
Theses and Dissertations

Spring 2011

Solution of two nucleon systems using vector variables in momentum space - an innovative approach

Saravanan Veerasamy
University of Iowa

Copyright 2011 Saravanan Veerasamy

This dissertation is available at Iowa Research Online: <http://ir.uiowa.edu/etd/1099>

Recommended Citation

Veerasamy, Saravanan. "Solution of two nucleon systems using vector variables in momentum space - an innovative approach." PhD (Doctor of Philosophy) thesis, University of Iowa, 2011.
<http://ir.uiowa.edu/etd/1099>.

Follow this and additional works at: <http://ir.uiowa.edu/etd>

 Part of the [Physics Commons](#)

SOLUTION OF TWO NUCLEON SYSTEMS USING VECTOR VARIABLES IN
MOMENTUM SPACE - AN INNOVATIVE APPROACH

by

Saravanan Veerasamy

An Abstract

Of a thesis submitted in partial fulfillment of the
requirements for the Doctor of Philosophy
degree in Physics in the
Graduate College of The
University of Iowa

May 2011

Thesis Supervisor: Professor Wayne Polyzou

ABSTRACT

An alternate formalism that uses vector variables to treat the two-body Lippmann-Schwinger equation for realistic nucleon-nucleon potentials in momentum space is discussed in this thesis. The formalism uses the symmetry properties of the nucleon-nucleon potential and expands the nucleon-nucleon potential in terms of six linearly independent spin operators. The alternate formalism discussed in this thesis brings to light the role of time-odd spin operators. The vector variable formalism's treatment of spin degrees of freedom heavily depends on the analytical computation of hundreds of algebraic expressions. A mathematical framework and computer algorithms for an automated symbolic reduction of algebraic expressions into scalar functions of vector variables are explained in this thesis. The vector variable formalism requires nucleon-nucleon potentials that are in operator form as input. The configuration space nucleon-nucleon potential Argonne V18 is one such potential that can be used for relativistic energies if it can be computed efficiently in momentum space. This thesis develops an efficient numerical technique using Chebyshev approximation to compute the Argonne V18 potential in momentum-space. The tools discussed in this thesis, the algebraic system and the efficient computation of the Argonne V18 potential in momentum space are tested by computing the binding energy and bound state wavefunctions of the deuteron using the vector variable approach. The results were successful and the first step towards a higher goal of using vector formalism of the three-body Faddeev equations for intermediate and high energies has been made.

Abstract Approved: _____
Thesis Supervisor

Title and Department

Date

SOLUTION OF TWO NUCLEON SYSTEMS USING VECTOR VARIABLES IN
MOMENTUM SPACE - AN INNOVATIVE APPROACH

by

Saravanan Veerasamy

A thesis submitted in partial fulfillment of the
requirements for the Doctor of Philosophy
degree in Physics in the
Graduate College of The
University of Iowa

May 2011

Thesis Supervisor: Professor Wayne Polyzou

Copyright by
SARAVANAN VEERASAMY
2011
All Rights Reserved

Graduate College
The University of Iowa
Iowa City, Iowa

CERTIFICATE OF APPROVAL

PH.D. THESIS

This is to certify that the Ph.D. thesis of

Saravanan Veerasamy

has been approved by the Examining Committee for the thesis requirement
for the Doctor of Philosophy degree in Physics at the May 2011
graduation.

Thesis Committee: _____
Wayne Polyzou, Thesis Supervisor

Charlotte Elster

Craig E. Pryor

Gerald Payne

Aaron Stump

...dedicated to my family and friends

ACKNOWLEDGMENTS

I would like to take this occasion to express my gratitude to people who have helped me succeed in crossing an important milestone in my academic career. First, I thank my advisor Prof. Wayne Polyzou. As an advisor his hands off approach gave me the opportunity and freedom to pursue my interests that has eventually translated into this thesis. I would like to thank Prof. Payne for being a member of my committee and for his helpful advice. I had the wonderful opportunity of meeting Prof. Elster in late summer of 2009. I thank her for introducing me to the field of vector variable scattering in few body systems. I also thank her for being a member of my committee and her interest in my work. I thank other committee members Prof. Aaron Stump and Prof. Craig Pryor. During the years I spent in Iowa there are faculty members and friends who have offered their help and support. I would specially like to thank Prof. Rodgers for his help and advice. I also thank Ms. Deborah Foreman the graduate secretary. Among my friends I thank Mr. Sailesh Tendolkar for his support. Lastly I thank my family for their support and patience.

ABSTRACT

An alternate formalism that uses vector variables to treat the two-body Lippmann-Schwinger equation for realistic nucleon-nucleon potentials in momentum space is discussed in this thesis. The formalism uses the symmetry properties of the nucleon-nucleon potential and expands the nucleon-nucleon potential in terms of six linearly independent spin operators. The alternate formalism discussed in this thesis brings to light the role of time-odd spin operators. The vector variable formalism's treatment of spin degrees of freedom heavily depends on the analytical computation of hundreds of algebraic expressions. A mathematical framework and computer algorithms for an automated symbolic reduction of algebraic expressions into scalar functions of vector variables are explained in this thesis. The vector variable formalism requires nucleon-nucleon potentials that are in operator form as input. The configuration space nucleon-nucleon potential Argonne V18 is one such potential that can be used for relativistic energies if it can be computed efficiently in momentum space. This thesis develops an efficient numerical technique using Chebyshev approximation to compute the Argonne V18 potential in momentum-space. The tools discussed in this thesis, the algebraic system and the efficient computation of the Argonne V18 potential in momentum space are tested by computing the binding energy and bound state wavefunctions of the deuteron using the vector variable approach. The results were successful and the first step towards a higher goal of using vector formalism of the three-body Faddeev equations for intermediate and high energies has been made.

TABLE OF CONTENTS

LIST OF TABLES	vii
LIST OF FIGURES	viii
CHAPTER	
1 INTRODUCTION	1
1.1 Format of the thesis	4
2 FORMALISM OF SCATTERING USING VECTOR VARIABLES	5
2.1 Spin independent interaction	5
2.1.1 Vector form of the Lippmann-Schwinger equation.	5
2.1.2 The three-body Faddeev equation	7
2.1.3 Introducing relativity	11
2.2 Spin-dependent nucleon-nucleon potentials	12
2.3 Structure of the formalism	14
2.3.1 Conclusions	19
2.4 What does this thesis offer?	21
3 THE NUCLEON-NUCLEON POTENTIAL - ARGONNE V18	24
3.1 Momentum-space representation	26
3.1.1 Operator : \mathbf{I}	27
3.1.2 Operator : $3(\vec{\sigma}_1 \cdot \hat{r})(\vec{\sigma}_2 \cdot \hat{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2$	28
3.1.3 Operator : $\vec{L} \cdot \vec{S}$	29
3.1.4 Operator : $\vec{L} \cdot \vec{L}$	30
3.1.5 Operator : $(\vec{L} \cdot \vec{S})^2$:	32
3.2 Conclusion	32
4 NUMERICAL EVALUATION OF INTEGRALS	34
4.1 Chebyshev approximation of integrals	38
4.2 $\mathbf{I}^1(\rho)$	40
4.3 $\mathbf{I}^2(\rho)$	47
4.4 $\mathbf{I}^3(\rho)$	50
4.5 $\mathbf{I}^4(\rho)$	58
5 A FORMALISM FOR AUTOMATED ALGEBRAIC REDUCTION	64
5.1 Description of reduction mechanism	64

5.2	Inverse transformation	67
5.2.1	Uniqueness	67
5.2.2	Structure of transformation	69
5.2.3	Elementary transformation	70
5.2.4	Illustration	72
5.3	Description of algorithm	72
5.3.1	Algorithm: 1	74
5.3.2	Algorithm: 2	75
5.3.3	Algorithm: 3	76
5.4	Conclusion	77
6	DEUTERON BOUND STATE OF ARGONNE V18	78
6.1	Numerical realization	78
6.2	Computation of traces	88
6.3	Conclusion	91
7	GENERAL REPRESENTATION OF BASIS OPERATORS	93
7.1	Basis operators	93
7.2	Representation	93
7.3	Type I	96
7.3.1	Time-odd operator and the basis	100
7.3.2	Conclusion of Type I	101
7.4	Orthogonal vectors - Type II	102
7.4.1	Time-odd basis elements	103
7.4.2	Conclusion for Type II	105
7.5	Conclusion	108
8	SUMMARY AND OUTLOOK	109
	APPENDIX A: TRIPLE TRACES USING AUTOMATED ALGEBRAIC SYSTEM	111
	REFERENCES	121

LIST OF TABLES

Table

2.1	Time reversal and space reflection symmetry	14
2.2	Symmetry transformations of the vectors	15
3.1	Argonne V18 operators in configuration space	24
3.2	Argonne V18 operators in configuration space	25
6.1	Energy values vs λ for $k_{max} = 10fm^{-1}$	83
6.2	Convergence test for k_{max}	84
6.3	Comparison of direct and Chebyshev integration.	86
6.4	Change in bound state energy with number of Chebyshev functions	87
7.1	Total symmetry (time-reversal and space-reflection of spin operators).	97
7.2	Effect of time and space-reflection operators on vectors.	103
7.3	Total symmetry (time-reversal and space- reflection) of spin operators.	107

LIST OF FIGURES

Figure		
4.1	Plot of $j_0(x)$, $j_1(x)$ and $j_2(x)$ with respect to x	35
4.2	Fourier-Bessel integral of $I_1^1(\rho)$	40
4.3	Fourier-Bessel integral of $I_2^1(\rho)$	41
4.4	Fourier-Bessel integral of $I_3^1(\rho)$	42
4.5	Fourier-Bessel integral of $I_4^1(\rho)$	43
4.6	Fourier-Bessel integral of $I_{15}^1(\rho)$	44
4.7	Fourier-Bessel integral of $I_{16}^1(\rho)$	45
4.8	Fourier-Bessel integral of $I_{18}^1(\rho)$	46
4.9	Fouurier-Bessel integral of $I_5^2(\rho)$	47
4.10	Fourier-Bessel integral of $I_6^2(\rho)$	48
4.11	Fourier-Bessel integral of $I_{17}^2(\rho)$	49
4.12	Fourier-Bessel integral of $I_7^3(\rho)$	50
4.13	Fourier-Bessel integral of $I_8^3(\rho)$	51
4.14	Fourier-Bessel integral of $I_9^3(\rho)$	52
4.15	Fourier-Bessel integral of $I_{10}^3(\rho)$	53
4.16	Fourier-Bessel integral of $I_{11}^3(\rho)$	54
4.17	Fourier-Bessel integral of $I_{12}^3(\rho)$	55
4.18	Fourier-Bessel integral of $I_{13}^3(\rho)$	56
4.19	Fourier-Bessel integral of $I_{14}^3(\rho)$	57
4.20	Fourier-Bessel integral of $I_9^4(\rho)$	58
4.21	Fourier-Bessel integral of $I_{10}^4(\rho)$	59
4.22	Fourier-Bessel integral of $I_{11}^4(\rho)$	60

4.23	Fourier-Bessel integral of $I_{12}^4(\rho)$	61
4.24	Fourier-Bessel integral of $I_{13}^4(\rho)$	62
4.25	Fourier-Bessel integral of $I_{14}^4(\rho)$	63
6.1	The s wave function of deuteron	85
6.2	The d wave function of deuteron	86

CHAPTER 1

INTRODUCTION

Few-body methods have provided the most detailed understanding of the microscopic properties of nuclear systems. The reason for this success is because few-nucleon systems are simple enough (1) to perform numerically exact calculations of all relevant observables using realistic models of these systems and (2) to perform almost complete experimental measurements of the observable properties of these systems. This has led to realistic potentials of the two-nucleon system. When these nucleon-nucleon potentials are used in systems of three or more nucleons they can lead to a quantitative understanding of most low-energy few-body observables. One of the most interesting energy scales in nuclear physics is the GeV scale. This is the scale where sub-nucleon degrees of freedom are expected to be relevant. If the dynamics is still governed by a small number of relevant degrees of freedom one expects that few-body tools may prove useful for understanding the relevant dynamics at this interesting energy scale. At this energy scale a relativistic treatment of the few-body dynamics is necessary. A number of problems need to be solved to perform realistic few-body calculations at these energies. These include constructing realistic model Hamiltonians with the relevant degrees of freedom, and numerically exact computational methods that can be successfully used at these scales.

The purpose of this thesis is to make modest first steps toward this goal. The two-body system is the simplest few-body system. The Lippmann-Schwinger equation is a reformulation of the two-body Schrödinger equation that is used for solving the bound state and scattering problems. Conventionally a rotationally invariant potential is expanded in a partial wave basis and the Lippmann-Schwinger equation is replaced by an infinite number of decoupled one-variable integral equations. The solution is obtained by adding the contribution from each partial wave basis[1]. At low energies accurate

solutions can be obtained from a small number of partial waves. For three-nucleon problems the Lippmann-Schwinger equation is replaced by the Faddeev equation [2], which is a reformulation of the three-body Schrödinger equation as an integral equation with a compact kernel. The kernel requires fully off-shell solutions of the Lippmann-Schwinger equation embedded in the three-body Hilbert space as input. Partial wave expansions also simplify low-energy three-body calculations. As the energy is increased the number of partial wave channels required for the solution to converge increases. For each energy the number of partial waves required for convergence needs to be established. At higher energies the increase in the number of partial waves results in oscillations of the functions in the kernel of the scattering equation. The numerical treatment of these oscillations for higher energies makes it difficult to use partial waves. Converged three-nucleon calculations using partial waves have been computed [3] for energies up to 250 MeV.

An alternative approach that may be useful at higher energies is to use direct integration methods. Instead of expanding the angular dependence in spherical harmonics, the angular variables are integrated directly and the variables are treated as vectors. The benefit of direct integration is that the equations have the same form at all energies and no convergence needs to be established for each energy with respect to the number of partial waves. Since the vector form of the Faddeev equation has the same structure for all energies, it is an attractive alternative to a partial wave formulation. Converged solutions of the vector form of the three-body Faddeev equation for spin-independent interactions have been performed by Liu and Elster[4]. At the interesting GeV energy scale relativistic effects cannot be ignored. Calculations of the relativistic Faddeev equation[5] in vector variables have also been performed for spin-independent interactions and convergence has been established for beam energies up to two GeV [6], [7].

Realistic calculations require high-quality spin-dependent nucleon-nucleon interactions. The high-precision nucleon-nucleon potentials that are available are Argonne V18 [8], CD-BONN [9] and Nijmegen [10] potentials. The high-precision CD-BONN and Nijmegen nucleon-nucleon potentials are available in momentum space and in different partial wave channels. They contain parameters fitted to different finite number of partial waves with respect to angular momentum and hence they cannot be transformed to operator form and are not suited for three-dimensional vector treatment of scattering. Argonne V18 nucleon-nucleon potential is a high precision configuration space nucleon-nucleon potential that is available in operator form. At present the best model interactions are phenomenological operators that are motivated by meson exchange physics with parameters fit to the world nucleon-nucleon scattering data. These non-relativistic nucleon-nucleon potentials can be reinterpreted as potentials in a relativistic rest-energy (mass) operator [11] fit to the same data. This identification implies that solutions of the non-relativistic Lippmann-Schwinger equation can be used directly to construct the kernel of the relativistic Faddeev equation, [12][6]. Thus, the required input for a vector treatment of the relativistic Faddeev equation is a vector treatment of the non-relativistic Lippmann-Schwinger equation for spin $\frac{1}{2}$ particles. In addition, relativistic treatments of the dynamics involve momentum-dependent spin rotation functions, so it is desirable to use momentum-space representations of the interactions. This thesis discusses the treatment of two-body scattering using vector variables in momentum-space for realistic nucleon-nucleon potentials. The Argonne V18 nucleon-nucleon potential is an ideal candidate to be used for relativistic few-body calculations. To use Argonne V18 in the momentum-space two-body scattering the two main problems are (1) constructing an accurate and easy to compute momentum-space representation of the Argonne V18 potentials and (2) developing methods to treat the spin coupling in the vector forms of the dynamical equations. The treatment of the spin relies on symbolic methods that are developed to formulate coupled integral equations. The solutions of both of these

problems are needed to formulate realistic relativistic few-body models.

1.1 Format of the thesis

The thesis explains the innovative methods adopted for the vector solution of spin dependent two-nucleon systems in momentum-space. The content of each chapter is summarized below

1. Chapter two discusses recent formalism of the vector treatment of two-nucleon scattering for a spin-dependent potential in momentum space. This chapter introduces the spin operators and the vector formulation of the Lippmann-Schwinger equation. The choice of spin operators in [13] and the conclusions of this work are also discussed in this chapter.
2. Chapter three derives the Fourier transform of the configuration space Argonne V18 potential.
3. Chapter four discusses the numerical method used to compute the Fourier transform and the Chebyshev approximation to the scalar coefficients in the Argonne V18 potential.
4. Chapter five discusses the motivation for constructing an automated reduction mechanism and the algorithm that was developed for this purpose.
5. Chapter six discusses the vector solution of deuteron bound state using the momentum-space V18 potential. This calculation uses the numerical and algebraic programs developed in this thesis to calculate the binding energy and bound state wave functions.
6. Chapter seven discusses the alternative formalism for the vector variable approach and discusses the role of time-odd operators in the formalism.

CHAPTER 2

FORMALISM OF SCATTERING USING VECTOR VARIABLES

2.1 Spin independent interaction

This section introduces the formalism of two-body and three-body scattering using vector variables for a spin independent nucleon-nucleon potential. This formalism has been successfully implemented for two-body and three-body systems. This includes the treatment of three-body systems with relativity. The first discussion is the vector formulation of the Lippmann-Schwinger equation for a spin-independent (scalar) potential followed by the embedding of this solution in the numerical realization of the vector formulation of the three-body Faddeev equation. This is followed by a discussion of the vector formulation of the relativistic Faddeev equations.

2.1.1 Vector form of the Lippmann-Schwinger equation.

The Lippmann-Schwinger equation for the transition operator is given by

$$T(z) = V + VG_0(z)T(z) \quad (2.1)$$

where $T(z)$ is the transition operator, V is the potential operator and $G_0(z)$ is the resolvent of the free center of mass Hamiltonian, H_0 ,

$$G_0 = \frac{1}{z - H_0} \quad (2.2)$$

with $z = E + i\epsilon$. In the non-relativistic case

$$H_0 = \frac{k^2}{2\mu}, \quad (2.3)$$

where k is the momentum of one of the particles in the rest frame of the two-nucleon system and μ is the reduced mass. For a spin-independent, translationally invariant interaction we work in a representation where the vector variables are the momentum of a particle in the center of momentum frame and total momenta of the particles, \vec{k}, \vec{p} . Because of the translational invariance and invariance with respect to Galilean boosts,

matrix elements of the interaction have the form

$$\langle \vec{p}, \vec{k} | V | \vec{p}', \vec{k}' \rangle = \delta(\vec{p} - \vec{p}') \langle \vec{k} | V | \vec{k}' \rangle. \quad (2.4)$$

If the potential is also rotationally invariant the reduced kernel has the form

$$\langle \vec{k} | V | \vec{k}' \rangle = V(k, k', u) \quad (2.5)$$

where $u = \hat{k} \cdot \hat{k}'$ is the cosine of the angle between \vec{k} and \vec{k}' , where \vec{k} is the initial relative momentum of the nucleons and \vec{k}' is the final relative momentum of the nucleons.

The transition operator has the same structure

$$\begin{aligned} \langle \vec{p}, \vec{k} | T(z) | \vec{p}', \vec{k}' \rangle = \\ \delta(\vec{p} - \vec{p}') \langle \vec{k} | T(z) | \vec{k}' \rangle \end{aligned} \quad (2.6)$$

with

$$\langle \vec{k} | T(z) | \vec{k}' \rangle = T(k, k', u, z) \quad (2.7)$$

and an additional energy variable, $z = E + i0^+$.

In all that follows the overall momentum conserving delta function, which factors out of all of the dynamical equations, is removed.

In this representation Lippmann-Schwinger equation becomes a two-variable singular integral equation

$$\begin{aligned} T(k, k', u, z) = V(k, k', u) + \int_0^\infty k''^2 dk''^2 \int_{-1}^1 du'' \int_0^{2\pi} d\phi \\ \frac{V(k, k'', uu'' + \sqrt{1-u^2}\sqrt{1-(u'')^2}\cos(\phi))}{\frac{k_0^2}{2\mu} - \frac{k''^2}{2\mu} + i\epsilon} T(k'', k', u'', z) \end{aligned} \quad (2.8)$$

where $E = \frac{k_0^2}{2\mu}$. The solution is needed for different choices of the relative momenta \vec{k} and \vec{k}' :

1. on shell $T(k_0, k_0, u, k_0^2/2\mu + i\epsilon)$,
2. half shell $T(k, k_0, u, k_0^2/2\mu + i\epsilon)$,
3. off shell $T(k, k', u, k_0^2/2\mu + i\epsilon)$.

The scattering amplitude can be expressed in terms of the on-shell transition matrix:

$$f(\vec{k}, \vec{k}') = -2\mu(2\pi)^2 T(k_0, k_0, u, k_0^2/2\mu + i\epsilon), \quad (2.9)$$

where $k^2 = k'^2 = k_0^2$. The differential cross-section can then be expressed in terms of the scattering amplitude,

$$\frac{d\sigma}{d\Omega} = |f(k, \hat{k} \cdot \hat{k}')|^2. \quad (2.10)$$

To solve for the on-shell transition matrix elements, the half-shell transition matrix elements are computed.

The kernel of the three-body Faddeev equation is constructed from the off-shell transition operator, $T(k, k', u, k_0^2/2\mu + i\epsilon)$, for $k \neq k' \neq k_0$. Ref [14] discusses the solution of this form of the Lippmann-Schwinger equation using a Malfliet-Tjon potential [15], which is the sum of an attractive and repulsive Yukawa potential.

2.1.2 The three-body Faddeev equation

This section discusses how the two-body transition amplitude is embedded in the three-nucleon Faddeev equation. A three-particle Hamiltonian with two-body interactions has the form

$$H = H_0 + V_{12} + V_{23} + V_{13} \quad (2.11)$$

where V_{ij} is the two body interaction between particle i and j and H_0 is the three-particle kinetic energy operator. This equation is usually written using “odd man out” notation

$$H = H_0 + \sum_{i=1}^3 V_i \quad (2.12)$$

where $V_i = V_{jk}$, $i \neq j \neq k$.

The Faddeev equation is a reformulation of the three-particle Schrödinger equation [2],[16] as a compact-kernel integral equation.

The Schrödinger equation for a three-body bound state is given by

$$(H_0 + \sum_{i=1}^3 V_i)|\psi\rangle = E|\psi\rangle. \quad (2.13)$$

The Schrödinger equation can be transformed into integral form

$$|\psi\rangle = G_0(E) \left(\sum_{i=1}^3 V_i \right) |\psi\rangle \quad (2.14)$$

where $G_0 = \frac{1}{E - H_0}$ is the resolvent of the free three-body Hamiltonian. The Faddeev

decomposition of the state vector is defined by

$$|\psi\rangle = \sum_{i=1}^3 |\psi_i\rangle \quad (2.15)$$

with

$$|\psi_i\rangle = G_0(E)V_i|\psi\rangle = G_0(E)V_i|\psi_i\rangle + G_0(E)V_i \sum_{i \neq j} |\psi_j\rangle. \quad (2.16)$$

Re-arranging terms gives

$$\begin{aligned} |\psi_i\rangle &= (1 - G_0(E)V_i)^{-1}G_0(E)V_i \sum_{i \neq j} |\psi_j\rangle \\ &= G_0(E)(1 - V_iG_0(E))^{-1}V_i \sum_{i \neq j} |\psi_j\rangle. \end{aligned} \quad (2.17)$$

The formal solution of the Lippmann-Schwinger equation for the interacting pair $i \neq (jk)$

$$T_i(z) = V_i + V_iG_0(z)T_i(z) \quad (2.18)$$

is

$$T_i(z) = (1 - V_iG_0(z))^{-1}V_i. \quad (2.19)$$

Using (2.19) in (2.17) gives the Faddeev equation for the bound states

$$|\psi_i\rangle = G_0T_i(E) \sum_{j \neq i} |\psi_j\rangle. \quad (2.20)$$

The condition $i \neq j$ ensures that the first iteration of the kernel is compact, which is a sufficient condition for the kernel to include the boundary conditions for a unique solution.

If the three particles are identical fermions then $|\psi\rangle$ is antisymmetric. The states $|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle$ have identical functional form and all that is required is to permute the particles. For example, when arbitrarily using $|\psi_1\rangle$.

$$|\psi_2\rangle = P_{12}P_{23}|\psi_1\rangle \quad (2.21)$$

$$|\psi_3\rangle = P_{13}P_{23}|\psi_1\rangle \quad (2.22)$$

where P_{ij} are transposition operators that interchange particles i and j .

The total wave function is now written as

$$|\psi\rangle = (1 + P)|\psi_1\rangle \quad (2.23)$$

where the permutation operator $P = P_{12}P_{23} + P_{13}P_{23}$ and

$$|\psi_1\rangle = G_0(E)T_1(E)(P_{12}P_{23} + P_{22}P_{23})|\psi_1\rangle \quad (2.24)$$

or

$$|\psi_1\rangle = G_0(E)T_1(E)P|\psi_1\rangle, \quad (2.25)$$

where the energy eigenvalue E has to be determined by the condition that the equation has a non-trivial solution. Using the component $|\psi_1\rangle$ does not restrict generality of the formulation.

For three-body scattering the scattering asymptotic conditions need to be imposed. For an initial state consisting of a free particle (also called the beam) and a bound two-body pair the state vector has the asymptotic form

$$|\phi_i\rangle = |\phi_d, \vec{q}_0\rangle_i, \quad (2.26)$$

where ϕ_d is the bound state of the bound two-body pair and $|\vec{q}_0\rangle$ the is a plane wave representing the beam particle i with momentum \vec{q}_0 . The result of a scattering reaction can be classified into 1.) elastic scattering, where in the final state the bound pair continues to exist and the final state has the same form as the initial state but with different relative momenta, 2.) breakup scattering, where all the particles in the final state are free.

For the elastic channel the final state is given by

$$|\phi'_i\rangle = |\phi_d, \vec{q}\rangle_i, \quad |q| = |q_0|, \quad (2.27)$$

where \vec{q} is the final relative momenta of the incident particle i . Without loss of generality particle (1) is taken to be the incident particle and particles (23) are bound. The asymptotic states are eigenstates of the channel Hamiltonians

$$H_i = H_0 + V_i, \quad (2.28)$$

where H_0 is the three-body kinetic energy operator and V_i is the pair interaction that forms the bound state:

$$H_i|\phi_i \vec{q}_i\rangle = (E_d + \frac{3}{4m}q_0^2)|\phi_i, \vec{q}_i\rangle, \quad (2.29)$$

E_d is the binding energy of the pair, $\frac{3}{4m}q_0^2$ is the relative kinetic energy of the beam particle, and m is the mass of each particle. The Schrödinger equation for the scattering

eigenstate can be put in the form

$$|\psi\rangle^+ = G_Z(E) \sum_i^3 V_i |\psi\rangle^+, \quad (2.30)$$

where $Z = E + i\epsilon^+$ and E is the energy of the initial incident state.

The Faddeev decomposition can be applied to equation (2.30)

$$|\psi\rangle^+ = \sum_{i=1}^3 |\psi_i\rangle^+, \quad (2.31)$$

with

$$|\psi_i\rangle^+ = G_0(E) V_i |\psi\rangle^+. \quad (2.32)$$

Similar to the bound state Faddeev equation, the Faddeev equation for the scattering state is

$$|\psi_1\rangle^+ = |\phi_1, \vec{q}_1\rangle + G_0(E) T_1(E) P |\psi_1\rangle^+. \quad (2.33)$$

The Faddeev equation of the three-body transition operator $\mathbf{T}(E)$:

$$\mathbf{T}(Z) = T_1(Z) P + T_1(Z) P G_0(Z) \mathbf{T}(Z). \quad (2.34)$$

The operator $T_1(Z)$ is the two-body transition operator embedded in the three-particle Hilbert space

$$\langle \vec{q}'_1, \vec{k}'_{23} | T_1(Z) | \vec{q}_1, \vec{k}_{23} \rangle = \delta(\vec{q}'_1 - \vec{q}_1) \langle \vec{k}'_{23} | T(Z - \frac{q^2}{3m}) | \vec{k}_{23} \rangle, \quad (2.35)$$

where \vec{k}, \vec{k}' are the relative initial and final momentum of the bound (23) particle system, \vec{q}_1 is the relative momentum of the incident free particle (1) with respect to the center of mass of the bound pair, and $\langle \vec{k}'_{23} | T(Z - \frac{q^2}{3m}) | \vec{k}_{23} \rangle$ is the kernel of the off-shell two-body transition operator.

The summary of the discussion is that the off-shell two-body transition matrix elements are needed as input to the Faddeev equations. The two-body transition operators embedded in the three particle Hilbert space are multiplied by an identity operator in the spectator spin. Further discussion of the three-body Faddeev equation using partial waves can be found in references [17],[3],[16]. The vector form of the Faddeev equation for spinless interactions is discussed in [18].

2.1.3 Introducing relativity

Relativistic three-body problems require the construction of a unitary representation of the Poincaré group [19] on the three-nucleon Hilbert space. The Poincaré group has two Casimir operators, the mass and spin. One way to construct a consistent relativistic three-body dynamics is to add interactions to the mass (rest energy operator) that commute with the three-body spin. The dynamical problem is then reduced to diagonalizing the mass operator [5]. Solutions of the Faddeev equation for the three-body mass operator give the required scattering eigenstates.

Two-body nucleon-nucleon interactions are constructed by fitting interactions motivated by meson-exchange models to scattering data that is properly Lorentz transformed to the two-body center of momentum of system. Because of this it follows that any nucleon-nucleon potential can be used to generate a relativistic mass (rest energy) operator for two interacting nucleons [11][6]:

$$M_{23} = m_{23} + v_r := \sqrt{k^2 + 2\mu V_{nr} + m_2^2} + \sqrt{k^2 + 2\mu V_{nr} + m_3^2}. \quad (2.36)$$

Because the M_{23} is a function of the non-relativistic rest Hamiltonian, both M_{12} and $H_{12} = k^2/2\mu + V_{nr}$ have identical wave functions and scattering phase shifts.

The relativistic form of the three-body equations involve the following replacements in the non-relativistic equation. The interaction V_1 is replaced by

$$\langle \vec{q}_1, \vec{k}_{23} | V_1 | \vec{q}'_1, \vec{k}'_{23} \rangle = \delta(\vec{q}_1 - \vec{q}'_1) \langle \vec{k}_{23} | [\sqrt{M_{23}^2 + q_1^2} - \sqrt{M_{230}^2 + q_1^2}] | \vec{k}'_{23} \rangle \quad (2.37)$$

where M_{230} is obtained from M_{23} by setting the two-body interaction to zero, the vectors \vec{q}_1 and \vec{k}_{23} are relativistic Jacobi-momenta obtained from the single particle momenta by replacing the Galilean boosts used to define standard Jacobi momenta by Lorentz boosts. The free resolvent $G_0(z)$ is replaced by

$$G_0(z) = (z - \sqrt{M_{230}^2 + q_1^2} - \sqrt{q_1^2 + m^2})^{-1} \quad (2.38)$$

and the two-body transition operator embedded in the three-particle Hilbert space is the solution to

$$T_1(z) = V_1 + V_1 G_0(z) T_1(z). \quad (2.39)$$

The relation between M_{12} and H_{12} can be used to express the half-shell solution to (2.39) by [12]

$$\langle \vec{q}'_1, \vec{k}'_{23} | T_1(E) | \vec{q}_1, \vec{k}_{23} \rangle = \frac{2\mu}{\omega_2\omega_3 + \omega'_2\omega'_3} \frac{(\omega_2 + \omega_3)^2 + (\omega'_2 + \omega'_3)^2}{\sqrt{(\omega_2 + \omega_3)^2 + q_1^2} + \sqrt{(\omega'_2 + \omega'_3)^2 + q_1^2}} \times \delta(\vec{q}'_1 - \vec{q}_1) \times \langle \vec{k}'_{23} | T_{nr}(k_{23}^2/2\mu) | \vec{k}_{23} \rangle \quad (2.40)$$

where

$$\omega_i = \sqrt{k_{23}^2 + m_i^2} \quad i \in \{2, 3\} \quad (2.41)$$

Here it should be emphasized, that the above expression requires the solution of the non-relativistic half-shell transition operator associated with the realistic non-relativistic interaction, V_{nr} . The fully off-shell relativistic two-body transition operators, which are needed in the relativistic Faddeev equations, can be constructed from the half shell transition operators by solving the first resolvent equations [12]

$$\bar{T}_1(z') = \bar{T}_1(z_0) + \bar{T}_1(z') \frac{(z' - z_0)}{(z' - M_0)(z_0 - M_0)} \bar{T}_1(z_0) \quad z' \neq z_0 \quad (2.42)$$

rather than directly solving the for the off-shell transition operators at each off-shell energy. The treatment of the spins in the transition operators remains unchanged, although the permutation operators that appear in the relativistic Faddeev equation get modified [6]. The vector formalism of the two-body scattering for spin-dependent nucleon-nucleon potential is discussed in the next section.

2.2 Spin-dependent nucleon-nucleon potentials

Different formalisms that treat realistic nucleon-nucleon scattering without using a partial wave decomposition were proposed in [20],[21],[22],[23],[24],[13]. A helicity based formalism is discussed in [21],[23]. The most recent formalism uses vector variables [24],[13]. This chapter discuss the formalism of 3D scattering with spin-dependent nucleon-nucleon potentials using vector variables. The basic foundation of this formalism is the property [25] that a general nucleon-nucleon potential which is invariant with respect to rotations, time reversal, space reflection and permutation symmetry can be

expanded in a basis of six rotationally invariant spin operators. This is expressed as

$$\mathbf{V}(\vec{k}', \vec{k}) = \sum_{i=1}^6 v_i(k, k', \hat{k} \cdot \hat{k}') w_i(\vec{k}, \vec{k}', \vec{\sigma}_1, \vec{\sigma}_2). \quad (2.43)$$

In (2.43), \mathbf{V} is the nucleon-nucleon potential which is a function of the initial and final momentum vectors \vec{k} and \vec{k}' , the scalar function v_i is the expansion coefficient function and w_i is the rotationally invariant spin operator. Nucleon-nucleon potentials expressed in the form

$$\mathbf{V}(\vec{k}, \vec{k}') = \sum_{i=1}^n V_i(k, k', \hat{k} \cdot \hat{k}') O_i(\vec{\sigma}_1, \vec{\sigma}_2, \vec{k}, \vec{k}') \quad (2.44)$$

are ideal candidates to be employed in this formalism. Here V_i is a scalar function and O_i is the corresponding spin operator and n the number of spin operators. The candidate selected in this thesis is the Argonne V18 nucleon-nucleon potential. It has eighteen operators, $n=18$. Examples of nucleon-nucleon potential's spin operators are given below:

$$1, \quad \vec{\sigma}_1 \cdot \vec{\sigma}_2, \quad i\vec{S} \cdot (\vec{k} \times \vec{k}'), \quad S^2, \quad \vec{\sigma}_1 \cdot (\vec{k}' - \vec{k}) \vec{\sigma}_2 \cdot (\vec{k}' - \vec{k}), \quad (\vec{S} \cdot \vec{k})(\vec{S} \cdot \vec{k}') \quad (2.45)$$

where $\vec{S} = \frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)$ is the total spin of the nucleon-nucleon system. These spin operators are invariant under rotation, time reversal and space reflection symmetry transformations. Realistic nucleon-nucleon potentials include the Bonn-B [26], NNLO[27] and Argonne V18 [8] potentials. Bonn-B and NNLO are momentum-space nucleon-nucleon potentials and Argonne V18 is a configuration-space potential.

The transition amplitude has the same properties as the nucleon-nucleon potential. This allows the expansion of the transition amplitude in terms of the six basis operators for off-shell values of the momenta. However, the on-shell transition amplitude requires only five operators [25]. This is because one of the basis elements, $\sigma_1 \cdot \sigma_2$, becomes linearly dependent on other elements of the basis or the coefficient of expansions of one element vanishes. The loss of linearly independence on-shell is explained in the later section of this chapter.

The operator w_i is constructed out of the scalar products of the Pauli matrices and linearly independent vectors \vec{P} , \vec{K} and \vec{N} constructed out of the momentum vectors.

Equation (2.43) shows that the nucleon-nucleon potential $\mathbf{V}(\vec{k}', \vec{k})$ preserves the discrete symmetry conditions if both the terms w_i and v_i are symmetry even or odd. The formalism using vector variables is tested with a basis of symmetry even spin operators in ref [13].

2.3 Structure of the formalism

This section discusses the formalism used to solve the Lippmann Schwinger equation in [16],[24] and [13]. As discussed earlier in this chapter, a nucleon-nucleon potential that is invariant under rotation, time reversal, permutation symmetry and space inversion symmetry transformations [25] can be expanded using six rotationally invariant spin operators (2.43). The Euclidean space is spanned by three linearly independent vectors constructed from the initial and final momenta \vec{k} and \vec{k}' . They are

$$\hat{P} = \frac{\vec{k} + \vec{k}'}{|\vec{k} + \vec{k}'|}, \quad \hat{K} = \frac{\vec{k} - \vec{k}'}{|\vec{k} - \vec{k}'|}, \quad \hat{N} = \frac{\vec{k} \times \vec{k}'}{|\vec{k} \times \vec{k}'|}. \quad (2.46)$$

The time reversal and space reflection operations on the vectors \vec{k} , \vec{k}' , $\vec{\sigma}_1$, $\vec{\sigma}_2$ are illustrated in Table[2.1].

Time reversal and space reflection symmetry		
Operator	Time	Parity
\vec{k}	$-\vec{k}'$	$-\vec{k}$
\vec{k}'	$-\vec{k}$	$-\vec{k}'$
$\vec{\sigma}_1$	$-\vec{\sigma}_1$	$\vec{\sigma}_1$
$\vec{\sigma}_2$	$-\vec{\sigma}_2$	$\vec{\sigma}_2$

Table 2.1: Time reversal and space reflection symmetry

The action of time reversal and space reflection on the three unit vectors is shown in Table[2.2].

Space inversion and time invariance of vectors		
Vector	Parity	Time invariance
\hat{P}	-1	-1
\hat{K}	-1	1
\hat{N}	1	-1

Table 2.2: Symmetry transformations
of the vectors

The scalar products of the unit vectors for off-shell values of \vec{k} and \vec{k}' are

$$\begin{aligned}
 \hat{P} \cdot \hat{N} &= 0 \\
 \hat{P} \cdot \hat{K} &\neq 0 \\
 \hat{N} \cdot \hat{K} &= 0.
 \end{aligned}
 \tag{2.47}$$

While on-shell values ($k = k'$)

$$\begin{aligned}
 \hat{P} \cdot \hat{N} &= 0 \\
 \hat{P} \cdot \hat{K} &= 0 \\
 \hat{K} \cdot \hat{N} &= 0
 \end{aligned}
 \tag{2.48}$$

The rotationally invariant spin operators required to expand the potential (2.43) are the scalar products of the Pauli matrices and the three linearly independent vectors. These are called spin-momentum operators. The spin-momentum operators that can be

formed by the product of Pauli matrices and the vectors are

$$\vec{\sigma}_1 \cdot \vec{\sigma}_2, (\vec{\sigma}_1 \pm \vec{\sigma}_2) \cdot \vec{A}, (\vec{A} \cdot \vec{\sigma}_1)(\vec{A} \cdot \vec{\sigma}_2), 1, (\vec{A} \cdot \vec{\sigma}_1)(\vec{B} \cdot \vec{\sigma}_2), (\vec{\sigma}_1 \times \vec{\sigma}_2) \cdot \vec{A}. \quad (2.49)$$

Here $\vec{A}, \vec{B} \in \{\vec{K}, \vec{P}, \vec{N}\}$. Since the nucleon-nucleon potential has spin operators that are even under discrete symmetry transformations it is simpler if the basis operators have the same even symmetry properties. From the above list, the following six linearly independent spin operators are invariant with respect to rotation, time reversal and space inversion [13]. They are

$$\begin{aligned} & (\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{N} \\ & (\vec{\sigma}_1 \cdot \vec{N})(\vec{\sigma}_2 \cdot \vec{N}) \\ & (\vec{\sigma}_1 \cdot \vec{P})(\vec{\sigma}_2 \cdot \vec{P}) \\ & (\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{K}) \\ & \vec{\sigma}_1 \cdot \vec{\sigma}_2 \\ & 1. \end{aligned} \quad (2.50)$$

These basis elements are the w_i s in (2.43) that are used to expand the nucleon-nucleon potential.

The transition operator has the same properties as the potential hence

$$T(\vec{k}', \vec{k}, z) = \sum_{i=1}^6 T^i(k', k, \vec{k} \cdot \vec{k}', z) w_i(\vec{k}, \vec{k}'). \quad (2.51)$$

The Lippmann-Schwinger equation in vector form is given by

$$\langle \vec{k}', \mu'_1, \mu'_2 | T | \vec{k}, \mu_1, \mu_2 \rangle = \langle \vec{k}', \mu'_1, \mu'_2 | V | \vec{k}, \mu_1, \mu_2 \rangle + \langle \vec{k}', \mu'_1, \mu'_2 | V \frac{2\mu}{E - k^2 + i\epsilon} T | \vec{k}, \mu_1, \mu_2 \rangle. \quad (2.52)$$

Using (2.43) in (2.52), (2.52) becomes

$$\begin{aligned} & \sum_{i=1}^6 t^i(k, k', \vec{k} \cdot \vec{k}', z) w_i(\vec{k}, \vec{k}') = \sum_{i=1}^6 v^i(k, k', \vec{k} \cdot \vec{k}') w_i(\vec{k}, \vec{k}') \\ & + \int \sum_{j=1}^6 v^j(\vec{k}, \vec{k}', \hat{k} \cdot \hat{k}') w_j(\vec{k}, \vec{k}') \frac{2\mu}{k^2 - k''^2 + i\epsilon} \sum_{l=1}^6 t^l(\vec{k}'', \vec{k}', \hat{k}' \cdot \hat{k}'', z) w_l(\vec{k}'', \vec{k}) d^3 \vec{k}''. \end{aligned} \quad (2.53)$$

Multiplying by the operators $w_k(\vec{k}, \vec{k}')$ and taking traces over both spins gives six coupled scalar equations for the six coefficient functions $t^i(k, k', \hat{k} \cdot \hat{k}', z)$.

$$\sum_i t^i(k', k, \hat{k} \cdot \hat{k}', z) A_{ip} = \sum_i v^i(k, k', \hat{k} \cdot \hat{k}') A_{ip} + \int \sum_{j=1}^6 v^j(k, k'', \hat{k} \cdot \hat{k}'') \frac{2\mu}{k^2 - k''^2 + i\epsilon}$$

$$\sum_l B_{jlp}(\vec{k}, \vec{k}'', \vec{k}') t^l(k'', k', \vec{k}'' \cdot \vec{k}', z) d^3 k'', \quad (2.54)$$

where

$$B_{jlp}(\vec{k}, \vec{k}'', \vec{k}') = \text{Tr}(w_j(\vec{k}, \vec{k}'') w_l(\vec{k}'', \vec{k}') w_p(\vec{k}, \vec{k}')) \quad (2.55)$$

$$A_{ip}(\vec{k}, \vec{k}') = \text{Tr}(w_i(\vec{k}, \vec{k}'), w_p(\vec{k}, \vec{k}')). \quad (2.56)$$

A_{ip} is the element of matrix \mathbf{A} . To compute the traces the properties of the Pauli spin matrices

$$(\vec{\sigma}_1 \cdot \vec{E})(\vec{\sigma}_1 \cdot \vec{F}) = \vec{E} \cdot \vec{F} + i\vec{\sigma}_1 \cdot (\vec{E} \times \vec{F}) \quad (2.57)$$

$$[\vec{\sigma}_1, \vec{\sigma}_2] = 0 \quad (2.58)$$

$$\text{Tr}(\sigma_i) = 0 \quad (2.59)$$

$$\text{Tr}((\vec{\sigma}_i \cdot \vec{E})(\vec{\sigma}_i \cdot \vec{F})) = 2\vec{E} \cdot \vec{F} \quad (2.60)$$

$$\begin{aligned} \text{Tr}((\vec{\sigma}_i \cdot \vec{D})(\vec{\sigma}_i \cdot \vec{F})(\vec{\sigma}_i \cdot \vec{G})) &= \text{Tr}(\sigma_{il} \sigma_{im} \sigma_{in}) D_l F_m G_n = \\ &= 2i(\vec{D} \times \vec{F}) \cdot \vec{G}. \end{aligned} \quad (2.61)$$

are used. Using properties of Pauli spin matrices the trace (2.56)

$$\mathbf{A} = \begin{pmatrix} 8(\vec{N} \cdot \vec{N}) & 0 & 0 & 0 & 0 & 0 \\ 0 & 4(\vec{K} \cdot \vec{K})^2 & 0 & 4(\vec{K} \cdot \vec{P})^2 & 4(\vec{K} \cdot \vec{K}) & 0 \\ 0 & 0 & 4(\vec{N} \cdot \vec{N})^2 & 0 & 4(\vec{N} \cdot \vec{N}) & 0 \\ 0 & 4(\vec{K} \cdot \vec{P})^2 & 0 & 4(\vec{P} \cdot \vec{P})^2 & 4(\vec{P} \cdot \vec{P}) & 0 \\ 0 & 4(\vec{K} \cdot \vec{K}) & 4(\vec{N} \cdot \vec{N}) & 4(\vec{P} \cdot \vec{P}) & 12 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 \end{pmatrix}.$$

can be computed. A set of operators must meet the criteria of linear independence to form a basis. A linearly independent set of operators has the property

$$\det|A| \neq 0. \quad (2.62)$$

At the on-shell point

$$k = k', \quad (2.63)$$

and

$$\vec{K} \cdot \vec{P} = \frac{k^2 - k'^2}{|\vec{k} - \vec{k}'||\vec{k} + \vec{k}'|} = 0, \quad (2.64)$$

and

$$\det|A| = -8192(N^2 + K^2 + P^2 - 3)N^4P^2K^2. \quad (2.65)$$

Since the vectors $\vec{N}, \vec{K}, \vec{P}$ are unit vectors, $N^2 + K^2 + P^2 = 3$, the result is $\det|A| = 0$.

This linear dependence arises from the fact that, for on-shell values the three vectors are orthogonal (2.48) and the spin operator $\vec{\sigma}_1 \cdot \vec{\sigma}_2$ can be expanded as

$$\vec{\sigma}_1 \cdot \vec{\sigma}_2 = (\vec{\sigma}_1 \cdot \hat{K})(\vec{\sigma}_2 \cdot \hat{K}) + (\vec{\sigma}_1 \cdot \hat{P})(\vec{\sigma}_2 \cdot \hat{P}) + (\vec{\sigma}_1 \cdot \hat{N})(\vec{\sigma}_2 \cdot \hat{N}). \quad (2.66)$$

This leaves only five linearly independent spin operators on-shell. They are

$$1, \quad i(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \hat{N}, \quad (\vec{\sigma}_1 \cdot \hat{K})(\vec{\sigma}_2 \cdot \hat{K}), \quad (\vec{\sigma}_1 \cdot \hat{P})(\vec{\sigma}_2 \cdot \hat{P}), \quad (\vec{\sigma}_1 \cdot \hat{N})(\vec{\sigma}_2 \cdot \hat{N}). \quad (2.67)$$

The solution of the Lippmann-Schwinger equation gives the matrix element

$$\langle \mu_1, \mu_2, \vec{k} | T(z) | \vec{k}', \mu'_1, \mu'_2 \rangle = \sum_{i=1}^6 t_i(k, k', \hat{k} \cdot \hat{k}') w_i(\vec{k}, \vec{k}') \quad (2.68)$$

of the 4×4 transition amplitude matrix \mathbf{T} and the 4×4 scattering amplitude matrix (defined on-shell)

$$\mathbf{M}(\vec{k}, \vec{k}') = -(2\pi)^2 \mu \mathbf{T}(\vec{k}, \vec{k}'). \quad (2.69)$$

Here $k = k'$. The general representation of \mathbf{M} [25] is

$$\begin{aligned} \mathbf{M} = & a + b(\vec{\sigma}_1 - \vec{\sigma}_2) \cdot \hat{N} + c(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \hat{N} + m(\vec{\sigma}_1 \cdot \hat{N})(\vec{\sigma}_2 \cdot \hat{N}) + (g + h)(\vec{\sigma}_1 \cdot \hat{P})(\vec{\sigma}_2 \cdot \hat{P}) \\ & + (g - h)(\vec{\sigma}_1 \cdot \hat{K})(\vec{\sigma}_2 \cdot \hat{K}). \end{aligned} \quad (2.70)$$

The nucleon-nucleon potentials are also isospin invariant.

$$\langle t, m_t | \mathbf{V} | t', m'_t \rangle = \mathbf{V}^{tm_t} \delta_{t,t'} \delta_{m_t, m'_t}. \quad (2.71)$$

In (2.71), t is the isospin and t_z is the z component of the isospin t . The symmetries of the potential imply that the Pauli exchange symmetry can be implemented by anti-symmetrizing the initial state (2.52). The anti-symmetrized state can be expressed as

$$|\vec{k}, \mu_1, \mu_2 \rangle = (1 - P_{12}) |\vec{k}, \mu_1, \mu_2, t, m_t \rangle, \quad (2.72)$$

where P_{12} is the permutation operator that interchanges the spin magnetic quantum

numbers of the two particles. The matrix elements of the scattering amplitude are [13]

$$M_{\mu'_1, \mu'_2, \mu_1, \mu_2}^{tm_t}(\vec{k}', \vec{k}) = -\mu(2\pi)^2 \langle \mu'_1, \mu'_2 | (t^{tm_t}(\vec{k}', \vec{k}) + (-)^t t^{tm_t}(\vec{k}', \vec{k}) P_{12}) | \mu_1, \mu_2 \rangle,$$

with

$$k = k' \tag{2.73}$$

This can be expressed as

$$\mathbf{M} = a + c(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \hat{N} + m(\vec{\sigma}_1 \cdot \hat{N})(\vec{\sigma}_2 \cdot \hat{N}) + (g+h)(\vec{\sigma}_1 \cdot \hat{P})(\vec{\sigma}_2 \cdot \hat{P}) + (g-h)(\vec{\sigma}_1 \cdot \hat{K})(\vec{\sigma}_2 \cdot \hat{K}). \tag{2.74}$$

The parameters { a, c, m, g+h, g-h } are called the Wolfenstein parameters [25] [16]. The five Wolfenstein parameters are obtained by taking the trace of $\mathbf{M}w_j$ where $j \in \{1, \dots, 5\}$ and w_j is the j^{th} operator in which \mathbf{M} is expanded. The five Wolfenstein parameters directly lead to the scattering and spin observables. One advantage of the vector formalism is that it can be used directly with the density matrices that experimentalists use to extract spin observables.

2.3.1 Conclusions

The formalism to solve the Lippmann-Schwinger equation using vector variables was discussed in this chapter. The formalism was employed in [13] to compute the scattering cross sections. The calculation was done using the spin-dependent Bonn-B [26] and the chiral NNLO [27] momentum space potentials. This thesis attempts to take an alternate approach to formulate the two-body scattering problem using vector variables. The approach taken solves for the following problems

1. The formalism discussed in this chapter requires a basis of six spin operators that are rotationally invariant to solve the Lippmann-Schwinger equation. The operators are selected by choosing rotationally invariant spin operators that are linearly independent and meet the required symmetry conditions. This choice is determined by the choice of three linearly independent vectors. If an orthonormal set of three vectors are used then the spin operator $\vec{\sigma}_1 \cdot \vec{\sigma}_2$ is a linear combination

of the other spin operators.

$$\vec{\sigma}_1 \cdot \vec{\sigma}_2 = (\vec{\sigma}_1 \cdot \hat{K})(\vec{\sigma}_2 \cdot \hat{K}) + (\vec{\sigma}_1 \cdot \hat{N})(\vec{\sigma}_2 \cdot \hat{N}) + (\vec{\sigma}_1 \cdot \hat{P})(\vec{\sigma}_2 \cdot \hat{P}).$$

One of the spin operators from the above equation needs to be removed from the list of possible spin operators that make the elements of the basis. A general representation of spin operators that can be used to construct a basis for any choice of three vectors \vec{K} , \vec{P} and \vec{N} is required. An important requirement is that at the on-shell point five basis elements instead of six elements are needed to expand the transition amplitude.

In general the symmetry conditions allow the product of a symmetry-odd expansion coefficient and the corresponding symmetry-odd spin-momentum operator. Hence this symmetry-odd spin operator can be an element of the basis. What role do these symmetry-odd spin operators play in the solution of Lippmann-Schwinger equation?

2. This formalism is dependent on computing the trace of the products of spin operators. Since the vector treatment of two-body scattering is aimed at solving the three-body problem at energies close to or above the pion production threshold it is efficient to analytically compute these trace equations. For a two-body problem, two hundred and sixteen trace expressions (2.55) need to be computed analytically. Using properties of Pauli matrices the trace equations can be expressed as scalar products of the vectors that are functions of \vec{k} and \vec{k}' . The vector functions can be numerically computed. However, expressing these trace expressions as scalar products of momenta, \vec{k} and \vec{k}' , can result in some expressions being zero [13] which improves the efficiency of computation. This process is however tedious and makes the vector variable approach difficult to implement.

3. The nucleon-nucleon potentials that were used are spin-dependent momentum-space nucleon-nucleon potentials Bonn-B and NNLO. The Argonne V18 nucleon-nucleon potential however is in configuration space and the numerical computation of the Fourier transform at every grid point is inefficient. A new technique for computing the Fourier transforms is required to use the Argonne V18 nucleon-nucleon potential in this formalism for both two-body and three-body scattering.

2.4 What does this thesis offer?

The vector treatment of the relativistic three-body problem requires realistic momentum space interactions in operator form. In this thesis the momentum space Argonne V18 nucleon-nucleon potential is expressed as an expansion in operators. This provides needed input to test the limits of meson exchange models in realistic relativistic few-nucleon calculations. A useful operator representation of this potential that is applicable to the most general potential involving two spin $\frac{1}{2}$ particles is introduced. Symbolic tools for performing all of the algebraic operations with these operators that are needed to formulate the relativistic two and three-body problems are developed. To the best of the author's knowledge this is one of the first symbolic programs written explicitly to perform complex algebra in nuclear physics problems. These contributions are discussed below:

1. Consider an example, a trace of product of Pauli spin matrices

$$\text{Tr}((\vec{\sigma}_1 \cdot \vec{P})(\vec{\sigma}_2 \cdot \vec{P})(\vec{\sigma}_1 \cdot \vec{K}_1)(\vec{\sigma}_2 \cdot \vec{K}_1)(\vec{\sigma}_1 \cdot \vec{N}_2)(\vec{\sigma}_2 \cdot \vec{N}_2)) = 4((\vec{P} \times \vec{K}_1) \cdot \vec{N}_2)^2 \quad (2.75)$$

where \vec{P} is a function of \vec{q}_1 and \vec{q}_2 , \vec{K}_1 is function of \vec{q}_2 and \vec{q}_3 and \vec{N}_2 is a function of \vec{q}_1 and \vec{q}_3 . The equation (2.75) can be numerically computed in two different ways.

- (a) \vec{P} , \vec{K}_1 and \vec{N}_2 are computed as functions of \vec{q}_1 , \vec{q}_2 and \vec{q}_3 and these are used

in (2.75). For example let

$$\begin{aligned}\vec{P} &= (\vec{q}_1 + \vec{q}_2) \times (\vec{q}_1 - \vec{q}_2), \\ \vec{K}_1 &= (\vec{q}_2 - \vec{q}_3), \\ \vec{N}_2 &= (\vec{q}_1 - \vec{q}_3) \times (\vec{q}_1 + \vec{q}_3) \times (\vec{q}_1 - \vec{q}_3).\end{aligned}$$

(b) Equation (2.75) is expanded in terms of \vec{q}_1, \vec{q}_2 and \vec{q}_3 , (2.75) is re expressed in a reduced form as

$$\begin{aligned}& -4((\vec{q}_1 \times \vec{q}_2) \cdot \vec{q}_3)^{(2)} - 4(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_3)^{(2)} + 4(\vec{q}_1 \cdot \vec{q}_2)(\vec{q}_1 \cdot \vec{q}_3)^{(2)} \\ & + 4(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_1 \cdot \vec{q}_2)(\vec{q}_2 \cdot \vec{q}_3) - 4(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_1 \cdot \vec{q}_3)(\vec{q}_2 \cdot \vec{q}_3) + 4(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_3)(\vec{q}_3 \cdot \vec{q}_3) \\ & + 4(\vec{q}_1 \cdot \vec{q}_2)(\vec{q}_1 \cdot \vec{q}_3)(\vec{q}_2 \cdot \vec{q}_3) - 4(\vec{q}_1 \cdot \vec{q}_2)(\vec{q}_1 \cdot \vec{q}_3)(\vec{q}_3 \cdot \vec{q}_3) - 4(\vec{q}_1 \cdot \vec{q}_2)^{(2)}(\vec{q}_1 \cdot \vec{q}_3). \quad (2.76)\end{aligned}$$

This equation is then computed for values of \vec{q}_1, \vec{q}_2 and \vec{q}_3 .

The numerical computation of (2.76) requires 20 % less cpu time than the computation of (2.75) using the first method. Reducing the trace expressions to explicit scalar functions results in an increase in efficiency thereby reducing the computational load in the three-body problem for spin-dependent potentials. The vector solution with a spin-dependent potential requires repeating this process hundreds of times for algebras that are far more complex than the example above. Reducing the trace expressions result in an increase in efficiency thereby reducing the computational load in the three-body problem for spin-dependent potentials. For two and three-body non-relativistic and relativistic scattering problems the vector treatment of the spins is a major algebraic complication. An algebraic system that can be used automate the reduction of the trace expression and can be easily integrated with the numerical codes will eliminate the difficulty of dealing with complex algebraic equations in the vector formulation of the two-body and three-body problems.

This thesis shares the view of the developers of the symbolic manipulation computer system GINAC[28] that the existing computer algebraic systems are not able

to handle large scale symbolic computations and the reduction techniques are not sufficient. Further discussions can be found in ref[28]. The GINAC algebraic system is used to achieve the reduction of large algebraic expressions for the vector treatment of two-body and three-body systems.

2. The Fourier transform of local momentum-space potentials involves two vector variables which require additional evaluations or interpolations. In this thesis the Fourier transforms are represented using Chebyshev expansions of the momentum space potential. These are fast to compute and do not require interpolations of explicit evaluations of the Fourier transform. This method is applied to Argonne V18 potential.
3. A new basis for expanding operators on the two-nucleon Hilbert space is introduced. These operators are similar to the operators that are used in the Wolfenstein parametrization of nucleon-nucleon scattering amplitudes, but lead to better behaved two-body equations. It was also observed that iterations of potentials can sometimes generate time-odd operators multiplied by time-odd coefficients which may need to be included in the representation of the transition operator, even if they do not appear in the potential. The need for additional time-odd operators can be established by considering the output of the symbolic code. The role of these time-odd operators in the dynamics merits further investigation.
4. The realistic momentum space Argonne V18 potential and the symbolic reduction system is used to compute the deuteron bound state. This tests the method developed in this thesis.

The next chapter discusses the Fourier transform of the Argonne V18 nucleon-nucleon potential.

CHAPTER 3

THE NUCLEON-NUCLEON POTENTIAL - ARGONNE V18

The Argonne V18 potential [8] is a realistic nucleon-nucleon potential that is expressed as a linear combination of 18 spin-isospin operators with rotationally invariant coefficient functions. It has the general form

$$\mathbf{V}(\vec{r}) = \sum_{i=1}^{18} O_i v_i(r) \quad (3.1)$$

where O_i is the spin-isospin operator and $v_i(r)$ is the scalar function. The Tables 3.1 3.2 below lists the eighteen operators, O_i .

Argonne V18 operators in configuration space	
Operator	V(r)
1	V_1
$(\vec{\tau}_1 \cdot \vec{\tau}_2)$	V_2
$\vec{\sigma}_1 \cdot \vec{\sigma}_2$	V_3
$(\vec{\sigma}_1 \cdot \vec{\sigma}_2)(\vec{\tau}_1 \cdot \vec{\tau}_2)$	V_4
$(3\vec{\sigma}_1 \cdot \hat{r}\vec{\sigma}_2 \cdot \hat{r} - \vec{\sigma}_1 \cdot \vec{\sigma}_2)$	V_5
$(3\vec{\sigma}_1 \cdot \hat{r}\vec{\sigma}_2 \cdot \hat{r} - \vec{\sigma}_1 \cdot \vec{\sigma}_2)(\vec{\tau}_1 \cdot \vec{\tau}_2)$	V_6

Table 3.1: Argonne V18 operators in configuration space

Argonne V18 operators in configuration space	
Operator	V(r)
$(\vec{L} \cdot \vec{S})$	V_7
$(\vec{L} \cdot \vec{S})(\vec{\tau}_1 \cdot \vec{\tau}_2)$	V_8
L^2	V_9
$L^2(\vec{\tau}_1 \cdot \vec{\tau}_2)$	V_{10}
$L^2\vec{\sigma}_1 \cdot \vec{\sigma}_2$	V_{11}
$L^2(\vec{\sigma}_1 \cdot \vec{\sigma}_2)(\vec{\tau}_1 \cdot \vec{\tau}_2)$	V_{12}
$(\vec{L} \cdot \vec{S})^2$	V_{13}
$(\vec{L} \cdot \vec{S})^2(\vec{\tau}_1 \cdot \vec{\tau}_2)$	V_{14}
$(3\tau_{1z}\tau_{2z} - \vec{\tau}_1 \cdot \vec{\tau}_2)$	V_{15}
$(3\tau_{1z}\tau_{2z} - \vec{\tau}_1 \cdot \vec{\tau}_2)\vec{\sigma}_1 \cdot \vec{\sigma}_2$	V_{16}
$(3\vec{\sigma}_1 \cdot \hat{r}\vec{\sigma}_2 \cdot \hat{r} - \vec{\sigma}_1 \cdot \vec{\sigma}_2)(3\tau_{1z}\tau_{2z} - \vec{\tau}_1 \cdot \vec{\tau}_2)$	V_{17}
$(\tau_{1z} + \tau_{2z})$	V_{18}

Table 3.2: Argonne V18 operators in configuration space

This potential is a local configuration space potential. Table 3.1 3.2 represents the different types of spin operators that appear in a typical realistic nucleon-nucleon potential. The next section derives the momentum-space nucleon-nucleon Argonne V18 potential.

3.1 Momentum-space representation

The momentum-space Argonne V18 nucleon-nucleon potential is an ideal candidate for areas of nuclear research that require the nucleon-nucleon potential to be computed at high energies. Examples of such studies are modeling relativistic effect in three-body systems and the problem of electron deuteron scattering. This section analytically derives the Argonne V18 potential in momentum-space, using its configuration space spin operators and the corresponding scalar functions (3.1). A local nucleon-nucleon potential in configuration space has the property

$$\langle \vec{r}' | \mathbf{V} | \vec{r} \rangle = \delta(\vec{r}' - \vec{r}) \mathbf{V}(\vec{r}) \quad (3.2)$$

where \vec{r} is the relative position between two nucleons. In momentum-space the Fourier transform of the potential is given by

$$\langle \vec{k}' | \mathbf{V} | \vec{k} \rangle = \frac{1}{(2\pi)^3} \int_0^\infty e^{(-i\vec{k}' \cdot \vec{r})} \mathbf{V}(\vec{r}) e^{(i\vec{k} \cdot \vec{r})} d^3\vec{r}. \quad (3.3)$$

Using (3.1) in (3.3) gives

$$\begin{aligned} \langle \vec{k}' | \mathbf{V} | \vec{k} \rangle &= \sum_{i=1}^{18} \frac{1}{(2\pi)^3} \int_0^\infty e^{(-i\vec{k}' \cdot \vec{r})} v_i(r) O_i e^{(i\vec{k} \cdot \vec{r})} d^3\vec{r} \\ &= \sum_{i=1}^{18} \langle \vec{k}' | v_i(r) O_i | \vec{k} \rangle = \sum_{i=1}^{18} V_i(\vec{k}', \vec{k}) \end{aligned} \quad (3.4)$$

where

$$V_i(\vec{k}', \vec{k}) = \frac{1}{(2\pi)^3} \int_0^\infty e^{(-i\vec{k}' \cdot \vec{r})} v_i(r) O_i e^{(i\vec{k} \cdot \vec{r})} d^3\vec{r}. \quad (3.5)$$

The type of spin operators O_i that appear in the Argonne V18 nucleon-nucleon potential are

$$I \quad (3.6)$$

$$3\vec{\sigma}_1 \cdot (\hat{r}) \vec{\sigma}_2 \cdot (\hat{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2 \quad (3.7)$$

$$(\vec{L} \cdot \vec{S}) \quad (3.8)$$

$$L^2 \quad (3.9)$$

$$S^2 \quad (3.10)$$

$$(\vec{L} \cdot \vec{S})^2 \quad (3.11)$$

The Argonne V18 potential is a linear combination of the product of isospin operators with the spin operators listed above. The Fourier transform of each type of operator is derived next.

3.1.1 Operator : I

The identity operator includes the O_i s in (3.1) that are not functions of the integral variables. Equation (3.5) can be written as

$$\begin{aligned} \langle \vec{k}' | \mathbf{V} | \vec{k} \rangle &= O_i \frac{1}{(2\pi)^3} \int_0^\infty e^{(-i\vec{k}' \cdot \vec{r})} v_i(r) e^{(i\vec{k} \cdot \vec{r})} d^3\vec{r}. \\ &= \left(\frac{1}{2\pi}\right)^3 O_i \int_0^\infty v_i(r) e^{-i(\vec{k}' - \vec{k}) \cdot \vec{r}} d^3r = V_i(\vec{k}', \vec{k}). \end{aligned} \quad (3.12)$$

Using the plane wave expansion

$$e^{(-i(\vec{k}' - \vec{k}) \cdot \vec{r})} = 4\pi \sum_{l,m} (-i)^l j_l(\rho r) Y_m^l(\hat{\rho}) Y_m^{*l}(\hat{r}) \quad (3.13)$$

where

$$\hat{\rho} = \frac{\vec{k}' - \vec{k}}{|\vec{k}' - \vec{k}|}, \quad \rho = \sqrt{k'^2 + k^2 - 2\vec{k} \cdot \vec{k}'} \quad (3.14)$$

and the relation

$$\int d\hat{\Omega}(\hat{r}) Y_m^l(\hat{r}) = \sqrt{4\pi} \delta_{l0} \delta_{m0} \quad (3.15)$$

in (3.12), the momentum-space representation becomes

$$V_i(\vec{k}', \vec{k}) = \frac{1}{2\pi^2} O_i \int_0^\infty v_i(r) j_0(\rho r) r^2 dr = O_i \mathbf{I}_i^1(\rho). \quad (3.16)$$

where

$$\mathbf{I}_i^1(\rho) = \frac{1}{2\pi^2} \int_0^\infty v_i(r) j_0(\rho r) r^2 dr \quad (3.17)$$

3.1.2 Operator : $3(\vec{\sigma}_1 \cdot \hat{r})(\vec{\sigma}_2 \cdot \hat{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2$

The operator $3(\sigma_1 \cdot \hat{r})(\sigma_2 \cdot \hat{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2$ contributes to the tensor force of the Argonne V18 nucleon-nucleon potential. This operator can be re-expressed as

$$3(\sigma_1 \cdot \hat{r})(\sigma_2 \cdot \hat{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2 = \quad (3.18)$$

$$\begin{pmatrix} -r_y^2 + 2r_z^2 - r_x^2 & 3r_z r_x + (-3r_z r_y)i & 3r_z r_x + (-3r_z r_y)i & -3r_y^2 + 3r_x^2 + (-6r_x r_y)i \\ 3r_z r_x + (3r_z r_y)i & r_y^2 - 2r_z^2 + r_x^2 & r_y^2 - 2r_z^2 + r_x^2 & -3r_z r_x + (3r_z r_y)i \\ 3r_z r_x + (3r_z r_y)i & r_y^2 - 2r_z^2 + r_x^2 & r_y^2 - 2r_z^2 + r_x^2 & -3r_z r_x + (3r_z r_y)i \\ -3r_y^2 + 3r_x^2 + (6r_x r_y)i & -3r_z r_x + (-3r_z r_y)i & -3r_z r_x + (-3r_z r_y)i & -r_y^2 + 2r_z^2 - r_x^2 \end{pmatrix}.$$

Using the spherical harmonics expressions for $Y_m^2(\hat{r})$ the matrix can be re-written as

$$\begin{pmatrix} \frac{4}{5}\sqrt{\pi}Y_0^2(\hat{r})\sqrt{5} & 3\sqrt{\pi}Y_{-1}^2(\hat{r})\sqrt{\frac{8}{15}} & 3\sqrt{\pi}Y_{-1}^2(\hat{r})\sqrt{\frac{8}{15}} & 3\sqrt{\pi}\sqrt{\frac{32}{15}}Y_{-2}^2(\hat{r}) \\ -3\sqrt{\pi}\sqrt{\frac{8}{15}}Y_1^2(\hat{r}) & -\frac{4}{5}\sqrt{\pi}Y_0^2(\hat{r})\sqrt{5} & -\frac{4}{5}\sqrt{\pi}Y_0^2(\hat{r})\sqrt{5} & -3\sqrt{\pi}Y_{-1}^2(\hat{r})\sqrt{\frac{8}{15}} \\ -3\sqrt{\pi}\sqrt{\frac{8}{15}}Y_1^2(\hat{r}) & -\frac{4}{5}\sqrt{\pi}Y_0^2(\hat{r})\sqrt{5} & -\frac{4}{5}\sqrt{\pi}Y_0^2(\hat{r})\sqrt{5} & -3\sqrt{\pi}Y_{-1}^2(\hat{r})\sqrt{\frac{8}{15}} \\ 3\sqrt{\pi}Y_2^2(\hat{r})\sqrt{\frac{32}{15}} & 3\sqrt{\pi}\sqrt{\frac{8}{15}}Y_1^2(\hat{r}) & 3\sqrt{\pi}\sqrt{\frac{8}{15}}Y_1^2(\hat{r}) & \frac{4}{5}\sqrt{\pi}Y_0^2(\hat{r})\sqrt{5} \end{pmatrix}.$$

The momentum-space representation of the term $v_i(r)(3(\sigma_1 \cdot \hat{r})(\sigma_2 \cdot \hat{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2)$, $i \in \{5, 6, 17\}$ is obtained by substituting $v_i(r)O_i$ in (3.5), then

$$\begin{aligned} V_i(\vec{k}', \vec{k}) &= \frac{1}{2\pi^2} \sum_{l,m} \int_0^\infty v_i(r) j^l(\rho r) (3(\sigma_1 \cdot \hat{r})(\sigma_2 \cdot \hat{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2) Y_m^l(\hat{\rho}) Y_m^{*l}(\hat{r}) d\Omega(\hat{r}) r^2 dr \\ &= \frac{1}{2\pi^2} \sum_{l,m} \int_0^\infty r^2 j_l(\rho r) v_i(r) \int d\Omega(\hat{r}) (-i)^l \end{aligned} \quad (3.19)$$

$$\begin{pmatrix}
\frac{4}{5}\sqrt{\pi}Y_0^2(\hat{r})\sqrt{5} & 3\sqrt{\pi}Y_{-1}^2(\hat{r})\sqrt{\frac{8}{15}} & 3\sqrt{\pi}Y_{-1}^2(\hat{r})\sqrt{\frac{8}{15}} & 3\sqrt{\pi}\sqrt{\frac{32}{15}}Y_{-2}^2(\hat{r}) \\
-3\sqrt{\pi}\sqrt{\frac{8}{15}}Y_1^2(\hat{r}) & -\frac{4}{5}\sqrt{\pi}Y_0^2(\hat{r})\sqrt{5} & -\frac{4}{5}\sqrt{\pi}Y_0^2(\hat{r})\sqrt{5} & -3\sqrt{\pi}Y_{-1}^2(\hat{r})\sqrt{\frac{8}{15}} \\
-3\sqrt{\pi}\sqrt{\frac{8}{15}}Y_1^2(\hat{r}) & -\frac{4}{5}\sqrt{\pi}Y_0^2(\hat{r})\sqrt{5} & -\frac{4}{5}\sqrt{\pi}Y_0^2(\hat{r})\sqrt{5} & -3\sqrt{\pi}Y_{-1}^2(\hat{r})\sqrt{\frac{8}{15}} \\
3\sqrt{\pi}Y_2^2(\hat{r})\sqrt{\frac{32}{15}} & 3\sqrt{\pi}\sqrt{\frac{8}{15}}Y_1^2(\hat{r}) & 3\sqrt{\pi}\sqrt{\frac{8}{15}}Y_1^2(\hat{r}) & \frac{4}{5}\sqrt{\pi}Y_0^2(\hat{r})\sqrt{5}
\end{pmatrix} Y_m^{*l}(\hat{r})Y_m^l(\hat{\rho}) \quad (3.20)$$

$$= \int_0^\infty r^2 j_2(\rho r) v_i(r) (-1)$$

$$\begin{pmatrix}
\frac{4}{5}Y_0^2(\hat{\rho})\sqrt{5}\sqrt{\pi} & 3Y_{-1}^2(\hat{\rho})\sqrt{\frac{8}{15}}\sqrt{\pi} & 3Y_{-1}^2(\hat{\rho})\sqrt{\frac{8}{15}}\sqrt{\pi} & 3Y_{-2}^2(\hat{\rho})\sqrt{\frac{32}{15}}\sqrt{\pi} \\
-3Y_1^2(\hat{\rho})\sqrt{\frac{8}{15}}\sqrt{\pi} & -\frac{4}{5}Y_0^2(\hat{\rho})\sqrt{5}\sqrt{\pi} & -\frac{4}{5}Y_0^2(\hat{\rho})\sqrt{5}\sqrt{\pi} & -3Y_{-1}^2(\hat{\rho})\sqrt{\frac{8}{15}}\sqrt{\pi} \\
-3Y_1^2(\hat{\rho})\sqrt{\frac{8}{15}}\sqrt{\pi} & -\frac{4}{5}Y_0^2(\hat{\rho})\sqrt{5}\sqrt{\pi} & -\frac{4}{5}Y_0^2(\hat{\rho})\sqrt{5}\sqrt{\pi} & -3Y_{-1}^2(\hat{\rho})\sqrt{\frac{8}{15}}\sqrt{\pi} \\
3\sqrt{\frac{32}{15}}\sqrt{\pi}Y_2^2(\hat{\rho}) & 3Y_1^2(\hat{\rho})\sqrt{\frac{8}{15}}\sqrt{\pi} & 3Y_1^2(\hat{\rho})\sqrt{\frac{8}{15}}\sqrt{\pi} & \frac{4}{5}Y_0^2(\hat{\rho})\sqrt{5}\sqrt{\pi}
\end{pmatrix}$$

$$= (-3(\vec{\sigma}_1 \cdot \hat{\rho}\vec{\sigma}_2 \cdot \hat{\rho}) + \vec{\sigma}_1 \cdot \vec{\sigma}_2) \frac{1}{2\pi^2} \int_0^\infty v_i(r) j_2(\rho r) r^2 dr. \quad (3.21)$$

The momentum-space representation of $(3(\sigma_1 \cdot \hat{r})(\sigma_2 \cdot \hat{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2)v_i(r)$ is given by

$$V_i(\vec{k}', \vec{k}) = (-3(\vec{\sigma}_1 \cdot \hat{\rho}\vec{\sigma}_2 \cdot \hat{\rho}) + \vec{\sigma}_1 \cdot \vec{\sigma}_2) \mathbf{I}_i^2(\rho) \quad (3.22)$$

where

$$\mathbf{I}_i^2(\rho) = \frac{1}{2\pi^2} \int_0^\infty v_i(r) j_2(\rho r) r^2 dr. \quad (3.23)$$

3.1.3 Operator: $\vec{L} \cdot \vec{S}$

The operator $\vec{L} \cdot \vec{S}$ can be expressed as

$$\vec{L} \cdot \vec{S} = \vec{S} \cdot (-i\vec{\nabla}_k \times \vec{k}) \quad (3.24)$$

The momentum-space representation of $v_i(r)\vec{L} \cdot \vec{S}$ is derived by substituting (3.24) in (3.5). This is shown below

$$V_i(\vec{k}', \vec{k}) = \left(\frac{1}{2\pi}\right)^3 \int_0^\infty v_i(r) e^{-i\vec{k}' \cdot \vec{r}} \vec{L} \cdot \vec{S} e^{i\vec{k} \cdot \vec{r}} d^3r. \quad (3.25)$$

Using the relation (3.24) in the above equation leads to

$$V_i(\vec{k}', \vec{k}) = \left(\frac{1}{2\pi}\right)^3 \int_0^\infty v_i(r) e^{-i\vec{k}' \cdot \vec{r}} \vec{S} \cdot (-i\nabla_{\vec{k}} \times \vec{k}) e^{i\vec{k} \cdot \vec{r}} d^3r, \quad (3.26)$$

and

$$\begin{aligned} V_i(\vec{k}', \vec{k}) &= \vec{S} \cdot (-i\nabla_{\vec{k}} \times \vec{k}) \sum_{l,m} \frac{1}{2\pi^2} \int_0^\infty dr r^2 v_i(r) j_l(\rho r) \int d\Omega (-i)^l (\hat{r}) Y_m^{*l}(\hat{r}) Y_m^l(\hat{\rho}) \\ &= \left(\frac{1}{2\pi^2}\right) \int_0^\infty r^2 (-i\nabla_{\vec{k}} \times \vec{k}) j_0(\rho r) v_i(r) dr. \end{aligned} \quad (3.27)$$

Using the following identities,

$$\nabla_{\vec{k}} j_0(\rho r) = \partial_{k_i} j_0(\rho r) = \frac{\partial j_0(\rho r)}{\partial \rho} \frac{\partial \rho}{\partial k_i}, \quad (3.28)$$

$$\frac{\partial j_0(\rho r)}{\partial \rho} = -r j_1(\rho r), \quad (3.29)$$

$$\frac{\partial \rho}{\partial k_i} = \frac{1}{\rho} (k_i - k'_i), \quad (3.30)$$

$$\nabla_{\vec{k}} j_0(\rho r) = -r j_1(\rho r) \frac{(\vec{k} - \vec{k}')}{\rho}, \quad (3.31)$$

$$(\nabla_{\vec{k}} \times \vec{k}) j_0(\rho r) = r j_1(\rho r) \frac{(\vec{k}' - \vec{k}) \times \vec{k}}{\rho}, \quad (3.32)$$

in (3.27) the momentum-space representation of $\vec{L} \cdot \vec{S} v_i(r)$ is given by

$$V_i(\vec{k}', \vec{k}) = -i\vec{S} \cdot (\vec{k}' \times \vec{k}) \frac{1}{2\pi^2 \rho} \int_0^\infty v_i(r) r^3 j_1(\rho r) dr. \quad (3.33)$$

Thus, the momentum-space representation of $v_i(r)\vec{L} \cdot \vec{S}$ is

$$V_i(\vec{k}', \vec{k}) = -i\vec{S} \cdot (\vec{k}' \times \vec{k}) \mathbf{I}_i^3(\rho) \quad (3.34)$$

where

$$\mathbf{I}_i^3(\rho) = \frac{1}{2\pi^2 \rho} \int_0^\infty v_i(r) r^3 j_1(\rho r) dr. \quad (3.35)$$

3.1.4 Operator : $\vec{L} \cdot \vec{L}$

The following relations are useful in the rest of the discussion.

$$\vec{\rho} = \vec{k}' - \vec{k}$$

$$\vec{\nabla}_\rho f(\rho) = f'(\rho) \frac{\vec{\rho}}{\rho} \vec{\nabla}_\rho^2 f(\rho) = f''(\rho) + f'(\rho) \frac{3}{\rho} - f'(q) \frac{1}{\rho} = f''(q) + \frac{2}{\rho} f'(\rho) \quad (3.36)$$

$$\begin{aligned} (\vec{a} \cdot \vec{\nabla}_\rho (\vec{b} \cdot \vec{\nabla}_\rho f(\rho)) &= f''(q) \frac{\vec{a} \cdot \vec{\rho} \vec{b} \cdot \vec{\rho}}{\rho} + f'(q) \frac{\vec{a} \cdot \vec{b}}{\rho} - f'(q) \frac{(\vec{a} \cdot \vec{\rho})(\vec{b} \cdot \vec{\rho})}{(\rho)^3} \\ &= \frac{\vec{a} \cdot \vec{\rho} \vec{b} \cdot \vec{\rho}}{\rho} (f''(\rho) - \frac{f'(\rho)}{\rho}) + \frac{\vec{a} \cdot \vec{b}}{\rho} f'(\rho). \end{aligned} \quad (3.37)$$

The momentum-space representation of $\vec{L} \cdot \vec{L} v_i(r)$ is given by

$$\begin{aligned} \frac{1}{(2\pi)^3} \int e^{-i\vec{k}' \cdot \vec{r}} V_i(r) (\vec{r} \times \vec{p}) \cdot (\vec{r} \times \vec{p}) e^{i\vec{k} \cdot \vec{r}} d\vec{r} &= \frac{1}{(2\pi)^3} \int e^{-i\vec{k}' \cdot \vec{r}} V_i(r) (\vec{r} \times \vec{k}') \cdot (\vec{r} \times \vec{k}) e^{i\vec{k} \cdot \vec{r}} d\vec{r} \\ &= (i\vec{\nabla}_\rho \times \vec{k}') \cdot (i\vec{\nabla}_\rho \times \vec{k}) \frac{1}{(2\pi)^3} \int V_i(r) e^{i\vec{k} \cdot \vec{r}} d\vec{r} = -(\vec{\nabla}_\rho \times \vec{k}') \cdot (\vec{\nabla}_\rho \times \vec{k}) \frac{4\pi}{(2\pi)^3} \int_0^\infty V_i(r) j_0(\rho r) r^2 dr. \end{aligned} \quad (3.38)$$

To compute the derivatives the following equations are used

$$(\vec{\nabla}_\rho \times \vec{k}') \cdot (\vec{\nabla}_\rho \times \vec{k}) = (\vec{k}' \cdot \vec{k}') (\vec{\nabla}_\rho \cdot \vec{\nabla}_\rho) - (\vec{k}' \cdot \vec{\nabla}_\rho) (\vec{k} \cdot \vec{\nabla}_\rho). \quad (3.39)$$

Using this in relation (3.38) gives

$$-(\vec{\nabla}_\rho \times \vec{k}') \cdot (\vec{\nabla}_\rho \times \vec{k}) \frac{4\pi}{(2\pi)^3} \int_0^\infty v_i(r) j_0(\rho r) r^2 dr = -\left((\vec{k}' \cdot \vec{k}') \nabla_\rho^2 - (\vec{k}' \cdot \vec{\nabla}_\rho) (\vec{k} \cdot \vec{\nabla}_\rho) \right) \mathbf{I}_i^1(\rho), \quad (3.40)$$

where Evaluating this gives

$$\begin{aligned} & -\left((\vec{k}' \cdot \vec{k}') \nabla_\rho^2 - (\vec{k}' \cdot \vec{\nabla}_\rho) (\vec{k} \cdot \vec{\nabla}_\rho) \right) \mathbf{I}_i^1(\rho) = \\ & -(\vec{k}' \cdot \vec{k}') (\mathbf{I}_i^{1''}(\rho) + \frac{2}{\rho} \mathbf{I}_i^{1'}(\rho)) + \mathbf{I}_i^{1'}(\rho) \left(\frac{\vec{k}' \cdot \vec{k}}{\rho} - \frac{(\vec{k}' \cdot \vec{\rho})(\vec{k} \cdot \vec{\rho})}{\rho^3} \right) + \mathbf{I}_i^{1''}(\rho) \frac{(\vec{k}' \cdot \vec{\rho})(\vec{k} \cdot \vec{\rho})}{\rho^2} \\ & = -(\vec{k}' \cdot \vec{k}') (\mathbf{I}_i^{1''}(\rho) + \frac{1}{\rho} \mathbf{I}_i^{1'}(\rho)) + \frac{(\vec{k}' \cdot \vec{\rho})(\vec{k} \cdot \vec{\rho})}{\rho^2} (\mathbf{I}_i^{1''}(\rho) - \frac{1}{\rho} \mathbf{I}_i^{1'}(\rho)). \end{aligned} \quad (3.41)$$

To eliminate the derivatives equations (3.43) and (3.44) are used.

$$\mathbf{I}_i^{1''}(\rho) - \frac{1}{\rho} \mathbf{I}_i^{1'}(\rho) = \frac{1}{2\pi^2} \int_0^\infty v_i(r) (j_0''(\rho r) r^2 - j_0'(\rho r) \frac{r}{\rho}) r^2 dr \quad (3.42)$$

$$= \frac{1}{2\pi^2} \int_0^\infty v_i(r) (j_0''(\rho r) - j_0'(\rho r) \frac{1}{\rho r}) r^4 dr = \frac{1}{2\pi^2} \int_0^\infty v_i(r) j_2(\rho r) r^4 dr$$

$$= \rho^2 \left\{ \frac{1}{2\pi^2 \rho^2} \int_0^\infty v_i(r) j_2(\rho r) r^4 dr \right\} = \mathbf{I}_i^4(\rho) \rho^2$$

$$\mathbf{I}_i^{1''}(\rho) + \frac{1}{\rho} \mathbf{I}_i^{1'}(\rho) = \frac{1}{2\pi^2} \int_0^\infty v_i(r) (j_0''(\rho r) - j_0'(\rho r) \frac{1}{\rho r} + 2j_0'(\rho r) \frac{1}{\rho r}) r^4 dr \quad (3.43)$$

$$= \frac{1}{2\pi^2} \int_0^\infty v_i(r) j_2(\rho r) r^4 dr - \frac{1}{2\pi^2} \frac{2}{\rho} \int_0^\infty v_i(r) j_1(\rho r) r^3 dr$$

$$= \mathbf{I}_i^4(\rho) \rho^2 - \frac{2}{\rho} \mathbf{I}_i^3(\rho)$$

This gives

$$\frac{1}{(2\pi)^3} \int e^{-i\vec{k}' \cdot \vec{r}} v_i(r) (\vec{r} \times \vec{p}) \cdot (\vec{r} \times \vec{p}) e^{i\vec{k} \cdot \vec{r}} d\vec{r} = -(\vec{k}' \cdot \vec{k})(\rho^2 \mathbf{I}_1^4(\rho) - 2\mathbf{I}_1^3(\rho)) + (\vec{k}' \cdot \vec{\rho})(\vec{k} \cdot \vec{\rho}) \mathbf{I}_1^4(\rho). \quad (3.44)$$

Re expressing (3.44) in terms of cross products, the momentum-space representation of $(\vec{L} \cdot \vec{L} v_i(r))$ is given by

$$V_i(\vec{k}', \vec{k}) = -\mathbf{I}_1^4(\rho)(\vec{k}' \times \vec{k}) \cdot (\vec{k}' \times \vec{k}) + 2(\vec{k}' \cdot \vec{k}) \mathbf{I}_1^3(\rho), \quad (3.45)$$

where

$$\mathbf{I}_1^4(\rho) = \frac{1}{2\pi^2 \rho^2} \int_0^\infty v_i(r) j_2(\rho r) r^4 dr. \quad (3.46)$$

3.1.5 Operator $:(\vec{L} \cdot \vec{S})^2$:

The momentum-space representation of $(\vec{L} \cdot \vec{S})^2 v_i(r)$ is derived by substituting the operator in (3.5). This leads to

$$\begin{aligned} \frac{1}{(2\pi)^3} \int e^{-i(\vec{k}' - \vec{k}) \cdot \vec{r}} v_i(r) (\vec{L} \cdot \vec{S})^2 d\vec{r} &= \frac{1}{(2\pi)^3} \int e^{-i(\vec{k}' - \vec{k}) \cdot \vec{r}} v_i(r) (\vec{S} \cdot (\vec{r} \times \vec{p}))^2 d\vec{r} \\ &= -\frac{4\pi}{(2\pi)^3} ((\vec{k}' \times \vec{S}) \cdot \vec{\nabla}_\rho) ((\vec{k} \times \vec{S}) \cdot \vec{\nabla}_\rho) \int j_0(\rho r) v_i(r) r^2 dr \\ &= -((\vec{k}' \times \vec{S}) \cdot \vec{\nabla}_\rho) ((\vec{k} \times \vec{S}) \cdot \vec{\nabla}_\rho) \mathbf{I}_1^1(\rho) = \\ &= -((\vec{k}' \times \vec{S}) \cdot \vec{\rho} ((\vec{k} \times \vec{S}) \cdot \vec{\rho})) \frac{1}{\rho^2} (\mathbf{I}_1''(\rho) - \frac{1}{\rho} \mathbf{I}_1'(\rho)) - (\vec{k}' \times \vec{S}) \cdot (\vec{k} \times \vec{S}) \frac{1}{\rho} \mathbf{I}_1'(\rho) = \\ &= -((\vec{k}' \times \vec{S}) \cdot \vec{\rho} ((\vec{k} \times \vec{S}) \cdot \vec{\rho})) \mathbf{I}_1^4(\rho) + (\vec{k}' \times \vec{S}) \cdot (\vec{k} \times \vec{S}) \mathbf{I}_1^3(\rho). \end{aligned} \quad (3.47)$$

The momentum-space representation of $(\vec{L} \cdot \vec{S})^2 v_i(r)$ is given by

$$V(\vec{k}', \vec{k}) = -((\vec{S} \cdot (\vec{k} \times \vec{k}'))^2 \mathbf{I}^4(\rho) + (\vec{k}' \times \vec{S}) \cdot (\vec{k} \times \vec{S}) \mathbf{I}^3(\rho). \quad (3.48)$$

3.2 Conclusion

The Fourier transform of the Argonne V18 potential for the different types of operators are computed using the equations

$$\mathbf{V}(\vec{k}', \vec{k}) = \sum_{i=1}^{18} f_i(\vec{\tau}_1, \vec{\tau}_2) V_i(\vec{k}', \vec{k}) \quad (3.49)$$

where $f_i(\vec{\tau}_1, \vec{\tau}_2)$ is the isospin component for index i and the spin-dependent functions $V_i(\vec{k}', \vec{k})$ are given by

$$V_i(\vec{k}', \vec{k}) = \mathbf{I}_i^1(\rho) \quad i \in \{1, 2, 3, 4, 15, 16, 18\},$$

$$V_i(\vec{k}', \vec{k}) = (-3(\vec{\sigma}_1 \cdot \hat{\rho} \vec{\sigma}_2 \cdot \hat{\rho}) + \vec{\sigma}_1 \cdot \vec{\sigma}_2) \mathbf{I}_i^2(\rho) \quad i \in \{5, 6, 17\},$$

$$V_i(\vec{k}', \vec{k}) = -i \vec{S} \cdot (\vec{k}' \times \vec{k}) \mathbf{I}_i^3(\rho) \quad i \in \{7, 8\},$$

$$V_i(\vec{k}', \vec{k}) = -\mathbf{I}_i^4(\rho) (\vec{k}' \times \vec{k}) \cdot (\vec{k}' \times \vec{k}) + 2(\vec{k}' \cdot \vec{k}) \mathbf{I}_i^3(\rho) \quad i \in \{9, 10, 11, 12\},$$

$$V_i(\vec{k}', \vec{k}) = -((\vec{S} \cdot (\vec{k} \times \vec{k}'))^2) \mathbf{I}_i^4(\rho) + (\vec{k}' \times \vec{S}) \cdot (\vec{k} \times \vec{S}) \mathbf{I}_i^3(\rho) \quad i \in \{13, 14\}.$$

In the next chapter the numerical technique used to compute the integrals $\mathbf{I}^1(\rho)$, $\mathbf{I}^2(\rho)$, $\mathbf{I}^3(\rho)$ and $\mathbf{I}^4(\rho)$ are discussed.

CHAPTER 4

NUMERICAL EVALUATION OF INTEGRALS

This chapter describes the numerical technique adopted to compute the integrals that appear in the momentum-space Argonne V18 nucleon-nucleon potential. The spin operators in the momentum-space Argonne V18 potential are multiplied by the following scalar functions of the magnitude of the momentum transfer, ρ , (3.14):

$$\mathbf{I}_i^1(\rho) = \frac{1}{2\pi^2} \int_0^\infty v_i(r) j_0(\rho r) r^2 dr, i \in \{1, 2, 3, 4, 15, 16, 18\} \quad (4.1)$$

$$\mathbf{I}_i^2(\rho) = \frac{1}{2\pi^2} \int_0^\infty v_i(r) j_2(\rho r) r^2 dr, i \in \{5, 6, 17\} \quad (4.2)$$

$$\mathbf{I}_i^3(\rho) = \frac{1}{2\pi^2 \rho} \int_0^\infty v_i(r) j_1(\rho r) r^3 dr, i \in \{7, 8, 9, 10, 11, 12, 13, 14\} \quad (4.3)$$

$$\mathbf{I}_i^4(\rho) = \frac{1}{2\pi^2 \rho^2} \int_0^\infty v_i(r) j_2(\rho r) r^4 dr, i \in \{9, 10, 11, 12, 13, 14\} \quad (4.4)$$

The indices $i = \{1, \dots, 18\}$ label the 18 scalar coefficient functions that appear in the Argonne V18 potential. To numerically compute these integrals a standard method like the Filon quadrature formula[29] could be used, but an alternative approach that exploits the properties of the potential and spherical Bessel functions is used in this thesis. The integrands in the above integrals are products of the form $P(r)j_n(\rho r)$ where

$$P_i(r) = V_i(r)r^2,$$

$$P_i(r) = V_i(r)r^3$$

or

$$P_i(r) = V_i(r)r^4 \quad (4.5)$$

and V_i is one of the 18 scalar coefficient functions that appear in the Argonne V18 potential.

The following properties of the functions in the integrand are used:

1. The value of the function $r^2 V_i(r)$ drops from its maximal value by at least a factor of $< 10^{-11}$ when r is 50 fm. The integral's upper limit is initially taken to be $r_{max} = 50 fm$. The integrals $\{\mathbf{I}_i^1(\rho), \mathbf{I}_i^2(\rho), \mathbf{I}_i^3(\rho), \mathbf{I}_i^4(\rho)\}$ are evaluated at $\rho = 0$. If

the value of r_{max} is reduced to $20fm$, the error between computed integrals with $r_{max} = 50$ and $r_{max} = 20$,

$$error = \frac{|I_{50} - I_{20}|}{|I_{50}|}. \quad (4.6)$$

is of the order, $error < 10^{-6}$, except in the component $i = 16$ which is of the order, $error < 10^{-4}$. The integrals used in this thesis are computed with $r_{max} = 20fm$.

2. The spherical Bessel functions are oscillatory and the plots for $j_0(x)$, $j_1(x)$ and $j_2(x)$ are shown in figure [4.1]. In the integrals

$$x = \rho r.$$

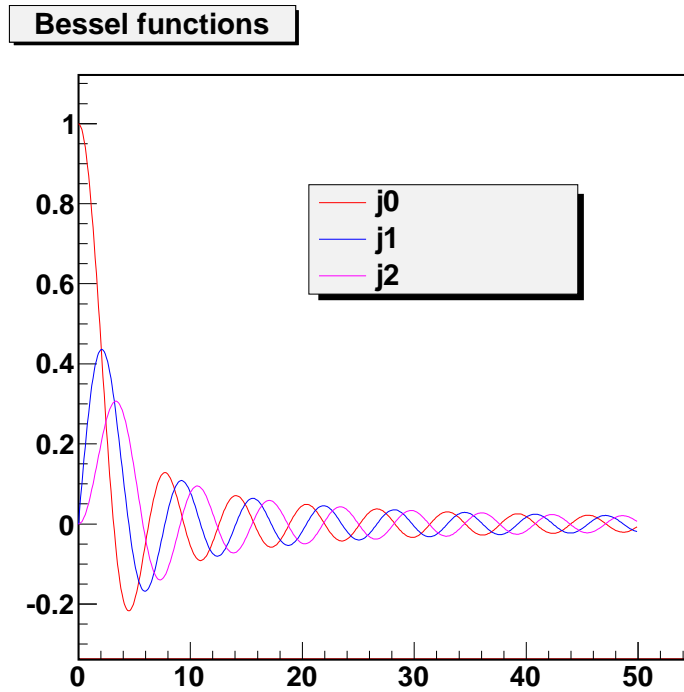


Figure 4.1: Plot of $j_0(x)$, $j_1(x)$ and $j_2(x)$
with respect to x

The maximum value of the momentum transfer ρ is limited to $\rho_{max} = 100fm^{-1}$. It

follows that the largest value of x that appears in the integrand for $r_{max} = 20fm$ is $x_{max} = 2000$. The zero values of all three spherical Bessel functions are computed for values of $x \leq x_{max}$ using standard numerical software [30].

The following steps are used for the numerical evaluation of the integrals.

1. The zeros between, $x = 0$ and $x = 2000$, of each spherical Bessel function $j_0(x), j_1(x), j_2(x)$ are computed and stored as three different arrays. The zeros are labeled in the array as

$$X_m = x_1, x_2, x_3, \dots, x_i, \dots, x_N, \quad (4.7)$$

where

$$m = \{j_0, j_1, j_2\},$$

and x_N is the largest zero $\leq x_{max} = \rho_{max}r_{max}$.

2. The number of zeros between zero and r_{max} is determined by the value of ρ . For example if

$$\rho = 0$$

then the integrand has no non-trivial zeros. Similarly if for all values of $\rho < 100fm^{-1}$

$$r_{max} < \frac{x_1}{\rho}$$

then the first zero is larger than $r_{max}\rho_{max}$ and the spherical Bessel function has no non-trivial zeros in the domain of integration.

In general for a given value of ρ , the values of r at the zeros of the spherical Bessel functions are given by

$$\mathbf{r} = \left\{ \frac{x_1}{\rho}, \dots, \frac{x_i}{\rho}, \dots, \frac{x_{lim}}{\rho} \right\}$$

where lim is the i^{th} position of the zero, which has the value

$$\frac{x_{lim}}{\rho} < r_{max} \leq \frac{x_{lim+1}}{\rho}.$$

3. For value of ρ where the spherical Bessel function has no zero in the domain of integration the integral is computed using 100 Gaussian quadrature points. The

number of points is large to remove any doubt that the integrals will converge. Later the number of Gaussian points are reduced. However, the final goal is to use Chebyshev polynomials to approximate the scalar functions and the coefficients are then extracted for computing the functions. For values of ρ satisfying

$$r_{max} > \frac{x_1}{\rho},$$

the region of integration is decomposed into intervals between successive zeros of the spherical Bessel functions. The lower and upper limits of each interval are

$$\delta = \left\{ \left(0, \frac{x_1}{\rho}\right), \left(\frac{x_1}{\rho}, \frac{x_2}{\rho}\right), \left(\frac{x_2}{\rho}, \frac{x_3}{\rho}\right), \dots, \left(\frac{x_{lim-1}}{\rho}, \frac{x_{lim}}{\rho}\right), \left(\frac{x_{lim}}{\rho}, r_{max}\right) \right\}. \quad (4.8)$$

The integral of each interval is evaluated using a Gauss-Legendre quadrature. The integrals $\mathbf{I}_i^1(\rho)$, $\mathbf{I}_i^2(\rho)$, $\mathbf{I}_i^3(\rho)$ and $\mathbf{I}_i^4(\rho)$ are then the sum of each integrated interval.

The integrals can be written as the sum

$$\begin{aligned} \int_0^{r_{max}} P_i(r) dr j_n(\rho r) &= \int_0^{\frac{x_1}{\rho}} P_i(r) j_n(\rho r) dr + \int_{\frac{x_1}{\rho}}^{\frac{x_2}{\rho}} P_i(r) j_n(\rho r) dr + \\ &\dots \int_{\frac{x_{lim-1}}{\rho}}^{\frac{x_{lim}}{\rho}} P_i(r) j_n(\rho r) dr + \int_{\frac{x_{lim}}{\rho}}^{r_{max}} P_i(r) j_n(\rho r) dr \end{aligned} \quad (4.9)$$

where the integrals on each interval can be approximated by

$$\int_{\frac{x_i}{\rho}}^{\frac{x_{i+1}}{\rho}} P_i(r) j_n(\rho r) \approx \sum_{t=0}^{t=NN} P_i(r_t) j_n(\rho r_t) w_t. \quad (4.10)$$

The number of Gauss-Legendre quadrature points used on intervals with right endpoint $r < 5$ was initially taken to be 40 and 100 for intervals with right endpoint $5 < r < 20$. These numbers were reduced to 20 Gauss points for right endpoint $r < 5fm$, 40 Gauss points for right endpoint $r < 10fm$ and 80 Gauss points for right endpoint $r < 20fm$. The maximum difference observed was 10^{-7} .

The plots of the computed integrals as functions of the momentum transfer ρ are shown in sections 4.2, 4.3, 4.4 and 4.5.

4.1 Chebyshev approximation of integrals

The numerical computation of integrals described above is not efficient for large calculations, where these integrals need to be evaluated many times. A more efficient representation is constructed by making polynomial approximations to the integrals as functions of momentum transfer over the range $\rho \in [0, 100 fm^{-1}]$. This interval is decomposed into three sub-intervals and the numerical values of the integrals are used to construct Chebyshev polynomial approximations to these integrals in each of the three-sub intervals. Chebyshev polynomials are useful for approximating functions because they vary strictly between -1 and 1 due to their relation to trigonometric polynomials. The coefficients of the Chebyshev expansion can be computed using a Clenshaw-Curtiss quadrature.

The function $f(x)$ is approximated on the interval $x \in [a, b]$ by Chebyshev polynomials, $T_n(y)$

$$f(x) \approx c_0/2 + \sum_{n=1}^{100} c_n T_n\left(-\frac{a+b}{b-a} + \frac{2}{b-a}x\right),$$

where

$$T_n(y) = \cos(n \cos^{-1}(y))$$

are the Chebyshev polynomials. The coefficients c_n , of the expansion, computed using the Clenshaw-Curtiss quadrature, are:

$$c_n = \frac{2}{N} \left(\frac{1}{2} f(b) + \sum_{j=1}^{N-1} f\left(\frac{a+b}{2} + \frac{b-a}{2} \cos(\pi j/N)\right) \cos(nj\pi/N) + (-)^n \frac{1}{2} f(a) \right). \quad (4.11)$$

The Chebyshev polynomials are computed using the recurrence relations

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad T_0(x) = 1, \quad T_1(x) = x.$$

This entire process is used in standard software package [30].

The approximation requires evaluations of the function $f(x)$ at the transformed Clenshaw-Curtiss quadrature points $x_j := \frac{a+b}{2} + \frac{b-a}{2} \cos(\pi j/N)$. The function $f(y)$ is replaced by each of the integrals, $\{\mathbf{I}_1^1(\rho), \mathbf{I}_1^2(\rho), \mathbf{I}_1^3(\rho), \mathbf{I}_1^4(\rho)\}$ and y by ρ . These functions are then approximated by expansions in Chebyshev polynomials on three different

intervals of the variable ρ , which are

$$0 \leq \rho < 10fm^{-1}, \quad 10 \leq \rho < 50fm^{-1}, \quad 50 \leq \rho < 100fm^{-1}. \quad (4.12)$$

A polynomial approximation of 101 terms is used for each of these intervals. The resulting expansion coefficients are stored, and used to with the polynomials to evaluate the functions and any value of $\rho \in [0, 100]fm^{-1}$.

The choice of intervals above is dictated by the Argonne V18 interaction. The first interval, $0 - 10fm^{-1}$, is where the potential structure is observed. The other two intervals provide an adequate range of values for most applications.

The Chebyshev functions reproduce the integrals with a uniform error ($I(\rho) - I_{chebyshev}(\rho)$) of the order 10^{-9} (there are some exceptions in the region between $0-1fm^{-1}$ of orders 10^{-5} for potential 4 and 6).

In the next chapter these Fourier transforms are tested by computing the wave functions and binding energy of the deuteron in momentum space. In addition, expansion in lesser numbers of Chebyshev polynomials are examined in the next chapter.

The remaining sections show the results of the numerical Fourier-Bessel transforms. The Fourier-Bessel equations

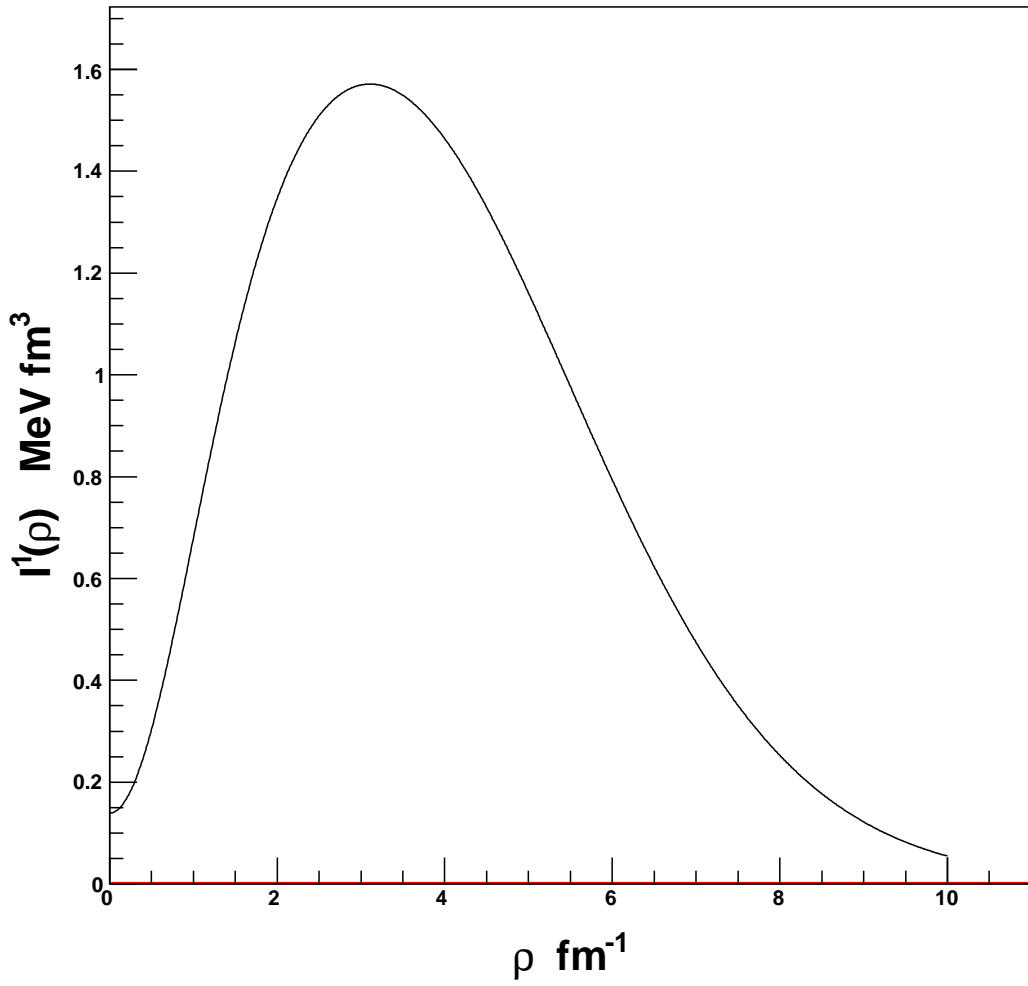
$$\mathbf{I}_i^1(\rho) = \frac{1}{2\pi^2} \int_0^\infty v_i(r) j_0(\rho r) r^2 dr, i \in \{1, 2, 3, 4, 15, 16, 18\} \quad (4.13)$$

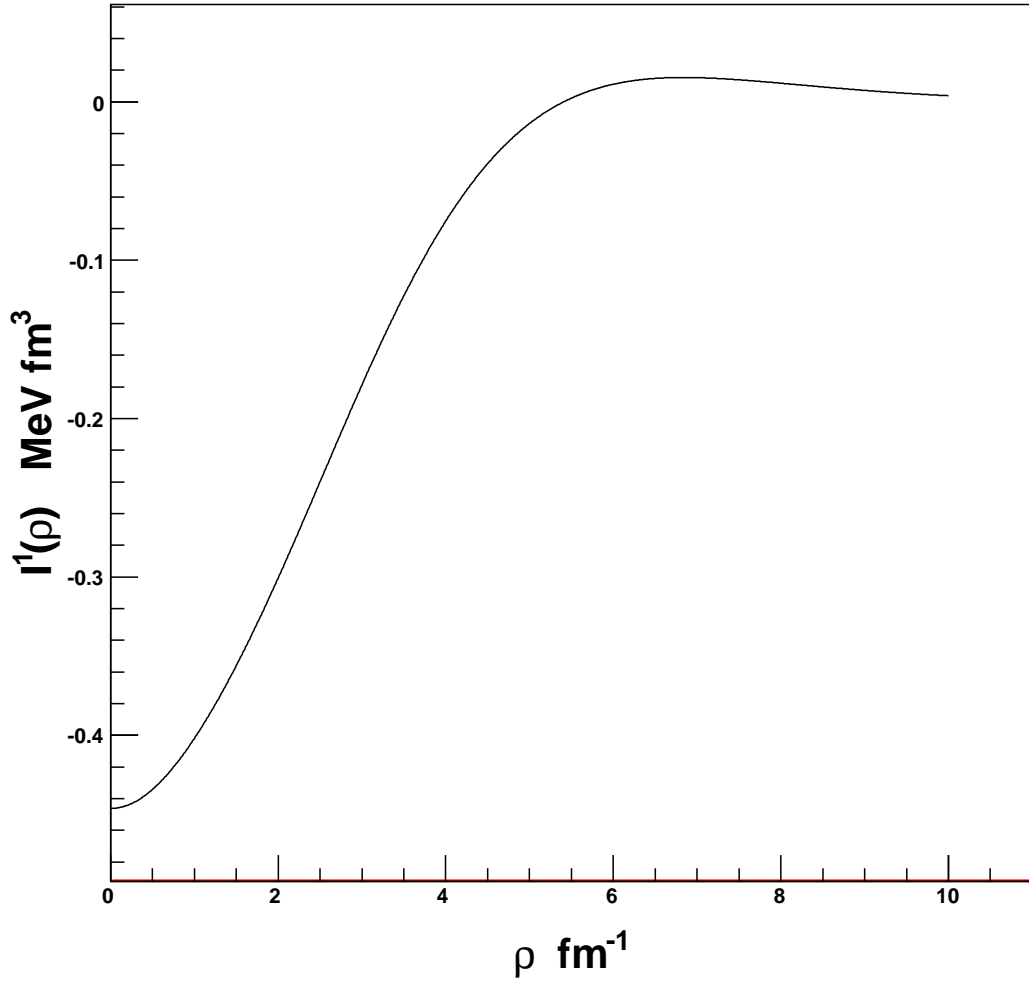
$$\mathbf{I}_i^2(\rho) = \frac{1}{2\pi^2} \int_0^\infty v_i(r) j_2(\rho r) r^2 dr, i \in \{5, 6, 17\} \quad (4.14)$$

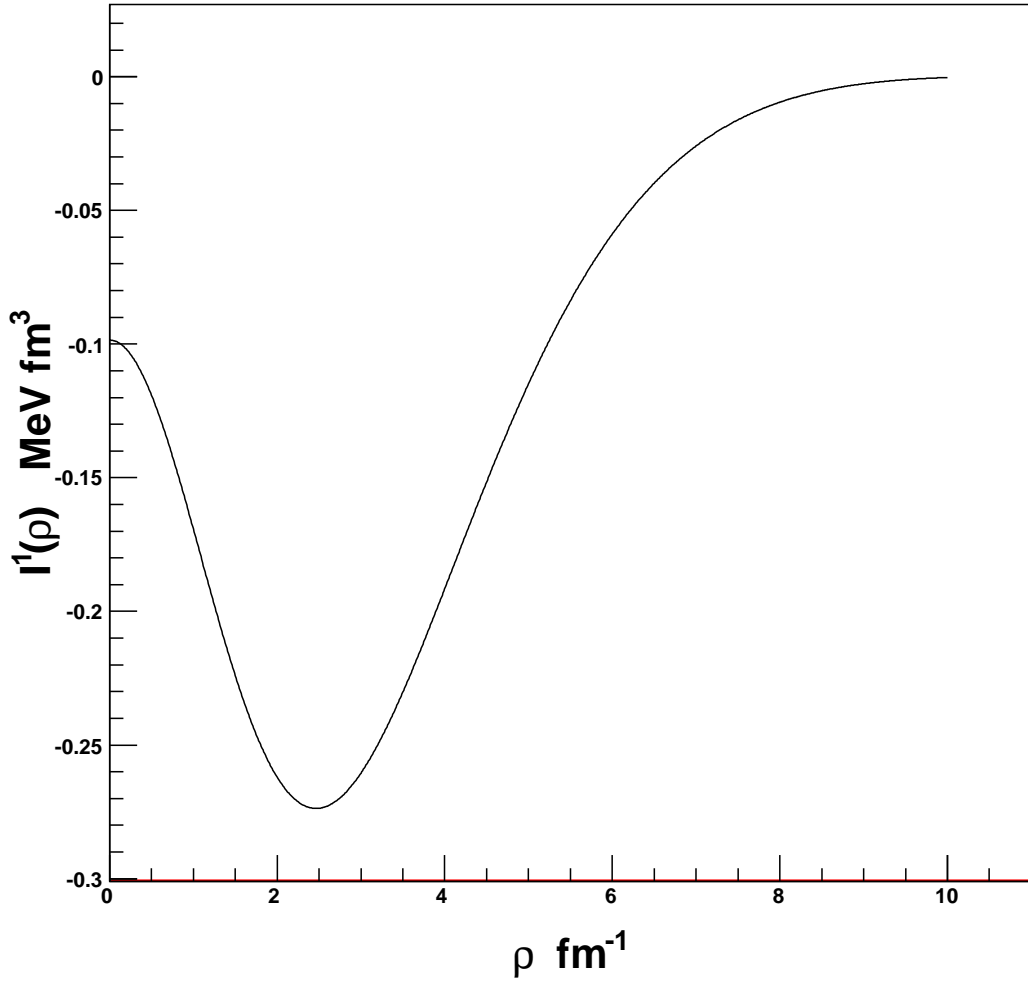
$$\mathbf{I}_i^3(\rho) = \frac{1}{2\pi^2 \rho} \int_0^\infty v_i(r) j_1(\rho r) r^3 dr, i \in \{7, 8, 9, 10, 11, 12, 13, 14\} \quad (4.15)$$

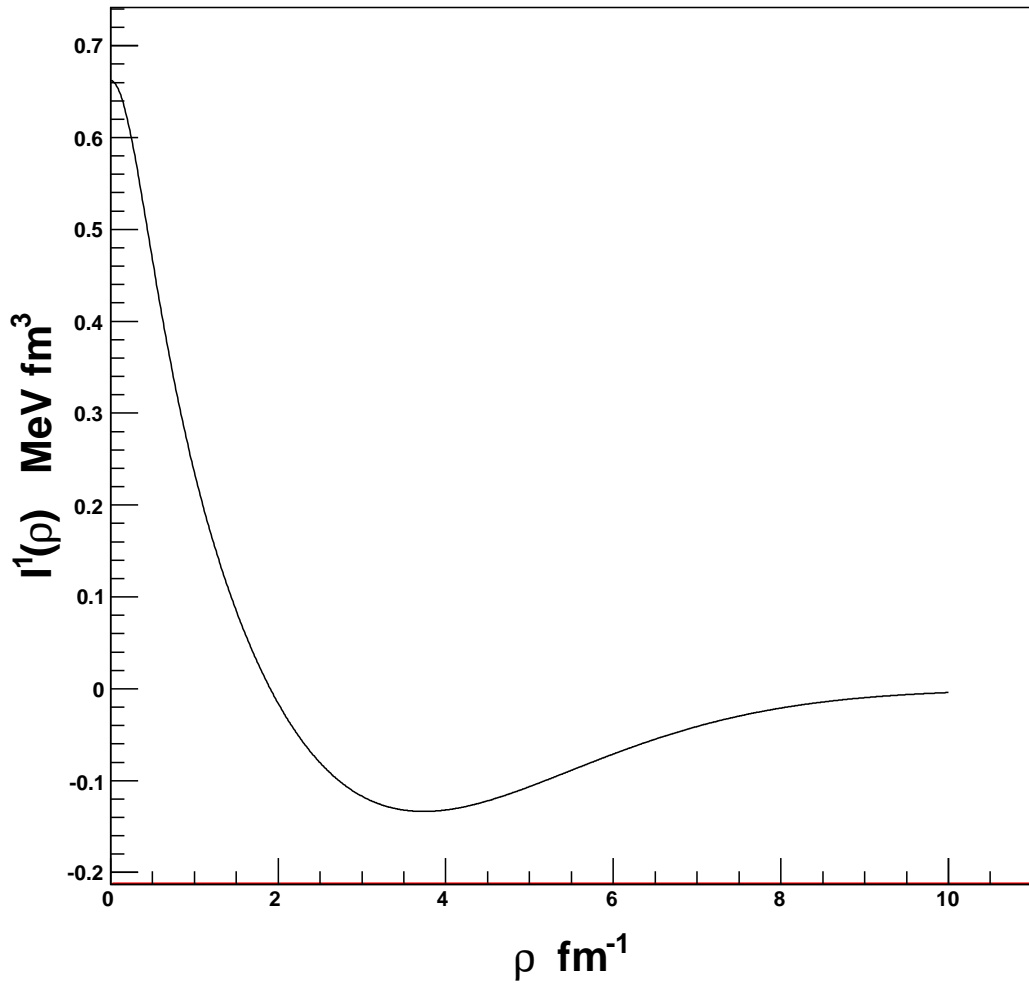
$$\mathbf{I}_i^4(\rho) = \frac{1}{2\pi^2 \rho^2} \int_0^\infty v_i(r) j_2(\rho r) r^4 dr, i \in \{9, 10, 11, 12, 13, 14\} \quad (4.16)$$

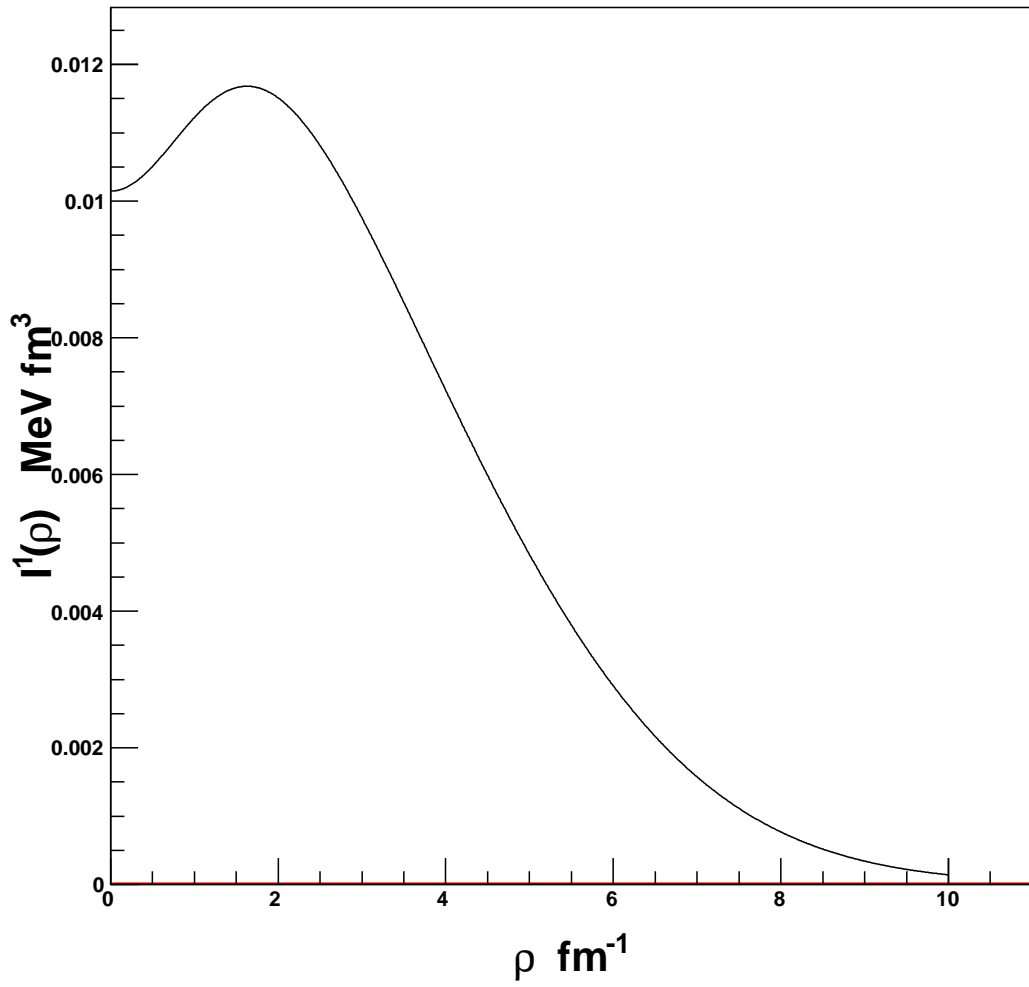
are numerically computed and the results are shown in the remaining sections. In these sections the functions $\{I_i^1(\rho), I_i^2(\rho), I_i^3(\rho), I_i^4(\rho)\}$ are computed for different values of ρ and the plots are shown.

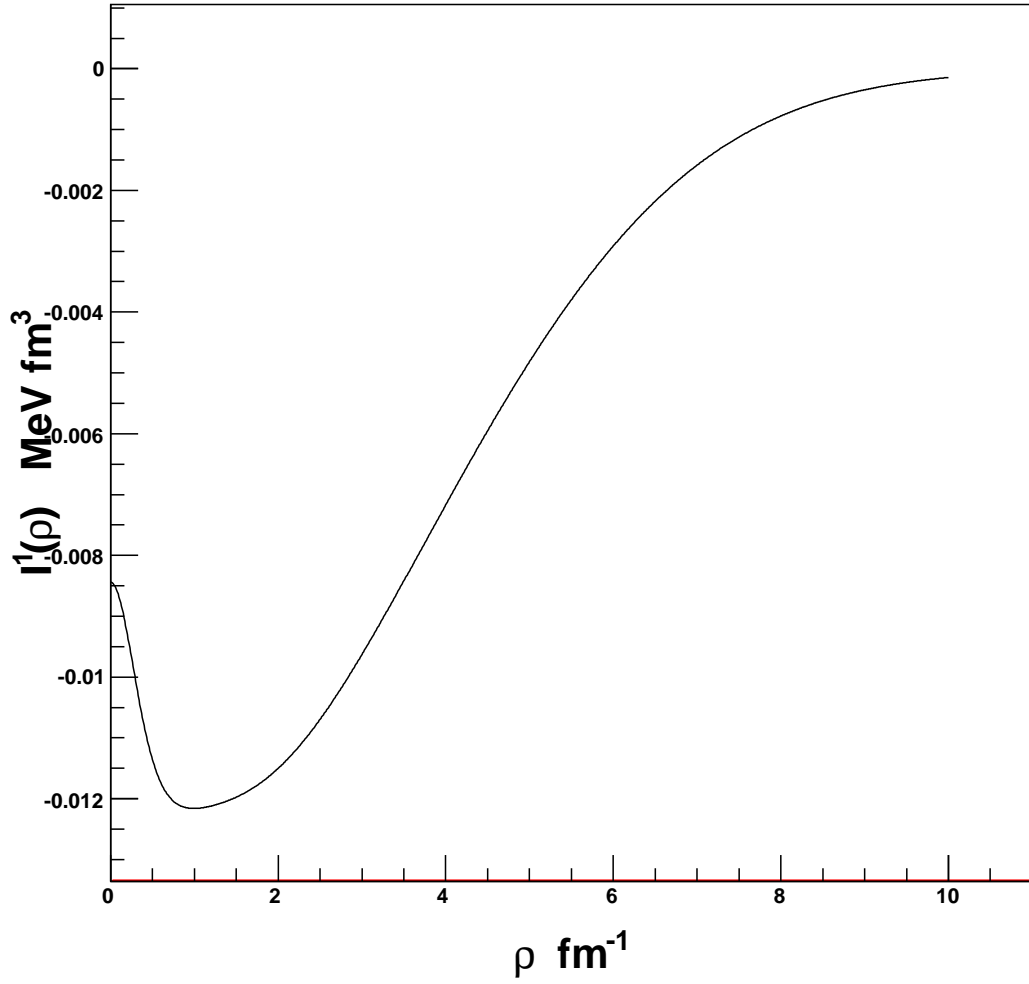
4.2 $I^1(\rho)$ **Argonne V18 1**Figure 4.2: Fourier-Bessel integral of $I_1^1(\rho)$

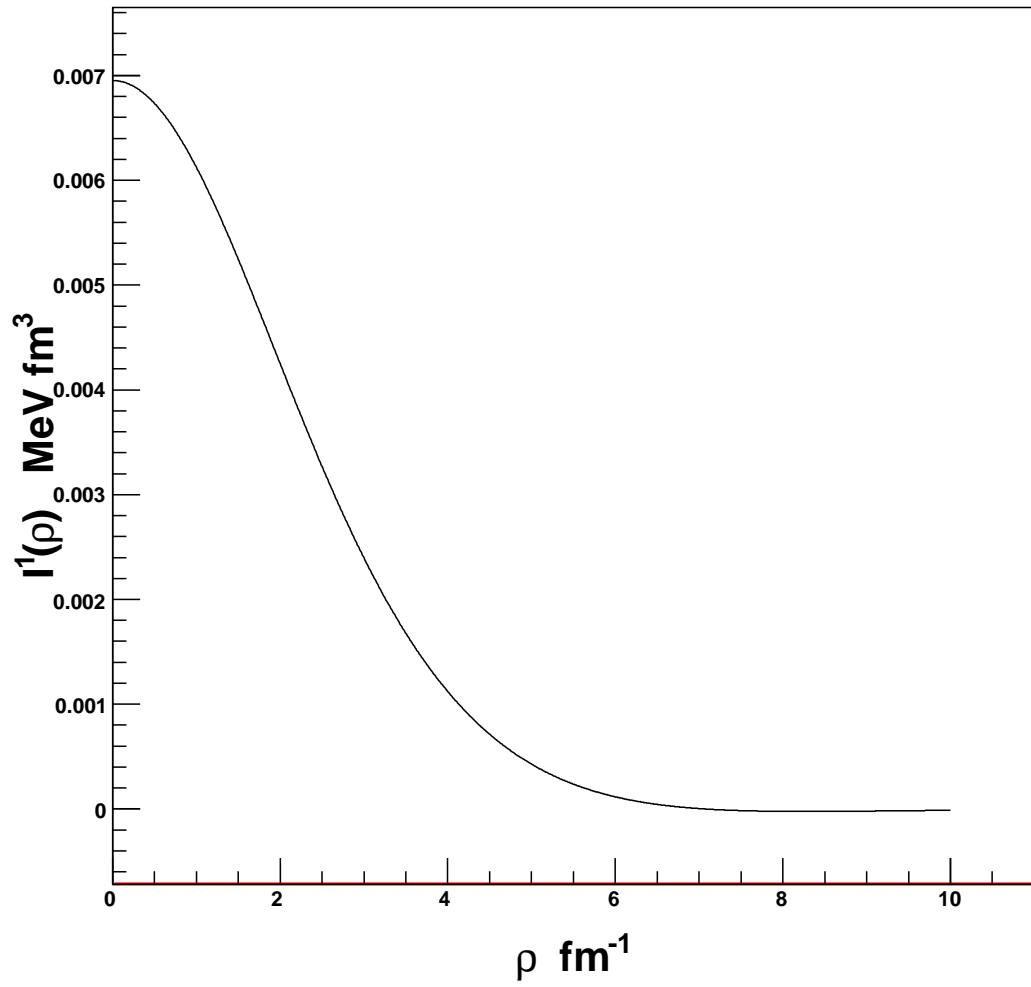
Argonne V18 2Figure 4.3: Fourier-Bessel integral of $I_2^1(\rho)$

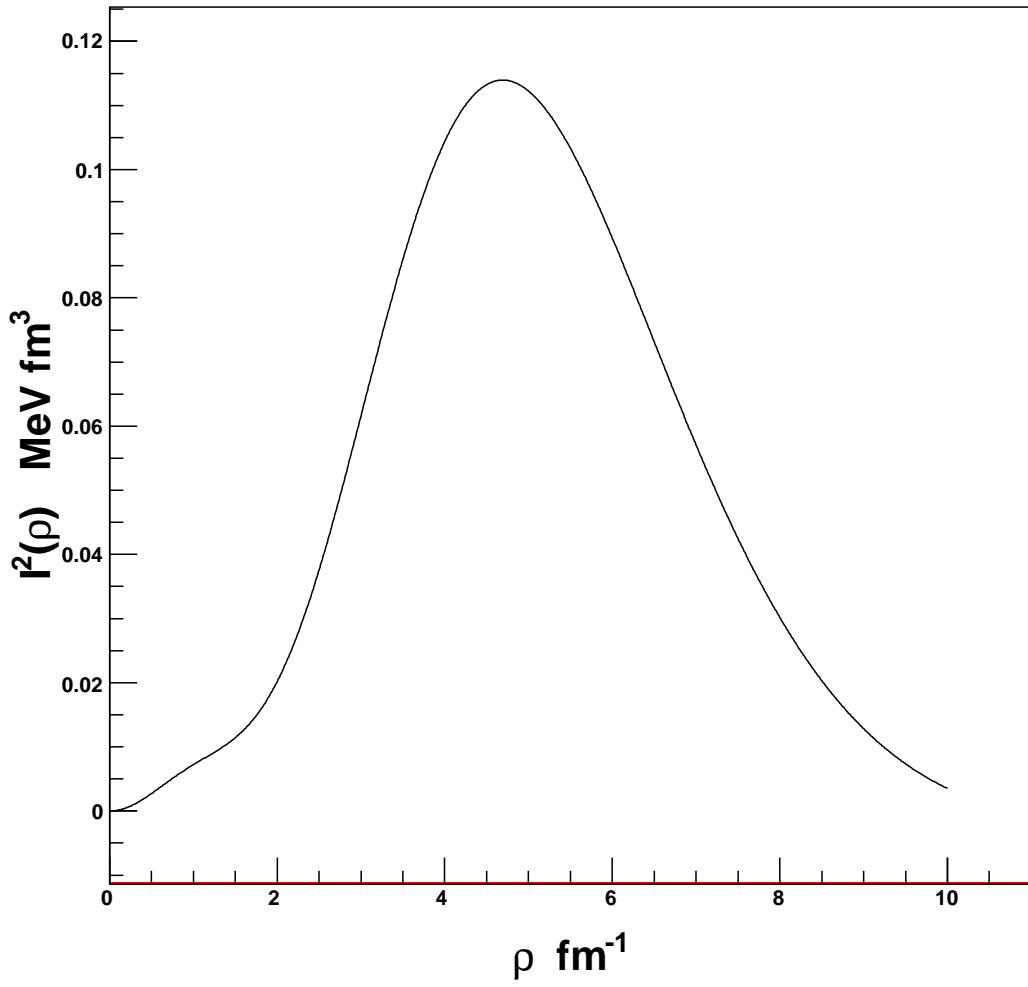
Argonne V18 3Figure 4.4: Fourier-Bessel integral of $I_3^1(\rho)$

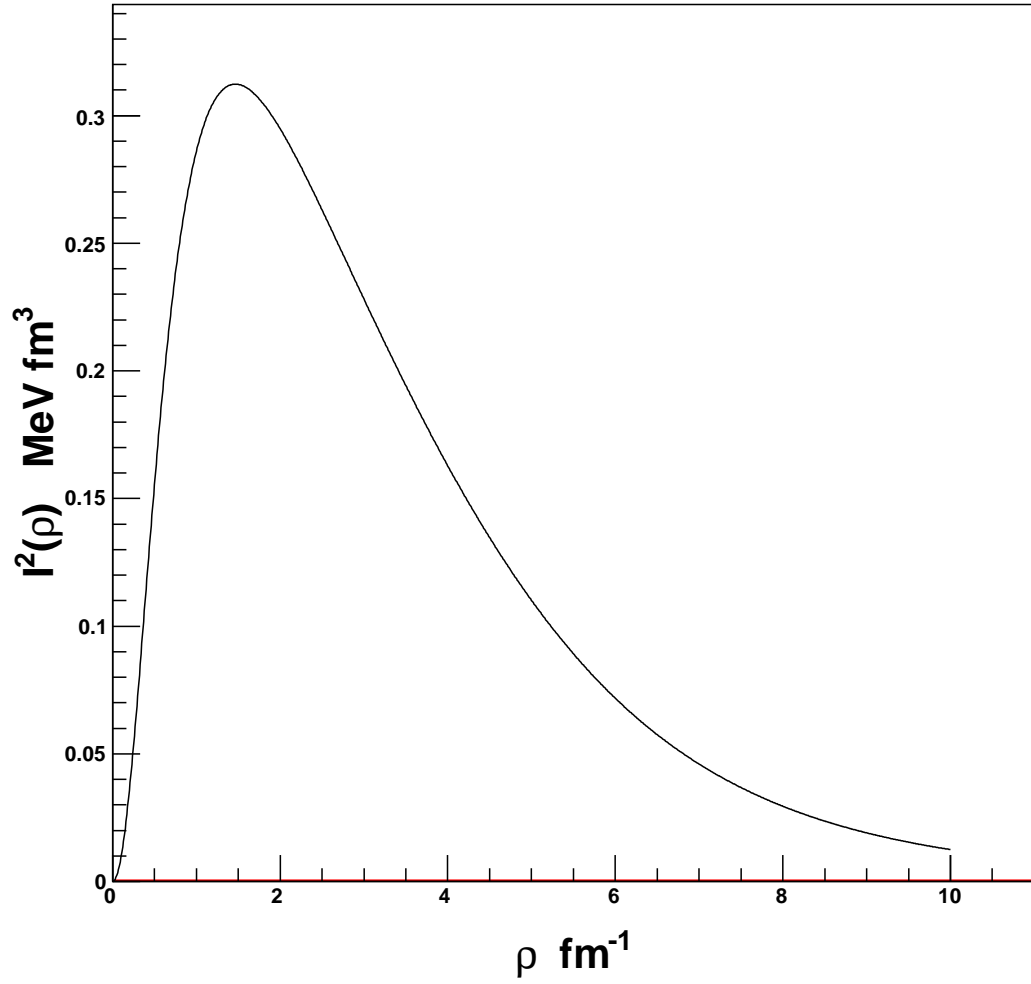
Argonne V18 4Figure 4.5: Fourier-Bessel integral of $I_4^1(\rho)$

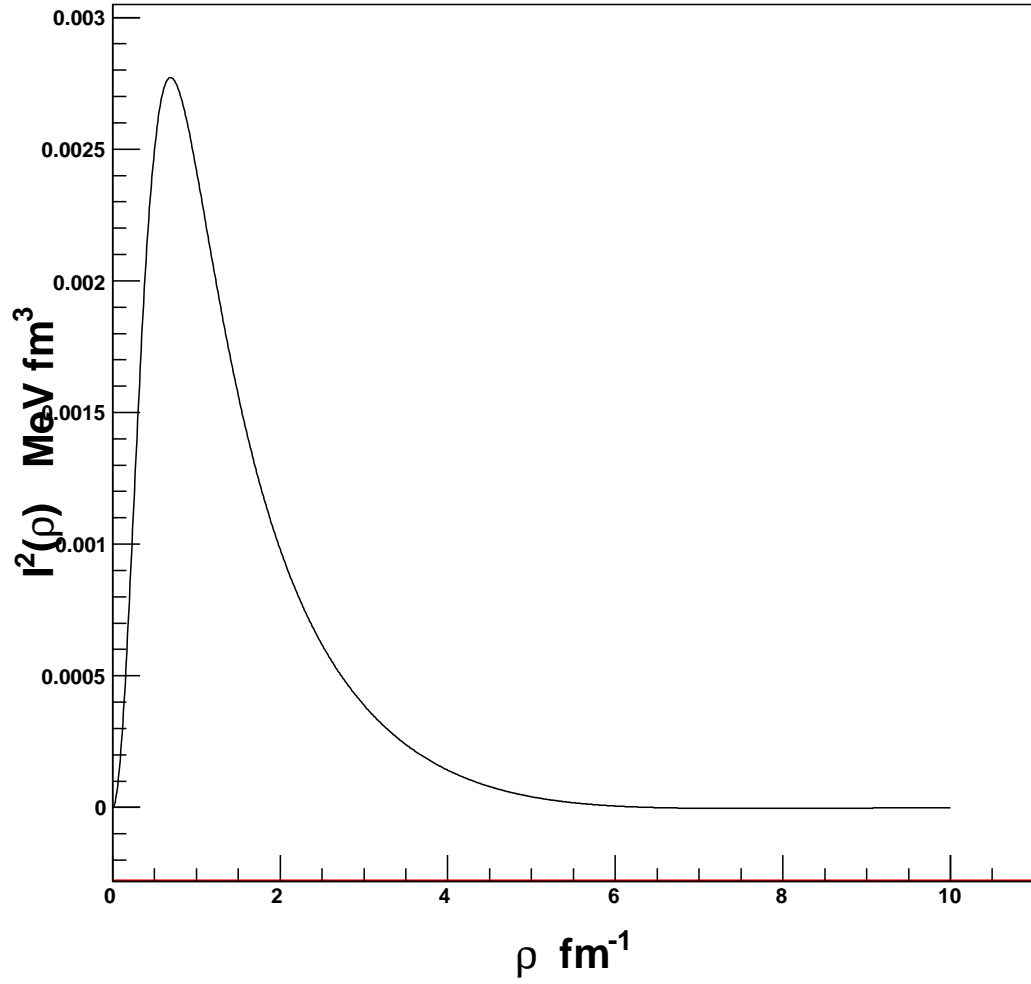
Argonne V18 15Figure 4.6: Fourier-Bessel integral of $I_{15}^1(\rho)$

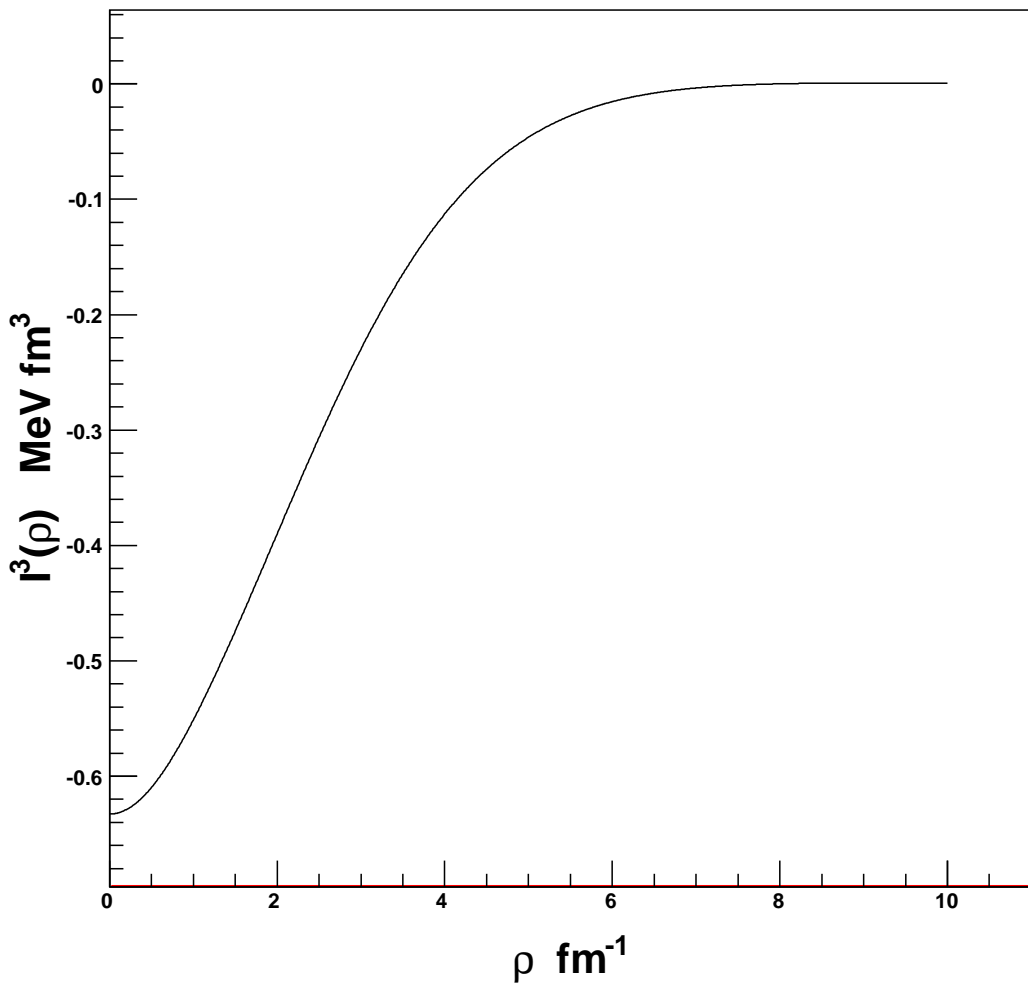
Argonne V18 16Figure 4.7: Fourier-Bessel integral of $I_{16}^1(\rho)$

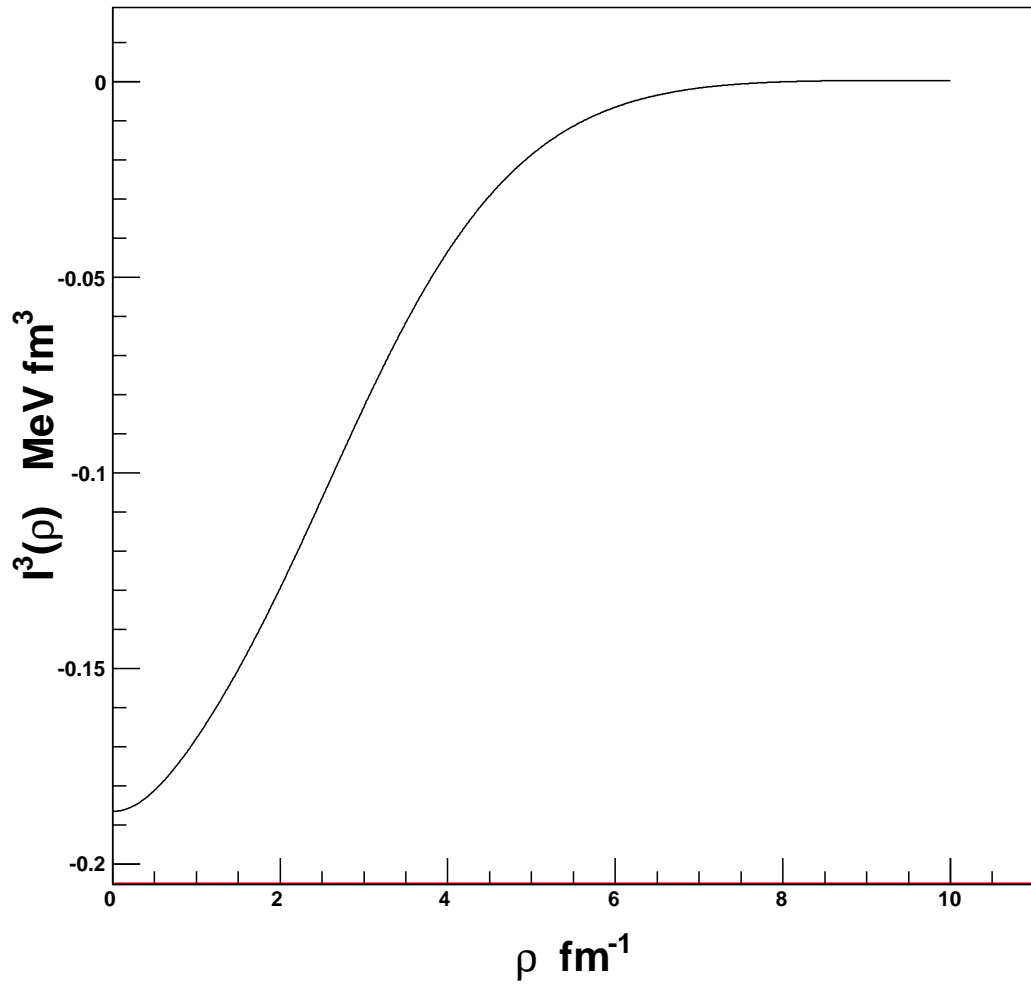
Argonne V18 18Figure 4.8: Fourier-Bessel integral of $I_{18}^1(\rho)$

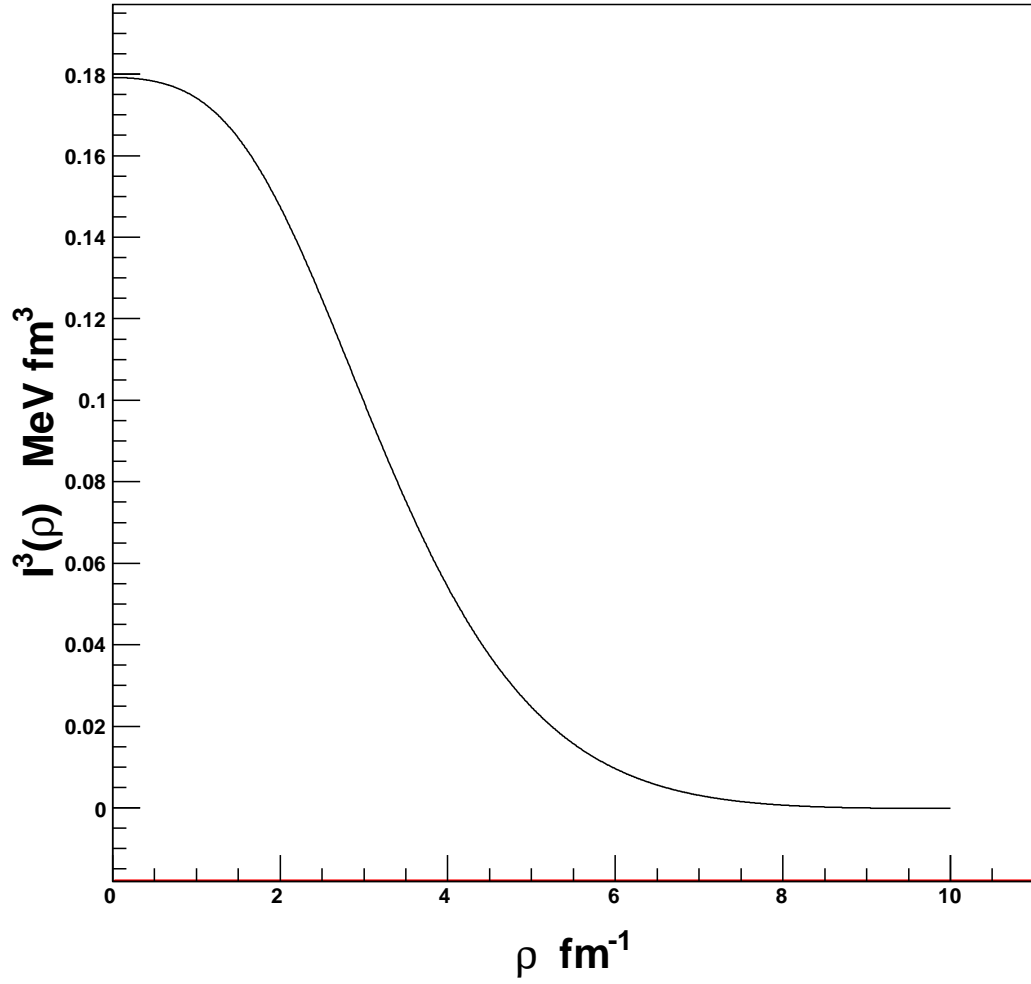
4.3 $I^2(\rho)$ **Argonne V18 5**Figure 4.9: Fouuier-Bessel integral of $I_5^2(\rho)$

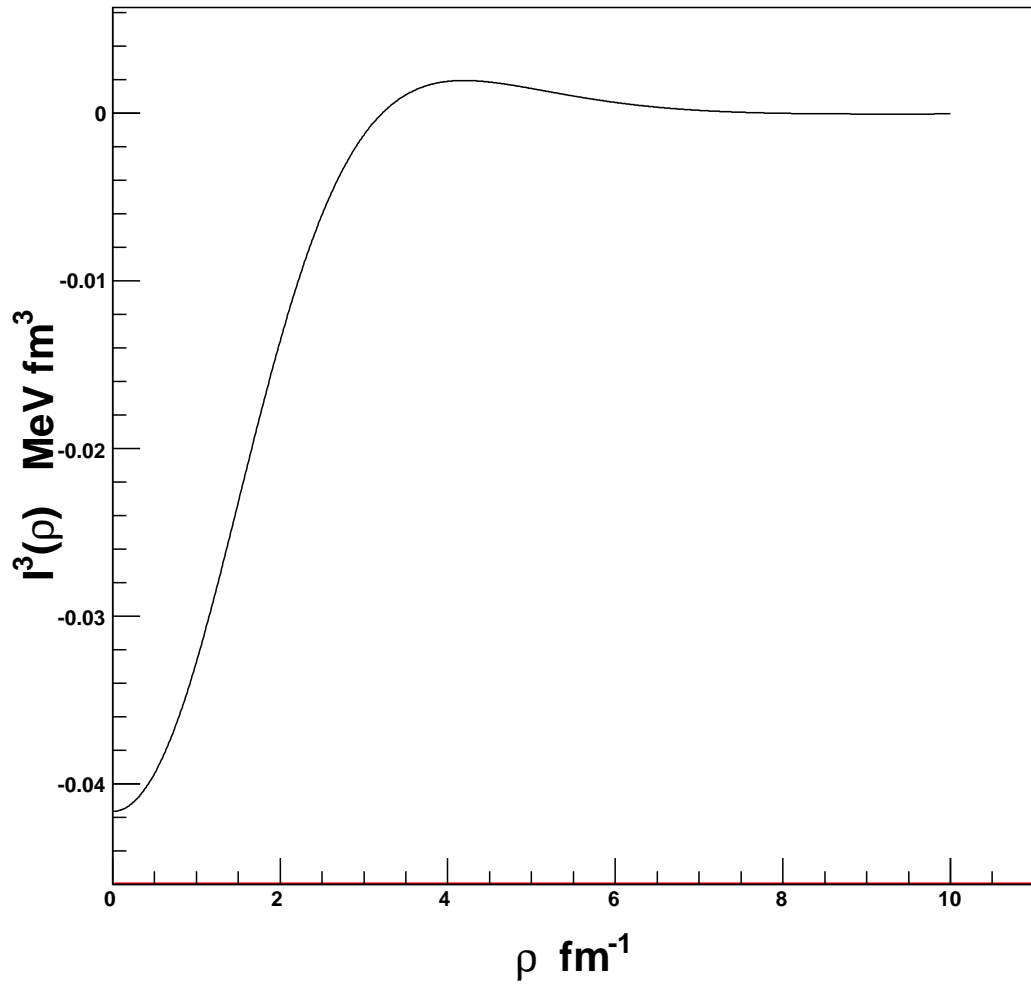
Argonne V18 6Figure 4.10: Fourier-Bessel integral of $I_6^2(\rho)$

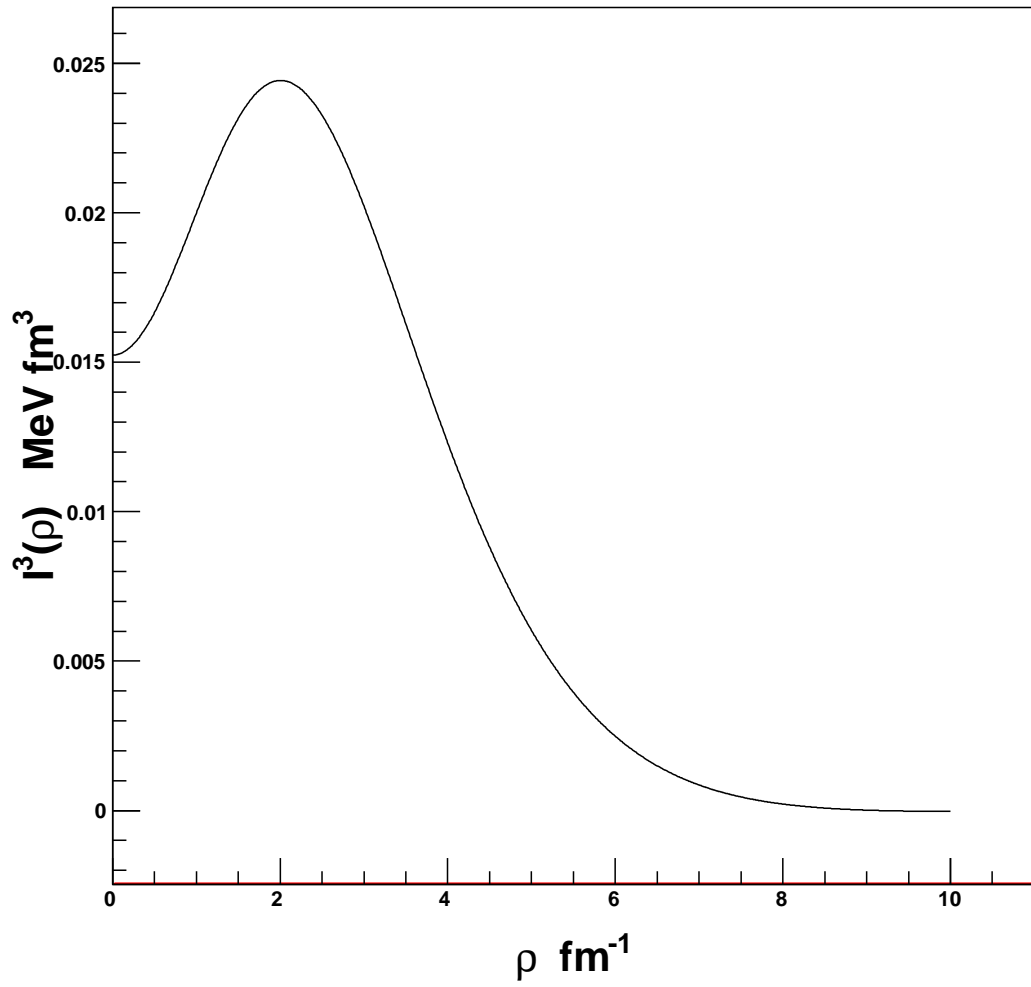
Argonne V18 17Figure 4.11: Fourier-Bessel integral of $I_{17}^2(\rho)$

4.4 $I^3(\rho)$ **Argonne V18 7**Figure 4.12: Fourier-Bessel integral of $I_7^3(\rho)$

Argonne V18 8Figure 4.13: Fourier-Bessel integral of $I_8^3(\rho)$

Argonne V18 9Figure 4.14: Fourier-Bessel integral of $I_9^3(\rho)$

Argonne V18 10Figure 4.15: Fourier-Bessel integral of $I_{10}^3(\rho)$

Argonne V18 11Figure 4.16: Fourier-Bessel integral of $I_{11}^3(\rho)$

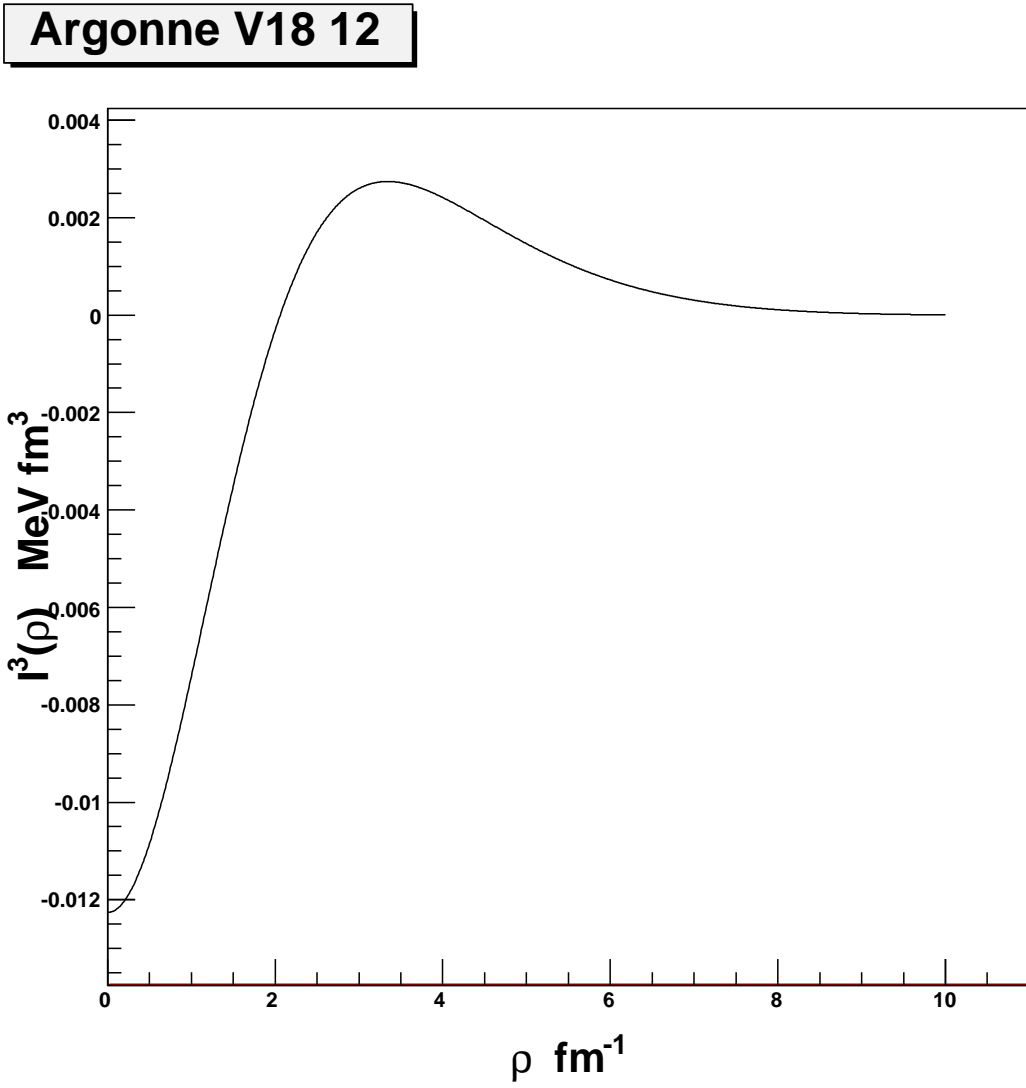
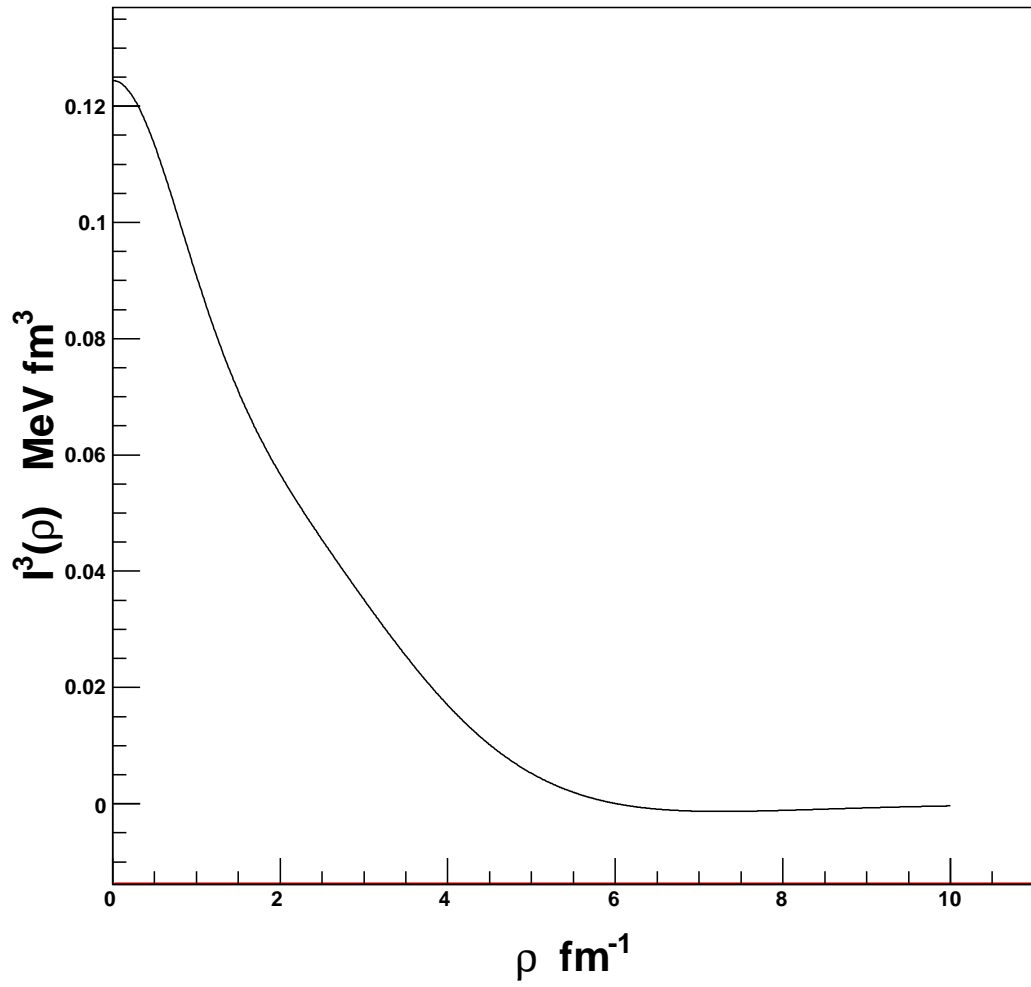
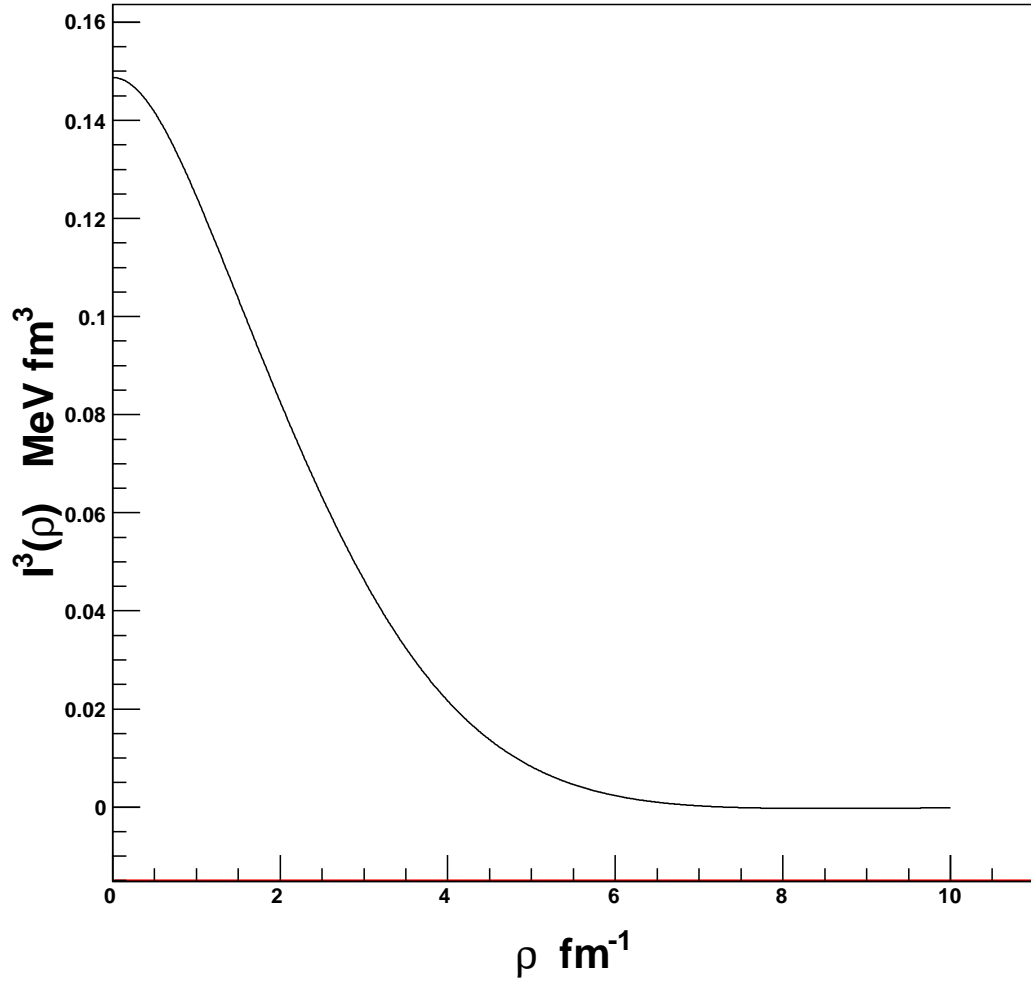
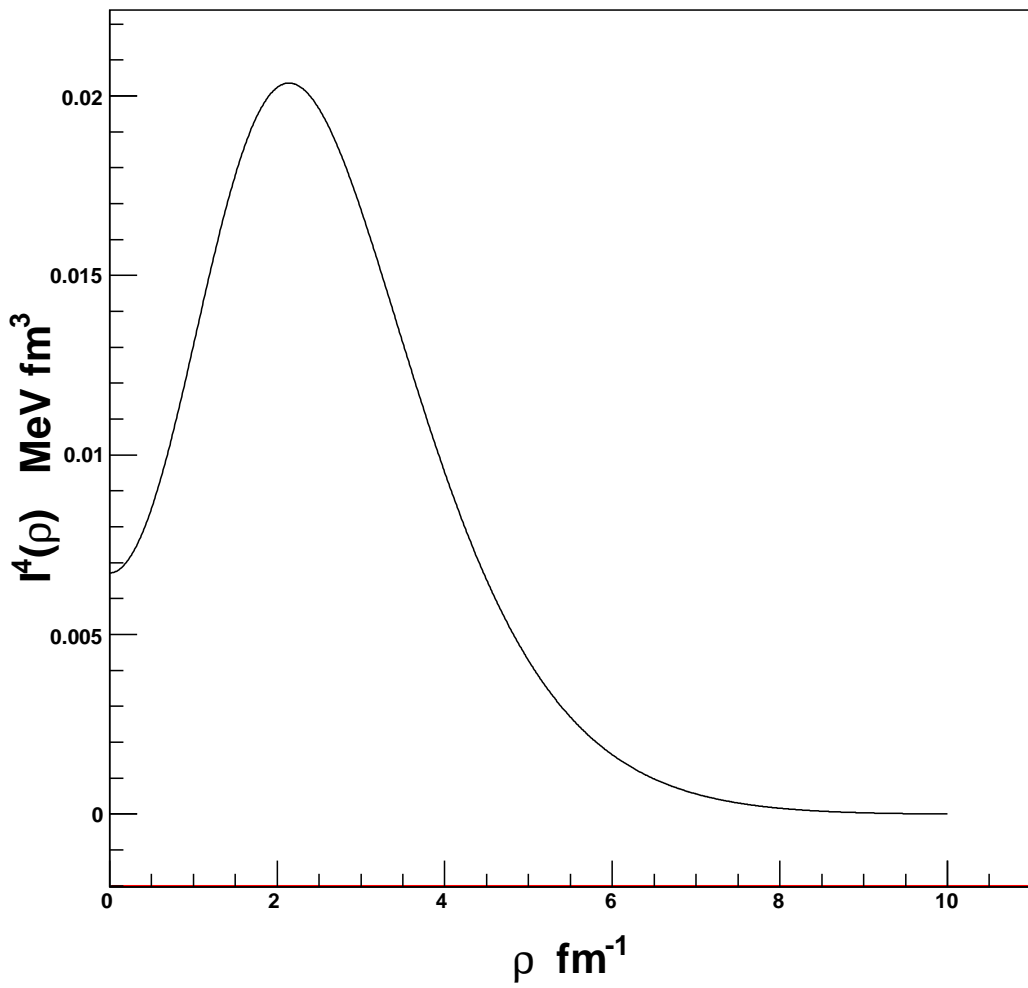


Figure 4.17: Fourier-Bessel integral of $I_{12}^3(\rho)$

Argonne V18 13Figure 4.18: Fourier-Bessel integral of $I_{13}^3(\rho)$

Argonne V18 14Figure 4.19: Fourier-Bessel integral of $I_{14}^3(\rho)$

4.5 $I^4(\rho)$ **Argonne V18 9**Figure 4.20: Fourier-Bessel integral of $I_9^4(\rho)$

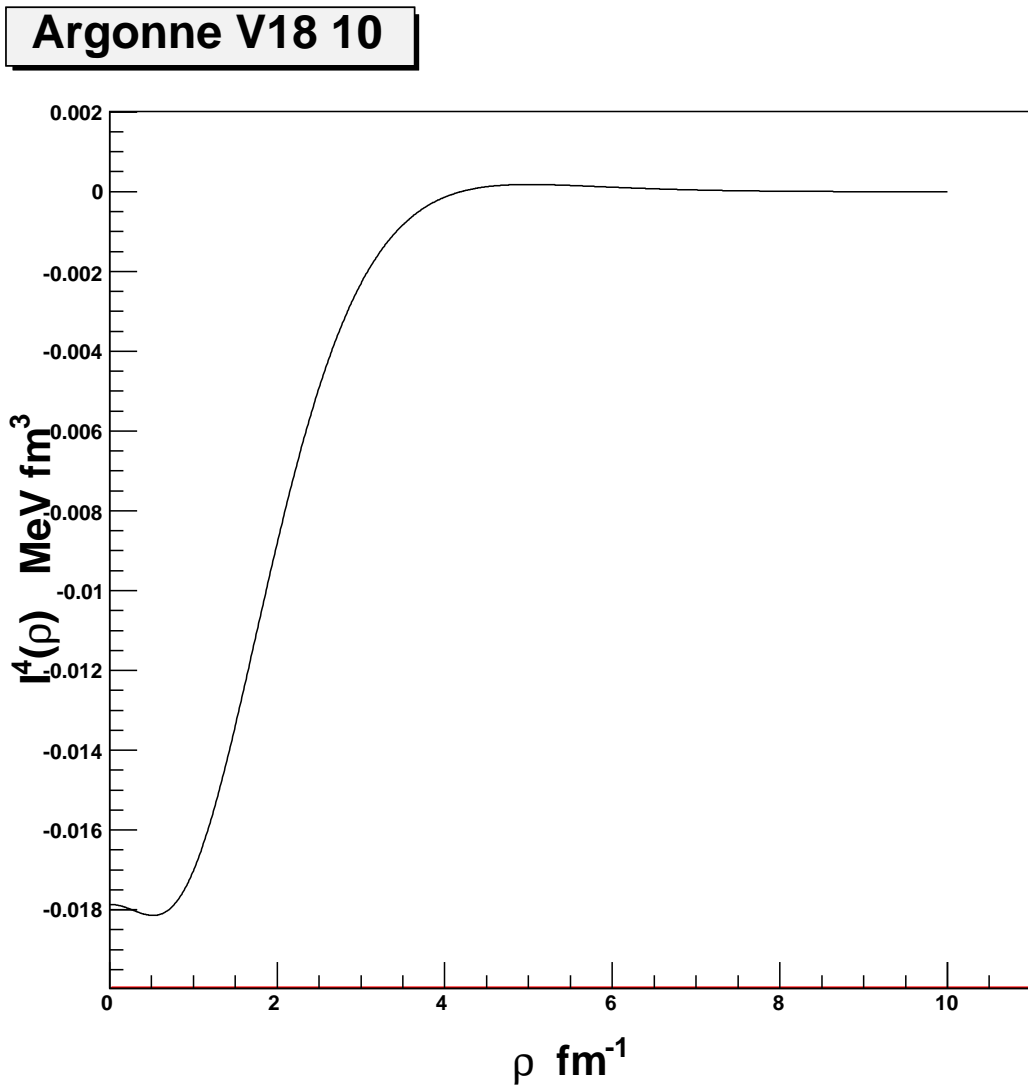
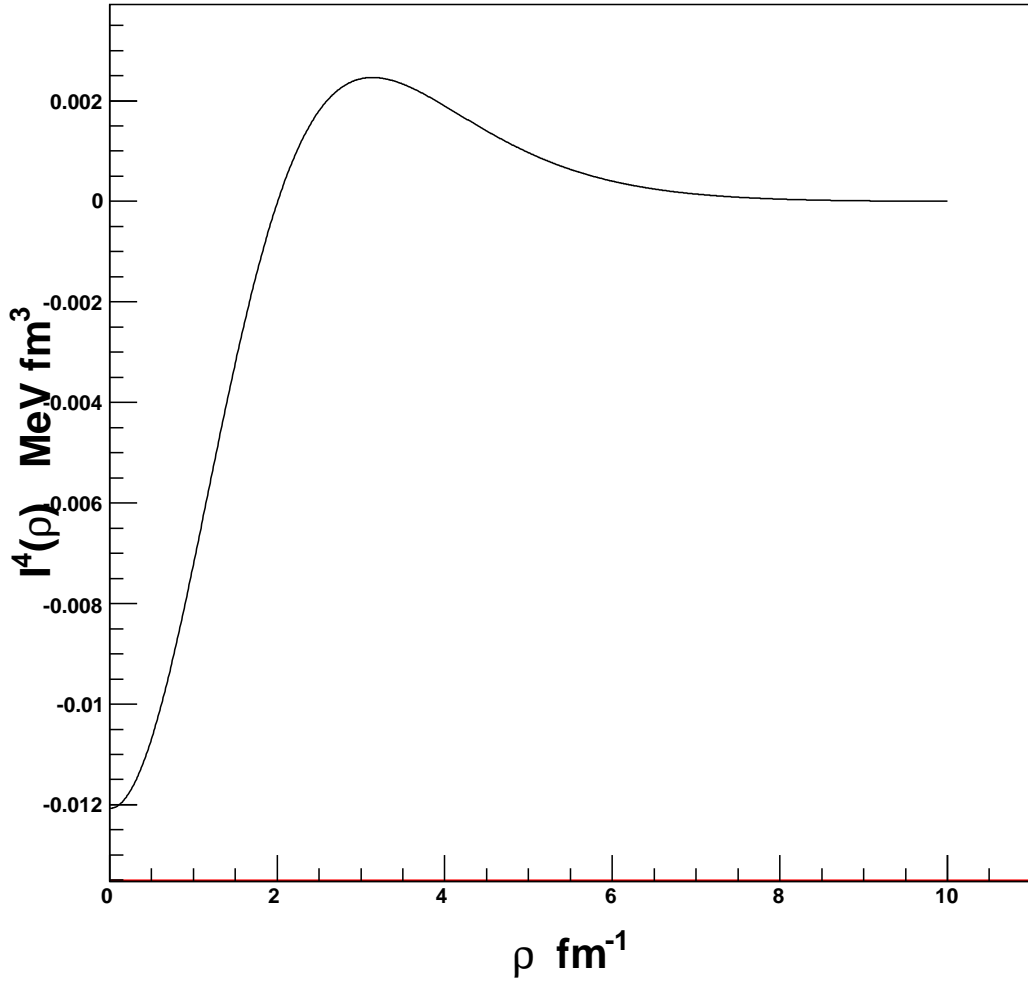
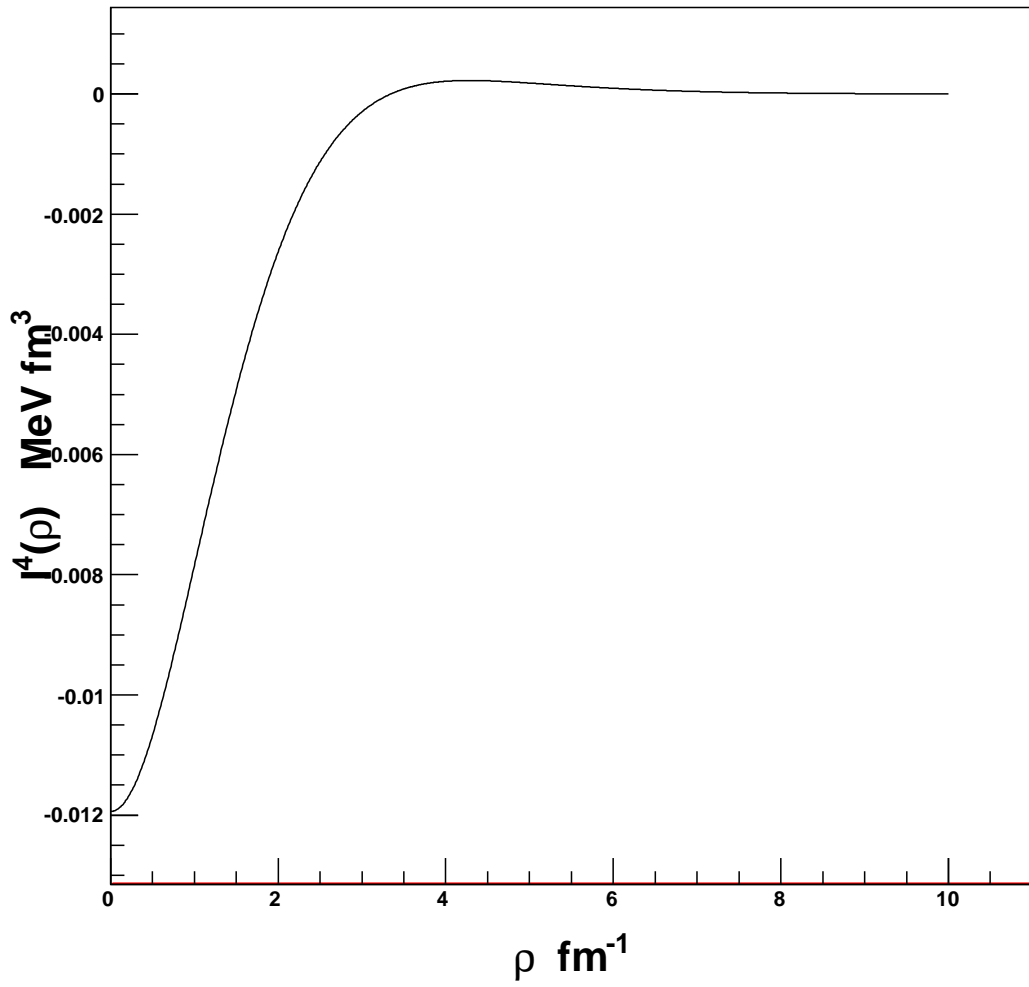
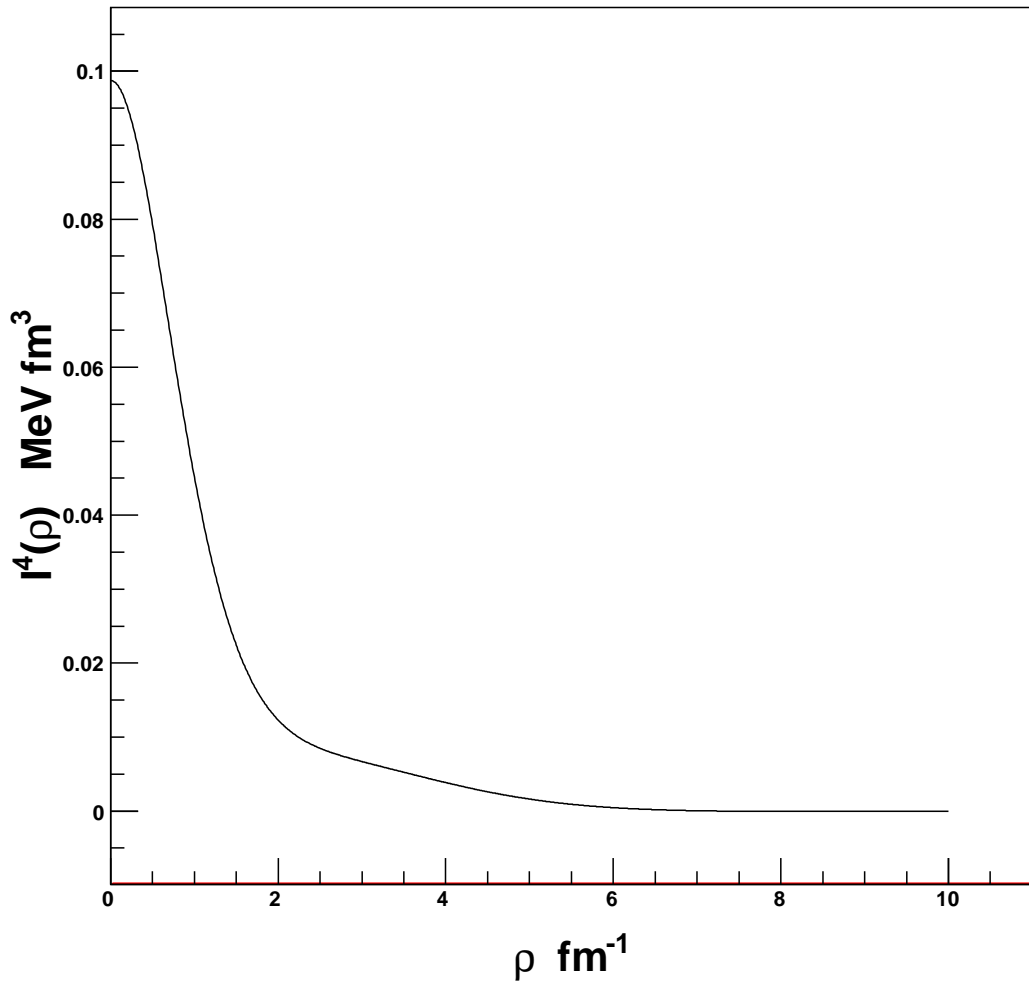


Figure 4.21: Fourier-Bessel integral of $I_{10}^4(\rho)$

Argonne V18 11Figure 4.22: Fourier-Bessel integral of $I_{11}^4(\rho)$

Argonne V18 12Figure 4.23: Fourier-Bessel integral of $I_{12}^4(\rho)$

Argonne V18 13Figure 4.24: Fourier-Bessel integral of $I_{13}^4(\rho)$

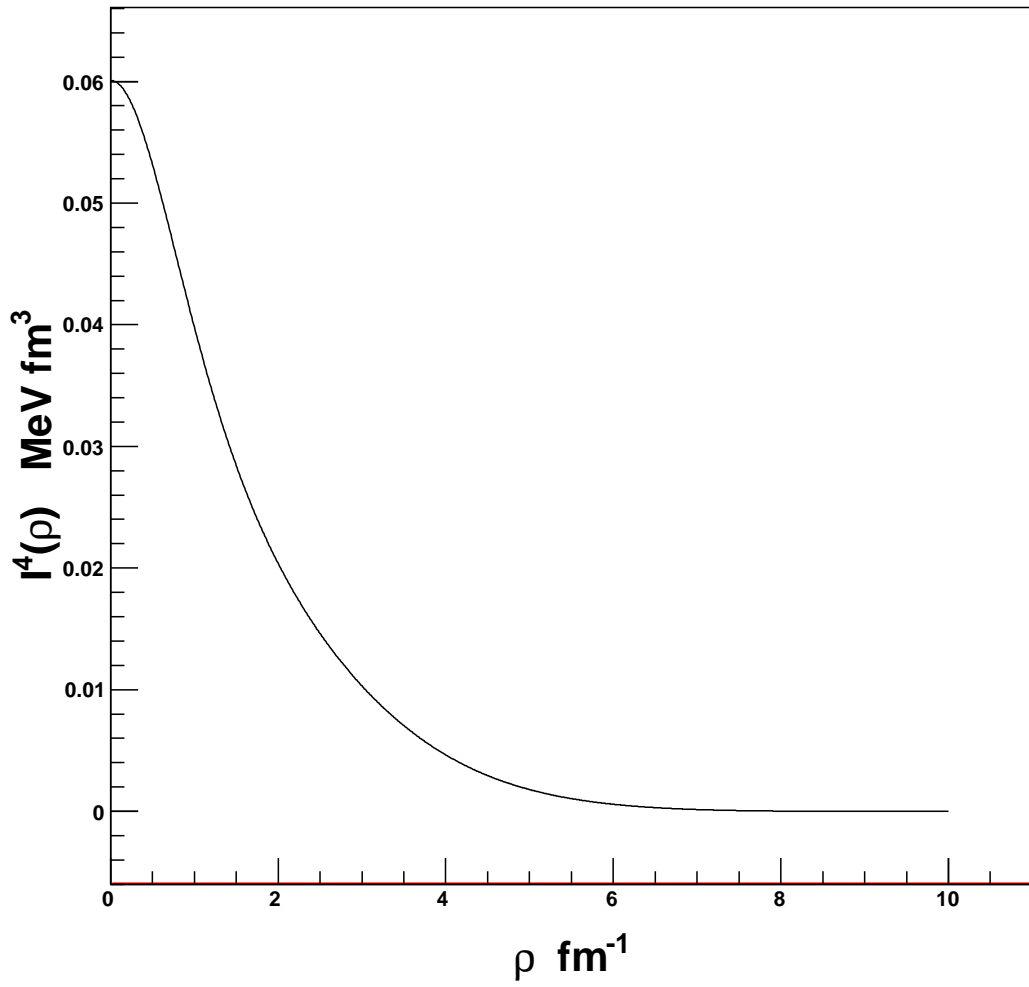
Argonne V18 14

Figure 4.25: Fourier-Bessel integral of $I_{14}^4(\rho)$

CHAPTER 5

A FORMALISM FOR AUTOMATED ALGEBRAIC REDUCTION

The solution of the three-body problem using vector variables stretches the limitations of existing computing resource. The three-body problem with a scalar potential has been successfully solved using the vector variable approach. This required state of the art super computing facilities. The solution of the two-body problem is embedded in the three-body Faddeev equation and hence an efficient code that would make the optimum use of the finite computing resource becomes an important aspect of solving the two-body problem. The vector variable formalism of two-body scattering for realistic nucleon-nucleon potentials with spin degrees of freedom requires the solution of six coupled equations. These equations are dependent on the trace expressions of Pauli matrices that are computed analytically. Hundreds of algebraic expressions are repeatedly computed for each grid point of the three dimensional integral. It has been shown in chapter two that these algebraic expressions if simplified, would result in reducing the time of computation. However manual reduction is time consuming and error prone. It is therefore ideal to build an automated system that can reduce these large algebraic expressions. This chapter describes an algorithm that can simplify these expressions.

5.1 Description of reduction mechanism

Let \mathbf{S} be the set of scalar polynomials to be constructed from a given set of vectors $\mathbf{V} : \{\vec{V}_1, \vec{V}_2, \vec{V}_3, \dots, \vec{V}_N\}$. Two types of representation can be used to express any element $x \in \mathbf{S}$. They are,

1. Irreducible scalars that can be constructed out of the set \mathbf{V} are classified as

Type	<i>I</i>	$\vec{V}_i \cdot \vec{V}_i$
Type	<i>II</i>	$\vec{V}_i \cdot \vec{V}_j$
Type	<i>III</i>	$(\vec{V}_i \times \vec{V}_j) \cdot \vec{V}_k$

where $\vec{V}_i \in \mathbf{V}$. It is then possible to define sets

$$\mathbf{s}_1 : \quad \{\vec{V}_1 \cdot \vec{V}_1, \vec{V}_2 \cdot \vec{V}_2, \dots, \vec{V}_n \cdot \vec{V}_n\} \quad (5.1)$$

$$\mathbf{s}_2 : \quad \{\vec{V}_1 \cdot \vec{V}_2, \vec{V}_2 \cdot \vec{V}_3, \dots, \vec{V}_i \cdot \vec{V}_j, \dots\} \quad i \neq j \quad i, j \in \{1, \dots, n\} \quad (5.2)$$

$$\mathbf{s}_3 : \quad \{(\vec{V}_1 \times \vec{V}_2) \cdot \vec{V}_3, \dots, (\vec{V}_i \times \vec{V}_j) \cdot \vec{V}_k, \dots\} \quad i \neq j \neq k \neq i \quad (5.3)$$

$$i, j, k \in \{1, \dots, n\}, \quad (5.4)$$

where $\mathbf{s}_1, \mathbf{s}_2$ and \mathbf{s}_3 are the sets of combinations of one, two and three variable irreducible scalars. The set of all the irreducible scalars is given by

$$\mathbf{s} = \mathbf{s}_1 \cup \mathbf{s}_2 \cup \mathbf{s}_3, \quad (5.5)$$

$$\mathbf{s} \subseteq \mathbf{S}. \quad (5.6)$$

Let $\mathbf{P}(\mathbf{s})$ be the set of polynomials in \mathbf{s} and $\mathbf{m}(\mathbf{s})$ is the set of all the multi variable monomials. Any element $\mathfrak{S}(\mathbf{s}) \in \mathbf{P}(\mathbf{s})$ can be expressed as

$$\mathfrak{S}(\mathbf{s}) = \sum_{i=0}^n d_i \beta_i(\mathbf{s}). \quad (5.7)$$

The i^{th} monomial $\beta_i(\mathbf{s}) \in \mathbf{m}(\mathbf{s})$ and $d_i \in \mathbb{R}$. Let $DEGP2(\mathfrak{S}(\mathbf{s}))$ be defined as the degree of the polynomial $\mathfrak{S}(\mathbf{s}) \in \mathbf{P}(\mathbf{s})$. For any element $x \in \mathbf{S}$ there exists an element $\mathfrak{S}(\mathbf{s}) \in \mathbf{P}(\mathbf{s})$ that represents x . In addition, $[\beta(\mathbf{s})] = \{\beta_1(\mathbf{s}), \dots, \beta_i(\mathbf{s}), \dots, \beta_n(\mathbf{s})\}$ is also defined. The rest of the thesis uses the notation $[\]$ for the set of all monomials in a polynomial.

2. A general representation of any vector \vec{V} is in terms of euclidean coordinates V_x, V_y and V_z . The set $\mathbf{v} : \{V_{1x}, V_{1y}, V_{1z}, V_{2x}, V_{2y}, \dots, V_{Nz}\}$ is the set of components of N vectors of the set \mathbf{V} . $\mathbf{P}(\mathbf{v})$ is the set of rotationally invariant polynomials in \mathbf{v} constructed from the scalars in \mathbf{S} . Let $\mathbf{m}(\mathbf{v})$ be the set of all possible multivariable

monomials for any element $x \in \mathbf{S}$. There exists an element $F(\mathbf{v}) \in \mathbf{P}(\mathbf{v})$ that represents x .

$$F(\mathbf{v}) = \sum_i^{i=n} c_i \alpha_i(\mathbf{v}), \quad (5.8)$$

where the i^{th} term is $\alpha_i(v) \in \mathbf{m}(\mathbf{v})$ and $c_i \in \mathbb{R}$. Let $[\alpha(\mathbf{v})] : \{\alpha_1(\mathbf{v}), \dots, \alpha_n(\mathbf{v})\}$. $\text{DEGP1}(F(\mathbf{v}))$ is the degree of $F(\mathbf{v})$ and $\text{LENTGH}(F(\mathbf{v}))$ is the length of the polynomial.

The reduction or "term re-writing" is a change of representation (or variables). This transformation is possible since every $x \in \mathbf{s}$ can be represented by an element in $\mathbf{P}(\mathbf{v})$. Let the representation of the irreducible sets $\mathbf{s}_1, \mathbf{s}_2$ and \mathbf{s}_3 be given by the corresponding sets $\mathbf{P}_1(\mathbf{v}) \subset \mathbf{P}(\mathbf{v})$, $\mathbf{P}_2(\mathbf{v}) \subset \mathbf{P}(\mathbf{v})$ and $\mathbf{P}_3(\mathbf{v}) \subset \mathbf{P}(\mathbf{v})$. The representation of the irreducible scalars by the elements of $\mathbf{P}(\mathbf{v})$ are given by

$$\text{Type I} \quad \vec{V}_i \cdot \vec{V}_i = V_{ix}^2 + V_{iy}^2 + V_{iz}^2 = p_1(\mathbf{v}), \quad (5.9)$$

$$\text{Type II} \quad \vec{V}_i \cdot \vec{V}_j = V_{ix}V_{jx} + V_{iy}V_{jy} + V_{iz}V_{jz} = p_2(\mathbf{v}), \quad (5.10)$$

$$\text{Type III} \quad (\vec{V}_i \times \vec{V}_j) \cdot \vec{V}_k = \epsilon_{i,j,k} V_i V_j V_k = p_3(\mathbf{v}). \quad (5.11)$$

Here, Type I is the length of a vector, Type II is the dot product and Type III is the triple product, $p_1(\mathbf{v}) \in \mathbf{P}_1(\mathbf{v})$, $p_2(\mathbf{v}) \in \mathbf{P}_2(\mathbf{v})$ and $p_3(\mathbf{v}) \in \mathbf{P}_3(\mathbf{v})$. Because of this relationship, it is possible to define sets of polynomials $\mathbf{Q}_1(\mathbf{v})$, $\mathbf{Q}_2(\mathbf{v})$ and $\mathbf{Q}_3(\mathbf{v})$ that represent the set of monomials $\mathbf{m}(\mathbf{s}_1)$, $\mathbf{m}(\mathbf{s}_2)$ and $\mathbf{m}(\mathbf{s}_3)$,

$$q_1(\mathbf{v}) \in \mathbf{Q}_1(\mathbf{v})$$

$$q_2(\mathbf{v}) \in \mathbf{Q}_2(\mathbf{v})$$

$$q_3(\mathbf{v}) \in \mathbf{Q}_3(\mathbf{v}).$$

Any monomial in $g(\mathbf{s}) \in m(\mathbf{s})$ can then be written as a product of

$$g(\mathbf{s}) = g_1(\mathbf{s}_1)g_2(\mathbf{s}_2)g_3(\mathbf{s}_3) \quad (5.12)$$

where $g_1(\mathbf{s}_1) \in \mathbf{m}(\mathbf{s}_1)$, $g_2(\mathbf{s}_2) \in \mathbf{m}(\mathbf{s}_2)$ and $g_3(\mathbf{s}_3) \in \mathbf{m}(\mathbf{s}_3)$. The representation of g in polynomials $p_{123} \in \mathbf{P}(\mathbf{v})$ is given by the equation

$$g(\mathbf{s}) = p_{123}(\mathbf{v}) = q_1(\mathbf{v})q_2(\mathbf{v})q_3(\mathbf{v}) \in \mathbf{Q}(\mathbf{v}), \quad (5.13)$$

where $\mathbf{Q}(\mathbf{v})$ represent all the possible products of q_1, q_2 and q_3 . A polynomial $\mathfrak{S}(\mathbf{s}) \in (\mathbf{P}(\mathbf{s}))$ is given by

$$\mathfrak{S}(\mathbf{s}) = \sum_{i=0}^n d_i \beta_i(\mathbf{s}) \quad (5.14)$$

where $d_i \in \mathbb{R}$ and $\beta_i(\mathbf{s}) \in \mathbf{m}(\mathbf{s})$. They can be represented by $F(\mathbf{v}) \in \mathbf{P}(\mathbf{v})$ by transforming all $\beta_i(\mathbf{s}) \in [\beta(\mathbf{s})]$ using (5.13). This can be formally expressed as

$$\begin{aligned} \mathfrak{S}(\mathbf{s}) &= \sum_{i=0}^n d_i \beta_i(\mathbf{s}) = \sum_{i=0}^n d_i p_{123}^i(v) = \sum_{j=0}^{n_1} c_j \alpha_j(\mathbf{v}) = F(\mathbf{v}), \\ p_{123}^i(\mathbf{v}) &= \sum_{j=0}^{n_i} \tilde{\beta}^j(\mathbf{v}). \end{aligned} \quad (5.15)$$

Here $\alpha_j(\mathbf{v}) \in \mathbf{m}(\mathbf{v})$ and $\forall \beta_i(\mathbf{s}) \in [\beta(\mathbf{s})]$ the representation in \mathbf{v} are the polynomials $p_{123}^i(\mathbf{v})$. The monomials of $p_{123}^i(\mathbf{v})$ are given by the set $[\tilde{\beta}_i(\mathbf{v})]$. The transformation is represented by the expression

$$\beta_i(\mathbf{s}) \xrightarrow{T} [\tilde{\beta}^i(\mathbf{v})] \quad (5.16)$$

The next section the transformation of elements $F(\mathbf{v}) \in \mathbf{P}(\mathbf{v})$ to $\mathfrak{S}(\mathbf{s}) \in \mathbf{P}(\mathbf{s})$ is discussed.

5.2 Inverse transformation

The process of transforming a polynomial $F(\mathbf{v})$ to a polynomial $\mathfrak{S}(\mathbf{s})$ is discussed in this section.

5.2.1 Uniqueness

Since the monomials $m(s) \in \mathbf{m}(\mathbf{s})$ are generated from three irreducible scalars, their representation is a polynomial $p(\mathbf{v}) \in \mathbf{Q}(\mathbf{v})$. Let the monomial $m_l(s) \in (\mathbf{m}(\mathbf{s}))$ be represented as

$$m_l(\mathbf{s}) = \sum_{i=1}^n w_i^l \tilde{\gamma}_i^l(\mathbf{v}), \quad (5.17)$$

where $\tilde{\gamma}_i^l(\mathbf{v}) \in \mathbf{m}(\mathbf{v})$. Since the polynomials are generated from three distinct polynomials that represent irreducible scalars, if any two monomials $m^p(s), m^q(s) \in \mathbf{m}(\mathbf{s})$

fulfil

$$[\tilde{\gamma}^p(\mathbf{v})] = [\tilde{\gamma}^q(\mathbf{v})] \quad (5.18)$$

then the set of coefficients $[w^p] = [w^q]$ and therefore the two monomials $m^p(s)$ and $m^q(s)$ give the same representation and either one can be used to represent the RHS of the (5.17).

Let the set of sets that represents the set of monomials in $\mathbf{m}(\mathbf{s})$ in \mathbf{v} be $\Gamma(\tilde{\mathbf{v}}) = \{[\tilde{\gamma}^1(\mathbf{v})], [\tilde{\gamma}^2(\mathbf{v})], \dots\}$. There is a one to one correspondence between $\mathbf{m}(\mathbf{s})$ and $\Gamma(\tilde{\mathbf{v}})$. This relationship is used to reconstruct the monomials $m_1(\mathbf{s}) \in \mathbf{m}(\mathbf{s})$ from the monomials $m(\mathbf{v}) \in \mathbf{m}(\mathbf{v})$. Re-writing (5.15) the polynomial $\mathfrak{S}(\mathbf{s})$ can be written as

$$\mathfrak{S}(\mathbf{s}) = \sum_{i=0}^n d_i \beta_i(\mathbf{s}) = \sum_{j=0}^{n_1} c_j \alpha_j(\mathbf{v}) = F(\mathbf{v}), \quad (5.19)$$

and

$$\beta_i(\mathbf{s}) \rightarrow [\tilde{\beta}^i(\mathbf{v})].$$

The elements of the set $[\alpha(\mathbf{v})]$ are also elements of $\psi = \bigcup_{i=0}^n [\beta(\tilde{\mathbf{v}})]$. To further investigate the relationship between $[\alpha(\mathbf{v})]$ and ψ , for the n sets $[\tilde{\beta}^i(\mathbf{v})]$, $i = 1 \dots n$ the sets

$$[c(\mathbf{v})^r] = [\tilde{\beta}^r(\mathbf{v})] \setminus \bigcup_{i=0, i \neq r}^n [\tilde{\beta}^i(\mathbf{v})], \quad (5.20)$$

$$[i(\mathbf{v})^r] = \bigcup_{i=0, i \neq r}^n ([\tilde{\beta}^r] \cap [\tilde{\beta}^i(\mathbf{v})]) \quad (5.21)$$

are defined. Here \setminus is the symbol for compliment. The set $[c(\mathbf{v})^r]$ is the set of elements that exists in $[\tilde{\beta}^r]$ but not in any other set. The set $[i(\mathbf{v})^r]$ represents the set of common elements that exist in the pairs $[\tilde{\beta}^r(\mathbf{v})]$, $[\tilde{\beta}^i(\mathbf{v})]$ with $i \neq r$. For $r = 1, \dots, n$ two sets

$$\begin{aligned} [C(\mathbf{v})] &= \bigcup_{r=0}^n [c^r(\mathbf{v})] \\ [I(\mathbf{v})] &= \bigcup_{r=0}^n [i^r(\mathbf{v})] \end{aligned} \quad (5.22)$$

are defined. Any set $[\alpha(\mathbf{v})]$ can be decomposed into $[\alpha(\mathbf{v})]^I$ and $[\alpha(\mathbf{v})]^C$

$$[\alpha(\mathbf{v})] = [\alpha(\mathbf{v})]^I \cup [\alpha(\mathbf{v})]^C \quad (5.23)$$

where $[\alpha(\mathbf{v})]^C = [C(\mathbf{v})]$ and $[\alpha(\mathbf{v})]^I \subseteq [I(\mathbf{v})]$. Decomposing the set $[\alpha(\mathbf{v})]$ into $[\alpha(\mathbf{v})]^I$ and $[\alpha(\mathbf{v})]^C$ plays an important role in the transformation of elements $F(\mathbf{v}) \in \mathbf{P}(\mathbf{v})$ to

$\mathfrak{S}(\mathbf{s}) \in \mathbf{P}(\mathbf{s})$ discussed in the next section.

5.2.2 Structure of transformation

The mathematical process of transforming $F(\mathbf{v})$ to $\mathfrak{S}(\mathbf{s})$ requires defining new sets $\mathbf{P}(\mathbf{M}) = \mathbf{P}(\mathbf{v}) \cup (\mathbf{P}(\mathbf{s}))$ as well as set

$$\mathbf{m}(\mathbf{M}) = \mathbf{m}(\mathbf{v}) \cup \mathbf{m}(\mathbf{s}).$$

Then (5.13) can be re-written as

$$g(\mathbf{s}) - (q_1(\mathbf{v}))(q_2(\mathbf{v}))(q_3(\mathbf{v})) = 0. \quad (5.24)$$

An example to illustrate this is shown in the next equation.

$$(\vec{V}_1 \cdot \vec{V}_2)^2 (\vec{V}_1 \cdot \vec{V}_2) - (V_{ix}^2 + V_{iy}^2 + V_{iz}^2)^2 (V_{ix}V_{jx} + V_{iy}V_{jy} + V_{iz}V_{jz}) = 0. \quad (5.25)$$

To inverse transform a scalar represented by polynomial $F(\mathbf{v}) \in P(\mathbf{v})$ to a polynomial $\mathfrak{S}(\mathbf{s})$,

$$F(\mathbf{v}) = \sum_{i=1}^l c_i \alpha_i(\mathbf{v}) \rightarrow \sum_{i=1}^{l_2} d_i \beta_i(\mathbf{s}), \quad (5.26)$$

is not a straight forward process. A monomial in $\mathbf{m}(\mathbf{v})$ is not rotationally invariant unlike the elements in $\mathbf{m}(\mathbf{s})$ and cannot be expressed in elements of $\mathbf{m}(\mathbf{s})$. Hence the starting point of the transformation is to find the elements in $\mathbf{m}(\mathbf{s})$ that may contain the monomial term in $\mathbf{m}(\mathbf{v})$. The number of terms are finite and this property is exploited to inverse transform $F(\mathbf{v})$ to $\mathfrak{S}(\mathbf{s})$. The replacement of a monomial $m_v \in [\alpha(\mathbf{v})]$ by polynomial $G(\mathbf{M})$ in $F(\mathbf{v})$ is called an elementary transformation. Here $G(\mathbf{M}) \in \mathbf{P}(\mathbf{M})$, has only one monomial $m_s \in \mathbf{m}(\mathbf{s})$ and the rest of the monomials are elements of $\mathbf{m}(\mathbf{v})$. The transformation is carried out through a sequence of elementary transformations. The transformation of a polynomial $F(\mathbf{v}) \in P(\mathbf{v})$ to $\mathfrak{S}(\mathbf{s}) \in \mathbf{P}(\mathbf{s})$ can be symbolically expressed as

$$F \xrightarrow{\mathbf{T}} \mathfrak{S}. \quad (5.27)$$

The transformation $\xrightarrow{\mathbf{T}}$ is carried out by a series of elementary transformation. This can be expressed as a recurrence relation

$$F(\mathbf{v}) \xrightarrow{\mathbf{T}} \mathfrak{S}(\mathbf{s}) = \chi^0(\mathbf{v}) \xrightarrow{\xi_i^0(v)} \chi^1(\mathbf{M}) \dots \chi^t(\mathbf{M}) \xrightarrow{\xi_j^t(v)} \chi^{t+1} \dots \chi^{n-1}(\mathbf{M}) \xrightarrow{\xi_k^{n-1}(v)} \chi_n(\mathbf{M}) \quad (5.28)$$

here " \rightarrow " represents the elementary transformations or "term re-writing", the term on the left side of the \rightarrow is the polynomial $\chi^t(\mathbf{M})$, the term on the right side of the \rightarrow is the initiating monomial $\xi_i^t(M)$ being transformed and the function at the end of the arrow is the polynomial $\chi_{t+1}(\mathbf{M})$ where the index t is the t^{th} transformation.

Since the transformations are done to simplify the expressions for computational purposes, the elementary transformation must satisfy

$$LENTGH(\chi_{t+1}(\mathbf{M})) < LENTGH(\chi_t(\mathbf{M})). \quad (5.29)$$

$\chi_0 = F(\mathbf{v})$ is the function to be transformed and $DEGP2(F(\mathbf{v})) = 0$, the transformed function after $n-1$ elementary transformations is $\chi_n = \mathfrak{S}(\mathbf{s})$ and $DEGP1(\mathfrak{S}(\mathbf{s})) = 0$. The condition that decides that transformation has been successful is called termination step and the terminating step is when $DEGP1 = 0$.

5.2.3 Elementary transformation

Let the j^{th} monomial of $F(\mathbf{v})$ (5.26), $\alpha_j(s)$ initiate the transformation. A finite set $\mathbf{H}^j(\mathbf{s}) : \{h_1^j(\mathbf{s}), h_2^j(\mathbf{s}), \dots, h_n^j(\mathbf{s})\}$ represents all the monomials in $m(\mathbf{s})$, whose representation in $\mathbf{P}(\mathbf{v})$ contains the monomial $\alpha_j(\mathbf{v})$. The element $h_i^j(\mathbf{s})$ is written as,

$$h_i^j(\mathbf{s}) = \sum_{l=0}^L w_l m_l(\mathbf{v}) = \sum_{l=0}^{q-1} w_l m_l(\mathbf{v}) + \sum_{l=q+1}^L w_l m_l(\mathbf{v}) + w_q m_q(\mathbf{v}) \quad (5.30)$$

where $m_l(\mathbf{v}) \in \mathbf{m}(\mathbf{v})$ and for $n = q$, $m_q(\mathbf{v}) = \alpha_j(\mathbf{v})$. If we take the coefficients into consideration then,

$$\frac{c_j}{w_q} h_i^j(\mathbf{s}) = \frac{c_j}{w_q} \left(\sum_{l=0}^{q-1} w_l m_l(\mathbf{v}) + \sum_{l=q+1}^L w_l m_l(\mathbf{v}) \right) + c_j m_q(\mathbf{v}) \quad (5.31)$$

where c_j is the coefficient of $\alpha_j(\mathbf{v})$. This can be re-expressed as

$$\frac{c_j}{w_q} h_i^j(\mathbf{s}) - \frac{c_j}{w_q} \left(\sum_{l=0}^{q-1} w_l m_l(\mathbf{v}) + \sum_{l=q+1}^L w_l m_l(\mathbf{v}) \right) - c_j m_q(\mathbf{v}) = 0 \quad (5.32)$$

An elementary transformation is described in the following steps:

1. The first step of the elementary transformation adds (5.32) to $F(\mathbf{v})$.

$$\begin{aligned}
 F(\mathbf{v}) + 0 &= \sum_i^{j-1} c_i \alpha_i(\mathbf{v}) + c_j \alpha_j(\mathbf{v}) + \sum_{i=j+1}^{l_2} c_i \alpha_i(\mathbf{v}) + \frac{c_i}{w_q} h_i(\mathbf{s}) \quad (5.33) \\
 &\quad - \frac{c_i}{w_q} \left(\sum_{l=0}^{q-1} w_l m_l^{\mathbf{v}} + \sum_{l=q+1}^n w_l m_l(\mathbf{v}) \right) - c_i m_q(v) \\
 &= \frac{c_i}{w_q} h_i(\mathbf{s}) + \sum_{i=0}^{l_3} o_i \gamma_i(\mathbf{v}) = \chi_1(\mathbf{M}).
 \end{aligned}$$

The above equation adds function $h_i^j(\mathbf{s})$ to the polynomial $F(\mathbf{v})$ and then subtracts the term $\alpha_i(\mathbf{v}) = m_q(\mathbf{v})$ and other monomials that are elements of the set $[m^l(\mathbf{v})] \cap [\alpha]$.

2. The set $[\beta(\mathbf{s})] : \{\beta^1(\mathbf{s}), \dots, \beta^n(\mathbf{s})\}$ has all the monomial elements of the polynomial $\mathfrak{S}(\mathbf{s})$. There are two cases that are being discussed:

- (a) Let $\Phi = [\beta(\mathbf{s})] \cap \mathbf{H}^j(\mathbf{s})$. If $|\Phi| = 1$ then there is one element in $\mathbf{H}(\mathbf{s})$ for which the condition (5.29) is satisfied. This can be extracted by transforming all of the elements in $H^j(\mathbf{s})$ until the element satisfies (5.29).
- (b) If $\Phi : \{h_l^j, h_{l+3}^j, \dots\}$, the number of elements is more than one, the condition (5.29) will not be met. This is because the monomial being transformed is $\alpha_j(\mathbf{v}) \in \alpha(\mathbf{v})^I$.

To avoid ambiguities that come from terms that are elements of $[\alpha(\mathbf{v})]^I$, the elementary transformation is carried out for all monomial terms $\alpha_i(\mathbf{v})$ and the polynomial $\{\chi^0(\mathbf{M})_{\alpha_u}\}$ (transformed by the term $\alpha_u(\mathbf{v})$) that has the least $LENGTH_{min}(\chi_{\alpha_u}^1(\mathbf{M}))$ is used for the next transformation. This ensures that only elements of $[\alpha(\mathbf{v})]^C$ are picked for elementary transformations. This is expressed as

$$\chi^0 \xrightarrow{\alpha_u(\mathbf{v})} \chi^1(\mathbf{M}) \quad (5.34)$$

The index α_u is understood implicitly.

The result $\chi^1(\mathbf{M})$ is tested for the termination condition. (This step can be done every time the elementary transformation condition (5.29) is met.) If the condition is not met the elementary transformation is done for all the terms in the polynomial $\chi^1(\mathbf{M})$ and this transformation process is repeated until the termination condition is satisfied.

In practice, it is simpler to fix an algorithm called A that reconstructs a certain type of scalar monomials and its representation in \mathbf{v} . The algorithm is used for the elementary transformation of all the monomials $\alpha_i(\mathbf{v})$ and the transformed polynomial with the least length $\chi_1^A(\mathbf{M})$. The next algorithm called B generates a different type of scalar monomials and the corresponding transformed polynomials are used. One of the possible combinations of the algorithms result in a transformed polynomial with the least length. This process is repeated till the termination condition is reached.

5.2.4 Illustration

The transformation from $F(\mathbf{v})$ to $\mathfrak{S}(\mathbf{v})$ is illustrated by an example. Consider the expression that is generated by (5.35)

$$\begin{aligned} F(\mathbf{v}) = & q_{1y}q_{2z}q_{3x} - q_{1z}q_{3x}q_{2y} + q_{2z}q_{1z} - q_{2z}q_{1x}q_{3y} + q_{1y}q_{2y} - q_{1y}q_{3z}q_{2x} \\ & + q_{1z}q_{2x}q_{3y} + q_{2x}q_{1x} + q_{3z}q_{1x}q_{2y}. \end{aligned} \quad (5.35)$$

The sequence of transformation of (5.35) are

$$F(\mathbf{v}) \xrightarrow{q_{1z}q_{2x}q_{3y}} q_{2z}q_{1z} + ((\vec{q}_3 \times \vec{q}_1) \cdot \vec{q}_2) + q_{1y}q_{2y} + q_{2x}q_{1x} \xrightarrow{q_{2z}q_{1z}} ((\vec{q}_3 \times \vec{q}_1) \cdot \vec{q}_2) + (\vec{q}_1 \cdot \vec{q}_2)$$

where $((\vec{q}_3 \times \vec{q}_1) \cdot \vec{q}_2) + (\vec{q}_1 \cdot \vec{q}_2)$ is the termination step or the reduced equation $\mathfrak{S}(\mathbf{s})$.

5.3 Description of algorithm

This section discusses the algorithms that are used for the elementary transformations. The algorithms follow the structure of scalar monomials $m(\mathbf{s}) \in \mathbf{m}(\mathbf{s})$ and $m(\mathbf{s}) = m_1(\mathbf{s})m_2(\mathbf{s})m_3(\mathbf{s})$ where $m_1(\mathbf{s}) \in \mathbf{m}_1(\mathbf{s})$, $m_2(\mathbf{s}) \in \mathbf{m}_2(\mathbf{s})$, $m_3(\mathbf{s}) \in \mathbf{m}_3(\mathbf{s})$. The

following rules are used in the algorithm

$$R_1^i \quad (V_l^i)^2 \rightarrow \vec{V}^i \cdot \vec{V}^i \quad (5.36)$$

$$R_2^{i,j} \quad V_l^i V_m^j \rightarrow \vec{V}^i \cdot \vec{V}^j \quad (5.37)$$

$$R_3^{i,j,k} \quad V_l^i V_m^j V_n^k \rightarrow (\vec{V}^i \times \vec{V}^j) \cdot (\vec{V}^k). \quad (5.38)$$

where $l, m, n = \{1, 2, 3\}$. R_1^i reconstructs the irreducible scalar of type I, $R_2^{i,j}$ reconstructs the irreducible scalar of type II, $R_3^{i,j,k}$ reconstructs the irreducible scalars of type III, where $i \neq j \neq k$. Using these rules, the algorithm reconstructs monomial $m_1(\mathbf{s})$, $m_2(\mathbf{s})$ and $m_3(\mathbf{s})$.

A monomial $\alpha_i(v)$ is expressed as

$$\alpha_i(\mathbf{v}) = \prod_{s=1}^n (V_x^s)^{n_s} \prod_{t=1}^n (V_y^t)^{n_t} \prod_{u=1}^n (V_z^u)^{n_u} \quad (5.39)$$

Here n_s, n_t, n_u are the powers of the components V_x^s, V_y^t, V_z^u where $s, t, u = \{1, 2, \dots, N\}$.

The elements of \mathbf{v} are decomposed into sets $\mathbf{X} = \{V_x^1, V_x^2, \dots, V_x^i, V_x^N\}$, $\mathbf{Y} = \{V_y^1, V_y^2, \dots, V_y^N\}$ and $\mathbf{Z} = \{V_z^1, V_z^2, \dots, V_z^N\}$. Three matrices XX, YY and ZZ of dimensions $(N \times N)$ are used for storing the degrees of elements $X_i \in \mathbf{X}, Y_i \in \mathbf{Y}$ and $Z_i \in \mathbf{Z}$.

The degrees of each component $X^i \in \mathbf{X}$ of the monomial α_v are stored in the diagonal of the matrix XX where the i^{th} position represents the i^{th} vector and $XX_{i,i}$ is the degree of the variable X_i . Similarly the degree of variables Y_i and Z_i are stored as diagonals in YY and ZZ . The degrees are elements of the set of non-negative integers. Let set $\mathbf{D} = [XX] \cup [YY] \cup [ZZ]$ represent all the diagonal elements in matrix XX, YY and ZZ given by set $[XX], [YY]$ and $[ZZ]$. In addition let

Algorithm **1** reconstruct monomials that are elements of $\mathbf{m}_1(\mathbf{s})$,

Algorithm **2** reconstruct monomials that are elements of $\mathbf{m}_2(\mathbf{s})$,

Algorithm **3** reconstruct monomials that are elements of $\mathbf{m}_3(\mathbf{s})$.

Let the combinations of algorithms be defined by set $ALGO : \{\mathbf{123}, \mathbf{231}, \dots\}$, which has six elements. These algorithms are used to reconstruct the scalar monomials in the set $\mathbf{H}^j(\mathbf{s})$ and their representation in \mathbf{v} . For an input $\alpha_i(\mathbf{v})$, any combination of algorithm

$ABC \in ALGO$, where A, B and C are elements of $\{\mathbf{1}, \mathbf{2}, \mathbf{3}\}$, reconstructs the scalars in the following steps

Algorithm A takes the input XX, YY and ZZ and reconstructs the monomial $m_A(\mathbf{s}) \in \mathbf{m}_A(\mathbf{s})$. For example A could be \mathbf{I} and element reconstructed is $m_A(\mathbf{s}) \in \mathbf{m}_A(\mathbf{s})$. The output consists of the matrices XX', YY' and ZZ' and the monomial $m_l(\mathbf{s})$. If the matrices XX', YY', ZZ' are null matrices then $m_l(\mathbf{s})$ is the required scalar and the algorithm terminates. Otherwise the algorithm continues to the next step.

Algorithm B takes the input XX', YY' and ZZ' and reconstructs the monomial $m_B(\mathbf{s}) \in \mathbf{m}_B(\mathbf{s})$. The output consists of the matrices XX'', YY'' and ZZ'' and the monomial $m_A(\mathbf{s})m_B(\mathbf{s})$. If the matrices XX'', YY'', ZZ'' are null matrices then $m_A(\mathbf{s})$ is the required scalar and the algorithm terminates. Other wise the algorithm continues to the next step.

This step is similar to previous steps and reconstructs $m_c(\mathbf{s}) \in \mathbf{m}_c(\mathbf{s})$. The output matrices are X''', Y''', Z''' . If $\{XX''', YY''', ZZ'''\}$ are null matrices then the output is a scalar monomial $h^j(s) = m_A(\mathbf{s})m_B(\mathbf{s})m_C(\mathbf{s})$.

If the matrices are not null matrices then the algorithm has failed to reconstruct $\alpha_i(\mathbf{v})$ and the process is repeated with another algorithm ACB .

The algorithms are discussed next.

5.3.1 Algorithm: $\mathbf{1}$

This algorithm reconstructs monomials that are elements of $\mathbf{m}_1(\mathbf{s})$ where

$$m_1(s) = \prod_{i=1}^{i=N} (\vec{V}_i \cdot \vec{V}_i)^{n_i}. \quad (5.40)$$

where n_i is the power of the i^{th} term. This algorithm uses rule R_1^i . To use this rule the condition

$$\exists x \in \mathbf{D} : x > 1 \quad (5.41)$$

must be satisfied.

If (5.41) is not satisfied the output of the algorithm is the input XX', YY' and ZZ' .

If the condition holds in then XX', YY' and ZZ' are decomposed into

$$XX' = XX'' + XX^{even} \quad (5.42)$$

$$YY' = YY'' + YY^{even} \quad (5.43)$$

$$ZZ' = ZZ'' + ZZ^{even}, \quad (5.44)$$

where matrices XX^{even} , YY^{even} and ZZ^{even} are given by the equations

$$\begin{aligned} \forall i \quad XX'_{i,i} > 1, \quad XX'_{i,i} = 2n_i^x + 1 \quad n_i^x = \{0, 1, 2, \dots\} \\ XX^{even}_{i,i} = 2n_i^x, \quad XX''_{i,i} = 1, \end{aligned} \quad (5.45)$$

and

$$\begin{aligned} \forall i, \quad XX'_{i,i} < 2 \\ XX^{even}_{i,i} = 0, \quad XX''_{i,i} = XX'_{i,i}. \end{aligned} \quad (5.46)$$

The same applies for YY' and ZZ' . The monomial $m_1(\mathbf{s}) \in \mathbf{m}_1(\mathbf{s})$ is reconstructed using rule R_1 .

$$m_1(s) = \prod_{i=0}^N (\vec{V}_i \cdot \vec{V}_i)^{\frac{(XX^{even}_{i,i} + YY^{even}_{i,i} + ZZ^{even}_{i,i})}{2}} \quad (5.47)$$

The monomial $m_1(\mathbf{s})$, the representation of $m_1(\mathbf{s})$ in \mathbf{v} and the matrices X'', Y'' and Z'' are the output of the algorithm.

5.3.2 Algorithm: 2

This algorithm reconstructs the monomials $m_2(\mathbf{s}) \in \mathbf{m}_2(\mathbf{s})$. Let the input matrices XX', YY' and ZZ' . This algorithm uses R_2 (5.38) to reconstruct $m_2(\mathbf{s})$. The matrices are decomposed as

$$\begin{aligned} XX'_{i,i} &= XX'_{i,i} - \text{minimum}(XX'_{i,i}, XX'_{j,j}) \quad i \neq j \\ XX'_{j,j} &= XX'_{j,j} - \text{minimum}(XX'_{i,i}, XX'_{j,j}) \end{aligned} \quad (5.48)$$

and

$$XX'_{i,j} = \text{minimum}(XX'_{i,i}, X'_{j,j}) \quad (5.49)$$

After rearranging the elements, the matrices XX' , YY' and ZZ' are decomposed into diagonal and non-diagonal matrices

$$\begin{aligned} XX' &= XX'' + XX^{nd} \\ YY' &= YY'' + YY^{nd} \\ ZZ' &= ZZ'' + ZZ^{nd}. \end{aligned} \quad (5.50)$$

Then rule R_2 is used to re-construct the scalars. The reconstruction equation is

$$m_2(s) = \prod_{i=0}^N \prod_{j=0}^N (\vec{V}_i \cdot \vec{V}_j)^{(XX^{nd}_{i,j} + YY^{nd}_{i,j} + ZZ^{nd}_{i,j})} \quad (5.51)$$

The output of the algorithm are $m_2(\mathbf{s})$, representation in \mathbf{v} and the matrices XX'' , YY'' and ZZ'' .

5.3.3 Algorithm: 3

The algorithm uses rule \mathbf{R}_3 (5.38). For this algorithm to be useful, the condition that there $\exists X_{i,i} \in [XX]$, $\exists Y_{j,j} \in [YY]$ and $\exists Z_{k,k} \in [ZZ]$ for any value of $\{i, j, k : i \neq j \neq k \neq i\}$ must be satisfied. Let 3DN be a three dimensional matrix of dimensions $(N \times N \times N)$. Defining

$$n_{i,j,k} = \text{minimum}(XX_{i,i}, YY_{j,j}, Z_{k,k}), \quad (5.52)$$

the new matrices are

$$XX''_{i,i} = X'_{i,i} - n_{i,j,k} \quad (5.53)$$

$$YY''_{j,j} = Y'_{j,j} - n_{i,j,k} \quad (5.54)$$

$$ZZ''_{k,k} = Z'_{k,k} - n_{i,j,k} \quad (5.55)$$

$$3DN_{i,j,k} = n_{i,j,k} \quad (5.56)$$

The scalar $m_3(s)$ is constructed by the equation

$$m_3(s) = \prod_{i=0, j=0, k=0}^{N, N, N} ((\vec{V}_i \times \vec{V}_j) \cdot \vec{V}_k)^{3DN_{i,j,k}} \quad (5.57)$$

The output of algorithm are $m_3(\mathbf{s})$, the representation in \mathbf{v} and matrices XX'' , YY'' and ZZ'' .

5.4 Conclusion

To test the algebraic reduction mechanism discussed in this chapter the reduction algorithms are tested first by generating the representation of a monomial $m(\mathbf{s}) \in \mathbf{m}(\mathbf{s})$ in \mathbf{v} and using the reduction algorithm to reproduce the monomial $m(\mathbf{s})$. The algorithm was successful in reproducing the monomial. An example of a test monomial is

$$m(\mathbf{s}) = (\vec{q}_1 \cdot \vec{q}_2)(\vec{q}_3 \cdot \vec{q}_4)(\vec{q}_5 \cdot \vec{q}_6) + 56(\vec{q}_1 \times \vec{q}_2)(\vec{q}_3 \times \vec{q}_4)(\vec{q}_5 \times \vec{q}_6) \quad (5.58)$$

The algorithms were successful in reducing the trace expressions (2.55) and the output is given in Appendix A of this thesis. These functions are re-expressed in terms of momenta variables and a random set is chosen to compare with the expressions in [13]. The test expressions reduced matched the same trace expressions in [13]. The algebraic system discussed in this chapter is used in solving the bound-state of the deuteron and in formalism of the two-body scattering using vector variables. They are discussed in later chapters of this thesis.

CHAPTER 6

DEUTERON BOUND STATE OF ARGONNE V18

This chapter discusses the computation of the binding energy and wave functions of the deuteron. The two-body bound state problem is solved using vector variable approach [31]. The realistic nucleon-nucleon potential used is the Argonne V18 potential. This calculation provides a test of all of the methods developed in this thesis. These calculations test

1. the Fourier transform of the Argonne V18 interaction in operator form,
2. the convergence of the Fourier-Bessel integrals,
3. the Chebyshev approximation of the Fourier-Bessel integrals,
4. the symbolic methods for treating the spin in the vector form of the dynamical equations.

6.1 Numerical realization

The Schrödinger equation for the two-nucleon system in the center of mass frame is given by

$$\left(\frac{k^2}{2\mu} + V\right)|\psi\rangle = E|\psi\rangle, \quad (6.1)$$

which leads to a momentum space integral equation,

$$\langle\vec{k}|\psi\rangle = \frac{1}{E_d - \frac{k^2}{2\mu}} \int_0^\infty d^3\vec{k}' \langle\vec{k}|V|\vec{k}'\rangle \langle\vec{k}'|\psi\rangle, \quad (6.2)$$

where k is the nucleon momentum in two-body rest frame, and E is the energy eigenvalue.

In general a vector representative of an isosinglet bound state will have four amplitudes corresponding to the four different spin combinations. Space reflection symmetry reduces this to two spin combinations. These properties can be encoded into the representation for the deuteron eigenstate. Ref [31] gives the following representation for the deuteron

eigenstate $|\psi\rangle$ in operator form:

$$\langle \vec{k} | \psi_d \rangle = \left(\phi_1(k) + \{(\sigma_1 \cdot \vec{k})(\sigma_2 \cdot \vec{k}) - \frac{k^2}{3}\} \phi_2(k) \right) |1, m_s\rangle. \quad (6.3)$$

This is for isospin $t = 0$, spin $S = 1$, $j = 1$ and

$$\psi_0(k) = \phi_1(k) \quad (6.4)$$

$$\psi_1(k) = \frac{4k^2}{3\sqrt{2}} \phi_2(k) \quad (6.5)$$

where $\psi_0(k)$ is the s wave function and $\psi_2(k)$ is the d wave function.

The vector $|1, m_s\rangle$ on the right side of this equation can be thought of as the Clebsch-Gordan coefficient $\langle \frac{1}{2}, \mu_1, \frac{1}{2}, \mu_2 | 1, m_s \rangle$ in the tensor product representation. When the operator on the left side of this expression acts on $|1, m_s\rangle$ it generates the linear combination of spin and spherical harmonic states corresponding to a spin 1 deuteron with magnetic quantum number $m_d = m_s$.

The following notation is used for the operators

1. Operator: $O_1(\vec{k})$ is the identity operator \mathbf{I}
2. Operator: $O_2(\vec{k})$ is $(\vec{\sigma}_1 \cdot \vec{k})(\vec{\sigma}_2 \cdot \vec{k}) - O_1(\vec{k})\frac{k^2}{3}$.

In this notation equation (6.2) becomes

$$\begin{aligned} & \left(\phi_1(k) O_1(\vec{k}) + O_2(\vec{k}) \phi_2(k) \right) |1, m_s\rangle = \\ & \frac{1}{E_d - \frac{k^2}{m}} \int_0^\infty d^3 \vec{k}' V (O_1(\vec{k}') \phi_1(k') + O_2(\vec{k}') \phi_2(k')) |1, m_s\rangle \end{aligned} \quad (6.6)$$

To solve the Schödinger equation the operators $O_i(\vec{k})$, where $i = \{1, 2\}$ are applied to both sides of (6.7) and the result is multiplied by a projection operator on the spin $S = 1$ subspace. This is expressed in the equation below

$$\begin{aligned} & \langle 1, m'_s | O_i(\vec{k}) \left(\phi_1(k) O_1(\vec{k}) + \phi_2(k) O_2(\vec{k}) \right) |1, m_s\rangle = \\ & \frac{1}{E_d - \frac{k^2}{m}} \langle 1, m'_s | O_i(\vec{k}) \int_0^\infty d^3 \vec{k}' V (\phi_1(k') O_1(\vec{k}') + \phi_2(k') O_2(\vec{k}')) |1, m_s\rangle \end{aligned} \quad (6.7)$$

which is a 3×3 matrix in spin projection m_s .

After the projection on the spin $S = 1$ states the 4×4 matrices that appear in

(6.7) are replaced by the following 3×3 matrices:

$$\langle 1, m'_s | O_i(\vec{k}) O_1(\vec{k}) | 1, m_s \rangle \rightarrow \mathbf{AA}_i(\vec{k}) \quad (6.8)$$

$$\langle 1, m'_s | O_i(\vec{k}) O_2(\vec{k}) | 1, m_s \rangle \rightarrow \mathbf{BB}_i(\vec{k}) \quad (6.9)$$

$$\langle 1, m'_s | O_i(\vec{k}) V O_1(\vec{k}') | 1, m_s \rangle \rightarrow \mathbf{CC}_i(k, k', \hat{k} \cdot \hat{k}') \quad (6.10)$$

$$\langle 1, m'_s | O_i(\vec{k}) V O_2(\vec{k}') | 1, m_s \rangle \rightarrow \mathbf{DD}_i(k, k', \hat{k} \cdot \hat{k}') \quad (6.11)$$

Equations for the wave functions $\phi_i(k)$ are obtained by taking the trace of (6.7) over m_s . The resulting equations are

$$\sum_{m_s=-1}^1 \langle 1, m_s | O_i(\vec{k}) \left(\phi_1(k) O_1(\vec{k}) + \phi_2(k) O_2(\vec{k}) \right) | 1, m_s \rangle = \sum_{m_s=-1}^1 \frac{1}{E_d - \frac{k^2}{m}} \langle 1, m_s | O_i(\vec{k}) \int_0^\infty d^3 k' V (\phi_1(k') O_1(\vec{k}') + \phi_2(k') O_2(\vec{k}')) | 1, m_s \rangle \quad (6.12)$$

and can be expressed in terms of the operators (6.11) as

$$\begin{aligned} & Tr(\mathbf{AA}_i) \phi_1(k) + Tr(\mathbf{BB}_i) \phi_2(k) = \\ & \frac{1}{E - \frac{k^2}{m}} \int_0^\infty \{ Tr(\mathbf{CC}_i(k, k', \hat{k} \cdot \hat{k}')) \phi_1(k') + Tr(\mathbf{DD}_i(k, k', \hat{k} \cdot \hat{k}')) \phi_2(k') \} d^3 k' \end{aligned} \quad (6.13)$$

The functions obtained by taking the traces are scalar functions of the form $F(k, k', \vec{k} \cdot \vec{k}')$.

These scalar functions are given by

$$\begin{aligned} Tr(\mathbf{AA}_i(k)) &= A_i(k), \\ Tr(\mathbf{BB}_i(k)) &= B_i(k), \\ Tr(\mathbf{CC}_i(k, k', \hat{k} \cdot \hat{k}')) &= C_i(k, k', \hat{k} \cdot \hat{k}'), \\ Tr(\mathbf{DD}_i(k, k', \hat{k} \cdot \hat{k}')) &= D_i(k, k', \hat{k} \cdot \hat{k}'). \end{aligned} \quad (6.14)$$

Inserting the traces into (6.14) gives a pair of coupled integral equations for $\phi_i(k')$:

$$\begin{aligned} & \frac{1}{E - \frac{k^2}{m}} \int_0^\infty \left\{ C_i(k, k', \hat{k} \cdot \hat{k}') \phi_1(k') + D_i(k, k', \hat{k} \cdot \hat{k}') \phi_2(k') \right\} k'^2 dk' d\Omega(\hat{k}') \\ &= A_i(k) \phi_1(k) + B_i(k) \phi_2(k). \end{aligned} \quad (6.15)$$

The trace expressions of these spin operators and the reduction of the trace expression into scalar products are carried out using the algebraic reduction mechanism discussed in chapter 5. In the next section the reduced expressions are given. The integral equation is solved by the collocation method. The collocation points are taken as Gauss Legendre

quadrature points where the upper limit of the integral is set to a finite value. The optimum value was determined through convergence tests. With this discretization the Schrödinger equation turn into the matrix equation,

$$\frac{2\pi}{E - \frac{k_l^2}{m}} \sum_{t=0}^{t=N} \sum_{tt=0}^{tt=N} \left\{ C_i(k_l, k_t, x_{tt})\phi_1(k_t) + D_i(k_l, k_t, x_{tt})\phi_2(k_t) \right\} k_t^2 w_t w_{tt} = A_i(k_l)\phi_1(k_l) + B_i(k_l)\phi_2(k_l) \quad (6.16)$$

The angular variable does not appear in the wavefunctions, so it can be integrated out without seperately. Defining

$$C_i(k_l, k_t) := \sum_{\substack{tt=0 \\ tt=N}}^{tt=N} C_i(k_l, k_t, x_{tt}) w_{tt} \quad (6.17)$$

$$D_i(k_l, k_t) := \sum_{tt=0}^{tt=N} D_i(k_l, k_t, x_{tt}) w_{tt} \quad (6.18)$$

gives

$$\frac{2\pi}{E - \frac{k_l^2}{m}} \sum_{t=0}^{t=N} \left(C_i(k_l, k_t)\phi_1(k_t) + D_i(k_l, k_t)\phi_2(k_t) \right) k_t^2 w_t = A_i(k_l)\phi_1(k_l) + B_i(k_l)\phi_2(k_l) \quad (6.19)$$

The Gauss-Legendre quadrature points and the weights for radial integral are k_t, k_m and w_t . Similarly, x_{tt} and w_{tt} are the Gauss Legendre quadrature points and weights for the angular integral. In abstract form, the integral equation is a matrix,

$$\begin{pmatrix} \mathbf{A}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{B}_2 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = \begin{pmatrix} \mathbf{E} & \mathbf{0} \\ \mathbf{0} & \mathbf{E} \end{pmatrix} \begin{pmatrix} \mathbf{C}_1 & \mathbf{C}_2 \\ \mathbf{D}_1 & \mathbf{D}_2 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \quad (6.20)$$

with size $(2N \times 2N)$. The matrices $\mathbf{A}_1, \mathbf{B}_2$ and \mathbf{E} are diagonal $N \times N$ matrices. The matrix element is a function of the energy eigenvalue

$$\mathbf{E}_{i,j} = \frac{2\pi}{E - \frac{k_i^2}{m}} \delta_{ij},$$

and the equation in matrix form is

$$\widehat{AB}\bar{\phi} = \widehat{E}\widehat{CD}\bar{\phi}$$

where \widehat{AB} is the matrix with A_i, B_i , \widehat{CD} is the matrix with C_i, D_i and $\bar{\phi}$ is the column vector. To solve for $\bar{\phi}$, the eigenvalue equation

$$\bar{\phi} = \lambda \widehat{AB}^{-1} \widehat{E}\widehat{CD}\bar{\phi}$$

is solved for λ as a function of E . E is varied until $\lambda = 1$, which results in E being an eigenvalue of H .

The equation (6.1) determines the wave function at the collocation points. Since these are also the quadrature points the solution can be evaluated at any point by inserting the discrete solution back into the integral equation.

For $\rho > 50fm^{-1}$ the Fourier-Bessel transformed integrals fall off with values of the order $I(\rho) < 10^{-7}fm^{-1}$ (except the integral $I_i^2(\rho)$ that has order of $10^{-5}fm^{-1}$). The integral can be approximated with an upper limit of k_{max} . The upper limits $k_{max} = \{50fm^{-1}, 30fm^{-1}, 10fm^{-1}, 5fm^{-1}\}$ are chosen to test for convergence of the integral. To compute the eigenvalue (6.1) the number of Gaussian quadrature points and weights for the radial integral is fixed at 60 and the angular integral is fixed at 40. The Gaussian quadrature points are sufficient for different k_{max} values and hence in the discussion of computing equation (6.1) the number of Gaussian quadrature points are fixed at 40 for angular integral and at 60 for radial integral. The eigenvalues are determined using the LAPACK [32] subroutine "dgeev". This subroutine computes the eigenvalues and eigenvectors for a real non-symmetric square matrix .

The eigenvalue λ is a function of energy and the bound state energy is when the solution results in $\lambda = 1$. To calculate the binding energy, the eigenvalue is computed for different energies. The smallest interval between $\lambda > 1.0$ and $\lambda < 1.0$ is where the bound state energy can be obtained. Table 6.1 gives the interval between energy values -2.235 MeV and -2.24 MeV. The eigenvalue for different energy values is then computed in this interval. Depending on the number of significant figures required for the bound state the process is repeated. An example is shown in Table[6.1]. Table[6.1] illustrates the dependence of the energy on the eigenvalue λ for a cutoff of $k_{max} = 10fm^{-1}$. Table[6.1] gives the energy for different values of the λ near $\lambda = 1$. $\lambda = 1$ is obtained at the energy value $E_b = -2.3829MeV$.

Energy values vs eigenvalue λ	
Energy(Mev)	λ
-2.22	1.00083
-2.225	1.00061
-2.23	1.00038
-2.235	1.00015
-2.24	0.999927
-2.245	0.999927
-2.25	0.999701
-2.255	0.999476
-2.26	0.99925
-2.265	0.999025

Table 6.1: Energy values vs λ for

$$k_{max} = 10fm^{-1}$$

Convergence: k_{max} vs binding energy	
$k_{max}(fm^{-1})$	$E_b(\text{Mev})$
10	-2.3829
20	-2.242212
30	-2.242212
40	-2.242212

Table 6.2: Convergence test for k_{max}

Table[6.2] shows the binding energy computed for different values of k_{max} . The binding energy converges to seven significant figures $E_b = -2.242219$ MeV and the eigenvalue $\lambda = 0.99999999$. This value of the binding energy is reached at $k_{max} = 20fm^{-1}$. The E_b results are constant after $20fm^{-1}$. As discussed before, the number of Gaussian quadrature grid points used is fixed for different k_{max} values. The Argonne V18 potential does not include the electromagnetic terms and the binding energy is computed for strong interaction. This is compared with a direct calculation of the deuteron binding energy using partial waves in configuration space which gives $E_b = -2.242211$ MeV. Reference [33] gives a binding energy of -2.224574 MeV. But this also includes the electromagnetic terms in the potential.

The s wave and d wave functions for the deuteron are computed and shown in Fig[6.1] and Fig[6.2]. The s state probability is $P_s = 0.942241$ and d state probability is $P_d = 0.0577595$.

Now that the Fourier transform of the Argonne V18 has been directly computed

and used for calculating the bound state of deuteron , an efficient method of computing these Fourier transforms using Chebyshev approximation is explored in the following discussions. The Chebyshev approximation of the Fourier-Bessel integrals reduce the time of computation. Table[6.3] shows the cpu (dual core 3Ghz pentium processor) time for the direct numerical computation of the Fourier-Bessel integrals compared with the same calculation using the Chebyshev approximations to these integrals. The total number of Chebyshev points used in the approximation is 303 with 101 polynomials used for each of the three intervals discussed on page 39 equation (4.12).

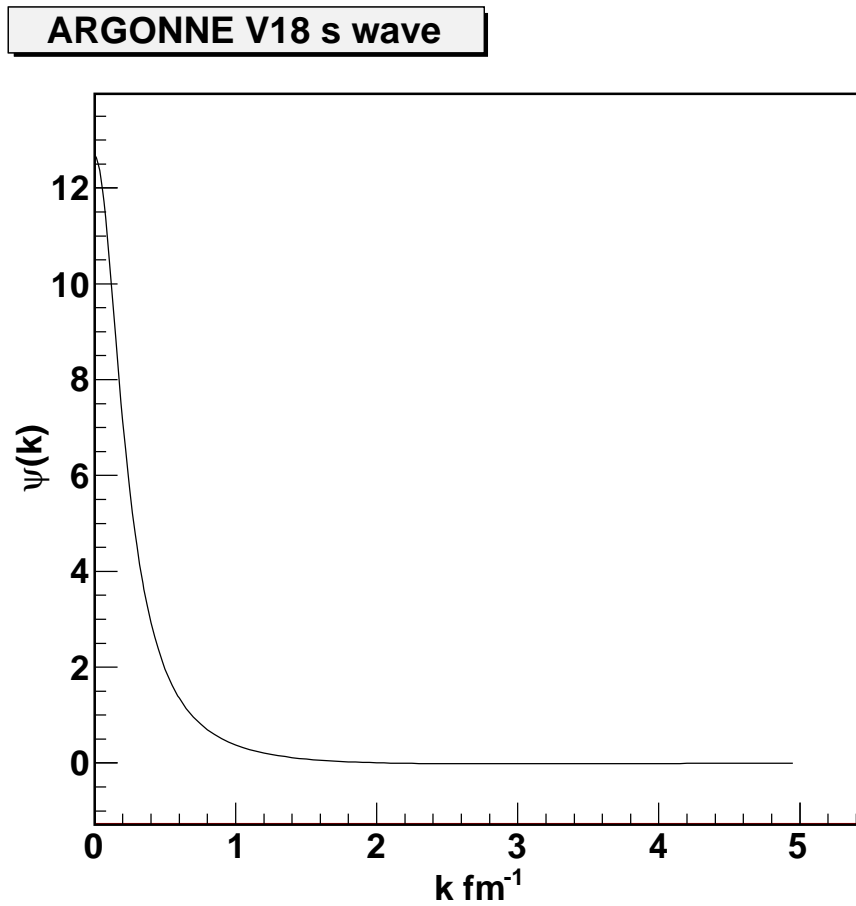


Figure 6.1: The s wave function of deuteron

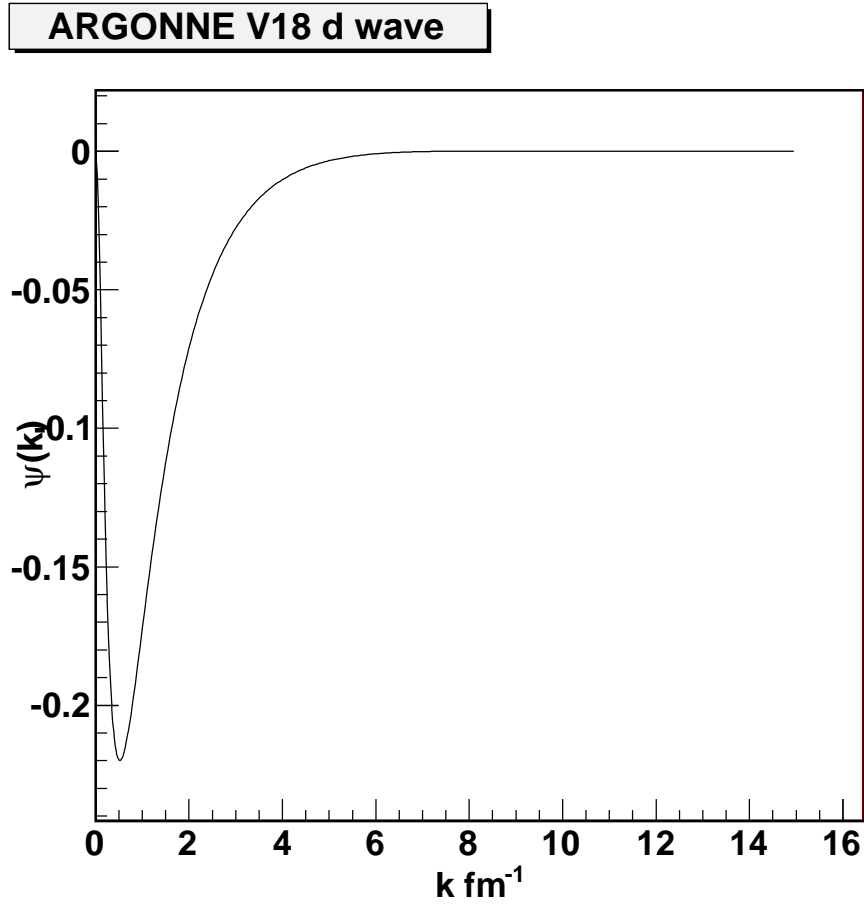


Figure 6.2: The d wave function of deuteron

Direct vs Chebyshev approximation		
Method	Binding Energy(Mev)	Time(in sec)
Direct	-2.242219	16915
Chebyshev	-2.242219	6

Table 6.3: Comparison of direct and Chebyshev integration.

The Chebyshev coefficients are extracted separately and used in the computation of deuteron binding energy. Now that the Chebyshev approximation has been successful, the dependence on the number of Chebyshev functions that are needed to accurately compute the deuteron binding energy are investigated next. The results of the number of Chebyshev functions and E_b are given in Table[6.4]

Number of Chebyshev functions vs E_b			
n1	n2	n3	E_b
100	100	100	-2.242219
50	50	50	-2.24225
50	30	30	-2.24225
30	50	50	-2.242402
30	30	30	-2.242402

Table 6.4: Change in bound state energy with number of Chebyshev functions

The investigation shows that it takes 93 Chebyshev functions to get a binding energy with an accuracy of 5 significant figures.

6.2 Computation of traces

In this chapter the deuteron two-body problem was solved for the bound state by taking traces of the spin matrices. Each expression is reduced to scalar products of momentum vectors \vec{k} and \vec{k}' . A variable change of $\vec{k}' \rightarrow \vec{q}_1$ and $\vec{k} \rightarrow \vec{q}_2$ is made. The traces involve the operators defined in the wave function given in (6.14)

$$O_1 = \mathbf{1}$$

$$O_2(\vec{P}) = (\vec{\sigma}_1 \cdot \vec{P})(\vec{\sigma}_2 \cdot \vec{P}) - \frac{1}{3}P^2 O_1 = A(\vec{P}) - \frac{1}{3}P^2 O_1$$

where $\vec{P} = \{\vec{q}_1, \vec{q}_2\}$ and $A(\vec{P}) = (\vec{\sigma}_1 \cdot \vec{P})(\vec{\sigma}_2 \cdot \vec{P})$. The spin operators of the momentum-space nucleon-nucleon potential Argonne V18 are listed below

$$w_1 = (\vec{\sigma}_1 \cdot \vec{\sigma}_2) \tag{6.21}$$

$$w_2 = \frac{(-3(\vec{\sigma}_1 \cdot (\vec{q}_2 - \vec{q}_1))(\vec{\sigma}_2 \cdot (\vec{q}_2 - \vec{q}_1)))}{Q^2} \tag{6.22}$$

$$w_3 = (-i((\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)) \cdot (\vec{q}_2 \times \vec{q}_1))) \tag{6.23}$$

$$w_4 = ((\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)) \cdot (\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2))) \tag{6.24}$$

$$w_5 = ((\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)) \cdot \vec{q}_2)((\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)) \cdot \vec{q}_1) \tag{6.25}$$

$$w_6 = ((\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)) \cdot (\vec{q}_2 \times \vec{q}_1))((\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)) \cdot (\vec{q}_2 \times \vec{q}_1)). \tag{6.26}$$

Here $Q = \sqrt{q_1^2 + q_2^2 - 2q_1 q_2 \hat{q}_1 \cdot \hat{q}_2}$. To calculate these traces and simplify the results the symbolic algebraic system is used. The symbolic program gives the following values for the traces of the operators. The left side of the equation is the operator and the right hand side of the equation is the trace of the operator (please note that the symbol used to represent imaginary numbers i is replaced by j) :

$$O_1 O_1 = 3.0. \tag{6.27}$$

$$O_1(\vec{\sigma}_1 \cdot \vec{\sigma}_2)O_1 = 3.0. \tag{6.28}$$

$$O_1 \frac{(-3(\vec{\sigma}_1 \cdot (\vec{q}_2 - \vec{q}_1))(\vec{\sigma}_2 \cdot (\vec{q}_2 - \vec{q}_1)))}{Q^2} O_1 = \frac{-3(\vec{q}_1 \cdot \vec{q}_1) - (6.0)(\vec{q}_1 \cdot \vec{q}_2) + 3(\vec{q}_2 \cdot \vec{q}_2)}{Q^2}. \tag{6.29}$$

$$O_1(-j((\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)) \cdot (\vec{q}_2 \times \vec{q}_1)))O_1 = 0. \tag{6.30}$$

$$O_1((\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)) \cdot (\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)))O_1 = 6.0. \tag{6.31}$$

$$O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_2\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_1\right)O_1 = 2(\vec{q}_1 \cdot \vec{q}_2) \quad (6.32)$$

$$\begin{aligned} O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)O_1 = \\ -(2.0)(\vec{q}_1 \cdot \vec{q}_2)^{(2,0)} + (2.0)(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_2) \\ -(\vec{q}_2 \cdot \vec{q}_2)O_1O_1\frac{1}{3} + O_1A(\vec{q}_2) = 0 \end{aligned} \quad (6.33)$$

$$-(\vec{q}_2 \cdot \vec{q}_2)O_1(\vec{\sigma}_1 \cdot \vec{\sigma}_2)O_1\frac{1}{3} + O_1(\vec{\sigma}_1 \cdot \vec{\sigma}_2)A(\vec{q}_2) = 0 \quad (6.34)$$

$$\begin{aligned} -(\vec{q}_2 \cdot \vec{q}_2)O_1\frac{(-3(\vec{\sigma}_1 \cdot (\vec{q}_2 - \vec{q}_1))(\vec{\sigma}_2 \cdot (\vec{q}_2 - \vec{q}_1)))}{Q^2}O_1\frac{1}{3} + O_1\frac{(-3(\vec{\sigma}_1 \cdot (\vec{q}_2 - \vec{q}_1))(\vec{\sigma}_2 \cdot (\vec{q}_2 - \vec{q}_1)))}{Q^2}A(\vec{q}_2) = \\ \frac{1}{3}\frac{-(36.0)(\vec{q}_1 \cdot \vec{q}_2)^{(2,0)} - (24.0)(\vec{q}_2 \cdot \vec{q}_2)^2 + 12.0(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_2)}{Q^2} \\ + \frac{(48.0)(\vec{q}_1 \cdot \vec{q}_2)(\vec{q}_2 \cdot \vec{q}_2)}{Q^2} \end{aligned}$$

$$\begin{aligned} -(\vec{q}_2 \cdot \vec{q}_2)O_1(-j\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right))O_1\frac{1}{3} \\ + O_1(-j\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right))A(\vec{q}_2) = 0 \end{aligned} \quad (6.35)$$

$$\begin{aligned} -(\vec{q}_2 \cdot \vec{q}_2)O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right)\right)O_1\frac{1}{3} \\ + O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right)\right)A(\vec{q}_2) = 0. \end{aligned}$$

$$\begin{aligned} -(\vec{q}_2 \cdot \vec{q}_2)O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_2\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_1\right)O_1\frac{1}{3} \\ + O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_2\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_1\right)A(\vec{q}_2) = \\ \left(\frac{1.0}{3} + 1.0\right)(\vec{q}_1 \cdot \vec{q}_2)(\vec{q}_2 \cdot \vec{q}_2) \end{aligned} \quad (6.36)$$

$$\begin{aligned} -(\vec{q}_2 \cdot \vec{q}_2)O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)O_1\frac{1}{3} \\ + O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)A(\vec{q}_2) = \\ -\frac{1}{3}(-2.0)(\vec{q}_1 \cdot \vec{q}_2)^{(2,0)} + (2.0)(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_2)(\vec{q}_2 \cdot \vec{q}_2) \end{aligned} \quad (6.37)$$

$$-(\vec{q}_1 \cdot \vec{q}_1)O_1O_1\frac{1}{3} + A(\vec{q}_1)O_1 = 0. \quad (6.38)$$

$$-(\vec{q}_1 \cdot \vec{q}_1)O_1(\vec{\sigma}_1 \cdot \vec{\sigma}_2)O_1\frac{1}{3} + A(\vec{q}_1)(\vec{\sigma}_1 \cdot \vec{\sigma}_2)O_1 = O.$$

$$\begin{aligned} -(\vec{q}_1 \cdot \vec{q}_1)O_1\frac{(-3(\vec{\sigma}_1 \cdot (\vec{q}_2 - \vec{q}_1))(\vec{\sigma}_2 \cdot (\vec{q}_2 - \vec{q}_1)))}{Q^2}O_1\frac{1}{3} \\ + A(\vec{q}_1)\frac{(-3(\vec{\sigma}_1 \cdot (\vec{q}_2 - \vec{q}_1))(\vec{\sigma}_2 \cdot (\vec{q}_2 - \vec{q}_1)))}{Q^2}O_1 = \end{aligned}$$

$$\frac{1}{3}\frac{-(24.0)(\vec{q}_1 \cdot \vec{q}_1)^2 - (36.0)(\vec{q}_1 \cdot \vec{q}_2)^{(2,0)} + (48.0)(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_1 \cdot \vec{q}_2) + 12(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_2)}{Q^2}. \quad (6.39)$$

$$-(\vec{q}_1 \cdot \vec{q}_1)O_1(-j\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right))O_1\frac{1}{3} + A(\vec{q}_1)(-j\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right))O_1 = O.$$

$$\begin{aligned}
& -(\vec{q}_1 \cdot \vec{q}_1)O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right)\right)O_1\frac{1}{3} \\
& + A(\vec{q}_1)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right)\right)O_1 = 0. \\
& -(\vec{q}_1 \cdot \vec{q}_1)O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_2\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_1\right)O_1\frac{1}{3} \\
& + A(\vec{q}_1)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_2\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_1\right)O_1 = \\
& \quad \left(\frac{1.0}{3} + 1.0\right)(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_1 \cdot \vec{q}_2) \tag{6.40}
\end{aligned}$$

$$\begin{aligned}
& -(\vec{q}_1 \cdot \vec{q}_1)O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)O_1\frac{1}{3} \\
& + A(\vec{q}_1)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)O_1 = \\
& -\frac{1}{3}\left(-2.0\right)(\vec{q}_1 \cdot \vec{q}_2)^{(2.0)} + (2.0)(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_2)(\vec{q}_1 \cdot \vec{q}_1) \tag{6.41}
\end{aligned}$$

$$\begin{aligned}
& -(\vec{q}_1 \cdot \vec{q}_1)O_1A(\vec{q}_2)\frac{1}{3} - (\vec{q}_2 \cdot \vec{q}_2)A(\vec{q}_1)O_1\frac{1}{3} + (\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_2)O_1O_1\frac{1}{9} + A(\vec{q}_1)A(\vec{q}_2) = \\
& (4.0)(\vec{q}_1 \cdot \vec{q}_2)^{(2.0)} - \left(\frac{1.0}{3} + 1.0\right)(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_2) \tag{6.42}
\end{aligned}$$

$$\begin{aligned}
& -(\vec{q}_1 \cdot \vec{q}_1)O_1(\vec{\sigma}_1 \cdot \vec{\sigma}_2)A(\vec{q}_2)\frac{1}{3} - (\vec{q}_2 \cdot \vec{q}_2)A(\vec{q}_1)(\vec{\sigma}_1 \cdot \vec{\sigma}_2)O_1\frac{1}{3} \\
& + (\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_2)O_1(\vec{\sigma}_1 \cdot \vec{\sigma}_2)O_1\frac{1}{9} + A(\vec{q}_1)(\vec{\sigma}_1 \cdot \vec{\sigma}_2)A(\vec{q}_2) = \\
& (4.0)(\vec{q}_1 \cdot \vec{q}_2)^{(2.0)} - \left(\frac{1.0}{3} + 1.0\right)(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_2) \tag{6.43}
\end{aligned}$$

$$\begin{aligned}
& -(\vec{q}_1 \cdot \vec{q}_1)O_1\frac{(-3(\vec{\sigma}_1 \cdot (\vec{q}_2 - \vec{q}_1))(\vec{\sigma}_2 \cdot (\vec{q}_2 - \vec{q}_1)))}{Q^2}A(\vec{q}_2)\frac{1}{3} \\
& -(\vec{q}_2 \cdot \vec{q}_2)A(\vec{q}_1)\frac{(-3(\vec{\sigma}_1 \cdot (\vec{q}_2 - \vec{q}_1))(\vec{\sigma}_2 \cdot (\vec{q}_2 - \vec{q}_1)))}{Q^2}O_1\frac{1}{3} \\
& + (\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_2)O_1\frac{(-3(\vec{\sigma}_1 \cdot (\vec{q}_2 - \vec{q}_1))(\vec{\sigma}_2 \cdot (\vec{q}_2 - \vec{q}_1)))}{Q^2}O_1\frac{1}{9} \\
& + A(\vec{q}_1)\frac{(-3(\vec{\sigma}_1 \cdot (\vec{q}_2 - \vec{q}_1))(\vec{\sigma}_2 \cdot (\vec{q}_2 - \vec{q}_1)))}{Q^2}A(\vec{q}_2) = \\
& \frac{1 - (48.0)(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_1 \cdot \vec{q}_2)(\vec{q}_2 \cdot \vec{q}_2) - (12.0)(\vec{q}_1 \cdot \vec{q}_1)^2(\vec{q}_2 \cdot \vec{q}_2) + (36.0)(\vec{q}_1 \cdot \vec{q}_2)^{(2.0)}(\vec{q}_2 \cdot \vec{q}_2)}{9Q^2} \\
& + \frac{(36.0)(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_1 \cdot \vec{q}_2)^{(2.0)} - 12(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_2)^2}{Q^2} \tag{6.44}
\end{aligned}$$

$$\begin{aligned}
& -(\vec{q}_1 \cdot \vec{q}_1)O_1(-j)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)A(\vec{q}_2)\frac{1}{3} - (\vec{q}_2 \cdot \vec{q}_2)A(\vec{q}_1)(-j)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)O_1\frac{1}{3} \\
& + (\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_2)O_1(-j)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)O_1\frac{1}{9} + A(\vec{q}_1)(-j)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)A(\vec{q}_2) = \\
& (4.0)(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_1 \cdot \vec{q}_2)(\vec{q}_2 \cdot \vec{q}_2) - (4.0)(\vec{q}_1 \cdot \vec{q}_2)^{(3.0)} \\
& -(\vec{q}_1 \cdot \vec{q}_1)O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right)\right)A(\vec{q}_2)\frac{1}{3} \\
& -(\vec{q}_2 \cdot \vec{q}_2)A(\vec{q}_1)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right)\right)O_1\frac{1}{3}
\end{aligned}$$

$$\begin{aligned}
& +(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_2)O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right)\right)O_1\frac{1}{9} \\
& +A(\vec{q}_1)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right)\right)A(\vec{q}_2) = \\
& (8.0)(\vec{q}_1 \cdot \vec{q}_2)^{(2.0)} - \left(\frac{2}{3} + 1.0\right)(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_2) \tag{6.45}
\end{aligned}$$

$$\begin{aligned}
& -(\vec{q}_1 \cdot \vec{q}_1)O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_2\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_1\right)A(\vec{q}_2)\frac{1}{3} \\
& -(\vec{q}_2 \cdot \vec{q}_2)A(\vec{q}_1)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_2\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_1\right)O_1\frac{1}{3} \\
& +(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_2)O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_2\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_1\right)O_1\frac{1}{9} \\
& +A(\vec{q}_1)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_2\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot \vec{q}_1\right)A(\vec{q}_2) = \\
& -\left(\frac{1}{3} + 3.0\right)(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_1 \cdot \vec{q}_2)(\vec{q}_2 \cdot \vec{q}_2) + (4.0)(\vec{q}_1 \cdot \vec{q}_2)^{(3.0)}. \tag{6.46}
\end{aligned}$$

$$\begin{aligned}
& -(\vec{q}_1 \cdot \vec{q}_1)O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)A(\vec{q}_2)\frac{1}{3} \\
& -(\vec{q}_2 \cdot \vec{q}_2)A(\vec{q}_1)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)O_1\frac{1}{3} \\
& +(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_2 \cdot \vec{q}_2)O_1\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)O_1\frac{1}{9} \\
& +A(\vec{q}_1)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)\left(\left(\frac{1}{2}(\vec{\sigma}_1 + \vec{\sigma}_2)\right) \cdot (\vec{q}_2 \times \vec{q}_1)\right)A(\vec{q}_2) = \\
& -(4.0)(\vec{q}_1 \cdot \vec{q}_2)^{(4.0)} - \left(\frac{2.0}{3} + \frac{1.0}{9} + 1.0\right)(\vec{q}_1 \cdot \vec{q}_1)^2(\vec{q}_2 \cdot \vec{q}_2)^2 + \left(\frac{2.0}{3} + \frac{1.0}{9} + 5.0\right)(\vec{q}_1 \cdot \vec{q}_1)(\vec{q}_1 \cdot \vec{q}_2)^{(2.0)}(\vec{q}_2 \cdot \vec{q}_2). \tag{6.47}
\end{aligned}$$

These traces serve as input to the computation of the deuteron bound state. The time for the program to execute and print these expressions was 13 seconds.

6.3 Conclusion

The vector solution of the deuteron bound state problem, discussed in this section provides a good test of all the tools developed in this thesis. These include

1. The Fourier transform of the Argonne V18 potential.
2. The numerical method for computing with oscillatory integrals in the Fourier-Bessel transformation.

3. The use of the Chebyshev expansion of the Fourier Bessel integrals to reduce the time of computation. Three hundred and three Chebyshev functions were used and employed for calculating the bound state energy of deuteron. When compared with the direct method, the Chebyshev functions reproduce the bound state energy calculated by the direct method but reduce the time of execution by a factor of 2800.
4. The algebraic system discussed in Chapter 5 was successful in computing traces and reducing them to simple scalar functions.

CHAPTER 7

GENERAL REPRESENTATION OF BASIS OPERATORS

7.1 Basis operators

This chapter adopts an alternative formulation of the two-nucleon problem using vector variables. A general representation that can be used to expand any nucleon-nucleon potential for a given choice of three linearly independent vectors is introduced. The representation to expand any nucleon-nucleon potential expressed in a form similar to the Argonne V18 potential is tested for two different choice of linearly dependent three vectors. The first choice is to construct the basis using the three vectors given by (2.46) in Chapter two. This choice is called Type I. Another choice that may be convenient is a basis of operators constructed using an orthogonal set of vectors. The second choice is called Type II. This chapter also investigates the contribution of time-odd operators in defining a basis and their importance in computing the Wolfenstein parameters. The algebraic system introduced in chapter four is used for computing the equations that appear throughout this chapter.

7.2 Representation

The representation that is used to solve the Lippmann-Schwinger equation in vector variables for scattering of two spin $\frac{1}{2}$ particles is discussed in this section. While in general there are four initial and four final spin states, the size of the system of coupled linear equations can be reduced by taking advantage of symmetries of the interaction. In order to take advantage of these symmetries the interaction is expressed as a linear combination of scalar coefficient functions multiplied by linearly independent rotationally invariant spin operators that have well-defined transformation properties with respect to time-reversal and space reflection. The spin operators for two spin $\frac{1}{2}$ particles are given by the set $\{S^i\} = \{\sigma_p^1 \otimes \sigma_q^2\}$ where $p, q = 0, 1, 2, 3$ and $i = \{1, 2, \dots, 16\}$. Rotationally

invariant spin operators are constructed by taking scalar products of the Pauli spin matrices with independent vectors. If $\vec{P}, \vec{K}, \vec{N}$ are three linearly independent unit vectors constructed from \vec{k} and \vec{k}' then the Pauli matrices for each particle can be replaced by the rotationally invariant spin operators

$$\sigma'_\mu{}^i = (\sigma_0^i, \quad \vec{\sigma}^i \cdot \vec{P}, \quad \vec{\sigma}^i \cdot \vec{K}, \quad \vec{\sigma}^i \cdot \vec{N}), \quad (7.1)$$

where

$$\sigma_\mu^i = (\sigma_0^i, \quad \sigma_1^i, \quad \sigma_2^i, \quad \sigma_3^i). \quad (7.2)$$

Tensor products of these spin operators for particle 1 and particle 2 give a set of sixteen rotationally invariant operators that can be used to expand any two-particle spin operator (also called spin momentum operators) represented in the $\frac{1}{2} \otimes \frac{1}{2}$ space. These spin operators are

$$\begin{aligned} & 1 \\ & (\vec{\sigma}_2 \cdot \vec{P}) \\ & (\vec{\sigma}_2 \cdot \vec{K}) \\ & (\vec{\sigma}_2 \cdot \vec{N}) \\ & (\vec{\sigma}_1 \cdot \vec{P}) \\ & (\vec{\sigma}_1 \cdot \vec{P})(\vec{\sigma}_2 \cdot \vec{P}) \\ & (\vec{\sigma}_1 \cdot \vec{P})(\vec{\sigma}_2 \cdot \vec{K}) \\ & (\vec{\sigma}_1 \cdot \vec{P})(\vec{\sigma}_2 \cdot \vec{N}) \\ & (\vec{\sigma}_1 \cdot \vec{K}) \\ & (\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{P}) \\ & (\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{K}) \\ & (\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{N}) \\ & (\vec{\sigma}_1 \cdot \vec{N}) \\ & (\vec{\sigma}_1 \cdot \vec{N})(\vec{\sigma}_2 \cdot \vec{P}) \\ & (\vec{\sigma}_1 \cdot \vec{N})(\vec{\sigma}_2 \cdot \vec{K}) \\ & (\vec{\sigma}_1 \cdot \vec{N})(\vec{\sigma}_2 \cdot \vec{N}). \end{aligned} \quad (7.3)$$

The sixteen operators form the basis for the expansion of a spin-dependent nucleon-nucleon given by (7.4)

$$\mathbf{V}(\vec{k}, \vec{k}') = \sum_{i=1}^{16} v_i(k, k', \hat{k} \cdot \hat{k}') w_i(\vec{k}, \vec{k}'), \quad (7.4)$$

where v_i and w_i are the i^{th} expansion coefficient function and the rotationally invariant spin operator. As discussed in chapter 2 the potential $\mathbf{V}(\vec{k}, \vec{k}')$ also preserves time-reversal and space-reflection symmetry ,

$$T^{-1} \mathbf{V} T = \mathbf{V} \implies T^{-1} v_i w_i T = v_i w_i, \quad (7.5)$$

$$P^{-1} \mathbf{V} P = \mathbf{V} \implies P^{-1} v_i w_i P = v_i w_i, \quad (7.6)$$

where T and P are the time-reversal and space-reflection operators. Those products, $v_i w_i$ in (7.4) that preserve time-reversal and space-reflection symmetry are selected for the basis. The product of $v_i w_i$ is invariant with respect to space-reflection and time-reversal if both terms v_i and w_i are even (or odd). The symmetry of the spin operator w_i and coefficient of expansion v_i are determined by three linearly independent vectors that define the scattering geometry. These three vectors are constructed from initial and final momentum vectors \vec{k} and \vec{k}' . The isospin invariance of the potential adds particle exchange symmetry to the existing list of symmetry conditions. These conditions are used to reduce the number of basis elements that expand the nucleon-nucleon potential from sixteen to six.

It is useful to chose three linearly independent vectors of the form \vec{A}, \vec{B} and $\vec{A} \times \vec{B}$. For this choice of three vectors a scalar that preserves the space-reflection symmetry is necessarily a scalar product of a pseudo-vector ($\vec{A} \times \vec{B}$) and a vector (\vec{A}) or (\vec{B}). This scalar product is always zero by geometry. A space-reflection odd expansion coefficient is a pseudo-scalar and is always zero. This leaves time-reversal odd basis elements as the only allowed symmetry odd basis elements.

In order to retain only those basis elements that preserve symmetry transformations, a maximal set of spin operators w_i that are even with respect to time-reversal and

space-reflection are initially selected. The additional time-odd symmetry coefficient-operator pairs are extracted by investigating the nucleon-nucleon potential.

7.3 Type I

This section uses the three linearly independent vectors (2.46) to construct the basis. The elements of the basis (7.3) can be classified by their symmetry transformation properties under time-reversal and space-reflection. This is listed in Table[7.1]. The ones that are symmetric with respect to space-reflection and time-reversal symmetry are given a value of 1 and those that do not have these symmetries are given a value of 0. As discussed in the earlier section, only the basis elements that are symmetric in time-reversal and space-reflection are retained. The time-odd symmetry basis elements are later extracted from the nucleon-nucleon potential. Five of these operators are even with respect to space-reflection and time-reversal. These operators are present in the list (2.50). The following 4×4 matrix representation is used to express these basis elements

σ_{1x} :

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

σ_{1y} :

$$\begin{pmatrix} 0 & (-1)i & 0 & 0 \\ (1)i & 0 & 0 & 0 \\ 0 & 0 & 0 & (-1)i \\ 0 & 0 & (1)i & 0 \end{pmatrix}$$

Operators vs Symmetry	
Operator	Invariance(time and space-reflection)
1	1
$((\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{K})$	0
$((\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{Q})$	1
$((\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{N})$	0
$((\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{K}))$	1
$((\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{Q}))$	0
$((\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{N}))$	0
$((\vec{\sigma}_1 \cdot \vec{Q})(\vec{\sigma}_2 \cdot \vec{K}))$	0
$((\vec{\sigma}_1 \cdot \vec{Q})(\vec{\sigma}_2 \cdot \vec{Q}))$	1
$((\vec{\sigma}_1 \cdot \vec{Q})(\vec{\sigma}_2 \cdot \vec{N}))$	0
$((\vec{\sigma}_1 \cdot \vec{N})(\vec{\sigma}_2 \cdot \vec{K}))$	0
$((\vec{\sigma}_1 \cdot \vec{N})(\vec{\sigma}_2 \cdot \vec{Q}))$	0
$((\vec{\sigma}_1 \cdot \vec{N})(\vec{\sigma}_2 \cdot \vec{N}))$	1

Table 7.1: Total symmetry (time-reversal and space-reflection of spin operators).

$$\sigma_{1z}: \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

$$\sigma_{2x}: \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

$$\sigma_{2y}: \begin{pmatrix} 0 & 0 & (-1)i & 0 \\ 0 & 0 & 0 & (-1)i \\ (1)i & 0 & 0 & 0 \\ 0 & (1)i & 0 & 0 \end{pmatrix}$$

$$\sigma_{2z}: \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

In this representation the time-even, parity-even spin operators are

$$w_1 = ((\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{N}) :$$

$$\begin{pmatrix} 2N_z & N_x + (-N_y)i & N_x + (-N_y)i & 0 \\ N_x + (N_y)i & 0 & 0 & N_x + (-N_y)i \\ N_x + (N_y)i & 0 & 0 & N_x + (-N_y)i \\ 0 & N_x + (N_y)i & N_x + (N_y)i & -2N_z \end{pmatrix} \quad (7.7)$$

$$w_2 = ((\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{K})) :$$

$$\begin{pmatrix} K_z^2 & K_x K_z + (-K_z K_y)i & K_x K_z + (-K_z K_y)i & K_x^2 - K_y^2 + (-2K_x K_y)i \\ K_x K_z + (K_z K_y)i & -K_z^2 & K_x^2 + K_y^2 & -K_x K_z + (K_z K_y)i \\ K_x K_z + (K_z K_y)i & K_x^2 + K_y^2 & -K_z^2 & -K_x K_z + (K_z K_y)i \\ K_x^2 - K_y^2 + (2K_x K_y)i & -K_x K_z + (-K_z K_y)i & -K_x K_z + (-K_z K_y)i & K_z^2 \end{pmatrix} \quad (7.8)$$

$$w_3 = ((\vec{\sigma}_1 \cdot \vec{N})(\vec{\sigma}_2 \cdot \vec{N})) :$$

$$\begin{pmatrix} N_z^2 & N_x N_z + (-N_y N_z)i & N_x N_z + (-N_y N_z)i & -N_y^2 + N_x^2 + (-2N_y N_x)i \\ N_x N_z + (N_y N_z)i & -N_z^2 & N_y^2 + N_x^2 & -N_x N_z + (N_y N_z)i \\ N_x N_z + (N_y N_z)i & N_y^2 + N_x^2 & -N_z^2 & -N_x N_z + (N_y N_z)i \\ -N_y^2 + N_x^2 + (2N_y N_x)i & -N_x N_z + (-N_y N_z)i & -N_x N_z + (-N_y N_z)i & N_z^2 \end{pmatrix} \quad (7.9)$$

$$w_4 = ((\vec{\sigma}_1 \cdot \vec{P})(\vec{\sigma}_2 \cdot \vec{P})) :$$

$$\begin{pmatrix} P_z^2 & P_x P_z + (-P_y P_z)i & P_x P_z + (-P_y P_z)i & -P_y^2 + P_x^2 + (-2P_y P_x)i \\ P_x P_z + (P_y P_z)i & -P_z^2 & P_y^2 + P_x^2 & -P_x P_z + (P_y P_z)i \\ P_x P_z + (P_y P_z)i & P_y^2 + P_x^2 & -P_z^2 & -P_x P_z + (P_y P_z)i \\ -P_y^2 + P_x^2 + (2P_y P_x)i & -P_x P_z + (-P_y P_z)i & -P_x P_z + (-P_y P_z)i & P_z^2 \end{pmatrix} \quad (7.10)$$

$$w_5 = 1 \quad (7.11)$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The operator $\vec{\sigma}_1 \cdot \vec{\sigma}_2$ is present in the tensor operator of the nucleon-nucleon interaction. To extract the time-odd operator and the corresponding coefficient of expansion this spin operator of the potential is investigated next.

7.3.1 Time-odd operator and the basis

Even though the time-odd operators are present in (7.1) the symmetry conditions of the nucleon-nucleon potential are met only if the expansion coefficient functions are also time-odd. The time-odd operators are obtained from the spin-spin operator $\sigma_1 \cdot \sigma_2$. $\vec{\sigma}_1 \cdot \vec{\sigma}_2$ is expanded in the basis (7.3) associated with the vectors \vec{K} , \vec{P} and \vec{N} . The result is

$$\begin{aligned} \vec{\sigma}_1 \cdot \vec{\sigma}_2 = & \frac{(\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{K}) + (\vec{\sigma}_1 \cdot \vec{P})(\vec{\sigma}_2 \cdot \vec{P})}{(1 - \vec{K} \cdot \vec{P})^2} + (\vec{\sigma}_1 \cdot \vec{N})(\vec{\sigma}_2 \cdot \vec{N}) \\ & - \frac{(\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{P})\{(\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{K}) + (\vec{\sigma}_1 \cdot \vec{P})(\vec{\sigma}_2 \cdot \vec{P})\}(\vec{K} \cdot \vec{P})^2}{(1 - \vec{K} \cdot \vec{P})^2} \\ & - \frac{(\vec{K} \cdot \vec{P})\{(\sigma_1 \cdot \vec{K})(\sigma_2 \cdot \vec{P}) + (\sigma_1 \cdot \vec{P})(\sigma_2 \cdot \vec{K})\}}{(1 - \vec{K} \cdot \vec{P})^2} + \frac{(\vec{K} \cdot \vec{P})^3\{(\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{P}) + (\vec{\sigma}_1 \cdot \vec{P})(\vec{\sigma}_2 \cdot \vec{K})\}}{(1 - \vec{K} \cdot \vec{P})^2}. \end{aligned} \quad (7.12)$$

In the above expression the expansion of the spin-spin interaction $\sigma_1 \cdot \sigma_2$ includes the linear operators $(\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{P})$ and $(\vec{\sigma}_1 \cdot \vec{P})(\vec{\sigma}_2 \cdot \vec{K})$. These operators are odd under time-reversal. These operators can appear in the expansion for the potential provided the coefficient function is also time-odd, as is the case in the above equation. While there are two time-odd operators, they are related by particle exchange-symmetry, so they always appear in exchange symmetric combinations. The time-odd scalar coefficients are proportional to $|k^2| - |k'^2|$ and hence the coefficient vanishes on shell.

7.3.2 Conclusion of **Type I**

Of the sixteen basis elements, only six have the required symmetry properties that can be used to expand nucleon-nucleon potentials. Five of the elements are invariant under time-reversal and space inversion transformations. The sixth is symmetry-odd with respect to time-reversal and symmetric with respect to space inversion. The basis elements are

$$\begin{aligned}
& (\vec{\sigma}_1 \cdot \vec{K} \vec{\sigma}_2 \cdot \vec{P}) + (\vec{\sigma}_1 \cdot \vec{P} \vec{\sigma}_2 \cdot \vec{K}) \\
& j(\vec{\sigma}_1 + \vec{\sigma}_2) \vec{N} \\
& (\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{K}) \\
& (\vec{\sigma}_1 \cdot \vec{N})(\vec{\sigma}_2 \cdot \vec{N}) \\
& (\vec{\sigma}_1 \cdot \vec{P})(\vec{\sigma}_2 \cdot \vec{P}) \\
& 1.
\end{aligned} \tag{7.13}$$

The matrix \mathbf{A} in this basis is

$$\mathbf{A} = \begin{pmatrix} 8(\vec{K} \cdot \vec{K})(\vec{P} \cdot \vec{P}) + 8(\vec{P} \cdot \vec{K})^2 & 0 & 8(\vec{K} \cdot \vec{K})(\vec{P} \cdot \vec{K}) & 0 & 8(\vec{P} \cdot \vec{K})(\vec{P} \cdot \vec{P}) & 0 \\ 0 & -8(\vec{N} \cdot \vec{N}) & 0 & 0 & 0 & 0 \\ 8(\vec{K} \cdot \vec{K})(\vec{P} \cdot \vec{K}) & 0 & 4(\vec{K} \cdot \vec{K})^2 & 0 & 4(\vec{P} \cdot \vec{K})^2 & 0 \\ 0 & 0 & 0 & 4(\vec{N} \cdot \vec{N})^2 & 0 & 0 \\ 8(\vec{P} \cdot \vec{K})(\vec{P} \cdot \vec{P}) & 0 & 4(\vec{P} \cdot \vec{K})^2 & 0 & 4(\vec{P} \cdot \vec{P})^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 \end{pmatrix} \tag{7.14}$$

The determinant of the matrix is computed as

$$\begin{aligned}
\det|A| &= 49152(\vec{K} \cdot \vec{K})^2(\vec{N} \cdot \vec{N})^3(\vec{P} \cdot \vec{K})^2(\vec{P} \cdot \vec{P})^2 \\
&\quad - 49152(\vec{K} \cdot \vec{K})(\vec{N} \cdot \vec{N})^3(\vec{P} \cdot \vec{K})^4(\vec{P} \cdot \vec{P}) - 16384(\vec{K} \cdot \vec{K})^3(\vec{N} \cdot \vec{N})^3(\vec{P} \cdot \vec{P})^3 \\
&\quad + 16384(\vec{N} \cdot \vec{N})^3(\vec{P} \cdot \vec{K})^6.
\end{aligned} \tag{7.15}$$

On on shell $\vec{K} \cdot \vec{P} = 0$ and the determinant reduces to

$$\det|A| = -16384(\vec{K} \cdot \vec{K})^3(\vec{N} \cdot \vec{N})^3(\vec{P} \cdot \vec{P})^3. \quad (7.16)$$

which is non zero at on shell. This shows that this basis has the same number of elements on shell. However, at the on shell point the coefficient of expansion of the time-odd operator is zero resulting in 5 operators for the on shell condition. The next section describes with a different basis derived from three orthogonal vectors.

7.4 Orthogonal vectors -Type II

A basis of spin operators using three orthogonal vectors is constructed.

$$\begin{aligned} \vec{K} &= \vec{k} - \vec{k}' \\ \vec{Q} &= (\vec{k} + \vec{k}') \times \vec{K} \\ \vec{N} &= (\vec{K} \times \vec{Q}). \end{aligned} \quad (7.17)$$

The vectors are not normalized for sake of convenience. For simplicity we use the abstract terms \vec{K}, \vec{Q} and \vec{N} . The identities

$$\begin{aligned} \vec{K} \cdot \vec{Q} &= 0, \quad \vec{K} \cdot \vec{N} = 0 \\ \vec{Q} \cdot \vec{k}' &= \vec{Q} \cdot \vec{k} = 0 \\ \vec{N} \cdot \vec{k} &= \vec{N} \cdot \vec{k}' \end{aligned} \quad (7.18)$$

are used in the rest of the discussion. The time and space-reflection symmetry properties of the vectors are given in Table[7.2].

For this choice of three linearly independent vectors the basis elements that are symmetric with respect to time-reversal and space-reflection symmetry properties are

$$\begin{aligned} w_1 &= j(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{Q} \\ w_2 &= (\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{K}) \\ w_3 &= (\vec{\sigma}_1 \cdot \vec{N})(\vec{\sigma}_2 \cdot \vec{N}) \\ w_4 &= (\vec{\sigma}_1 \cdot \vec{Q})(\vec{\sigma}_2 \cdot \vec{Q}) \\ w_5 &= 1. \end{aligned} \quad (7.19)$$

Symmetry properties of three Vectors		
Vector	Time	Space-Reflection
K	1	-1
Q	-1	1
N	-1	-1

Table 7.2: Effect of time and space-reflection operators on vectors.

7.4.1 Time-odd basis elements

As explained before basis elements that are symmtery odd with respect to time-reversal are extracted by investigating the nucleon-nucleon potential. The spin operator

$$((\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{k})((\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{k}') \quad (7.20)$$

is expanded in terms of the basis listed in Table [7.3].

$$\begin{aligned}
((\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{k})((\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{k}') &= 2 \frac{(\vec{K} \cdot \vec{\sigma}_1)(\vec{K} \cdot \vec{\sigma}_2)(\vec{k} \cdot \vec{K})(\vec{k}' \cdot \vec{K})}{(\vec{K} \cdot \vec{K})^2} + 2 \frac{(\vec{N} \cdot \vec{\sigma}_1)(\vec{N} \cdot \vec{\sigma}_2)(\vec{k} \cdot \vec{N})(\vec{k}' \cdot \vec{N})}{(\vec{N} \cdot \vec{N})^2} \\
&+ \frac{(\vec{K} \cdot \vec{\sigma}_1)(\vec{N} \cdot \vec{\sigma}_1)(\vec{k} \cdot \vec{K})(\vec{k}' \cdot \vec{N})}{(\vec{K} \cdot \vec{K})(\vec{N} \cdot \vec{N})} + \frac{(\vec{K} \cdot \vec{\sigma}_1)(\vec{N} \cdot \vec{\sigma}_1)(\vec{k} \cdot \vec{N})(\vec{k}' \cdot \vec{K})}{(\vec{K} \cdot \vec{K})(\vec{N} \cdot \vec{N})} + \frac{(\vec{K} \cdot \vec{\sigma}_1)(\vec{N} \cdot \vec{\sigma}_2)(\vec{k} \cdot \vec{K})(\vec{k}' \cdot \vec{N})}{(\vec{K} \cdot \vec{K})(\vec{N} \cdot \vec{N})} \\
&+ \frac{(\vec{K} \cdot \vec{\sigma}_1)(\vec{N} \cdot \vec{\sigma}_2)(\vec{k} \cdot \vec{N})(\vec{k}' \cdot \vec{K})}{(\vec{K} \cdot \vec{K})(\vec{N} \cdot \vec{N})} + \frac{(\vec{K} \cdot \vec{\sigma}_2)(\vec{N} \cdot \vec{\sigma}_1)(\vec{k} \cdot \vec{K})(\vec{k}' \cdot \vec{N})}{(\vec{K} \cdot \vec{K})(\vec{N} \cdot \vec{N})} + \frac{(\vec{K} \cdot \vec{\sigma}_2)(\vec{N} \cdot \vec{\sigma}_1)(\vec{k} \cdot \vec{N})(\vec{k}' \cdot \vec{K})}{(\vec{K} \cdot \vec{K})(\vec{N} \cdot \vec{N})} \\
&+ \frac{(\vec{K} \cdot \vec{\sigma}_2)(\vec{N} \cdot \vec{\sigma}_2)(\vec{k} \cdot \vec{K})(\vec{k}' \cdot \vec{N})}{(\vec{K} \cdot \vec{K})(\vec{N} \cdot \vec{N})} + \frac{(\vec{K} \cdot \vec{\sigma}_2)(\vec{N} \cdot \vec{\sigma}_2)(\vec{k} \cdot \vec{N})(\vec{k}' \cdot \vec{K})}{(\vec{K} \cdot \vec{K})(\vec{N} \cdot \vec{N})} + \frac{(\vec{K} \cdot \vec{\sigma}_1)^2(\vec{k} \cdot \vec{K})(\vec{k}' \cdot \vec{K})}{(\vec{K} \cdot \vec{K})^2} \\
&+ \frac{(\vec{K} \cdot \vec{\sigma}_2)^2(\vec{k} \cdot \vec{K})(\vec{k}' \cdot \vec{K})}{(\vec{K} \cdot \vec{K})^2} + \frac{(\vec{N} \cdot \vec{\sigma}_1)^2(\vec{k} \cdot \vec{N})(\vec{k}' \cdot \vec{N})}{(\vec{N} \cdot \vec{N})^2} + \frac{(\vec{N} \cdot \vec{\sigma}_2)^2(\vec{k} \cdot \vec{N})(\vec{k}' \cdot \vec{N})}{(\vec{N} \cdot \vec{N})^2}, \quad (7.21)
\end{aligned}$$

$$\begin{aligned}
((\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{k})((\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{k}') &= 2 \frac{(\vec{K} \cdot \vec{\sigma}_1)(\vec{K} \cdot \vec{\sigma}_2)(\vec{k} \cdot \vec{K})(\vec{k}' \cdot \vec{K})}{(\vec{K} \cdot \vec{K})^2} + 2 \frac{(\vec{N} \cdot \vec{\sigma}_1)(\vec{N} \cdot \vec{\sigma}_2)(\vec{k} \cdot \vec{N})(\vec{k}' \cdot \vec{N})}{(\vec{N} \cdot \vec{N})^2} \\
&+ \frac{(\vec{K} \cdot \vec{\sigma}_1)(\vec{N} \cdot \vec{\sigma}_1)(\vec{k} \cdot \vec{K})(\vec{k}' \cdot \vec{N})}{(\vec{K} \cdot \vec{K})(\vec{N} \cdot \vec{N})} + \frac{(\vec{K} \cdot \vec{\sigma}_1)(\vec{N} \cdot \vec{\sigma}_1)(\vec{k} \cdot \vec{N})(\vec{k}' \cdot \vec{K})}{(\vec{K} \cdot \vec{K})(\vec{N} \cdot \vec{N})} + \frac{(\vec{K} \cdot \vec{\sigma}_1)(\vec{N} \cdot \vec{\sigma}_2)(\vec{k} \cdot \vec{K})(\vec{k}' \cdot \vec{N})}{(\vec{K} \cdot \vec{K})(\vec{N} \cdot \vec{N})}
\end{aligned}$$

$$\begin{aligned}
& +\{w_1\}\left\{\frac{(\vec{k}\cdot\vec{K})(\vec{k}'\cdot\vec{N})}{(\vec{K}\cdot\vec{K})(\vec{N}\cdot\vec{N})}+\frac{(\vec{k}\cdot\vec{N})(\vec{k}'\cdot\vec{K})}{(\vec{K}\cdot\vec{K})(\vec{N}\cdot\vec{N})}\right\}+w_5\{2(\vec{k}\cdot\vec{K})(\vec{k}'\cdot\vec{K})+2(\vec{k}\cdot\vec{N})(\vec{k}'\cdot\vec{N})\} \\
& +\{(\vec{K}\cdot\vec{\sigma}_1)(\vec{N}\cdot\vec{\sigma}_2)+(\vec{K}\cdot\vec{\sigma}_2)(\vec{N}\cdot\vec{\sigma}_1)\}\frac{(\vec{k}\cdot\vec{K})(\vec{k}'\cdot\vec{N})+(\vec{k}'\cdot\vec{K})(\vec{k}\cdot\vec{N})}{(\vec{K}\cdot\vec{K})(\vec{N}\cdot\vec{N})}
\end{aligned} \tag{7.28}$$

Here w_1, w_2, w_4, w_5 are the basis elements that are symmetric with respect to time-reversal and space inversion (7.19). In addition, the spin operator $\{(\vec{K}\cdot\vec{\sigma}_1)(\vec{N}\cdot\vec{\sigma}_2)+(\vec{K}\cdot\vec{\sigma}_2)(\vec{N}\cdot\vec{\sigma}_1)\}$ is required for the expansion of $((\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{k})(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{k}'$. This operator is a linear combination of two basis elements that are symmetry-odd under time-reversal and symmetry even under space inversion. Due to particle exchange symmetry of the nucleon-nucleon potential, the two time-odd elements are combined. The expansion coefficient of this operator (7.29) is a scalar function with the same symmetry properties

$$\frac{(\vec{k}\cdot\vec{K})(\vec{k}'\cdot\vec{N})+(\vec{k}'\cdot\vec{K})(\vec{k}\cdot\vec{N})}{(\vec{K}\cdot\vec{K})(\vec{N}\cdot\vec{N})} \tag{7.29}$$

The product of the basis element $\{(\vec{K}\cdot\vec{\sigma}_1)(\vec{N}\cdot\vec{\sigma}_2)+(\vec{K}\cdot\vec{\sigma}_2)(\vec{N}\cdot\vec{\sigma}_1)\}$ and its coefficient of expansion (7.29) is symmetric with respect to space-reflection and time-reversal. The coefficient of expansion for the time-odd operator is given by

$$\begin{aligned}
(\vec{k}\cdot\vec{K})(\vec{k}'\cdot\vec{N})+(\vec{k}'\cdot\vec{K})(\vec{k}\cdot\vec{N}) &= -2(\vec{k}\cdot\vec{k})^2(\vec{k}'\cdot\vec{k}')-2(\vec{k}\cdot\vec{k}')^{(2)}(\vec{k}'\cdot\vec{k}') \\
&+2(\vec{k}\cdot\vec{k})(\vec{k}\cdot\vec{k}')^{(2)}+2(\vec{k}\cdot\vec{k})(\vec{k}'\cdot\vec{k}')^2.
\end{aligned} \tag{7.30}$$

For $|k'|=|k|$ (the on shell point)

$$(\vec{k}\cdot\vec{K})(\vec{k}'\cdot\vec{N})+(\vec{k}'\cdot\vec{K})(\vec{k}\cdot\vec{N})=0. \tag{7.31}$$

Equation (7.31) shows that similar to the coefficient of time-odd operator in Type I the time-odd expansion coefficients vanish on shell.

7.4.2 Conclusion for **Type II**

Orthogonal vectors $\vec{N}, \vec{K}, \vec{Q}$ were used to construct a rotationally invariant basis (7.3). This basis is used to expand the nucleon-nucleon potential (particle exchange symmetry is also included). Only those elements of the basis that preserve the symmetry conditions of the nucleon-nucleon potential are retained. This condition is met by

1. five basis elements that are symmetric with respect to time-reversal and space invariance,
2. the sixth basis element and its expansion coefficient is symmetry-odd with respect to time-reversal and and symmetry even with respect to space-reflection,
3. the expansion coefficient function of the sixth element vanishes on shell.

The basis elements are

$$\begin{aligned}
& (\vec{K} \cdot \vec{\sigma}_1)(\vec{N} \cdot \vec{\sigma}_2) + (\vec{K} \cdot \vec{\sigma}_2)(\vec{N} \cdot \vec{\sigma}_1) \\
& \quad j(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{Q} \\
& \quad (\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{K}) \\
& \quad (\vec{\sigma}_1 \cdot \vec{N})(\vec{\sigma}_2 \cdot \vec{N}) \\
& \quad (\vec{\sigma}_1 \cdot \vec{Q})(\vec{\sigma}_2 \cdot \vec{Q}) \\
& \quad 1
\end{aligned} \tag{7.32}$$

The matrix \mathbf{A} for this basis is given by

$$\mathbf{A} = \begin{pmatrix} 8(\vec{K} \cdot \vec{K})(\vec{N} \cdot \vec{N}) & 0 & 0 & 0 & 0 & 0 \\ 0 & -8(\vec{Q} \cdot \vec{Q}) & 0 & 0 & 0 & 0 \\ 0 & 0 & 4(\vec{K} \cdot \vec{K})^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4(\vec{N} \cdot \vec{N})^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4(\vec{Q} \cdot \vec{Q})^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 \end{pmatrix}$$

Operators vs Symmetry	
Operator	Invariance(time and space-reflection)
1	1
$((\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{K})$	0
$((\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{Q})$	1
$((\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{N})$	0
$((\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{K}))$	1
$((\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{Q}))$	0
$((\vec{\sigma}_1 \cdot \vec{K})(\vec{\sigma}_2 \cdot \vec{N}))$	0
$((\vec{\sigma}_1 \cdot \vec{Q})(\vec{\sigma}_2 \cdot \vec{K}))$	0
$((\vec{\sigma}_1 \cdot \vec{Q})(\vec{\sigma}_2 \cdot \vec{Q}))$	1
$((\vec{\sigma}_1 \cdot \vec{Q})(\vec{\sigma}_2 \cdot \vec{N}))$	0
$((\vec{\sigma}_1 \cdot \vec{N})(\vec{\sigma}_2 \cdot \vec{K}))$	0
$((\vec{\sigma}_1 \cdot \vec{N})(\vec{\sigma}_2 \cdot \vec{Q}))$	0
$((\vec{\sigma}_1 \cdot \vec{N})(\vec{\sigma}_2 \cdot \vec{N}))$	1

Table 7.3: Total symmetry (time-reversal and space-reflection) of spin operators.

7.5 Conclusion

This chapter introduces a general representation for constructing a basis of operators that can expand a nucleon-nucleon potential. For any linearly independent three vectors (the third is perpendicular to the other two) the elements of the basis can be constructed Table[7.3]. From this general representation the following procedure can be used to obtain the elements that can be used to expand a nucleon-nucleon potential which is symmetric with respect to time-reversal, rotations, space-reflection and particle exchange symmetries.

1. The number of basis elements (or spin momentum operators) are six.
2. Five of them conserve time-reversal invariance and space-reflection symmetry.
3. The sixth is symmetry-odd with respect to time-reversal and symmetric with respect to space-reflection.
4. The time-odd expansion coefficient vanish on shell. At the on shell point the number of basis elements required are five.

The investigation used the algebraic system developed in this thesis .

CHAPTER 8

SUMMARY AND OUTLOOK

A summary of the modest contributions made by this thesis to the field of scattering of nucleon-nucleon systems using the vector variable approach are discussed in this chapter.

This thesis adopts an alternate formalism of the vector variable approach. The formalism develops a systematic way of choosing the linearly independent and rotationally invariant operators. The formalism does not restrict itself to only operators that are invariant under time and parity but also includes the time-odd operators. Chapter 7 shows that one time odd operator is needed to make the matrix A in (2.56) non-singular at the on-shell point. The coefficient of this time-odd operator vanishes on-shell, fulfilling the condition that an on-shell transition amplitude is expanded in terms of five linearly independent operators. The formalism is formulated in momentum-space since the ultimate goal is to use this vector variable approach to solve relativistic three-body systems that are readily treated in momentum space.

The discussion turns towards the nucleon-nucleon potentials that can be used as input for this formalism. The configuration space Argonne V18 nucleon-nucleon potential was used as an input for this formalism. The analytical Fourier transform and an efficient method to compute the Argonne V18 potential in momentum space are discussed in Chapter 3 and Chapter 4. A Chebyshev approximation of the Fourier-Bessel integrals listed in Chapter 4 (4.4) achieve the goal of a computationally efficient representation of the Argonne V18 potential in momentum space.

The next discussion is the treatment of spin degrees of freedom. As explained in Chapter 2 the spin traces are analytically computed. This results in large-scale algebraic expressions that need to be reduced to scalar functions of vector variables. Apart from dealing with the spin algebraic systems, the expansion of the nucleon-nucleon potential in a basis of six linearly independent operators may also require algebraic

manipulations to extract the scalar coefficient for basis operators. To compute these algebraic expressions and reduce them to scalar functions of vector variables, an algebraic system that can automate the computation and reduction of large scale expressions becomes indispensable for the implementation of the vector variable formalism. To meet this goal, Chapter 5 discusses the mathematical framework that allows the possibility of an automated algebraic reduction system.

Having developed the tools, the algebraic reduction system and the efficient computation of the Fourier transform, are tested in a realistic calculation of the deuteron binding energy and bound-state wave functions. The automated algebraic reduction mechanism is used to treat the spin degrees of freedom. The test was successful and Chapter 6 discusses the results of the calculation. The cpu time utilized by the Chebyshev approximated momentum space Argonne V18 potential is efficient by a factor of 2800 compared to the direct numeric computation of the momentum space Argonne V18. The success of the bound state calculation is the first milestone in the development of the tools and techniques for the vector variable approach.

With the successful computation of the deuteron binding energy and wave functions, the next step is to calculate the scattering observables with the Argonne V18 potential as input. At this point the discussion comes to an end with the hope that a successful calculation of the scattering observables for two nucleons with the tools and methods explained in this thesis will lead the way towards applying the vector variable formalism to relativistic three-body systems.

APPENDIX A: TRIPLE TRACES USING AUTOMATED ALGEBRAIC SYSTEM

The computer output of the results for the input choice of vectors [13] and in 14 is given below. The trace of operators given equation (2.55) in Chapter 2 is shown in the next few pages.

Matrix $A =$

$$\begin{pmatrix} 8(\vec{N} \cdot \vec{N}) & 0 & 0 & 0 & 0 & 0 \\ 0 & 4(\vec{K} \cdot \vec{K})^2 & 0 & 4(\vec{K} \cdot \vec{P})^2 & 4(\vec{K} \cdot \vec{K}) & 0 \\ 0 & 0 & 4(\vec{N} \cdot \vec{N})^2 & 0 & 4(\vec{N} \cdot \vec{N}) & 0 \\ 0 & 4(\vec{K} \cdot \vec{P})^2 & 0 & 4(\vec{P} \cdot \vec{P})^2 & 4(\vec{P} \cdot \vec{P}) & 0 \\ 0 & 4(\vec{K} \cdot \vec{K}) & 4(\vec{N} \cdot \vec{N}) & 4(\vec{P} \cdot \vec{P}) & 12 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 \end{pmatrix}$$

<i>operator</i>	<i>Trace</i>
$((\vec{\sigma}_1 \cdot \vec{P}_1)(\vec{\sigma}_2 \cdot \vec{P}_1))((\vec{\sigma}_1 \cdot \vec{N}_2)(\vec{\sigma}_2 \cdot \vec{N}_2))$	$4(\vec{P}_1 \cdot \vec{N}_2)^2$
$((\vec{\sigma}_1 \cdot \vec{P}_1)(\vec{\sigma}_2 \cdot \vec{P}_1))((\vec{\sigma}_1 \cdot \vec{P}_2)(\vec{\sigma}_2 \cdot \vec{P}_2))$	$4(\vec{P}_1 \cdot \vec{P}_2)^2$
$((\vec{\sigma}_1 \cdot \vec{P}_1)(\vec{\sigma}_2 \cdot \vec{P}_1))(\vec{\sigma}_1 \cdot \vec{\sigma}_2)$	$4(\vec{P}_1 \cdot \vec{P}_1)$
$((\vec{\sigma}_1 \cdot \vec{P}_1)(\vec{\sigma}_2 \cdot \vec{P}_1))$	0
$(\vec{\sigma}_1 \cdot \vec{\sigma}_2)((\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{N}_2)$	0
$(\vec{\sigma}_1 \cdot \vec{\sigma}_2)((\vec{\sigma}_1 \cdot \vec{K}_2)(\vec{\sigma}_2 \cdot \vec{K}_2))$	$4(\vec{K}_2 \cdot \vec{K}_2)$
$(\vec{\sigma}_1 \cdot \vec{\sigma}_2)((\vec{\sigma}_1 \cdot \vec{N}_2)(\vec{\sigma}_2 \cdot \vec{N}_2))$	$4(\vec{N}_2 \cdot \vec{N}_2)$
$(\vec{\sigma}_1 \cdot \vec{\sigma}_2)((\vec{\sigma}_1 \cdot \vec{P}_2)(\vec{\sigma}_2 \cdot \vec{P}_2))$	$4(\vec{P}_2 \cdot \vec{P}_2)$
$(\vec{\sigma}_1 \cdot \vec{\sigma}_2)(\vec{\sigma}_1 \cdot \vec{\sigma}_2)$	12
$(\vec{\sigma}_1 \cdot \vec{\sigma}_2)$	0
$((\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \vec{N}_2)$	0
$((\vec{\sigma}_1 \cdot \vec{K}_2)(\vec{\sigma}_2 \cdot \vec{K}_2))$	0
$((\vec{\sigma}_1 \cdot \vec{N}_2)(\vec{\sigma}_2 \cdot \vec{N}_2))$	0
$((\vec{\sigma}_1 \cdot \vec{P}_2)(\vec{\sigma}_2 \cdot \vec{P}_2))$	0
$(\vec{\sigma}_1 \cdot \vec{\sigma}_2)$	0
1	4

REFERENCES

- [1] J.J.Sakurai, “Modern quantum mechanics,”
- [2] L.D.Faddeev *Sov.Phys,JETP*, vol. 12, p. 1014, 1961.
- [3] W. Glockle, H. Witala, D. Hber, H. Kamada, and J.Golak *Phys.Rep*, vol. 274, p. 107, 1996.
- [4] H. Liu, C. Elster, and W. Glockle, “Three-Body Scattering without Partial Waves,” *AIP Conf. Proc.*, vol. 768, pp. 430–432, 2005.
- [5] F. Coester, “Scattering theory for relativistic particles,” *Helv. Phys. Acta*, vol. 38, pp. 7–23, 1965.
- [6] W. N. Polyzou, T. Lin, C. Elster, and W. Glockle, “Three-body scattering in Poincaré invariant quantum mechanics,” *Few Body Syst.*, vol. 44, pp. 287–289, 2008.
- [7] C. Elster, T. Lin, W. N. Polyzou, and W. Glockle, “Poincare Invariant Three-Body Scattering,” *Few Body Syst.*, vol. 45, pp. 157–160, 2009.
- [8] V. G. J. S. R. B. Wiringa and R. Schiavilla *Phys. Rev.*, vol. C51, 1995.
- [9] R. Machleidt, “High-precision, charge-dependent bonn nucleon-nucleon potential,” *Phys. Rev. C*, vol. 63, p. 024001, Jan 2001.
- [10] V. G. J. Stoks, R. A. M. Klomp, M. C. M. Rentmeester, and J. J. de Swart, “Partial-wave analysis of all nucleon-nucleon scattering data below 350 mev,” *Phys. Rev. C*, vol. 48, pp. 792–815, Aug 1993.
- [11] F. Coester, S. C. Pieper, and F. J. D. Serduke, “Relativistic effects in phenomenological nucleon-nucleon potentials and nuclear matter,” *Phys. Rev.*, vol. C11, pp. 1–18, 1975.
- [12] B. D. Keister and W. N. Polyzou, “Quantitative Relativistic Effects in the Three-Nucleon Problem,” *Phys. Rev.*, vol. C73, p. 014005, 2006.
- [13] J. Golak *et al.*, “The Two-Nucleon System in Three Dimensions,” 2010.
- [14] C. Elster, J. H. . Thomas, and W. Gloeckle, “Two-body T-matrices without angular-momentum decomposition: Energy and momentum dependences,” *Few Body Syst.*, vol. 24, pp. 55–79, 1998.
- [15] R. A. Malfliet and J. A. Tjon *Nucl.Phys.*, vol. A127, 1969.
- [16] W. Gloeckle, *The Quantum Mechanical Few-Body Problem*. Springer-Verlag, Berlin-Heidelberg, 1983.
- [17] J. L. Friar, G. L. Payne, W. Glockle, D. Huber, and H. Witala, “Benchmark solutions for n-d breakup amplitudes,” *Phys. Rev.*, vol. C51, pp. 2356–2359, 1995.

- [18] H. Liu, C. Elster, and W. Gloeckle, “Three-Body Elastic and Inelastic Scattering at Intermediate Energies,” *Nucl. Phys.*, vol. A790, pp. 262–266, 2007.
- [19] E. P. Wigner, “On Unitary Representations of the Inhomogeneous Lorentz Group,” *Annals Math.*, vol. 40, pp. 149–204, 1939.
- [20] M. Rodriguez-Gallardo, A. Deltuva, E. Cravo, R. Crespo, and A. C. Fonseca, “Two-body scattering without angular-momentum decomposition,” *Phys. Rev.*, vol. C78, p. 034602, 2008.
- [21] I. Fachruddin, C. Elster, and W. Gloeckle, “Nucleon-Nucleon Scattering in a Three Dimensional Approach,” *Phys. Rev.*, vol. C62, p. 044002, 2000.
- [22] I. Fachruddin and I. Abdulrahman, “Scattering of Spin-Zero and Spin-Half Particles in Momentum-Helicity Basis,” 2007.
- [23] S. Bayegan, M. A. Shalchi, and M. R. Hadizadeh, “The three dimensional calculations of NN bound and scattering states with chiral potential up to N3LO,” *Phys. Rev.*, vol. C79, p. 057001, 2009.
- [24] W. Gloeckle *et al.*, “A New Treatment of 2N and 3N Bound States in Three Dimensions,” *Few Body Syst.*, vol. 47, pp. 25–38, 2010.
- [25] L. Wolfenstein, “Possible Triple-Scattering Experiments,” *Phys. Rev.*, vol. 96, pp. 1654–1658, 1954.
- [26] R. Machleidt *Adv. Nucl. Phys.*, vol. 19, 1989.
- [27] E. Epelbaum *Prog. Part. Nucl. Phys.*, vol. 57, 2006.
- [28] GINAC. Accessed November 10, 2010. Available at <http://www.ginac.de/>.
- [29] J. M. Abramowitz, “Handbook of Mathematical Functions.”
- [30] Gnu scientific library numerical library for C and C++ programmers. Accessed November 10, 2010. Available at <http://www.gnu.org/software/gsl/>.
- [31] I. Fachruddin, C. Elster, and W. Gloeckle, “New Forms of Deuteron Equations and Wave Function Representations,” *Phys. Rev.*, vol. C63, p. 054003, 2001.
- [32] LAPACK (Linear algebra package) version 3. Accessed November 10, 2010. Available at <http://www.netlib.org/lapack/>.
- [33] Deuteron wave functions of Argonne V18. Accessed November 10, 2010. Available at <http://www.phy.anl.gov/theory/research/av18/deut.wf/>.