8-1994

A Procedure for G-Matrix Calculation from a Momentum Space Potential

Zhaohui Gao Busche
Western Michigan University

A PROCEDURE FOR G-MATRIX CALCULATION FROM A MOMENTUM SPACE POTENTIAL

by

Zhaohui Gao Busche

A Thesis
Submitted to the
Faculty of The Graduate College
in partial fulfillment of the
requirements for the
Degree of Master of Arts
Department of Physics

Western Michigan University
Kalamazoo, Michigan
August 1994

ACKNOWLEDGMENTS

A special thanks is due to my committee chairman, Dr. Dean Halderson, and the other members of my committee, Dr. Alvin Rosenthal and Dr. Paul Pancella. Their technical guidance and writing style suggestions made this a successful and rewarding thesis.

Finally, I appreciated the suggestions and support of my husband, Michael Busche, in the final stage of my thesis.

Zhaohui Gao Busche

A PROCEDURE FOR G-MATRIX CALCULATION FROM A MOMENTUM SPACE POTENTIAL

Zhaohui Gao Busche, M.A.

Western Michigan University, 1994

In this work a numerical procedure was found to calculate the G-matrix in momentum space with a momentum space potential. The integral equation for the G-matrix was solved by conversion to a matrix equation. Two numerical integral methods, three-point Simpson method and Gaussian integral method, were employed in this process to determine the more efficient method.

The resulting G-matrix in momentum space was Fourier transformed into coordinate space. This was compared with the results of the G-matrix calculated from coordinate space directly as well as the results from solving the Bethe-Goldstone equation. A 2% accuracy was achieved with both the three-point Simpson and Gaussian methods, but the Gaussian method proved to be three times more efficient.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

CHAPTER I

INTRODUCTION

A principal objective of nuclear physics has been to understand the interaction between nucleons (N). With the discovery of additional baryons, this objective has been extended to understanding the interaction between baryons in general. A great deal of research has, for example, been performed on the lambda-nucleon (ΛN) interaction.

Theoretical and phenomenological models have been developed to represent these interactions. The parameters of these models are fixed by fits to baryon-nucleon scattering data. Here baryon can be a nucleon, a hyperon, etc. The off-shell behavior of these models is tested by comparing the calculated properties of a nucleus containing the baryon to experimental values for the same system. Hypernuclei, created by adding a strange baryon to a nucleus, are examples of such system.

The properties of a nucleus containing a baryon are determined by calculating an effective baryon-nucleon interaction. Early forms of the baryon-nucleon potential were given in coordinate space, and procedures were developed to calculate the effective interaction from

these potentials. More recent versions are given in momentum space. The purpose of this present work is to test a procedure by which one can calculate the effective baryon-nucleon interaction for finite nuclei with a momentum space potential.

There are several approaches which can be used to calculate the effective baryon-nucleon interaction. The Green's function method of statistical mechanics, invented by Martin and Schwinger, has been applied by Puff (1961). Lee and Yang's theory of quantum statistics has been developed and applied by Mohling (1962) to numerous problems. There is also Jastrow's method of correlated basis functions, a variational method, in which the trial wave function is taken to be a Slater determinant multiplied by a product of two-particle correlation functions --one correlation function for each pair of particles. The modified Jastrow's method has been developed by Feenberg, Clark, et al. (Washington University, St. Louis) (1966). Further development of this method has recently been done by Pandharipanda Smith and Lomnitz-Adler(1981). The method employed in this work is the Brueckner-Goldstone expansion (Day, 1967).

The G-matrix is the basic quantity in Brueckner-Goldstone theory. It represents the effective interaction described above. It satisfies,

$$G = v - v\frac{Q}{e}v + v\frac{Q}{e}v\frac{Q}{e}v - + \ldots\ldots . \qquad (1.1)$$

or the equivalent integral equation,

$$G = v - v\frac{Q}{e}G . \qquad (1.2)$$

Here v is the realistic baryon-nucleon interaction which fits scattering data. The two-particle operators, Q and e, are defined by the equations,

$$Q|rs\rangle = \begin{cases} |rs\rangle & \text{if } k_r > k_f \text{; and } k_s > k_f \qquad (1.3a) \\ 0 & \text{otherwise} \qquad (1.3b) \end{cases}$$

$$e|rs\rangle = (E_r + E_s - W)\,|rs\rangle \qquad (1.4)$$

where:

1. $|rs\rangle = \Phi_{rs} = \phi_r \phi_s$

2. Φ_{rs} is the unperturbed two-particle wave function.

3. ϕ_r, ϕ_s are the unperturbed one-particle wave functions.

4. k_f is the Fermi momentum.

5. k_r, k_s are the momenta of the states r and s.

6. W is the starting energy of the two particles.

7. E_r, E_s are the energies of the states r and s respectively.

When one calculates G-matrix elements for nuclear matter, the unperturbed one-particle wave functions are plane wave functions. For the calculation of G-matrix elements in finite nuclei, the unperturbed one-particle wave functions are usually taken to be harmonic-oscillator wave functions. The Pauli operator Q annihilates a two-particle state unless both particles are above the Fermi sea, and e gives the energy difference between the two-particle state and the starting energy. G always operates on two-particle wave function Φ_{rs}. It is not only a function of the two states r and s, but also a function of the starting energy W.

When the interaction, υ, is provided in coordinate space, the G-matrix elements can be calculated by defining a correlated wave function and solving the resulting differential equation. However, when υ is only given in momentum space, it is not always possible to obtain a convenient analytic form in coordinate space. Therefore a different procedure to calculate the G-matrix in momentum space directly is required. The procedure employed in this work is due to Brown, Jackson and Kuo (1969) and was developed for solving the Lipmann Schwinger equation.

First, this procedure is employed to calculate G-matrix elements in momentum space directly with a simple momentum space potential. Then the G-matrix is transformed from the momentum space into the coordinate space. Finally, to determine whether the method is correct, the Fourier transform of this simple potential is used to calculate the G-matrix elements in the coordinate space. If same results are achieved, then the procedure to calculate the G-matrix in momentum space is correct.

The simple baryon-nucleon interaction, used in this work, is in the form,

$$\upsilon = \frac{\upsilon_0 \exp(-r/r_0)}{r/r_0} . \qquad (1.5)$$

Although this is not a realistic potential, its Fourier transform is easy to calculate. Two integration methods, the three-point Simpson and the Gaussian integral method, are used to calculate the momentum integration. For different potential ranges (r_0), the range and step-size for υ-matrix elements calculation, and the range and step-size for the momentum space integral are tested.

CHAPTER II

G-MATRIX ELEMENTS IN COORDINATE SPACE

In section one, the differential G-matrix equation which is used for the calculation in coordinate space is derived. In section two, the form of the test simple potential is defined; and the numerical method used for the G-matrix calculation is reviewed.

The G-matrix Formalism for Finite Nuclei In Coordinate Space

The G-matrix has been defined above,

$$G = v - v\frac{Q}{e}G . \tag{2.1}$$

A matrix element of above equation gives,

$$\langle \Phi_{pq} | G | \Phi_{rs} \rangle = \langle \Phi_{pq} | v - v\frac{Q}{e}G | \Phi_{rs} \rangle . \tag{2.2}$$

Φ_{pq} and Φ_{rs} are the unperturbed two-particle wave functions, and

$$\Phi_{pq} = \phi_p \phi_q , \tag{2.3a}$$

$$\Phi_{rs} = \phi_r \phi_s . \tag{2.3b}$$

where ϕ_p, ϕ_q, ϕ_r and ϕ_s are the unperturbed one-particle wave functions.

For finite nuclei the unperturbed one-particle wave functions are harmonic-oscillator wave functions(HOWFs) (Baranger 1962), $|n_1 l_1\rangle$ and $|n_1 l_1\rangle$. HOWFs are known to be good approximations to radial wave functions, especially in light nuclei. Of course, the tails of the wave functions are not well represented by HOWFs, but the tails are not important for many nuclear properties. All of the recent sophisticated Brueckner calculations of finite nuclei with modern two-particle potentials have utilized HOWFs.

For finite nuclei, the solutions for the G-matrix elements in equation (2.2) are carried out in the reference spectrum approximation (Bethe, Brandow, Petschek, 1963). Therefore the Pauli operator Q is replaced by 1, however, the unperturbed one-particle Hamiltonian H_0 taken to be the harmonic-oscillator Hamiltonian,

$$H_0 = \mathbf{p}^2/2m + 1/2\, m\Omega^2 \mathbf{r}^2 . \qquad (2.4)$$

The two-particle Hamiltonian H can be separated neatly into a center-of-mass part and a relative part,

$$H = H_{c.m.} + H_r . \qquad (2.5)$$

Specifically,

$$H = \mathbf{p}_1^2/2m_1 + \mathbf{p}_2^2/2m_2 + \frac{1}{2}m_1\Omega^2\mathbf{r}_1^2 + \frac{1}{2}m_2\Omega^2\mathbf{r}_2^2$$

$$= \mathbf{P}^2/2M + \mathbf{p}^2/2\mu + 1/2M\Omega^2\mathbf{R}^2 + 1/2\mu\Omega^2\mathbf{r}^2 . \qquad (2.6)$$

Then it can be identified by,

$$H_{c.m.} = \mathbf{P}^2/2M + 1/2M\Omega^2\mathbf{R}^2 , \qquad (2.7)$$

and,

$$H_r = \mathbf{p}^2/2\mu + 1/2\mu\Omega^2\mathbf{r}^2 , \qquad (2.8)$$

where,

$$\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2 , \qquad \mathbf{p} = \mu\left(\frac{\mathbf{p}_1}{m_1} - \frac{\mathbf{p}_2}{m_2}\right), \qquad M = m_1 + m_2 ,$$

$$\mathbf{R} = \left(\frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}\right), \qquad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 , \qquad \mu = \frac{m_1 m_2}{m_1 + m_2} . \qquad (2.9)$$

Here $\mathbf{P}$ is the total momentum, $\mathbf{p}$ is relative momentum, $\mathbf{R}$ is the center-of-mass coordinate, $\mathbf{r}$ is relative coordinate, M is the total mass, μ is the reduced mass.

Since the two-particle potential is independent of the center-of-mass variables, $H_{c.m.}$, in the denominator of equation (2.1), commutes with everything and can be considered as just a number. If one defines,

$$W_r = W - H_{c.m.} , \qquad (2.10)$$

then equation (2.1) can be rewritten as

$$G_r = v - v\frac{1}{e}G_r$$

$$= v - v\frac{1}{H - W}G_r$$

$$= v - v\frac{1}{H_r - W_r}G_r . \qquad (2.11)$$

Here G_r means the G-matrix with reference spectrum approximation.

The unperturbed two-particle state for finite nuclei can be expanded in terms of products of a function of the center-of-mass coordinate and a function of the relative coordinate. Here the well known Talmi(1952)-Moshinsky(1959) transformation is used,

$$|n_1 l_1 n_2 l_2, \lambda\mu>$$

$$= \sum M\lambda(n_1 l_1 n_2 l_2; NLnl)|NLnl, \lambda\mu>, \qquad (2.12)$$

in which $\lambda\mu$ are the total orbital angular momentum quantum numbers. The Moshinsky brackets $M\lambda$ have been thoroughly studied and tabulated (Body, Moshinsky 1960; Baranger, Davies, 1966; Kumar,1966). Hence $\langle pq|G_r(W_r)|rs\rangle$ is reduced to a linear combination of matrix elements of the type,

$$< \mathrm{NLn}l,\lambda;\mathrm{ST};\mathrm{J}\left|\mathrm{G_r}(\mathrm{W_r})\right|\mathrm{N'L'n'}l',\lambda';\mathrm{ST};\mathrm{J} >, \qquad (2.13)$$

where J is the total angular momentum of the relative motion, obtained by adding the total orbital angular momentum λ and the total spin S. The angular momenta can be recoupled to the form,

$$\langle \mathrm{NLn}l;\mathrm{ST};\mathrm{JJ};\mathrm{J}\left|\mathrm{G_r}(\mathrm{W_r})\right|\mathrm{N'L'n'}l';\mathrm{ST};\mathrm{JJ};\mathrm{J}\rangle \qquad (2.14)$$

where JJ is the total angular momentum of the relative motion, obtained by adding l and S. Then J is obtained by adding L and JJ.

Since $\mathrm{G_r}(\mathrm{W_r})$ commutes with $\mathrm{H_{c.m.}}$, the matrix elements will be diagonal in N and L, so that:

$$\langle \mathrm{NLnl};\mathrm{ST};\mathrm{JJ};\mathrm{J}\left|\mathrm{G_r}(\mathrm{W_r})\right|\mathrm{N'L'n'l'};\mathrm{ST};\mathrm{JJ};\mathrm{J}\rangle$$

$$= \delta_{\mathrm{NN'}}\cdot\delta_{\mathrm{LL'}}\cdot\delta_{\mathrm{JJ'}}\cdot\langle \mathrm{nl};\mathrm{ST};\mathrm{JJ}\left|\mathrm{G_r}(\mathrm{W_r})\right|\mathrm{n'l'};\mathrm{ST};\mathrm{JJ}\rangle \qquad (2.15)$$

Similarly, matrix elements of the operators in equation (2.11) becomes

$$\langle \mathrm{nl}\left|\mathrm{G_r}(\mathrm{W_r})\right|\mathrm{n'l'}\rangle$$

$$= \langle \mathrm{nl}\left|\upsilon - \upsilon/(\mathrm{H_r} - \mathrm{W_r})\,\mathrm{G_r}(\mathrm{W_r})\right|\mathrm{n'l'}\rangle . \qquad (2.16)$$

Thus the problem is reduced to the calculation of $\mathrm{G_r}(\mathrm{W_r})$ between relative wave functions.

The equation(2.16) can be rewritten as:

$$\left[1-\upsilon\frac{1}{W_r-H_r}\right]G_r=\upsilon \tag{2.17}$$

$$G_r=\left[1-\upsilon\frac{1}{W_r-H_r}\right]^{-1}\upsilon \tag{2.18}$$

where:

$$H_r=\mathbf{p}^2/2\mu+1/2\mu\Omega^2\mathbf{r}^2$$

$$=(h/2\pi)^2/2\mu\nabla^2 r+1/2\mu\Omega^2\mathbf{r}^2\,. \tag{2.19}$$

Equation (2.18) may be considered a matrix equation which, if the matrix elements of υ are finite, may be solved for the G-matrix elements.

In order to compare the results from this method with the momentum calculation, it is necessary to use the kinetic energy $T=\mathbf{p}^2/2\mu$, instead of total energy H_r. Such a substitution is, in fact, common. A justification is developed in the Appendix A. The substitution gives a new G-matrix

$$G_r'=\upsilon-\frac{\upsilon}{T-W_r}G_r' \tag{2.20}$$

It is $G_r^{'}$, which is compared by using two different methods. Equation (2.20) is used to solve G-matrix elements in coordinate space. More clearly, equation (2.20) can be written as

$$G_r^{'} = \left[1 - \frac{\upsilon}{W_r - T}\right]^{-1} \upsilon. \qquad (2.21)$$

The technique to solve this equation is introduced in next section.

Procedure for Numerical Calculation

When $H_r = (h/2\pi)^2/2\mu\nabla^2_r + 1/2\mu\Omega^2 r^2$ operates on the harmonic-oscillator function $|nl\rangle$, it gives

$$\langle nl|H_r|n'l'\rangle = \delta_{nn'}\delta_{ll'}(h/2\pi)\omega(2n+l+3/2) \qquad (2.22)$$

If only kinetic energy is considered, then

$$\langle nl|T|n'l'\rangle$$

$$= \delta_{nn'}\delta_{ll'}(h/2\pi)\omega(2n+l+3/2) - \langle nl|1/2\mu\Omega^2 r^2|n'l'\rangle \qquad (2.23)$$

From Bertsch (1972), one has

$$\langle nl|r^2|nl\rangle = 1/\nu(2n+l+3/2), \text{ and} \qquad (2.24)$$

$$\langle nl|r^2|n+1l\rangle = -1/\nu[(n+1)(n+l+3/2)]^{1/2} \qquad (2.25)$$

where, $v = \mu\Omega/(h/2\pi)$.

Then,

$$\langle nl|1/2\mu\Omega^2 r^2|nl\rangle = 1/2(h/2\pi)\Omega(2n+l+3/2) \qquad (2.26)$$

$$\langle nl|1/2\mu\Omega^2 r^2|n+1l\rangle = -1/2(h/2\pi)\Omega[(n+1)(2n+l+3/2)]^{1/2} \qquad (2.27)$$

and

$$\langle nl|T|n'l'\rangle$$

$$= \begin{cases} 1/2(h/2\pi)\Omega(2n+l+3/2) & \text{if } n = n' \qquad (2.28) \\ 1/2(h/2\pi)\Omega[(n+1)(n+l+3/2)]^{1/2} & \text{if } n' = n+1 \qquad (2.29) \end{cases}$$

Now equation (2.21) can be treated as a matrix equation in a harmonic oscillator basis, and the $\dot{v}$-matrix is given by,

$$\langle nl|\dot{v}|n'l'\rangle. \qquad (2.30)$$

The operator D is defined as W_r-T and its matrix elements are

$$\langle nl|D|n'l'\rangle \equiv \langle nl|W_r - T|n'l'\rangle. \qquad (2.31)$$

which can be calculated by using the results of equation (2.28) and (2.29). So,

$$G = [1 - \upsilon D^{-1}]^{-1}\upsilon \qquad (2.32)$$

Equation (2.32) is used to calculate the G-matrix in the harmonic-oscillator basis. Here υ, the coordinate interaction, is

$$\upsilon = \upsilon_0 \exp(-r/r_0)/(r/r_0). \qquad (2.33)$$

Even though this interaction is not realistic in that it does not have the spin dependence or radial flexibility necessary to fit the baryon-nucleon phase shifts, it is easy to test the method by using a simple interaction.

CHAPTER III

G-MATRIX ELEMENTS IN MOMENTUM SPACE

In section one of this chapter, the appropriate G-matrix equation in nuclear matter is developed. Since nuclear matter calculations employ the plane-wave basis, which has conserved total linear momentum, then the G-matrix derivation in momentum space is the same as in nuclear matter. Also, the derivation in nuclear matter is simpler and easier to understand. In section two, the υ-matrix and the G-matrix in momentum space are defined. Then the G-matrix equation obtained from section one is further derived so that the G-matrix numerical calculation in momentum space can be accomplished. In section three, the G-matrix in momentum space is transformed into coordinate space. In section four, a numerical method to solve the differential G-matrix equation in momentum space is reviewed.

The G-matrix Formalism for Nuclear Matter

The unperturbed two-particle wave function for nuclear matter is $\Phi_{rs}(r_1,r_2)=\phi_r(r_1)\phi_s(r_2)$. ϕ_r and ϕ_s, the unperturbed one-particle wave functions, are plane wave

functions. This means that the two-particle wave function depends only trivially on the center-of-mass coordinate of the two interacting particles. This trivial dependence on the center-of-mass coordinate can be separated from the more important dependence of the relative position vector. So the unperturbed two-particle wave function can be written as,

$$\Phi_{rs}(\mathbf{r}_1,\mathbf{r}_2) = \Omega^{-1}\exp(i\mathbf{k}_r\cdot\mathbf{r}_1)\exp(i\mathbf{k}_s\cdot\mathbf{r}_2)$$

$$= \Omega^{-1}\exp(i\mathbf{K}_{rs}\cdot\mathbf{R})\exp(i\mathbf{k}_{rs}\cdot\mathbf{r}), \qquad (3.1)$$

Where

$$\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}, \qquad \mathbf{K}_{rs} = \mathbf{k}_r + \mathbf{k}_s ,$$

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 , \qquad \mathbf{k}_{rs} = \mu\left(\frac{\mathbf{k}_r}{m_1} - \frac{\mathbf{k}_s}{m_2}\right),$$

$$M = m_1 + m_2 , \qquad \mu = \frac{m_1 m_2}{m_1 + m_2} . \qquad (3.2)$$

Here Ω is the volume, $\mathbf{R}$ is the center-of-mass coordinate of the two interacting particles, $\mathbf{r}$ is the relative position vector, $\mathbf{K}_{rs}$ is the total momentum, $\mathbf{k}_{rs}$ is the relative momentum, $\mathbf{k}_r$, $\mathbf{k}_s$ are the individual momentum vectors, μ is the reduced mass, M is the total mass.

In terms of the total and relative momenta, the

operators e and Q can be written as

$$e|rs\rangle = [E(\mathbf{k}_r) + E(\mathbf{k}_s) - W]|rs\rangle$$

$$= e(\mathbf{k}_{rs}, \mathbf{K}_{rs})|rs\rangle , \qquad (3.3)$$

$$Q|rs\rangle = \begin{cases} |rs\rangle & \text{If } \mathbf{k}_r > \mathbf{k}_f \text{ and } \mathbf{k}_s > \mathbf{k}_f \\ 0 & \text{otherwise} \end{cases}$$

$$= Q(\mathbf{k}_{rs}, \mathbf{K}_{rs})|rs\rangle . \qquad (3.4)$$

Equation (2.2) for nuclear matter can be solved in the reference spectrum approximation by setting $Q=1$, and the single particle Hamiltonian taken as $\mathbf{p}^2/2m$ plus a constant. Then only the energy denominator, e, depends of $\mathbf{K}_{rs}$, and e is diagonal in this variable. The center-of-mass dependence can be integrated out and one obtains the relative G-matrix equation,

$$\langle \mathbf{k}_{pq}|G|\mathbf{k}_{rs}\rangle = \langle \mathbf{k}_{pq}|v - v/e(\mathbf{K}_{pq})G|\mathbf{k}_{rs}\rangle \qquad (3.5)$$

Introducing the unit operator

$$1 = \sum_n |n\rangle\langle n| = \frac{1}{(2\pi)^3}\int e^{-i\mathbf{k}\cdot\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}'} d^3\mathbf{k} , \qquad (3.6)$$

equation (3.5) can also be written as

$$\langle \mathbf{k}_{pq}|G|\mathbf{k}_{rs}\rangle = \langle \mathbf{k}_{pq}|\upsilon - \upsilon/e(\mathbf{K}_{pq})G|\mathbf{k}_{rs}\rangle$$

$$= \langle \mathbf{k}_{pq}|\upsilon|\mathbf{k}_{rs}\rangle - \frac{1}{(2\pi)^3}\int \frac{1}{e(\mathbf{k},\mathbf{K})} d^3\mathbf{k} \langle \mathbf{k}_{pq}|\upsilon|\mathbf{k}\rangle \langle \mathbf{k}|G|\mathbf{k}_{rs}\rangle . \qquad (3.7)$$

equation (3.7) is used to determine the G-matrix in momentum space in the following section.

Differential G-matrix Equation in Momentum Space

The G-matrix equation (3.7) is obtained in nuclear matter, and it can be used in momentum space. One re-writes equation (3.7) as,

$$\langle \mathbf{k}|G|\mathbf{k}'\rangle$$

$$= \langle \mathbf{k}|G|\mathbf{k}'\rangle - \frac{1}{(2\pi)^3}\int \frac{1}{e(\mathbf{q},\mathbf{K})} d^3\mathbf{q} \langle \mathbf{k}|\upsilon|\mathbf{q}\rangle \langle \mathbf{q}|G|\mathbf{k}'\rangle . \qquad (3.8)$$

This equation must be solved for the simple potential in equation (2.33). One begins with Fourier transformation for the υ-matrix,

$$\int \exp(-i\mathbf{k}\cdot\mathbf{r})\upsilon(r)\exp(-i\mathbf{k}'\cdot\mathbf{r})\, d^3\mathbf{r}$$

$$= \int \sum_{lm} (4\pi)\, j_l(kr)\, Y_{lm}(\mathbf{k})\, Y^*_{lm}(\mathbf{r})\, i^l \upsilon(r)$$

$$\times \sum_{l'm'} (4\pi)\, j_{l'}(k'r)\, Y^*_{l'm'}(\mathbf{k}')\, Y_{l'm'}(\mathbf{r})\, i^{l'} d^3\mathbf{r}$$

$$= (16\pi^2)\sum_{lm}\int j_l(k'r)\, j_l(kr)\upsilon(r)\, r^2 dr\, Y_{lm}(\mathbf{k})\, Y^*_{lm}(\mathbf{k}')\, i^{2l}$$

$$= (16\pi^2)\sum_{l}[Y_l(\mathbf{k})\cdot Y_l(\mathbf{k}')]\int j_l(k'r)\, j_l(kr)\upsilon(r)\, i^{2l} r^2 dr \qquad (3.9)$$

where the spherical harmonics are used to satisfy,

$$\int Y^*_{lm}(\mathbf{r})\, Y_{l'm'}(\mathbf{r})\, d\Omega_r = \delta_{l'l}\delta_{m'm} \qquad (3.10)$$

$$\sum_{l} Y_l(\mathbf{k})\cdot Y_l(\mathbf{k}') = \sum_{lm} Y_{lm}(\mathbf{k})\, Y^*_{lm}(\mathbf{k}') . \qquad (3.11)$$

Then the υ-matrix in momentum space is defined by,

$$\upsilon_l(k,k') = \int j_l(k'r)\, j_l(kr)\upsilon(r)\, i^{2l} r^2 dr . \qquad (3.12)$$

Substitution of Fourier transformations into equation (3.8) gives,

$$(16\pi^2)\sum_{l}[Y_l(\mathbf{k})\cdot Y_l(\mathbf{k}')]G_l(k,k')$$

$$= (16\pi^2)\sum_{l}[Y_l(\mathbf{k})\cdot Y_l(\mathbf{k}')]\upsilon_l(k,k')$$

$$-\frac{1}{(2\pi)^3}\int d^3q \frac{1}{e(\mathbf{q},\mathbf{K})}\times\left[(16\pi^2)\sum_{l'} Y_{l'}(\mathbf{k})\cdot Y_{l'}(\mathbf{q})\,\upsilon_{l'}(k,q)\right]$$

$$\times\left[(16\pi^2)\sum_{l''} Y_{l''}(\mathbf{q})\cdot Y_{l''}(\mathbf{k}')G_{l''}(q,k')\right]$$

$$= (16\pi^2)\sum_{l}[Y_l(\mathbf{k})\cdot Y_l(\mathbf{k}')]\upsilon_l(k,k')$$

$$-\frac{2}{\pi}\int q^2 dq \frac{1}{e(q,K)} \times \left[(16\pi^2) \sum_{l'} Y_{l'}(\hat{k}) \cdot Y_{l'}(\hat{k}') v_{l'}(k,q) G_{l'}(q,k') \right]. \quad (3.13)$$

Equation (3.13) can be simplified as,

$$G_l(k,k') = v_l(k,k') - \frac{2}{\pi}\int q^2 dq\, v_l(k,q) G_l(q,k') \frac{1}{e(q,K)}, \quad (3.14)$$

where,

$$\int \sum_{l'm'} Y_{l'm'}(\hat{k}) Y^*_{l'm'}(\hat{q}) \sum_{l''m''} Y_{l''m''}(\hat{q}) Y^*_{l''m''}(\hat{k}') d\Omega_q$$

$$= \delta_{l'l''}\delta_{m'm''} \sum_{l'm'} Y_{l'm'}(\hat{k}) Y^*_{l'm'}(\hat{k}') \quad (3.15)$$

has been used. The reference spectrum approximation is applied, and only the kinetic energy is employed in the energy denominator. This means that.

$$e(q,K) = \frac{q^2}{2\mu} - W_r, \quad (3.16)$$

Thus,

$$G^r_{rl}(k,k') = v_l(k,k') - \frac{2}{\pi}\int q^2 dq\, v_l(k,q) G^r_{rl}(q,k') \frac{1}{q^2/2\mu - W_r}. \quad (3.17)$$

Here $G^r_{rl}(k,k')$ represents the G-matrix element in momentum space with reference spectrum approximation and a kinetic

energy denominator. This is the equation used for the G-matrix calculations in momentum space. The specific numerical method is introduced in section four.

Transformation of G-matrix From Plane Wave to Harmonic-oscillator Basis

To compare the results from this method and the method introduced in Chapter II, $G'_{rl}(k,k')$ must be transformed into a harmonic-oscillator basis. The required transformation is,

$$G'_{rl}(n,n') = \int d^3\mathbf{r}\, \Phi^*_{nl}(\mathbf{r}) G'_{rl}(n,n',r) \Phi_{n'l}(\mathbf{r})$$

$$= \frac{1}{(2\pi)^3} \int \Psi^*_{nl}(\mathbf{k}) \exp(i\mathbf{k}\cdot\mathbf{r}) G'_{rl}(n,n',r)$$

$$\times \Psi_{n'l}(\mathbf{k}') \exp(-i\mathbf{k}'\cdot\mathbf{r})\, d^3\mathbf{r}\, d^3\mathbf{k}\, d^3\mathbf{k}'$$

$$= \frac{1}{(2\pi)^3} \int \Psi^*_{nl}(\mathbf{k})(16\pi^2) \sum_{lm} Y_{lm}(\mathbf{k})\, Y^*_{lm}(\mathbf{k}')$$

$$\times G'_{rl}(k,k') \Psi_{n'l}(\mathbf{k}')\, d^3\mathbf{k}\, d^3\mathbf{k}'$$

$$= \frac{2}{\pi} \int \psi^*_{nl}(\mathbf{k}) G'_{rl}(k,k') \psi_{n'l}(\mathbf{k}')\, k^2 k'^2\, dk\, dk', \qquad (3.18)$$

where:

$$\Psi_{n'l}(\mathbf{k}') = \psi_{n'l}(k')\, Y_{lm}(\mathbf{k}') . \qquad (3.19)$$

Ψ_{nl}, $\Psi_{n'l}$ are harmonic-oscillator wave functions in momentum space; ψ_{nl}, $\psi_{n'l}$ are radial part of harmonic-oscillator wave functions in momentum space. ψ_{nl} satisfies,

$$\psi_{nl}(k) = (-i)^l(-)^n \phi_{nl}(1/\alpha, k). \tag{3.20}$$

Here $\phi_{nl}(1/\alpha, k)$ is radial part of the harmonic-oscillator wave function in coordinate space with k replacing r and $1/\alpha$ replacing α.

Procedure for Numerical Calculations

For numerical calculations of the integral in equation (3.17) is replaced by a sum. Equation (3.17) yields,

$$G'_{rl}(k,k') = \upsilon_l(k,k') - \frac{2}{\pi}\sum_i q_i^2 \omega(i) \upsilon_l(k,q_i) G'_{rl}(q_i,k') \frac{1}{q_i^2/2\mu - W_r}. \tag{3.21}$$

where q_i and $\omega(i)$ are points and weights appropriate to the integration. Then $2/\pi q_i^2 w(i)/(q_i^2/2\mu - W_r)$ can be treated as a diagonal matrix D such that,

$$D_{ij} = \frac{2}{\pi} \frac{\delta_{ij} q_i^2 w(i)}{q_i^2/2\mu - W_r}. \tag{3.22}$$

Equation (3.21) can be treated as a matrix equation and written as:

$$G'_{rl}\begin{pmatrix} q_{11} & q_{12} & \cdots & q_{1k'} \\ q_{21} & q_{22} & \cdots & q_{2k'} \\ \cdots & \cdots & \cdots & \cdots \\ q_{k1} & q_{k2} & \cdots & q_{kk'} \end{pmatrix} = \upsilon_l \begin{pmatrix} q_{11} & q_{12} & \cdots & q_{1k'} \\ q_{21} & q_{22} & \cdots & q_{2k'} \\ \cdots & \cdots & \cdots & \cdots \\ q_{k1} & q_{k2} & \cdots & q_{kk'} \end{pmatrix} -$$

$$\upsilon_l \begin{pmatrix} q_{11} & q_{12} & \cdots & q_{1n} \\ q_{21} & q_{22} & \cdots & q_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ q_{k1} & q_{k2} & \cdots & q_{kn} \end{pmatrix} \times D \begin{pmatrix} D_{11} & & & \\ & D_{22} & & \\ & & & \\ & & & D_{nn} \end{pmatrix}$$

$$\times G'_{rl} \begin{pmatrix} q_{11} & q_{12} & \cdots & q_{1k'} \\ q_{21} & q_{22} & \cdots & q_{2k'} \\ \cdots & \cdots & \cdots & \cdots \\ q_{n1} & q_{n2} & \cdots & q_{nk'} \end{pmatrix} \qquad (3.23)$$

So,

$$G'_{rl} = \upsilon_l - \upsilon_l \times D \times G'_{rl}, \qquad (3.24)$$

$$G'_{rl}(1 + \upsilon_l \times D) = \upsilon_l, \text{ and} \qquad (3.25)$$

$$G'_{rl} = (1 + \upsilon_l \times D)^{-1} \upsilon_l . \qquad (3.26)$$

Equation (3.26) can be used to solve for the G-matrix in momentum space. Then by putting the results back into equation (3.26), the G-matrix elements in the harmonic oscillator basis can be obtained.

Equation (3.26) is solved by first calculating the υ-matrix with equation (3.12). Then the following two

different techniques are used to do the momentum integration for equation (3.17) or calculation of the D-matrix: (1) three-point Simpson(TPS), and (2) Gaussian integral method. The integration is done by using the three-point Simpson method first. The range and step-size for the momentum integral are tested. Then the Gaussian integral method is used. Since it is determined from the TPS method that the contribution from the integrand is mainly from a region less than $q=R_q$, the following transformation is used to calculate the D-matrix elements:

$$\omega_i = w_i R_q / 2 , \tag{3.27}$$

$$q_i = (R_q \times x_i + R_q)/2 . \tag{3.28}$$

Here w_i, x_i are standard tabulated Gaussian integral weights and points; the ω_i and q_i are the weights and points for the momentum integral for the matrix equation (3.21).

CHAPTER IV

RESULTS

The G-matrix obtained either by using equation (2.32), or equation (3.18) and (3.26), is dependent on (a) the starting energy, W_r, (b) the oscillator parameter α or $(h/2\pi)\Omega$, (c) the reduced mass μ, (d) the strength(v_0) of the simple potential, and the range (r_0) of the simple potential. In this work parameters, W_r, α, μ and v_0 are all fixed at typical values for light hypernuclei. The values are:

W_r = -10 Mev

$(h/2\pi)\Omega = [(h/2\pi)c]^2/[\mu c^2]*\alpha^2$, α = 0.5 fm,

μ = 509.7 Mev/c^2, which is the reduced mass of a nucleon and a lambda, and

v_0 = -40 Mev.

Because convergence of the integrals may depend on the range of the test potential, two different ranges, r_0 = 1.0 fm and r_0 = 0.5 fm are used to calculate G-matrix elements in both coordinate space and momentum space.

In order to calculate G-matrix elements in an harmonic-oscillator basis from a plane wave function basis, the following steps are used:

1. The υ-matrix elements are calculated in the plane wave basis from equation (3.12).

2. The D-matrix is calculated from equation (3.22).

3. The G-matrix in momentum space is obtained from equation (3.26).

4. Equation (3.18) is used to transform G-matrix elements from a plane wave function basis into an harmonic-oscillator basis.

In step 1, all the ranges and step-sizes for the υ-matrix element calculation are tested for r_0=1.0 fm and r_0=0.5 fm. The results for υ_l (k=0.1 fm^{-1}, k'=0.1 fm^{-1}) and υ_l(k=5 fm^{-1}, k'=5 fm^{-1}) (here l can be either 0 or 1) are shown in Tables 1-4. The results of this work, which employs a five-point Simpson algorithm, are checked by comparing to the trapezoid integral program which is available from the software package Speakeasy (Speakeasy Corp. 1978). The conclusion is that for this work a range of 15 fm and step-size of 0.1 fm for the υ-matrix elements integral are accurate to 0.01% for either r_0=1.0 fm, or r_0=0.5 fm; and for either l=0, or l=1.

Table 1

The Range and Step-size Test for υ-matrix Elements Integral at r_0=1.0 fm for l=0

Trapezoid Method*			
Range(fm)	Step-Size(fm)	$\upsilon_0(0.1,0.1)$	$\upsilon_0(5,5)$
15	0.1	39.19	1.812
15	0.05	39.21	1.838
15	0.01	39.22	1.846
15	0.005	39.22	1.846
20	0.1	39.19	1.812
20	0.05	39.21	1.838
20	0.01	39.22	1.846
Five Point Simpson Method**			
10	0.1	39.22	1.846

* Calculated with Speakeasy IV software.
** Calculated by the FORTRAN program written in this master's thesis.

Table 2

The Range and Step-size Test for υ-matrix Elements Integral at r_0=1.0 fm for l=1

Range(fm)	Step-Size(fm)	$\upsilon_{l}(0.1,0.1)$	$\upsilon_{l}(5,5)$
		Trapezoid Method*	
15	0.1	0.2563	1.083
15	0.05	0.2563	1.083
15	0.01	0.2563	1.083
20	0.1	0.2564	1.083
20	0.05	0.2564	1.083
20	0.01	0.2564	1.083
		Five Point Simpson Method**	
15	0.1	0.2563	1.083

* Calculated with Speakeasy IV software.
** Calculated by the FORTRAN program written in this master's thesis.

Table 3

The Range and Step-size Test for υ-matrix Elements Integral at r_0=0.5 fm for l=0

Range(fm)	Step-Size(fm)	$\upsilon_0(0.1,0.1)$	$\upsilon_0(5,5)$
Trapezoid Method*			
10	0.1	4.959	0.6349
10	0.05	4.971	0.6475
10	0.01	4.975	0.6515
15	0.1	4.959	0.6495
15	0.05	4.971	0.6475
15	0.01	4.975	0.6415
Five Point Simpson Method**			
10	0.1	4.975	0.6516

* Calculated with Speakeasy IV software.
** Calculated by the FORTRAN program written in this master's thesis.

Table 4

The Range and Step-size Test for υ-matrix Elements Integral at r_0=0.5 fm for l=1

Range(fm)	Step-Size(fm)	$\upsilon_{ll}(0.1,0.1)$	$\upsilon_{ll}(5,5)$
Trapezoid Method*			
10	0.1	0.008251	0.3038
10	0.05	0.008251	0.3038
15	0.1	0.008251	0.3038
Five Point Simpson Method**			
10	0.1	0.008251	0.3038

* Calculated with Speakeasy IV software.
** Calculated by the FORTRAN program written in this master's thesis.

In step 2, the D-matrix is constructed using the three-point Simpson method. Results for $G'_{n}(1,1)$ at different r_0 and different l are calculated and compared by using different ranges and step-sizes for the momentum integration of equation (3.17). Here $G'_{n}(1,1)$ is the G-matrix element in the harmonic-oscillator basis with n=1, n'=1. Results are shown in Table 5. It is found that an integral range of 10 fm^{-1} and step-size of 0.1 fm^{-1} gives at least 0.5% accuracy for the momentum integral for both values of r_0 and l.

Next, the D-matrix is calculated by using a Gaussian integral method. Then the following transformation is made,

$$\omega_i = w_i R_q / 2,$$

$$q_i = (R_q \times x_i + R_q)/2.$$

Here w_i, x_i are tabulated Gaussian integral weights and points; R_q is momentum integral range found from the Three Point Simpson method and is 10 fm^{-1}; the ω_i and q_i are the weights and points for the momentum integral for the matrix equation (3.21). The number of points required for the momentum integral of equation (3.17) are tested and results are shown in Table 5. It is very

Table 5

The Range And Step-size Test for
The Momentum Integral

(fm^{-1}) Range	(fm^{-1}) Points	r_0=1.0 fm $G'_{r0}(1,1)$	$G'_{r1}(1,1)$	r_0=0.5 fm $G'_{r0}(1,1)$	$G'_{r1}(1,1)$
Three Point Simpson Method					
5	25	8.15	1.72	1.18	0.157
5	50	8.16	1.71	1.18	0.157
5	100	8.15	1.71	1.18	0.157
10	50	8.20	1.72	1.18	0.157
10	100	8.22	1.71	1.18	0.157
10	200	8.22	1.71	1.18	0.157
15	150	8.22	1.71	1.18	0.157
Gaussian Integral Method					
10	48	8.22	1.71	1.18	0.157
10	32	8.22	1.71	1.18	0.157

clear that the Gaussian integral method is more efficient in that it only needs 32 points to do the momentum integral instead of the 100 points required by the three-point Simpson method.

Finally results of G-matrix element $G'_{rl}(1,1)$ at different potential ranges r_0 and different quantum numbers l are compared in Table 6 by using four different methods, that results in a 2% accuracy:

1. The procedure employed in this work with using the three-point Simpson method to do the momentum integral.

2. The procedure employed in this work with using the Gaussian integral method to do the momentum integral.

3. Calculating G-matrix elements in coordinate space directly.

4. Solving Bethe-Goldstone equation directly as described in Appendix B. (Only values for $G'_{r0}(1,1)$ and $G'_{r1}(1,1)$ at r_0=1.0 fm are provided in this case.)

Table 6

The Comparison of The Results From Four Methods

(fm^{-1}) Range	(fm^{-1}) Points	r_0=1.0 fm $G'_{r0}(1,1)$	$G'_{r1}(1,1)$	r_0=0.5 fm $G'_{r0}(1,1)$	$G'_{r1}(1,1)$
Three Point Simpson Method					
10	100	8.22	1.71	1.18	0.157
Gaussian Integral Method					
10	32	8.22	1.71	1.18	0.157
Coordinate Space Method					
/	/	8.07	1.71	1.17	0.157
Bethe-Goldstone Equation Method					
/	/	8.18	1.72	/	/

CHAPTER V

CONCLUSION

This work has demonstrated a procedure to calculate G-matrix elements of harmonic oscillator wave functions from a simple baryon-nucleon potential given in momentum space. Two numerical integration methods are employed to solve the integral equation, the three-point Simpson method and the Gaussian integral method. The range and step-size of the integration are tested. The Gaussian integral method is determined to be more efficient than the three-point Simpson method, in that it requires fewer than one-half the integration points for the same accuracy.

The results of $G'_n(1,1)$, the G-matrix element in the harmonic-oscillator basis with reference spectrum approximation applied and only a kinetic energy denominator, are compared by using four different methods:

1. The momentum space procedure employed in this work using the three-point Simpson method to do the momentum integral.

2. The procedure employed in this work using the Gaussian integral method to do the momentum integral.

3. Calculating G-matrix elements in coordinate space directly.

4. Direct integration of the Bethe-Goldstone equation.

Now that this work has demonstrated a method for calculating the baryon-baryon G-matrix for a model potential in momentum space, the method can be applied to realistic potentials. Future research should employ potentials such as the Bonn models A and B (Machleidt, Holinde, and Elster 1987). The resulting G-matrix elements in the harmonic oscillator basis can then be used to predict the properties of hypernuclei.

Appendix A

A Justification for Using T in the G-matrix Equation Instead of H

The main concern of this work is to test the method of calculating G-matrix elements in momentum space. The use of kinentic T instead of the total energy H_r does not influence this purpose. In fact it is reasonable to do this in binding energy calculations for finite nuclei. The Bethe-Goldstone theory is based on the Goldstone expansion(Brandow 1967), which is a linked-cluster perturbation series for the ground-state energy of a many body system. For a system of a certain number A of particles, which can be nucleons, or baryons, the Hamiltonian is the sum of the kinetic energies of all the particles plus the sum of the two-body interactions between them, i.e.,

$$H = \sum_{i=1}^{A} T_i + \sum_{i<j}^{A} v_{ij} = H_0 + H_1 . \qquad (A.1)$$

Equation (A.1) splits H into two parts. The unperturbed Hamiltonian is,

$$H_0 = \sum_{i}^{A} (T_i + U_i) . \qquad (A.2)$$

The perturbation is,

$$H_1 = \sum_{i<j}^{A} v_{ij} - \sum_{i=1}^{A} U_i \,. \qquad (A.3)$$

Here U is the single-particle potential. The introduction of U is intended to make numerical calculations easier. The final result should be independent of U. When the equation (1.1), or (1.2) is derived, the influence of U is not considered. Actually the consequence of U is small. However to be more accurate, the graph (Figure 1) of the second term of equation (1.1) should be replaced by a series of graphs (Figure 2) that include -U insertions. Then Q/e is replaced by the series,

$$\frac{Q}{e} - \frac{Q}{e}(-U)\frac{Q}{e} + \frac{Q}{e}(-U)\frac{Q}{e}(-U)\frac{Q}{e} - + \ldots$$

$$= \frac{Q}{e}\left[1 - (-U)\frac{Q}{e} + (-U)\frac{Q}{e}(-U)\frac{Q}{e} - + \ldots\ldots\right]$$

$$= \frac{Q}{e}\frac{1}{\left[1 + (-U)Q/e\right]}$$

$$= \frac{Q}{\left(e - eUQ/e\right)} \qquad (A.4)$$

After using the reference spectrum approximation, equation(A.4) becomes,

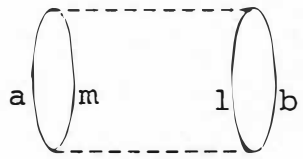

Figure 1. The Second Term of Equation(1.1) Without Considering -U Interaction

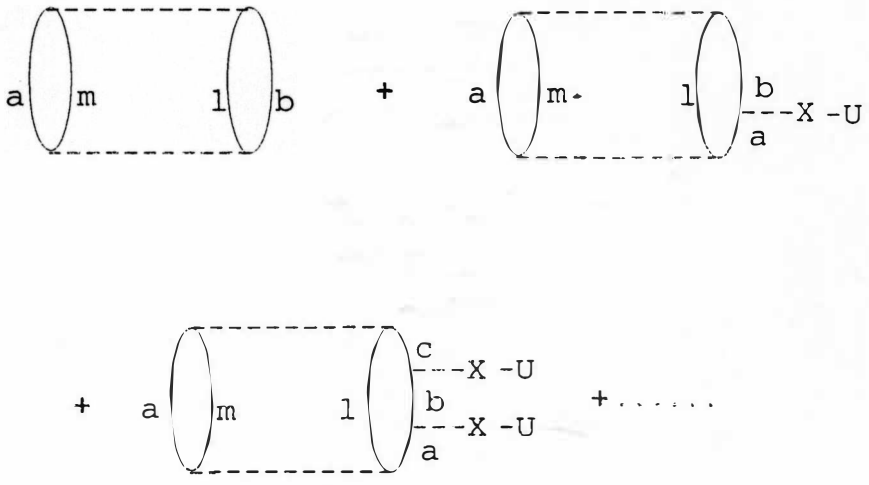

Figure 2. The Second Term of Equation(1.1) With Considering -U Interaction

$$\frac{1}{e-U}$$

$$= \frac{1}{T+U-W-U}$$

$$= \frac{1}{T-W}. \qquad (A.5)$$

So the second term of equation(1.1) can be replaced by,

$$-\upsilon\frac{1}{T-W}\upsilon.$$

The same is true for the third term, fourth term, etc., except the graphs become more complicated. After using equation(A.5) to replace Q/e, one can write equation(1.1) as,

$$G_r = (\upsilon - U) - \upsilon\frac{1}{T-W}\upsilon + \upsilon\frac{1}{T-W}\upsilon\frac{1}{T-W}\upsilon. \qquad (A.6)$$

Of course there are some terms like,

$$U\frac{Q}{e}U - U\frac{Q}{e}U\frac{Q}{e}U + -..... \qquad (A.7)$$

The sum of this series is small, and will not be considered (Baranger 1962). U term in equation(A.6) does not influence the form of the integral equation(2.1) and

$$G_r' = \upsilon - \upsilon \frac{1}{T - W_r} G_r', \qquad \text{(A.8)}$$

where G_r' now include the effect of diagonal -U insertions. It is the G-matrix with reference spectrum approximation and now includes only a kinetic energy term in the energy denominator.

Appendix B

The Derivation of Bethe-Goldstone Equation

The results of $G'_{rl}(1,1)$ by solving the Bethe-Goldstone equation directly are used to compare to the results from coordinate space method and momentum space method. In this appendix the Bethe-Goldstone equation is derived from equation (2.1) by define a correlated wave function, ψ, such that $G\phi = \upsilon\psi$. With setting Q=1, equation (2.1) becomes,

$$G\phi = \upsilon\phi - \upsilon\frac{1}{e}G\phi, \text{ or} \tag{B.1}$$

$$\upsilon\psi = \upsilon\phi - \upsilon\frac{1}{e}\upsilon\psi. \tag{B.2}$$

Operating with υ^{-1}, one obtains the Bethe-Goldstone equation,

$$\psi = \phi - \frac{1}{e}\upsilon\psi. \tag{B.3}$$

This is a differential equation for ψ which can be solved by standard numerical methods. The G-matrix can then be calculated by,

$$\int\phi' G\phi\, d^3\mathbf{r} = \int\phi'\upsilon\psi\, d^3\mathbf{r} \tag{B.4}$$

BIBLIOGRAPHY

Baranger, M. P511--614. Nuclear Structure and Nuclear Reaction editor, M.J. Raricci, Academic Press. (1969).

Baranger, M. and Davies, K.T.R. Nucl. Phys. 79, 403 (1966).

Bertsch, George F. The Practitioner's Shell Model American Elsevier Publishing Company, Inc. New York,(1972).

Bethe, H.A., Brandow, B.H. and Petschek, A.G. Phys. Rev. 129, 225(1963).

Body, T.A. and Moshinsky, M. Tables of Transformation Brackets (Monografias del Instituto de Fisica, Mexico) (1960).

Brandow, B.H., Rev. Mod. Phys. 39, 771(1967), See Appendeix C.

Brown, G.E., Jackson, A.D. and Kuo, T.T.S. Nucl. Phys. A133, 481-492(1969).

Clark, J.W. and Westhaus, P., Phys. Rev. 141, 833(1966).

Day, B.D., Rev. Mod. Phys. 39,719(1967).

Kumar, K. Journ. Math. Phys. 7, 671(1966).

Machleidt, R., Holinde, K., and Elster, Ch., Phys. Rep. 149, 1(1987).

Mohling, F., Phys. Rev. 124, 583(1961); 128, 1365(1962).

Moshinsky, M. Nucl. Phys. 13, 104(1959).

Pandharipanda, Z.R., Smith, R.A., Lomnitz-Adler, J., Nucl. Phys. A361, 399(1981).

Puff, R.D., Ann. Phys(N.Y.) 13, 317(1961).

Talmi, I. Helv. Phys. Acta, 25, 185(1952)

Zeta, Speakeasy IV, Speakeasy Computing Corporation (1978).