficient \( Z[(\lambda_1 \mu_1)(\lambda_2 \mu_2)(\lambda_3 \mu_3); (\lambda_{12} \mu_{12}) \rho_{12} \rho_{12,3} (\lambda_{13} \mu_{13}) \rho_{13} \rho_{13,2}] \) which is defined through the following relation [119]:

\begin{align*}
\left\{ \left[ (\lambda_1 \mu_1) \times (\lambda_2 \mu_2) \right]^{\rho_{12} (\lambda_{12} \mu_{12})} \times (\lambda_3 \mu_3) \right\}^{\rho_{12,3} (\lambda_\mu) \alpha} \\
= \sum_{\{(\lambda_{13} \mu_{13}) p_{13} p_{13,2}\}} Z[(\lambda_2 \mu_2)(\lambda_1 \mu_1)(\lambda_3 \mu_3); (\lambda_{12} \mu_{12}) \rho_{12} \rho_{12,3} (\lambda_{13} \mu_{13}) \rho_{13} \rho_{13,2}].
\end{align*}
The $U$- and $Z$-functions depend only in the SU(3) representations involved in the coupling and not on the specific subgroup chain chosen to specify the states. Most of the SU(3) recoupling coefficients that are needed for ds-shell nuclear shell model calculations have been tabulated by K. T. Hecht [91], and a computer code that evaluates SU(3) Racah coefficients for arbitrary couplings and multiplicity was developed by Akiyama and Draayer [1]. Special cases and special symmetry properties of the SU(3) coefficients can be found in [98].

Relations between SU(3) Racah and Wigner coefficients

A straightforward generalization of the relations between SU(2) unitary recoupling coefficients and SU(3) Wigner coefficients [169] leads to the corresponding relationships between SU(3) unitary (Racah) recoupling and SU(3) Wigner coefficients [91]. In particular, the SU(3) $U$-coefficient can be expressed in terms of unitary 6j-symbols $U(j_1 j_2 j_3; j_{12} j_{23})$ and SU(3) Wigner coefficients. For $\alpha = \epsilon \Lambda M_\Lambda$, Hecht gives the following relation [91]:

$$U[(\lambda_1 \mu_1) (\lambda_2 \mu_2) (\lambda_3 \mu_3); (\lambda_{12} \mu_{12}) (\lambda_{23} \mu_{23})] = \sum_{\{-\}} U(\Lambda_1 \Lambda_2 \Lambda_3; \Lambda_{12} \Lambda_{23}) \langle (\lambda_1 \mu_1) \epsilon_1 \Lambda_1; (\lambda_2 \mu_2) \epsilon_2 \Lambda_2; (\lambda_3 \mu_3) \epsilon_3 \Lambda_3 \rangle \langle (\lambda_{12} \mu_{12}) \epsilon_{12} \Lambda_{12} \rangle_{\rho_{12}} \times \langle (\lambda_{23} \mu_{23}) \epsilon_{23} \Lambda_{23} \rangle_{\rho_{23}}$$

with the summation going over $\{-\} = \{\Lambda_1, \Lambda_2, \Lambda_3, \Lambda_{12}, \Lambda_{23}, \epsilon_1, \epsilon_2, \epsilon_3, \epsilon_{12}, \epsilon_{23}\}$. For $\alpha = \kappa \ell m$, the SU(3) Racah coefficient can be expressed as:

$$U[(\lambda_1 \mu_1) (\lambda_2 \mu_2) (\lambda_3 \mu_3); (\lambda_{12} \mu_{12}) (\lambda_{23} \mu_{23})] = \sum_{\{-\}} U(\Lambda_1 \Lambda_2 \Lambda_3; \Lambda_{12} \Lambda_{23}) \langle (\lambda_1 \mu_1) \epsilon_1 \Lambda_1; (\lambda_2 \mu_2) \epsilon_2 \Lambda_2; (\lambda_3 \mu_3) \epsilon_3 \Lambda_3 \rangle \langle (\lambda_{12} \mu_{12}) \epsilon_{12} \Lambda_{12} \rangle_{\rho_{12}} \times \langle (\lambda_{23} \mu_{23}) \epsilon_{23} \Lambda_{23} \rangle_{\rho_{23}}$$

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\[
\begin{align*}
&= \sum_{\{-\}} U(l_1l_2l_3; l_{12}l_{23}) \langle (\lambda_1\mu_1)\kappa_1l_1; (\lambda_2\mu_2)\kappa_2l_2\rangle \langle \lambda_{12}\mu_{12}\kappa_{12}l_{12}\rangle \rho_{12} \\
&\quad \times \langle (\lambda_1\mu_1)\kappa_1l_1; (\lambda_3\mu_3)\kappa_3l_3\rangle \langle \lambda_{13}\mu_{13}\kappa_{13}l_{13}\rangle \rho_{13,3} \\
&\quad \times \langle (\lambda_2\mu_2)\kappa_2l_2; (\lambda_3\mu_3)\kappa_3l_3\rangle \langle \lambda_{23}\mu_{23}\kappa_{23}l_{23}\rangle \rho_{23} \\
&\quad \times \langle (\lambda_1\mu_1)\kappa_1l_1; (\lambda_{23}\mu_{23})\kappa_{23}l_{23}\rangle \langle \lambda_{12}\mu_{12}\kappa_{12}l_{12}\rangle \rho_{1,2,3} ,
\end{align*}
\]  
(C.35)

with the summation going over \{-\} = \{l_1, l_2, l_3, l_{12}, l_{23}, \kappa_1, \kappa_2, \kappa_3, \kappa_{12}, \kappa_{23}\}. The \(Z\)- and \(U\)-coefficients are related to each other as follows [8]:

\[
\begin{align*}
Z(\lambda_2\mu_2)(\lambda_1\mu_1)(\lambda_3\mu_3); (\lambda_{12}\mu_{12})\rho_{12}\rho_{12,3} (\lambda_{13}\mu_{13})\rho_{13}\rho_{13,2} \\
= \sum_{\{l_{23}\mu_{23}\}p_{23}p_{1,2,3}} U(\lambda_1\mu_1)(\lambda_2\mu_2)(\lambda_3\mu_3); (\lambda_{12}\mu_{12})\rho_{12}\rho_{12,3} (\lambda_{23}\mu_{23})\rho_{23}\rho_{1,2,3} \\
\times \sum_{\rho_{13}} \Phi_{\rho_{13}} \rho_{13}^2 (\lambda_2\mu_2), (\lambda_3\mu_3); (\lambda_{23}\mu_{23}) \\
\times \sum_{\rho_{13}} U(\lambda_2\mu_2)(\lambda_3\mu_3)(\lambda_1\mu_1); (\lambda_{23}\mu_{23})\rho_{12,23} (\lambda_{13}\mu_{13})\rho_{13}\rho_{13,2} \\
\end{align*}
\]  
(C.36)

with the geometrical phase \(\Phi_{\rho\rho'}\) as defined in Equation C.19.

Furthermore, several useful relations for the \(U\)- and \(Z\)-recoupling coefficients are given in [91] for the SU(3) \(\supset\) SU(2) \(\otimes\) U(1) chain:

\[
\begin{align*}
\sum_{\rho_{1,2,3}} ( (\lambda_1\mu_1)\epsilon_1\Lambda_1; (\lambda_{23}\mu_{23})\epsilon_{23}\Lambda_{23} \parallel (\lambda_\mu)\epsilon_\Lambda ) \rho_{1,2,3} \\
\times U( (\lambda_1\mu_1)(\lambda_{23}\mu_{23})(\lambda_\mu)\epsilon_\Lambda; (\lambda_{12}\mu_{12})\rho_{12,23} (\lambda_{23}\mu_{23})\rho_{1,2,3} ) \\
= \sum_{\{-\}} ( (\lambda_2\mu_2)\epsilon_2\Lambda_2; (\lambda_3\mu_3)\epsilon_3\Lambda_3 \parallel (\lambda_{23}\mu_{23})\epsilon_{23}\Lambda_{23} ) \rho_{23} \\
\times ( (\lambda_1\mu_1)\epsilon_1\Lambda_1; (\lambda_2\mu_2)\epsilon_2\Lambda_2 \parallel (\lambda_{12}\mu_{12})\epsilon_{12}\Lambda_{12} ) \rho_{12} \\
\times ( (\lambda_{12}\mu_{12})\epsilon_{12}\Lambda_{12}; (\lambda_3\mu_3)\epsilon_3\Lambda_3 \parallel (\lambda_\mu)\epsilon_\Lambda ) \rho_{12,3} \\
\times U(\Lambda_1\Lambda_2\Lambda_3\Lambda_{12}\Lambda_{23} ) .
\end{align*}
\]  
(C.37)

where \{-\} = \{\epsilon_2, \epsilon_3, \epsilon_{12}, \Lambda_2, \Lambda_3, \Lambda_{12}\}. The analogous expression for the SU(3) \(\supset\) SO(3) chain is
given in [173]:

$$
\sum_{\rho_{123}} \langle (\lambda_1 \mu_1) \kappa_1 \lambda_1; (\lambda_2 \mu_2) \kappa_2 \lambda_2 \vert (\lambda \mu) \kappa \lambda \rangle_{\rho_{123}} \\
\times U((\lambda_1 \mu_1) (\lambda_2 \mu_2) (\lambda \mu) (\lambda_3 \mu_3); (\lambda_1 \mu_1 \lambda_2 \mu_2 \lambda_3 \mu_3 \lambda)_{\rho_{123}} (\lambda_1 \mu_1 \mu_2 \lambda_2)_{\rho_{123}})
$$

$$
= \sum_{\{-\}} \langle (\lambda_1 \mu_1) \kappa_1 \lambda_1; (\lambda_3 \mu_3) \kappa_3 \lambda_3 \vert (\lambda_2 \mu_2) \kappa_2 \lambda_2 \rangle_{\rho_{123}} \\
\times ((\lambda_1 \mu_1) \kappa_1 \lambda_1; (\lambda_2 \mu_2) \kappa_2 \lambda_2 \vert (\lambda_1 \mu_1 \lambda_2 \mu_2)_{\rho_{123}})
$$

where $\{\\{-\}\} = \{\kappa_2, \kappa_3, \kappa_4, \lambda_2, \lambda_3, \lambda_4\}$, and a similar relation is given by Millener [119] for the $Z$-coefficients:

$$
\sum_{\rho_{13.2}} \langle (\lambda_1 \mu_1 \lambda_1 \lambda_1; \lambda_1 \mu_2 \lambda_2 \vert (\lambda \mu \epsilon \lambda) \rangle_{\rho_{13.2}} \\
\times Z((\lambda_2 \mu_2) (\lambda_1 \mu_1) (\lambda \mu) (\lambda_3 \mu_3); (\lambda_1 \mu_1 \lambda_2 \mu_2 \lambda_3 \mu_3 \lambda)_{\rho_{13.2}} (\lambda_1 \mu_1 \mu_2 \lambda_2)_{\rho_{13.2}})
$$

$$
= \sum_{\{-\}} \langle (\lambda_1 \mu_1) \epsilon_1 \lambda_1; (\lambda_3 \mu_3) \epsilon_3 \lambda_3 \vert (\lambda_1 \mu_1 \lambda_2 \mu_2 \lambda_3 \mu_3 \lambda)_{\rho_{13.2}} \rangle_{\rho_{13.2}} \\
\times ((\lambda_1 \mu_1) \epsilon_1 \lambda_1; (\lambda_2 \mu_2) \epsilon_2 \lambda_2 \vert (\lambda_1 \mu_1 \lambda_2 \mu_2)_{\rho_{13.2}})
$$

where $\{\\{-\}\} = \{\epsilon_1, \epsilon_2, \epsilon_1, \lambda_1, \lambda_2, \lambda_3, \lambda_4\}$.

**C.2.3 SU(3) 9-($\lambda \mu$) coefficients: Coupling of four SU(3) irreps**

If the coupling of four SU(3) irreps $(\lambda_1 \mu_1), (\lambda_2 \mu_2), (\lambda_3 \mu_3)$ and $(\lambda_4 \mu_4)$ is required, the resulting irrep $(\lambda \mu)$ may be constructed in three different ways, depending on the order of the coupling:

i) $(\lambda_1 \mu_1) \otimes (\lambda_2 \mu_2) \otimes (\lambda_3 \mu_3) \otimes (\lambda_4 \mu_4) \rightarrow (\lambda \mu), \text{ or}$

ii) $(\lambda_1 \mu_1) \otimes (\lambda_3 \mu_3) \otimes (\lambda_2 \mu_2) \otimes (\lambda_4 \mu_4) \rightarrow (\lambda \mu), \text{ or}$
iii) \( \{(\lambda_1 \mu_1) \otimes (\lambda_4 \mu_4)\} \otimes \{(\lambda_2 \mu_2) \otimes (\lambda_3 \mu_3)\} \rightarrow (\lambda \mu). \)

In analogy to the SU(2) Jahn-Hope (or unitary 9-j) symbol it is thus possible to define a unitary SU(3) or 9-(\(\lambda \mu\)) symbol \([119]\), which effects the transformation from one coupling order to another.

In particular, for the transition from scheme i) to ii) we have:

\[
\begin{align*}
\left\{\left\{ (\lambda_1 \mu_1) \times (\lambda_2 \mu_2) \right\} \rho_{12} (\lambda_{12} \mu_{12}) \times \left\{ (\lambda_3 \mu_3) \times (\lambda_4 \mu_4) \right\} \rho_{34} (\lambda_{34} \mu_{34}) \right\} \rho_{12,34} (\lambda_\mu) a \\
= \sum \left\{ \begin{array}{ccc}
(\lambda_1 \mu_1) & (\lambda_2 \mu_2) & (\lambda_{12} \mu_{12}) & \rho_{12} \\
(\lambda_3 \mu_3) & (\lambda_4 \mu_4) & (\lambda_{34} \mu_{34}) & \rho_{34} \\
(\lambda_{13} \mu_{13}) & (\lambda_{24} \mu_{24}) & (\lambda_\mu) & \rho_{13,24} \\
\rho_{14} & \rho_{23} & \rho_{12,34}
\end{array} \right\} \\
\times \left\{ \left\{ (\lambda_1 \mu_1) \times (\lambda_3 \mu_3) \right\} \rho_{13} (\lambda_{13} \mu_{13}) \times \left\{ (\lambda_2 \mu_2) \times (\lambda_4 \mu_4) \right\} \rho_{24} (\lambda_{24} \mu_{24}) \right\} \rho_{13,24} (\lambda_\mu) a
\end{align*}
\]  

where \(\{-\} = \{\rho_{13}(\lambda_{13} \mu_{13}), \rho_{24}(\lambda_{24} \mu_{24})\}. \) Similarly, we obtain for the transformation from scheme i) to iii):

\[
\begin{align*}
\left\{\left\{ (\lambda_1 \mu_1) \times (\lambda_2 \mu_2) \right\} \rho_{12} (\lambda_{12} \mu_{12}) \times \left\{ (\lambda_3 \mu_3) \times (\lambda_4 \mu_4) \right\} \rho_{14} (\lambda_{34} \mu_{34}) \right\} \rho_{12,34} (\lambda_\mu) a \\
= \sum \left\{ \begin{array}{ccc}
(\lambda_1 \mu_1) & (\lambda_2 \mu_2) & (\lambda_{12} \mu_{12}) & \rho_{12} \\
(\lambda_4 \mu_4) & (\lambda_3 \mu_3) & (\lambda_{34} \mu_{34}) & \rho_{34} \\
(\lambda_{14} \mu_{14}) & (\lambda_{23} \mu_{23}) & (\lambda_\mu) & \rho_{14,23} \\
\rho_{14} & \rho_{23} & \rho_{12,34}
\end{array} \right\} \\
\times \sum \phi_{\rho_{14} \rho_{23} \rho_{14,23}} ((\lambda_3 \mu_3), (\lambda_4 \mu_4); (\lambda_{34} \mu_{34})) \\
\times \left\{ \left\{ (\lambda_1 \mu_1) \times (\lambda_3 \mu_3) \right\} \rho_{13} (\lambda_{13} \mu_{13}) \times \left\{ (\lambda_2 \mu_2) \times (\lambda_4 \mu_4) \right\} \rho_{24} (\lambda_{24} \mu_{24}) \right\} \rho_{13,24} (\lambda_\mu) a
\end{align*}
\]  

where \(\{-\} = \{\rho_{14}(\lambda_{14} \mu_{14}), \rho_{23}(\lambda_{23} \mu_{23})\}. \)
The unitary 9-(\(\lambda \mu\)) symbols can be expressed as a sum over SU(3) Wigner coupling coefficients:

\[
\begin{pmatrix}
(\lambda_1 \mu_1) & (\lambda_2 \mu_2) & (\lambda_{12}; \mu_{12}) & \rho_{12} \\
(\lambda_3 \mu_3) & (\lambda_4 \mu_4) & (\lambda_{34}; \mu_{34}) & \rho_{34} \\
(\lambda_{13}; \mu_{13}) & (\lambda_{24}; \mu_{24}) & (\lambda, \mu) & \rho_{13,24} \\
\rho_{13} & \rho_{24} & \rho_{12,34}
\end{pmatrix}
\]

\[
= \sum_{\alpha_1, \alpha_4} \left( (\lambda_1 \mu_1) \alpha_1; (\lambda_2 \mu_2) \alpha_2 | (\lambda_{12} \mu_{12}) \alpha_{12} \right) \rho_{13} \left( (\lambda_3 \mu_3) \alpha_3; (\lambda_4 \mu_4) \alpha_4 | (\lambda_{34} \mu_{34}) \alpha_{34} \right) \rho_{34} \\
\times \left( (\lambda_{13}; \mu_{13}) \alpha_{13}; (\lambda_{24}; \mu_{24}) \alpha_{24} | (\lambda, \mu) \alpha \right) \rho_{13,24} \left( (\lambda_1 \mu_1) \alpha_1; (\lambda_3 \mu_3) \alpha_3 | (\lambda_{13}; \mu_{13}) \alpha_{13} \right) \rho_{13} \\
\times \left( (\lambda_2 \mu_2) \alpha_2; (\lambda_4 \mu_4) \alpha_4 | (\lambda_{24}; \mu_{24}) \alpha_{24} \right) \rho_{34} \left( (\lambda_{12}; \mu_{12}) \alpha_{12}; (\lambda_{34}; \mu_{34}) \alpha_{34} | (\lambda, \mu) \alpha \right) \rho_{13,24}.
\]

(C.42)

with \(\alpha\) labeling the additional quantum numbers, as before. Using the \(Z\) and \(U\) coefficients defined above, the 9-(\(\lambda \mu\)) symbol can be expressed as [119]:

\[
\begin{pmatrix}
(\lambda_1 \mu_1) & (\lambda_2 \mu_2) & (\lambda_{12}; \mu_{12}) & \rho_{12} \\
(\lambda_3 \mu_3) & (\lambda_4 \mu_4) & (\lambda_{34}; \mu_{34}) & \rho_{34} \\
(\lambda_{13}; \mu_{13}) & (\lambda_{24}; \mu_{24}) & (\lambda, \mu) & \rho_{13,24} \\
\rho_{13} & \rho_{24} & \rho_{12,34}
\end{pmatrix}
\]

\[
= \sum_{\{-\}} U[\left(\lambda_{13};\mu_{13}\right)(\lambda_2 \mu_2)(\lambda_4 \mu_4); (\lambda_0 \mu_0) \rho_{13,24} \rho_{24} \rho_{13,24}] \\
\times Z[\left(\lambda_2 \mu_2\right)(\lambda_1 \mu_1)(\lambda_0 \mu_0)(\lambda_3 \mu_3); (\lambda_{12};\mu_{12}) \rho_{12} \rho_{12,3} \rho_{13,3} \rho_{13,2}] \\
\times U[\left(\lambda_{12};\mu_{12}\right)(\lambda_3 \mu_3)(\lambda_4 \mu_4); (\lambda_0 \mu_0) \rho_{12,3} \rho_{24} \rho_{34} \rho_{12,34}].
\]

(C.43)

where \(\{-\} = \{(\lambda_0 \mu_0) \rho_{13,2} \rho_{24} \rho_{13,24}\}\). Various symmetry relations and special cases of the 9-(\(\lambda \mu\)) coefficients can be found in [97] and [98], and a computer code has been developed which provides numerical values for these recoupling coefficients [1].
C.3 Operators and their Matrix Elements in the SU(3)-scheme

C.3.1 Operators in the SU(3) scheme

A general one-body operator that acts symmetrically on a system of A identical particles is given by

\[ \mathcal{F} = \sum_s f(\vec{r}_s, \vec{\sigma}_s). \]  \hspace{1cm} (C.44)

where \( \vec{r}_s \) and \( \vec{\sigma}_s \) represent the position and spin (or spin-isospin) coordinates, respectively, of the \( s \)-th particle. In a fermion second quantization formulation this one-body operator takes the form:

\[ \mathcal{F} = \sum_{\rho,\rho'} \langle \rho' | f(\vec{r}, \vec{\sigma}) | \rho \rangle \ a_{\rho'}^\dagger \ a_\rho \]  \hspace{1cm} (C.45)

(for details see Appendix B). In Equation C.45 the symbol \( \rho \) labels the available single-particle states and \( a_{\rho}^\dagger \) and \( a_\rho \) are single-particle creation and annihilation operators that satisfy the usual fermion anti-commutation relations:

\[ \{a_\rho, a_{\rho'}^\dagger\} = \delta_{\rho, \rho'} \]

\[ \{a_\rho, a_{\rho'}\} = \{a_{\rho'}^\dagger, a_\rho^\dagger\} = 0. \]  \hspace{1cm} (C.46)

For fermions in a harmonic oscillator potential, \( \rho \) stands for a set of quantum numbers \( \rho = \eta l m_\frac{1}{2} \sigma \) or \( \rho = \eta l \frac{1}{2} j m_j \), depending on whether the states are characterized by an LS- or \( jj \)-coupling scheme, respectively. Here \( \eta \) is the principal quantum number (major oscillator shell) of the single-particle level; \( l, \frac{1}{2}, \) and \( j \) label the orbital, spin, and total angular momenta with projections \( m \), \( \sigma \), and \( m_j \), respectively. (In a spin-isospin formalism, one has \( \rho = \eta l m_\frac{1}{2} \sigma \frac{1}{2} \tau \) or \( \rho = \eta l \frac{1}{2} j m_j \frac{1}{2} \tau \), respectively, where the additional \( \frac{1}{2} \) denotes the isospin quantum number with projection \( \tau \).) For
our purposes it is most convenient to use the LS-coupling scheme, and this is what we will focus on from here on.

Since the single-particle harmonic oscillator wave functions, \( |\eta m_{1/2}\sigma\rangle = d_{\eta m_{1/2}\sigma}^{\dagger} |\rangle \), where \( |\rangle \) denotes the particle vacuum, transform irreducibly under a set of physically relevant SU(3) and SU(2) symmetry group operations, the fermion creation operator \( d_{\eta m_{1/2}\sigma}^{\dagger} \) is a double irreducible tensor operator of rank \( (\lambda \mu) = (\eta 0) \) in SU(3), which labels its orbital character (with subgroup labels \( l \) and \( m \)), and of rank \( s = \frac{1}{2} \) in SU(2) for the spin part (with subgroup label \( \sigma \)):

\[
a_{\eta m_{1/2}\sigma}^{\dagger} \rightarrow a_{(\eta 0)lm_{1/2}\sigma}^{\dagger}.
\]

It turns out that \( a_{\rho} = (a_{\mu}^{\dagger})^{\dagger} \) is not a proper irreducible tensor operator with respect to the above group transformations. One can, however, show that

\[
\tilde{a}_{(\eta 0)lm_{1/2}\sigma} = (-1)^{\eta + l + m + \frac{1}{2} + \sigma} a_{(\eta 0)lm_{1/2} - \sigma}.
\]

is a double irreducible tensor operator of rank \( (\lambda \mu) = (0 \eta) \) in SU(3) and rank \( s = \frac{1}{2} \) in (spin-)SU(2).

Hence it becomes possible to construct tensor products from \( a^{\dagger} \) and \( \tilde{a} \), such as

\[
\{a_{(\eta 0)}^{\dagger} \| \tilde{a}_{(\eta 0)} \}_{\frac{1}{2}} \times \Gamma_{\lambda \mu \Sigma} = \sum_{\alpha_{1} \alpha_{2} \sigma_{1} \sigma_{2}} \langle (\eta 1) \alpha_{1} (\eta 2) \alpha_{2} (\lambda \mu) \nu \Sigma \rangle \frac{1}{2} \sigma_{1} \frac{1}{2} \sigma_{2} a_{(\eta 1) \alpha_{1} \frac{1}{2} \sigma_{1}}^{\dagger} a_{(\eta 2) \alpha_{2} \frac{1}{2} \sigma_{2}}.
\]

which moves a particle from the \( \eta_{2}-\)th major oscillator shell to the \( \eta_{1}-\)th shell. The possible \( (\lambda \mu) \) values are given by the coupling rule \( (\eta_{1} 0) \times (0 \eta_{2}) = \bigoplus_{k=0}^{m_{(\eta_{1} \eta_{2})}} (\eta_{1} - k, \eta_{2} - k) \) and \( \alpha_{i} \) is an abbreviation for the set of possible subgroup labels \( \alpha_{i} = \kappa_{i} l_{i} m_{i} \), where \( \kappa_{i} = 1 \) must hold here. The total intrinsic spin \( S \) can take the values 0 or 1 with projection \( \Sigma = 0 \) or \( \Sigma = 0, \pm 1 \), respectively.

Using the second quantization formalism it is possible to express a general one-body operator in terms of single-particle creation and annihilation operators. Applying this procedure to a one-body
operator possessing good SU(3) symmetry yields:

\[ F_{\kappa LM, M_\sigma}^{(\lambda \mu) S} = \sum_{\{ - \}} \left\{ (\eta'(0)) l' m' \frac{1}{2} m'_{\sigma} \right\} f_{\kappa LM, M_\sigma}^{(\lambda \mu) S} \left| (\eta(0)) l m \frac{1}{2} m_{\sigma} \right\} a^+_{(\eta(0)) l m', \frac{1}{2} m', a_{(\eta(0)) l m, \frac{1}{2} m}. \] (C.50)

with the abbreviation \{ - \} = \{ \eta, l, m, m_{\sigma}, \eta', l', m', m'_{\sigma} \}. The sum over \eta is restricted because the SU(3)-coupling \{(\eta', 0) \times (0, \eta)\} \rightarrow (\lambda, \mu) must be allowed. Additionally, it is sometimes useful to drop the sum over \eta, \eta' and define an operator

\[ (\eta') F_{\kappa L M', M_\sigma}^{(\lambda \mu) S} = \sum_{\{ - \}} \left\{ (\eta'(0)) l' m' \frac{1}{2} m'_{\sigma} \right\} f_{\kappa L M', M_\sigma}^{(\lambda \mu) S} \left| (\eta(0)) l m \frac{1}{2} m_{\sigma} \right\} a^+_{(\eta(0)) l m', \frac{1}{2} m', a_{(\eta(0)) l m, \frac{1}{2} m}. \] (C.51)

with the abbreviation \{ - \} = \{ l, m, m_{\sigma}, l', m', m'_{\sigma} \}.

As an example for the SU(3) labeling of many-body operators, we list the relevant expressions for the orbital angular momentum

\[ L_{1\mu} \equiv F^{(1,1) 0}_{11 \mu 0}. \] (C.52)

and for the spin

\[ S_{1\mu} \equiv F^{(0,0) 1}_{00 \mu 1}. \] (C.53)

Since we want to make use of the SU(3) symmetry, we manipulate Equation C.51 to have the creation and annihilation operators coupled to good SU(3) quantum numbers. Therefore we employ the annihilation operator of Equation C.48 which has the proper SU(3) transformation properties. Next, we use the SU(3)-coupled product of the creation and annihilation operators given in Equation C.49.

The left-hand side of equation C.49 is a frequently occurring SU(3) unit tensor which we will abbreviate as:

\[ T_{\kappa LM, \Sigma}^{(\lambda \mu) S} = \left\{ a^+_{(\eta(0)), \frac{1}{2}} \times a_{(\eta(0)), \frac{1}{2}} \right\}^{(\lambda \mu) S}_{\kappa LM, \Sigma}. \] (C.54)
Using Equation C.51, one thus obtains

\[
\eta^2 \eta^2 \frac{\tau_{(\lambda\mu)S}}{\alpha L M \Sigma} = \left( \frac{2 \text{dim}(\eta 0)}{(2S + 1) \text{dim}(\lambda\mu)} \right)^{\frac{1}{2}} \langle \eta 0 \rangle, \frac{1}{2} \| f_{(1)}^{(\lambda \mu)} || (\eta 0), \frac{1}{2} \sigma_{(1)0} \alpha_{(0)0} \rangle \langle (1)0 \rangle \frac{1}{2} \left( \frac{25 + 1}{2} \right) \text{dim} (\lambda\mu)/ \Sigma^2 \, \text{dim} (\lambda\mu) \right)
\]

(C.55)

or, equivalently,

\[
\eta^2 \eta^2 \frac{\tau_{(\lambda\mu)S;J}}{\alpha L I : M J} = \left( \frac{2 \text{dim}(\eta 0)}{(2S + 1) \text{dim}(\lambda\mu)} \right)^{\frac{1}{2}} \langle \eta 0 \rangle, \frac{1}{2} \| f_{(1)}^{(\lambda \mu)} || (\eta 0), \frac{1}{2} \sigma_{(1)0} \alpha_{(0)0} \rangle \langle (1)0 \rangle \frac{1}{2} \left( \frac{25 + 1}{2} \right) \text{dim} (\lambda\mu) / (S;J) \left( \frac{\lambda\mu}{\Sigma;J} \right).
\]

(C.56)

Here we have introduced the SU(3) reduced (or triple-bar) matrix element (\(\eta ||\eta||\eta\)) (which will be defined in the next section). The task that remains at this point is to evaluate these triple-bar matrix elements. An example for such a calculation is given in Subsection 3.2.4, where fermionic expressions for the symplectic generators are derived. Further examples can be found in [26], where the single-particle triple-bar matrix elements for the orbital angular momentum, spin, and quadrupole operators are listed.

The two-body operators can be treated in an analogous fashion by using the techniques of second quantization (see Appendix B) and the appropriate recoupling coefficients. An example for the expansion of a two-body operator in terms of SU(3) irreducible tensor operators is given in Subsection 3.2.4, where spurious center-of-mass excitations are removed from the symplectic raising and lowering operators by subtracting the appropriate two-body contributions.

### C.3.2 Matrix elements and the Wigner-Eckart Theorem for SU(3)

Figure C.2 illustrates how group theory can be used to define a state by a sequence of irreducible representations (irreps) of physically relevant groups and additional multiplicity labels, like \(\alpha\) and \(\kappa\) which are needed to distinguish states belonging to the same irrep chain. The most striking advantage of the group-theoretical formulation, however, lies in the calculation of matrix elements.
By means of Racah’s fractional parentage techniques and the SU(3) irreducible tensor formalism, the relevant terms in the Hamiltonian under consideration can be decomposed into parts with well-defined group-theoretical transformation properties. The use of the Wigner-Eckart theorem - the theorem being applied not only to SO(3) (as in the standard angular momentum context) but also to higher symmetry groups - then allows one to express matrix elements of one- and two-body operators as products of reduced Wigner coefficients, Racah coefficients (also referred to as $6(\lambda\mu)$-symbols), and coefficients of fractional parentage (usually written as triple-bar matrix elements).

The Wigner-Eckart theorem for the group SU(2) yields SO(3)-reduced (double-bar) matrix elements $\langle l_3 \| T^{l_2} \| l_1 \rangle$ of an SO(3) irreducible tensor operator $T^{lm}$ [118, 169]:

$$\langle l_3 m_3 \| T^{l_2 m_2} \| l_1 m_1 \rangle = \langle l_1 m_1 l_2 m_2 l_3 m_3 \| T^{l_2} \| l_3 \rangle \langle l_3 \| T^{l_1} \| l_1 \rangle . \quad (C.57)$$

The generalized Wigner-Eckart theorem allows one to express matrix elements of SU(3) irreducible tensor operators as a sum over $\rho$ of the product of a $\rho$-dependent generalized reduced matrix element multiplied by the corresponding Wigner coefficient. Specifically, for the SU(3) $\supset$ SU(2) $\times$ U(1) subgroup chain, we have [47]:

$$\langle (\lambda_3 \mu_3) \ell_3 \Lambda_3 M_\Lambda_3 | T^{(\lambda_2 \mu_2) \ell_2 \Lambda_2 M_\Lambda_2} | (\lambda_1 \mu_1) \ell_1 \Lambda_1 M_\Lambda_1 \rangle = \sum_\rho \langle (\lambda_1 \mu_1) \ell_1 \Lambda_1 M_\Lambda_1 ; (\lambda_2 \mu_2) \ell_2 \Lambda_2 M_\Lambda_2 | (\lambda_3 \mu_3) \ell_3 \Lambda_3 M_\Lambda_3 \rangle \rho \langle (\lambda_3 \mu_3) \ell_3 \Lambda_3 M_\Lambda_3 | T^{(\lambda_2 \mu_2) \ell_2 \Lambda_2 M_\Lambda_2} | (\lambda_1 \mu_1) \ell_1 \Lambda_1 M_\Lambda_1 \rangle \rho . \quad (C.58)$$

For the SU(3) $\supset$ SU(2) chain, the Wigner-Eckart theorem takes the following form:

$$\langle (\lambda_3 \mu_3) \ell_3 m_3 | T^{(\lambda_2 \mu_2) \ell_2 m_2} | (\lambda_1 \mu_1) \ell_1 m_1 \rangle$$
From Equations C.58 and C.59 it becomes clear that the triple-bar matrix elements must be independent of the chosen subgroup chain.

**Reduction Rules**

In analogy to the well-known reduction rules for SU(2) [118, 169], one can derive expressions for the triple-bar matrix elements of a SU(3)-coupled tensor product acting on a two-component system [125]:

(C.60)
\[
\{N_\pi [f_\nu] \alpha_\pi (\lambda_\pi, \mu_\pi); N_\nu [f_\nu] \alpha_\nu (\lambda_\nu, \mu_\nu)\} (\lambda, \mu) \rho \kappa L, \{S_\pi, S_\nu\} S; J
\]

\[
= \left\{ \begin{array}{ccc}
L & L_0 & L' \\
S & S_0 & S'
\end{array} \right\} \left\{ \begin{array}{ccc}
S_\pi & S_{\pi_0} & S'_{\pi}
\end{array} \right\} \sum_\rho \langle (\lambda, \mu) \kappa L, (\lambda_0, \mu_0) \kappa_0 L_0 \| (\lambda', \mu') \kappa' L' \rangle \rho
\]

\[
\times \sum_{\rho_\pi, \rho_\nu} \left( \begin{array}{ccc}
(\lambda_\pi, \mu_\pi) & (\lambda_0, \mu_0) & (\lambda', \mu') \rho_\pi \\
(\lambda_\nu, \mu_\nu) & (\lambda_0, \mu_0) & (\lambda', \mu') \rho_\nu \\
(\lambda_\pi, \mu_\pi) & (\lambda_\nu, \mu_\nu) & (\lambda_0, \mu_0) \rho \rho_\pi \rho_\nu
\end{array} \right)
\]

\[
x (N'_\pi [f'_\nu] \alpha'_\pi (\lambda'_\pi, \mu'_\pi), S'_{\pi} \| \mathcal{F}(\lambda_\pi, \mu_\pi \| \mathcal{S}_\nu \| N_\nu [f_\nu] \alpha_\nu (\lambda_\nu, \mu_\nu), S_\nu)_{\rho_\pi}
\]

\[
x (N'_\nu [f'_\nu] \alpha'_\nu (\lambda'_\nu, \mu'_\nu), S'_{\nu} \| \mathcal{F}(\lambda_\nu, \mu_\nu \| \mathcal{S}_\nu \| N_\nu [f_\nu] \alpha_\nu (\lambda_\nu, \mu_\nu), S_\nu)_{\rho_\nu},
\]  \hspace{1cm} \text{(C.61)}

where the coupled tensor operator is defined as

\[
\mathcal{F}_{\kappa_\nu L_\nu}^{\rho_\nu (\lambda_\nu, \mu_\nu) S_\nu; J_\nu} \equiv \left\{ \mathcal{F}(\lambda_\nu, \mu_\nu \| \mathcal{S}_\nu \| \mathcal{F}(\lambda_\nu, \mu_\nu \| \mathcal{S}_\nu \| N_\nu [f_\nu] \alpha_\nu (\lambda_\nu, \mu_\nu), S_\nu)_{\rho_\nu} \right\}_{\kappa_\nu L_\nu}.
\]  \hspace{1cm} \text{(C.62)}
Vita

Jutta Escher was born on November 7, 1966, in Boppard, Germany. She attended high school in Boppard, Germany, and studied physics at the University of Bonn, where she received her Vordiplom in 1988. She completed a master's thesis in physics and obtained her master of science degree from Louisiana State University in 1993. Her Doctor of Philosophy degree in physics will be awarded in May of 1997.

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