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I. Introduction

A general form of a collective model was developed in a fundamental paper by J. A. Wheeler in 1937.[1]

In this theory, any state of a nucleus is regarded as a superposition of all possible kinds of nucleon clusters, continually broken and re-formed in new ways, the interchange of neutrons and protons between the groups being largely responsible for the intergroup forces. Such a state is called by Wheeler a "resonating group structure." To make the calculation feasible, no more than two clusters are considered, and the intergroup separation variable $\vec{r}$ (joining the centers of mass of the two clusters) is the main one of the problem, the scattering function being $F(\vec{r})$. After an exchange of nucleons between the clusters, $\vec{r}$ becomes $\vec{r}'$. It can then be shown that for any type of interaction we get an equation of the form

$$\left(\frac{\hbar^2}{2\mu}\nabla_r^2 + E_{inc}\right) F(\vec{r}) = U(r)\, F(\vec{r}) + \int K(\vec{r}, \vec{r}')\, F(\vec{r}')\, d\vec{r}'. \qquad (1)$$

Because of the principle of conservation of energy, $K(\vec{r}, \vec{r}')$ is symmetric in $\vec{r}$ and $\vec{r}'$.

The three-nucleon problem (n-d scattering) was tackled first by Buckingham and Massey in 1941,[2] using a central potential of exponential shape and the Massey and Mohr wave function[3] for the ground state of the deuteron.

Since then, and also in this paper, Gaussian have been preferred both for the potential shape and for the nuclear wave function because the analysis is easier and can be carried out further. But even when the Gaussian shape is used, the solution of Eq. (1) still requires the help of a powerful computer to tabulate the kernels and to solve Eq. (1) using finite-difference approximations.[4] Both programs have been written for the Ferranti Mercury digital computer by Dr. Philip G. Burke, and are now available at London University Computer Unit.[5]

The work presented here is half way between the fundamental Wheeler paper on resonating group structure and Burke's programs for tabulating kernels and solving the equations.

The reactions involved in the following scheme are considered here.

$$\begin{pmatrix} D(A,Z) \rightarrow D(A,Z) & D(A,Z) \rightarrow n(A+1,Z+1) & D(A,Z) \rightarrow p(A+1,Z) \\ n(A+1,Z+1) \rightarrow D(A,Z) & n(A+1,Z+1) \rightarrow n(A+1,Z+1) & n(A+1,Z+1) \rightarrow p(A+1,Z) \\ p(A+1,Z) \rightarrow D(A,Z) & p(A+1,Z) \rightarrow n(A+1,Z+1) & p(A+1,Z) \rightarrow p(A+1,Z) \end{pmatrix}$$

This is written in abbreviated form as

$$\begin{pmatrix} AA & AB & AC \\ BA & BB & BC \\ CA & CB & CC \end{pmatrix}$$

For A=2 we have the full three-channel d-d reactions;[6] for A=3 we have the two-channel d-t reactions[7] or d-He^3 reactions; for A=4 we have the single-channel d-He^4 elastic scattering.

The minor of AA of the type N(A, Z) (N being a nucleon, either a neutron, n or proton, p), and most of the possible cases have already been published. The n-d case of course, has been extensively studied; the Gaussian formulation with central forces of interest in connection with this paper has been carried out separately for n-d,[8] n-He^3 and n-T,[9] N-He^4,[10] and finally the two-channel n-He^3 case.[11]

In each of the above papers is a formulation corresponding to the reaction studied; all the formulations published (or to be published) can be found herein, so that Wheeler's model appears with full effect namely, covering a very large quantity of experimental data with only three parameters: V_0 (potential depth), $\rho_0 = 1/\sqrt{\mu}$ (range of the nuclear forces), and the type of exchange. However, one must keep in mind that the formulation is only the minor part of these problems, the far greater one being to get out numerical results, and in that respect the machine programs are much more valuable.

The limitation $A \leqslant 4$ is due to the symmetry property of the ground-state nuclear wave functions, namely factorization of spin and space part with invariance of the space part under any permutation of the nucleons inside the nucleus. This important property allows for a relabeling of the nucleons, which considerably simplifies the analysis.

Among the possible types of functions consistent with that property, Gaussian functions have been preferred. We take, for the potential shape,

$$V(r) = V_0 \, e^{-\mu r^2};$$

for the deuteron wave function,

$$\phi(A+1,\ A+2) = \phi(\rho_1) = \frac{1}{N_D}\left[\exp(-\alpha\rho_1^{\,2}) + c\,\exp(-\beta\rho_1^{\,2})\right];$$

and for any other nuclei,

$$\phi(A, Z) = \phi(1, 2, \cdots A) = \frac{1}{N_A}\ \exp\left[-(\lambda/2\sum (ij)^2\right].$$

As we have $A \leqslant 4$, we can denote protons by even numbers and neutrons by odd numbers. Also we assume 1 and A+1 to be of the same nature, as well as 2 and A+2.

From the form of $\phi(A, Z)$ it is obvious that AC can be deduced from AB, and similarly BB and CC from BC, by appropriate changes of λ.

Finally, owing to the symmetry property of the scattering matrix, we have $BA = (AB)^{\dagger}$, $CA = (AC)^{\dagger}$, $CB = (BC)^{\dagger}$, and we need to consider only the three terms

AA, AB, BC.

In the minor of AA, the nucleus involved contains A+1 nucleons; when dealing with it, to simplify the formulae, we write only A, so that we have at once the formulae ready for the two channels N(A, Z). The method is detailed in that case, and only tables are given for AA and AB and for BC.

Chapter II of this paper defines the central two-body interaction used in the formulation, and deals with the space-part wave function of the nuclei (A, Z). Chapter III gives the wave function, written according to the resonating-group-structure method, and the corresponding equations that the wave function must satisfy. Chapter IV deals mainly with the BC term, and in the appendix are given the corresponding Table II and Tables III for AA and AB terms built up by following the same method. Chapter V is a brief review of the method for getting the cross sections; this topic is dealt with in detail in other papers.[12, 13]

In appendices are given some details of the algebra involved in the calculations, and the results are listed in Tables II and III.

II. The Two-Body Potential and the Nuclear Wave Functions

1. The Exchange-Dependent Two-Body Potential

The potential used is a central two-body potential with Gaussian shape and exchange dependence. It can be written equally well in two forms, and the connection between these two forms is reviewed here.

The interaction between two nucleons can be written (using the same shape for all exchange potentials) as

$$V(r_{ij}) = (wW_{ij} + mM_{ij} + bB_{ij} + hH_{ij})\ V(r_{ij}) + \epsilon_{ij} \cdot \frac{e^2}{r_{ij}},$$

where $\epsilon_{ij} = 1$ if i and j are protons, and zero otherwise, $r_{ij} = |\vec{r}_i - \vec{r}_j|$, W_{ij} is an identity operator, and

M_{ij}, B_{ij}, H_{ij} are the usual Majorana, Bartlett, and Heisenberg operators exchanging space, spin, and spin-and-space co-ordinates of particles i and j such that $H\,B\,M\ \psi = W\,\psi = \psi$.

According to the Pauli principle, the total wave function must be totally

antisymmetric in space, spin, and isotopic spin so that, since $H' = \frac{1}{2}(1 + \vec{\tau}_i \cdot \vec{\tau}_j)$ is the operator exchanging the isotopic spin, we have $H' B M \psi = - \psi$. Consequently we have $H' = - H$, and $H_{ij} = - \frac{1}{2} (1 + \vec{\tau}_i \cdot \vec{\tau}_j)$.

As $B_{ij} = \frac{1}{2}(1 + \vec{\sigma}_i \cdot \vec{\sigma}_j)$, we deduce $M_{ij} = - \frac{1}{4} (1 + \vec{\sigma}_i \cdot \vec{\sigma}_j)(1 + \vec{\tau}_i \cdot \vec{\tau}_j)$.

Either from their very definition or from the above expressions, we deduce the following multiplication table:

	W_{ij}	M_{ij}	B_{ij}	H_{ij}
W_{ij}	W_{ij}	M_{ij}	B_{ij}	H_{ij}
M_{ij}	M_{ij}	W_{ij}	H_{ij}	B_{ij}
B_{ij}	B_{ij}	H_{ij}	W_{ij}	M_{ij}
H_{ij}	H_{ij}	B_{ij}	M_{ij}	W_{ij}

Here w, m, b, and h are constants that determine the relative importance of each type of exchange; they are chosen according to the different theories of nuclear forces, and it is hoped that the comparison of the final results with the experimental data lead to a reasonable choice.

Let us write $V(r_{ij}) = V_0 f(\mu, r_{ij})$,

where V_0 and μ give the depth and the range of this well,

and $\psi_{ij} = \sum_{\ell, s} \phi_\ell (r_{ij}) Y_{\ell, m}(\theta, \phi) \sigma_s (ij)$

is a wave function for the two nucleons i and j.

Then $V(r_{ij})$ acting on ψ_{ij} will give an effective potential ${}^{2S+1}V_{2T+1}^{(-1)^\ell}$, such that

$${}^{2S+1}V_{2T+1}^{(-1)^\ell} = [\, w + (-1)^\ell m + (-1)^{s+1} b + (-1)^{\ell+s+1} h\,]\, V_0\, f(\mu, r_{ij}).$$

We take $w + m + b + h = 1$,

so that V_0 is the depth of the well of the deuteron in the ^3S state. Also,

$$w + m - b - h = x$$

is the ratio of the ^1S to ^3S interaction.

The value of x is usually taken to be 0.6.[14]

We have

$$w + m = \frac{1+x}{2} = \frac{^3V + {}^1V}{2(^3V)} = 1 - g;$$

$$b + h = \frac{1-x}{2} = \frac{^3V - {}^1V}{2(^3V)} = g.$$

Using the previous definitions of W_{ij}, M_{ij}, E_{ij}, and H_{ij}, we can write the nuclear interaction,

$$V(r_{ij}) = \left[w + m\, M_{ij} + b \left(\frac{1+\vec{\sigma}_i \cdot \vec{\sigma}_j}{2}\right) + h\, M_{ij} \left(\frac{1+\vec{\sigma}_i \cdot \vec{\sigma}_j}{2}\right)\right] V(r_{ij}).$$

As M_{ij} had no effect on even states, we have, for the states of even parity only,

$$\left[w + m + \frac{b}{2} + \frac{h}{2} + \left(\frac{b+h}{2}\right) \vec{\sigma}_i \cdot \vec{\sigma}_j\right] V(r_{ij}) = \left[1 - \frac{1}{2} g + \frac{1}{2} g\, (\vec{\sigma}_i \cdot \vec{\sigma}_j)\right] V(r_{ij}).$$

The potential for states of odd parity is suggested by meson theory:

(a) Ordinary forces or neutral meson theory:

$V_{odd} = V_{even}$, i.e., $m = h = o$, $w = 1/2(1+x)$, $b = 1/2(1-x)$.

(b) Exchange forces or charged-meson theory:

$V_{odd} = (-1)^{\ell} V_{even}$, i.e., $w = b = o$, $m = 1/2(1+x)$, $h = 1/2(1-x)$.

(c) Symmetric forces or M H W B:

$V_{odd} = -1/3\, (\vec{\tau}_i \cdot \vec{\tau}_j)\, (\vec{\sigma}_i \cdot \vec{\sigma}_j)_{even}$, i.e., $^3V_{odd} = -1/3\, {}^3V_{even}$ and $^1V_{odd} = -3\, {}^1V_{even}$, or

$m = 2b = (1/3)(1+3x)$, $h = 2w = (1/3)(1-3x)$.

(because here $\vec{\tau}_i \cdot \vec{\tau}_j$ goes as $\vec{\sigma}_i \cdot \vec{\sigma}_j$, and $\vec{\sigma}_i \cdot \vec{\sigma}_j = +1$ for triplet states and $\vec{\sigma}_i \cdot \vec{\sigma}_j = -3$ for singlet states).

(d) Serber empirical forces:

$V_{odd} = 0$, $\quad w = m = (1/4)(1+x)$, $\quad b = h = (1/4)(1-x)$.

(e) Biel's force, a mixture of Serber and symmetrical exchange (which has given good results for the binding energy of the first 4n nuclei and the α-α scattering):

$V_{Biel} = 1/3\ V_{sym} + 2/3\ V_{Serber}$, $\quad w = b = 5/18$, $\quad h = 5/18 - x/2$. $\quad m = 5/18 + x/2$

That the deuteron has a quadrupole moment implies that the nuclear force is not merely a central one.

However, so that preliminary results may be obtained in a reasonable time, this work does not include a tensor force or a spin-orbit coupling. Using the central force not only saves labor but also allows us to consider the total spin s of the system and the angular momentum l as good quantum numbers; thus it is possible to solve, for each value of l, the system of equations obtained for each value of s. The phases and the cross sections are deduced according to the classical method of partial waves.

At low energy, the results are rather insensitive to the shape of the well, as we have seen from the Blatt and Jackson formula.

The potential shape used in this work is Gaussian,

$$V_0\, f(\mu, r) = V_0\, e^{-\mu r^2},$$

this form being the one which allows us to perform most of the algebra. The value of $\mu(\mu = 0.2669\ 10^{26}\text{cm}^{-2})$ is that derived by Breit,, Hoisington, and Share[15] from analysis of low-energy proton-proton scattering, and has been used in previous four- and five-nucleon calculations (see Bransden review paper[16]). Assuming that the nuclear forces are charge-independent, this range can be used indifferently for p-p, n-n, or n-p interaction. The corresponding range $\rho_0 = 1/\sqrt{\mu} = 1.936\ 10^{-13}$cm is larger than normal and in that respect can account, to a certain extent, for the effect of the neglected noncentral forces.

The corresponding value of the depth V_0 (that is, $V_0 = -46.8$ Mev) was interpolated from the results obtained by Burke[17] for the determination of the well depth required to give the observed binding energy of the deuteron for a Gaussian well using $\mu = 0.2\ (0.1)\ 0.6$.

2. Trial Functions and the Variational Principle

With the interaction $V(r_{ij})$ defined previously, and T being the appropriate kinetic energy operator, the Hamiltonian will be

$$H = T + \sum_{\text{all pairs}} V(r_{ij}) .$$

The wave function ψ to choose for the different nuclei in their ground states (D, T, He^3, He^4) should be the exact solution of the Schrodinger equation,

$$(H - E)\,\psi = 0,$$

E being the corresponding binding energy.

As is well known, it is not possible, using Gaussian potential, to solve these equations and express the eigenfunctions in an analytical form. To allow for an analytical evaluation of most of the integrals, a trial function is chosen for the space part.

As the total wave function must be totally antisymmetric, and as the product of the spin and isotopic spin parts can be antisymmetrized for any number of nucleons up to four, it is possible to take a space part completely symmetric with respect to permutation of the nucleons. Among this class of function, the Gaussian form has been chosen.

Deuteron: $\phi = (1/N_0)[\exp^{-\alpha r^2} + c \exp^{-\beta r^2}]$;

T, He^3, He^4: $\phi = 1/N \exp[-(\lambda/2) \sum (ij)^2]$

where N is the corresponding normalizing factor.

Writing $\psi = \phi\,\sigma$, and with λ being any of the parameters $\alpha, \beta, c, \lambda$, we have

$$E(\lambda) = \frac{\int \psi^{+} H \psi \, d\tau}{\int \psi^{+} \psi \, d\tau},$$

the integral sign involving the appropriate sums over the spin variables.

Then, according to the variational method, the parameters of the trial functions given above are determined so that

$$\delta E(\lambda) = \sum_i \frac{\partial E}{\partial \lambda_i} \delta \lambda_i = 0,$$

whatever the $\delta\lambda_i$ may be. This gives a system of simultaneous equations and therefore the values of λ_i.

The corresponding mean value E_{min} so obtained is an upper limit for the binding energy E and verifies the equation

$$\int \psi^{+} (H - E_{min}) \psi \, d\tau = 0.$$

This integral equation satisfied by the nuclear wave function is used later on to simplify the equations of the scattering problem.

The Gaussian form is

$$\phi = 1/N \exp\left[- \lambda/2 \sum_{i<j} (ij)^2 \right],$$

where (ij) is any two-by-two combination of the $(1, 2, \cdots A)$ nucleons. Using the elementary relation of the moment of inertia,

$$\sum_i m_i \, MA_i^{\,2} = \left(\sum_i m_i\right) MG^2 + \sum_i m_i \, GA_i^{\,2},$$

we get

$$\sum_{i<j} (ij)^2 = \sum_{p=1}^{A-1} \frac{A(A-p)}{A-p+1} \, R_p^{\,2},$$

with

$$\vec{R}_p = \vec{r}_p - \frac{\vec{r}_{p+1} + \vec{r}_{p+2} \cdots + \vec{r}_A}{A - p}.$$

By use of the formula given in the appendix, the normalizing factor is easily deduced:

$$N^2 = \prod_{p=1}^{A-1} \left(\frac{\pi (A-p+1)}{\lambda A (A-p)} \right)^{3/2}$$

where π means the product of all terms obtained by using successively $p = 1, 2, \cdots A-1$.

The kinetic energy is given by

$$- \frac{\hbar^2}{M} \sum_{p=1}^{A-1} \frac{A-p+1}{2(A-p)} \nabla^2_{R_p} .$$

For each $\vec{R}_p$ we get the contribution $\frac{\hbar^2}{M} \frac{3}{4} \lambda A$, and as we have $(A-1)$ different vectors $\vec{R}_p$, we get

$$\langle \phi \mid K.E. \mid \phi \rangle = \frac{\hbar^2}{M} \frac{3}{4} \lambda A (A-1).$$

The nuclear potential shape being $V(r) = V_0 e^{-\mu (ij)^2}$, we get

$$\langle \phi \mid V \mid \phi \rangle = \frac{A(A-1)}{2} (m + w) V_0 \left(\frac{A\lambda}{A\lambda + 2\mu} \right)^{3/2} .$$

The Coulomb potential gives

$$\langle \phi \mid V^c \mid \phi \rangle = \frac{Z(z-1)}{2} \frac{2 e^2}{\sqrt{\pi}} \left(\frac{A\lambda}{2} \right)^{1/2}$$

And finally the binding energy is

$$B E(A, Z) = \frac{3}{4} \frac{\hbar^2}{M} \lambda A (A-1) + \frac{A(A-1)}{2} (m+w) V_0 \frac{A\lambda}{A\lambda+2\mu} + \frac{z(z-1}{2} \frac{2 e^2}{\sqrt{\pi}} \left(\frac{A\lambda}{2} \right)^{1/2} .$$

By making $A = 2, 3, 4$ one can get all the formulae needed for deuterons, tritons, He^3, and He^4.

Table I

Summary of Chapter II. Parameters used in the trial wave functions and corresponding calculated and experimental binding energies.

Nucleus	λ	E_{min} (Mev)	E_{exp} (Mev)
d	$\alpha = 0.0299\times10^{26}\,cm^{-2}$	-2.133	-2.226
	$\beta = 0.186\times10^{26}\,cm^{-2}$		
	$c = 2.73$		
t	0.15715	-6.744	-8.3
He^3	0.15400	-5.975	-7.55
He^4	0.15780	-27.315	-28.2

The potential range $\rho_0 = \frac{1}{\sqrt{\mu}} = 1.936\times10^{-13}$ cm (from $\mu = 0.2669\times10^{26}\,cm^{-2}$) and depth $V_0 = -46.8$ Mev chosen can account for the binding energies of all the light nuclei we intend to deal with in our scattering problems. This is very important when dealing with coupled equations of a complete (elastic and nonelastic) system which has to be described with consistent parameters.

The values of the physical constants (h, e, etc.) used in the calculation are those given by DuMond and Cohen.[18]

III. Total Wave Function and Coupled Equations

A resonating-group wave function of correct symmetry may be written as

$$\psi_s(A+1, A+2; 1, 2, \cdots A) = (1-P_{A+1,1}-P_{A+1,3}-\cdots)(1-P_{A+2,2}-P_{A+2,4}-\cdots)$$

$$\phi(A+1, A+2)\ \phi(1, 2, \cdots A)\ \sigma_s(A+1, A+2; 1, 2, \cdots A)\ F_s(A+1, A+2; \cdots A)$$

$$+(1-P_{A+1,1}-P_{A+1,3}-\cdots)\ \phi(A+2, 1, 2, 3 \cdots A)\ \sigma_s(A+1; A+2, 1, 2, 3, \cdots A) G_s(A+1; A+2, 1, 2, \cdots A)$$

$$+(1-P_{A+2,2}-P_{A+2,4}-\cdots)\phi(A+1, 1, 2, 3, \cdots A)\ \sigma_s(A+1, 1, 2, 3, \cdots A) H_s(A+2; A+1, 1, 2, \cdots A).$$

Here P_{ij} are exchange operators of Heisenberg type;

σ_s is the spin function corresponding to the total spin S of the system of A+2 nucleons. As is well known, even though all spin orientations are contained in the usual beam, we may take only one definite spin orientation m_s for the spin function $\sigma_s^{m_s}$ because different values of m_s lead to incoherent contributions. In fact, we have taken $m_s = S$ and dropped the superscript;

F, G, H are the scattering functions (to be replaced by plane wave in Born approximation), which we are going to determine by the partial-wave method, as described in Mott and Massey.[12]

The general way of deriving the coupled equations through the variational principle is given in Wheeler's fundamental paper, and the application to the case of A=2 is given in detail in Burke and Laskar.[6]

The variational method leads to an integration over internal variables, and the appropriate differential volume elements are:

$$d\tau_1 = d(A+1, A+2)\ dR_1\ dR_2 \cdots dR_{A-1},$$

$$d\tau_2 = d(R_{A+2})_0\ dR_1\ dR_2 \cdots dR_{A-1},$$

$$d\tau_3 = d(R_{A+1})_0\ dR_1\ dR_2 \cdots dR_{A-1},$$

where we define

$$\begin{pmatrix} \vec{R}_{A+2} \\ \text{or } A+1 \end{pmatrix}_o = \begin{matrix} \vec{r}_{A+2} \\ \text{or } A+1 \end{matrix} - \frac{\vec{r}_1 + \vec{r}_2 + \cdots + \vec{r}_A}{A} .$$

The basic intergroup separation variables are

$$\vec{v} = \frac{\vec{r}_{A+1} + \vec{r}_{A+2}}{2} - \frac{\vec{r}_1 + \vec{r}_2 + \cdots + \vec{R}_A}{A} \quad \text{for AA, AB, AC;}$$

$$\vec{v}_{1,2} = \vec{r}_{A+1,2} - \frac{\vec{r}_{A+2,1} + \vec{r}_1 + \vec{r}_2 \cdots + \vec{r}_A}{A+1} \quad \text{for the other elements.}$$

The exchange operators P_{ij} replace this set of $\vec{v}$ by a set of $\vec{r}'$, and special care must be given to AA, AB, AC terms because of the occurrence of two types of exchanges.

First type of exchange:

$$\text{AA: } r' = \frac{\vec{r}_1 + \vec{r}_{A+2}}{2} - \frac{\vec{r}_{A+1} + \vec{r}_2 + \vec{r}_3 + \cdots \vec{r}_A}{A} ,$$

$$\text{AB: } \vec{r}' = \vec{r}_{A+1} - \frac{\vec{r}_{A+2} + \vec{r}_1 + \vec{r}_2 \cdots + \vec{r}_A}{A+1} .$$

Second type of exchange:

$$AA: \quad \vec{r}' = \frac{\vec{r}_1 + \vec{r}_2}{2} - \frac{\vec{r}_{A+1} + \vec{r}_{A+2} + \vec{r}_3 + \cdots + \vec{r}_A}{A}$$

$$AB: \quad \vec{r}' = \vec{r}_1 - \frac{\vec{r}_{A+2} + \vec{r}_{A+1} + \vec{r}_2 + \cdots + \vec{r}_A}{A+1} .$$

As already mentioned, BC belongs to the type N(A, Z), and on that basis we have a single type of exchange:

$$\vec{r}' = \vec{r}_1 - \frac{\vec{r}_{A+1} + \vec{r}_2 + \cdots + \vec{r}_A}{A} .$$

Consider now all the $\frac{(A+1)(A+2)}{2}$ interactions (n-p). They fall into different classes which can be listed and indicated as follows (where appearance of the same symbol indicates that the expressions are the same; the dagger is the classical adjoint symbol):

	AA		AB		BC
Type	First type of exchange	Second type of exchange	First type of exchange	Second type of exchange	
(A-1, A)	v	v	v	v	v
(1, i)	x	x	v	x	x
(A+1, i)	$x^\dagger$	v	0	∇	$x^\dagger$
(A+2, i)	∇	∇	∇	∇	...
(1, A+1)	0	∇	0	0	0
(1, A+2)	$\square^\dagger$	∇	∇	0	...
(A+1, A+2)	$\square$	x	$\square$	$\square$	...
(1, j)	...	ϕ			
(2, j)	...	ϕ			
(A+1, j)	...	$\phi^\dagger$			
(A+2, j)	...	$\phi^\dagger$			

The BC term will be dealt with in detail later on to illustrate the method. In this table $i = 2, 3, \cdots A$ except in (AA | II) and BC where $i = 2$ only;

$j = 3, \cdots A$.

Within a given column (AA, first type of exchange, for instance), all kernels corresponding to the same symbol are the same; for instance the $\frac{(A-1)(A-2)}{2}$ kernels interactions of the type (A-1, A) (in which neither neutron nor proton is A+1, A+2, or 1), are all the same.

Within a given column, (AA, first type of exchange for instance) the dagger signs correspond to the adjoint of the one without dagger; for instance

$[AA|1|A+1, A+2] = [AA|1|1, A+2]^{\dagger}$.

The notation $[AA|1|np]$ speaks for itself: it means the kernel corresponding to the interaction np, in AA, first type of exchange.

The correspondence between kernels shown above is self-evident as soon as the interaction (np) is expressed in terms of the variables $v, r', R_2, \cdots R_{A-1}$, and allows for tremendous simplification in the formulation.

The following notations will be used:

$$\mathcal{E} = E_{min}(D) + E_{min}(A, Z) + E_d = E_{min}(A+1, Z) + E_p = E_{min}(A+1, Z+1) + E_n,$$

$$k^2 = \frac{2\mu_{d, n, or\ p}}{\hbar^2} E_{d, n, or\ p},$$

where $E_{d, n, or\ p}$ is the kinetic energy of the corresponding particle in the center-of-mass frame,

and $\frac{1}{\mu_d} = \frac{1}{M(D)} + \frac{1}{M(A, Z)} = \frac{A+2}{2AM}$,

$$\frac{1}{\mu_{n\ or\ p}} = \frac{1}{M} + \frac{1}{(A+1)M} = \frac{A+2}{(A+1)M},$$

So that $\mathcal{E} = \mathcal{E}(k)$.

Also, $\mathcal{P}$ is the kernel arising from the product of the initial-state wave function on the one hand and the final-state wave function after exchange on the other hand.

For a given value of the total spin S, the system of coupled equations can then be written:

$$0 = -\left\{\frac{(A+2)\hbar^2}{4AM} + E(d)\right\} F(v) + F(v)\int \phi^2(\rho_1)\phi^2(A, Z)\left\{ZV_c^{A+2,2} + (\omega' w + \mu' m + \beta' b + t' h)V^{A+1,1}\right\} d\tau_1$$

$$+ J_{AA}^{s}\int \left\{ \gamma_{AA}^{s} \left[T - \mathcal{E}\mathcal{N}\right] + ((A+2,2))_c + ((A+1,1))_c \right.$$

$$\left. + ((A-1,A)) + ((1,A+1)) + ((A+1,A+2\,|+|\,1,A+2)) + ((A+2,2)) + ((1,2\,|+|\,A+1,2)) \right\} F(r')dr'$$

$$+ J_{AA}^{D}\int \left\{ \gamma_{AA}^{D} \left[T - \mathcal{E}\mathcal{N}\right] + ((A+2,2))_c + ((A+2,4))_c \right.$$

$$\left. + ((A-1,A)) + ((1,A+1)) + ((A+1,A+2)) + ((1,3\,|+|\,A+1,3)) \right\} F(r')dr'$$

$$+ J_{AA}^{s}\int \left\{ \gamma_{AB}^{s} \left[T - \mathcal{E}\mathcal{N}\right] + ((A+2,2))_c + ((A+2,4))_c \right.$$

$$\left. + ((A-1,A)) + ((1,A+1)) + ((A+1,A+2)) + ((A+2,2)) \right\} G(r')dr'$$

$$+ J_{AB}^{D}\int \left\{ \gamma_{AB}^{D} \left[T - \mathcal{E}\mathcal{N}\right] + ((A+2,2))_c + ((A+2,4))_c \right.$$

$$\left. + ((A-1,A)) + ((1,A+1)) + ((A+1,A+2)) + (A+2,2)) + ((1,2)) \right\} G(r')dr'$$

+ AC terms deduced from AB by interchanging conveniently A+1 and A+2 and also replacing G(r') by H(r').

$$0 = BA - \left\{\frac{(A+2)\hbar^2}{2(A+1)M} + E(n)\right\} G(v) + G(v)(\omega w + \mu m + \beta b + th)\int \phi^2(A+1, Z+1)\, V^{A+1,1}\, d\tau_2$$

$$+ J_{BB}\int \left\{ \gamma_{BB} \left[T - \mathcal{E}\mathcal{N}\right] + ((A+2,2))_c + ((A+2,4))_c \right.$$

$$\left. + ((A-1,A)) + ((1,A+1)) + ((1,2\,|+|\,A+1,2)) \right\} G(r')dr'$$

$$+ H(v)(\omega'' w + \mu'' m + \beta'' b + t'' h)\int \phi(A+1, Z+1)\, V^{A+1,1}\, \eta(A+1, Z)\, d\tau_2$$

$$+ J_{BC}\int \left\{ \gamma_{BC} \left[T - \mathcal{E}\mathcal{N}\right] + ((A+2))_c + ((A+2,4))_c + ((A-1,A)) + ((1,A+1)) + ((1,2\,|+|\,A+1,2)) \right\} H(r')dr'$$

$$0 = CA + CB - \left\{\frac{(A+2)\hbar^2}{2(A+1)M} + E(p)\right\} H(v) + H(v)(\omega w + \mu m + \beta b + th)\int \eta^2(A+1, Z)\, V^{A+2,2}\, d\tau_3$$

$$+ J_{CC}\int \left\{ \gamma_{CC} \left[T - \mathcal{E}\mathcal{N}\right] + ((A+2,2))_c + ((A+2,4))_c + ((A-1,A)) + ((2,A+2)) + ((2,1\,|+|\,A+2,1)) \right\} H(r')dr'.$$

The equation for D-He^4 scattering (which exists only for total spin 1) is given as an example: $DH_e^4 \equiv (56)(1234)$.

$$\frac{3\hbar^2}{8M}\left\{\frac{d^2}{dr^2} - \frac{\ell(\ell-1)}{r^2} + k^2\right\} f_\ell(r) = \left\{2V_c^{62} + (8w - 2m + 4b - 4h)\, V^{15}\right\} f_\ell(r)$$

$$- \int_0^\infty \Big\{ 2\Big(T - \mathcal{E}W^0 + (I|62)_c + (I|51)_c + (I|16+1|56)\Big) + 6(w+m)\Big((I|12+I|52) + (I|34)\Big)$$
$$+ (2w-8m+4b-4h)(I|15) + (6w-4m+2b-6h)(I|26)\Big\} f_\ell(r')\, dr'$$
$$+ \int_0^\infty \Big\{ T - \mathcal{E}W^0 + 2(II|62)_c + 2(II|12) + (II|34) + (4w-6m+6b-2h)(II|15)$$
$$+ (4w+4m-2b-2h)(II|13+II|53)\Big\} f_\ell(r')\, dr'.$$

For each value of the total spin S of the system of (A+2) nucleons we get a system of the type shown above. In this system, the Jacobian has been kept in front of each integral to show from where it arises. To simplify the writing of the equations, we use a notation explained by the example

$$((n,p)) = (\omega w + \mu m + \beta b + th)\,[\,AA\,|\,I \text{ or } II\,|\,np\,],$$

where ω, μ, β, and t are appropriate numerical coefficients depending on spin. Finally, for the whole system we use the abbreviated notation

$$\begin{pmatrix} AA & AB & AC \\ BA & BB & BC \\ CA & CB & CC \end{pmatrix} \begin{pmatrix} F \\ G \\ H \end{pmatrix} = 0.$$

Some relations between the spin-dependent coefficients can easily be obtained by using the multiplication table given in the definition of the potential. For instance, we have, before any direct term,

$$\omega w + \mu m + \beta b + th,$$

and before the corresponding kernel,

$$\mu w + \omega m + tb + \beta h .$$

Also

$$((AA|\,I\,|\,A+2,2)) = (\omega' w + \mu' m + \beta' b + t'h)\,[\,AA\,|\,I\,|\,A+2,2\,]$$

$$((AA|II\,|\,A+1,1)) = (\mu' w + \omega' m + t'b + \beta' h)\,[\,AA\,|II\,|\,A+1,1\,]$$

These spin-dependent coefficients will be analyzed in a more detailed manner for the BB case considered as a N(A, Z) problem.

IV. The Gaussian Formulation of the Different Terms

The method is fully explained for N(A, Z) and results are also given for D(A, Z).

1. The direct potential term

As all the (ij) couples involving (1, 2, $\cdots$A) disappear when we use the integral equation verified by the nuclei wave function

$$\int \phi\,(H = E_{min})\,\phi\, d\tau = 0,$$

we are left with couples of the form (A+1, i), where $i = 1, 2, \cdots A$, and (A+1) is the incident nucleon. All these terms give the same contribution, as we can always relabel the nucleons, and it is enough to calculate the contribution of one of them, say (1, A+1). Now in a cross term it is the space-part wave function of the newly formed nucleus $\eta(A+1, 2, 3, \cdots A)$ after exchange $(A+1 \rightleftarrows 1)$ which is involved.

Therefore, calling $\vec{v} = \vec{r}_{A+1} - \dfrac{\vec{r}_1 + \vec{r}_2 \cdots + \vec{r}_A}{A}$,

we have

$$(A+1, 1) = \vec{r}_1 = \vec{r}_{A+1} = \left(\frac{A-1}{A}\right)\vec{R}_1 = v,$$

and the corresponding contribution is

$$\int \phi\,(1, 2, \cdots A)\, V_0\, \exp[-\mu(A+1, 1)^2]\, \eta(A+1, 2 \cdots A) d\vec{R}_1 d\vec{R}_2 \cdots d\vec{R}_{A-1},$$

where $(A+1, 2, 3, \cdots A)$ is the space-part wave functions of (A, Z-1); we get

$$V_0 \int \exp\left[-\frac{\lambda+\nu}{2} \sum_{p=1}^{A-1} \left(\frac{A(A-p)}{A-p+1}\right) R_p^2 - \mu(A+1, 1)^2\right] d\vec{R}_1 d\vec{R}_2 \cdots d\vec{R}_{A-1} =$$

$$\langle\!\langle V^{A+1, 1} \rangle\!\rangle = V_0 \left\{\left[\frac{4\lambda\nu A^2}{(\lambda+\nu)^2 A^2 + 2(A-1)(\lambda+\nu)\mu}\right]\left(\frac{2\sqrt{\lambda\nu}}{\lambda+\nu}\right)^{A-3}\right\}^{3/2} \exp\left[-\frac{\mu(\lambda+\nu)A^2}{(\lambda+\nu)A^2 + 2\mu(A-1)} v^2\right].$$

In particular, for A = 2, 3, and 4 one gets the direct terms given for n-d, n-He^3, and n-He^4 respectively.

When N is a neutron obviously there is no Coulomb direct term.

When N is a proton a straightforward calculation gives (e.g., for the CC term)

$$\frac{z\,e^2}{|v|}\,\bar{\Phi}\left(A\sqrt{\frac{\lambda}{A-1}}\,v\right),$$

where

$$\bar{\Phi}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}\,dt,$$

and $\phi(x)$ is the well-known error function.

In the D(A, Z) case, one gets for the nuclear and Coulomb direct AA term respectively,

$$U_2(v) = V_0\,\frac{c}{N_D^2}\left(\frac{4\pi\lambda}{4(\alpha+\beta)\left[\lambda+\mu\frac{A-1}{A^2}\right]+\lambda\mu}\right)^{3/2}\exp\left[-\frac{4(\alpha+\beta)\,\lambda\mu v^2}{4(\alpha+\beta)\left[\lambda+\mu\frac{A-1}{A^2}\right]+\lambda\mu}\right]$$

$$C_2(v) = e^2\,\frac{c}{N_D^2}\,\frac{2\pi A(A-1)}{\lambda}\int_0^1 dt\left(\frac{4\lambda}{4(\alpha+\beta)(A-1)+t^2\lambda A^2}\right)^{3/2}\exp\left[-\frac{4(\alpha+\beta)\lambda A^2 t^2 v^2}{4(\alpha+\beta)(A-1)+t^2\lambda A^2}\right],$$

where the integral is computed numerically by any suitable method (six-point Gaussian integration formula, for instance).[19]

2. The Kinetic Energy Kernals in BC

The original intergroup separation variable being called $\vec{v}$ (defined in the preceding section), the intergroup separation variable after exchange is $\vec{r}'$:

$$r' = r_1 - \frac{r_{A+1} + r_2 + r_3 \quad + r_A}{A},$$

as a relabeling of the nucleons can let us call 1 the exchanged nucleon.

Therefore $\vec{R}_1 = \vec{r}_1 - \frac{\vec{r}_2+\vec{r}_3\cdots+\vec{r}_A}{A-1} = \frac{A}{A^2-1}(A\vec{r}' + \vec{v}) = U(\vec{r}', \vec{v})$.

The change of variable from $\vec{R}_1$ to $\vec{r}'$ brings the Jacobian

$$|J| = \left(\frac{A^2}{A^2-1}\right)^3,$$

and $d\vec{R}_1\, d\vec{R}_2\, d\vec{R}_3 \cdots d\vec{R}_{A-1} = \left(\frac{A^2}{A^2-1}\right)^3 d\vec{r}'\, d\vec{R}_2\, d\vec{R}_3 \cdots d\vec{R}_{A-1}$.

In conjunction with $\vec{R}_1$ let us define $\vec{R}_{A+1}$:

$$\vec{R}_{A+1} = \vec{r}_{A+1} - \frac{\vec{r}_2+\vec{r}_3+\cdots+\vec{r}_A}{A-1} = \frac{A}{A^2-1}(\vec{r}'+A\vec{v}) = V(\vec{r}', \vec{v}) = U^\dagger(\vec{r}', \vec{v}) = U(\vec{v}, \vec{r}').$$

Consider the product $\phi(1, 2\cdots A)\eta\,(A+1,\ 2\cdots A)$.

We have

$$\phi(1, 2, \cdots A)\eta(A+1, 2, \cdots A) = \frac{1}{N_\phi N_\eta} \exp\left[-\frac{\lambda+\nu}{2}\sum_{p=2}^{A-1}\frac{A(A-p)}{A-p+1}R_p^2 - \frac{A-1}{2}(\nu U^2+\lambda V^2)\right].$$

The kinetic energy operator is

$$-\frac{\hbar^2}{M}\left\{\sum_{p=2}^{A-1}\frac{A-p+1}{2(A-p)}\nabla^2_{R_p} + \frac{A}{2(A-1)}\nabla^2_{v} + \frac{A+1}{2A}\nabla^2_{r'}\right\}.$$

Using the method given in the Appendix, we obtain a kinetic energy kernel, and the result is given in the general table.

3. The Potential Kernels in BC

We have to consider a central two-body interaction $V(r) = V_0 e^{-\mu(ij)^2}$ between all the two-by-two combinations of the (A+1) nucleons (A from the target nucleus and one incident). These couples can be separated in three basic groups: First, the ones involving neither 1 nor (A+1); they are of the type (A-1, A); e.g., (i, j), i or j, for $i = 2, \cdots A$.

Second, the ones involving nucleon 1; they are (A-1) of this type, e.g., (1, i) for $i = 2, 3, \cdots A$

(the ones involving nucleon A+1; they are also (A-1) of this type,

e.g., $(A+1, i)$ for $i = 2, 3, \cdots A$,

and they are the transposed of the corresponding one with the exchange $1 \rightleftarrows A+1$,

$$K_{BC}^{A+1,i}(\vec{r}', \vec{v}) = \left[K_{cB}^{1,i}(\vec{r}', \vec{v}) \right]^{\dagger} = K_{cB}^{1,i}(\vec{v}, \vec{r}')\Big)$$

Third and last, we have the single kernel (A+1, 1) which has to be calculated for its own sake.

In each group all the kernels give the same contribution as can be explained by the relabeling argument or by direct calculation, using the formula

$$(A-p, A-p+k) = \vec{R}_{A-p} + \frac{1}{p}\vec{R}_{A-p+1} + \frac{1}{p-1}\vec{R}_{A-p+2} + \cdots + \frac{1}{p-k+2}\vec{R}_{A-p+k-1} - \left(\frac{p-k}{p-k+1}\right)\vec{R}_{A-p+k}.$$

We have now to calculate

$$J \int \phi(1, 2, \cdots A) V_0 \, e^{-\mu(ij)^2} \eta(A+1, 2, \cdots A) \, d\vec{r}' \, d\vec{R}_2 \, d\vec{R}_3 \quad d\vec{R}_{A-},$$

with the Jacobian $J = \left(\frac{A^2}{A^2-1}\right)^3$, as already seen. The product $\phi\eta$ is given in the preceding section and for (i, j), the three basic couples, i.e.

$$\begin{aligned} (A-1, A) &= \vec{R}_{A-1}, \\ (1, 2) &= \vec{U} - \frac{A-2}{A-1}\vec{R}_2; \quad (A+1, 2) = \vec{V} - \frac{A-2}{A-1}R_2 = (12)^{\dagger}; \\ (A+1, 1) &= \vec{U} - \vec{V}. \end{aligned}$$

The results we get for the kinetic energy and the potential kernels, using the method given in the Appendix, are given in the Tables II and III (also in the Appendix), which can be used as follows.

A. The general form of the kernels given in Appendix I is adopted so that F, D, $a_1 \equiv [\beta^{pq}]$, $a_2 \equiv [\gamma^{pq}]$, A_1, A_2, B, and E have the same definition throughout.

B. $\mu = 0$ in an potential kernel gives the energy-dependent kernel $\mathcal{N}$.

C. In the following table it must be noted that $A' = A+1$. By making $\lambda = \nu$ one gets the kernels of an elastic scattering problem.

Then if we make $A = 2, 3, 4$ one gets the corresponding kernels for n-D, nHe^3, and $n\text{-}He^4$ respectively.

D. The kernels occurring in AA and AB can be calculated in the same way as the previous ones, using Table I for the change of variables; results given in Table III.

E. Tables II and II are given in Appendix III.

4. The Coefficients of w, m, b, h in BB

We consider now the elastic case only. From the foregoing sections and for a given value of the total spins of th A+1 nucleons, and after integration over the internal variables, we get

$$0 = -\frac{\hbar^2}{2\mu}[\nabla_v^2 + k^2]\, F(\vec{v}) + (\omega w+\mu m+\beta b+th)\, F(\vec{v}) \int \phi^2 (A, Z)\, V^{1, A+1}\, d\tau$$

$$+\int \Big\{ \gamma[T - \mathcal{E}(k)\mathcal{N}] + \frac{(A-1)(A-2)}{2}(\omega' w+\mu' m+\beta' b+t' h)\, K^{A-1, A} + (\mu w+\omega m+tb+\beta h)\, K^{1, A+1}$$

$$+ (\omega'' w+\mu'' m+\beta'' b+t'' h)[K^{12}+K^{A+1, 2}] \Big\}\, F(\vec{r})\, d\vec{r}',$$

with $k^2 = E(N)\, \frac{2\, A\, M}{\hbar^2 (A+1)}$,

$\mathcal{E}(k) = E(A, Z) + E(N)$.

It is possible to give a general formula for ω, μ, β, and t and, at least for the others, to say that they only need to be calculated for a single couple: (A-1, A) for ω', μ', β', and t', and (12) for ω'', μ'', β'', and t''.

Consider first the single kernel $K^{1, A+1}$.

Using the multiplication table (p. 7) we see that μ and t are now the coefficients of w and b.

Therefore $\mu = - \sigma_s^{s}(A+1;\ 1,2,\cdots A) \cdot \sigma_s^{s}(1\ ;\ A+1,\ 1,2,\cdots A)$,

where σ_s^{s}'s are the spin function of the $(A+1)$ nucleons before and after exchange.

Also $\gamma = \mu$.

From the definition of the Bartlett operator, we have

$$B_{A+1,1}\sigma_s^{s}(1\ ;\ A+1,\ 1,2,\cdots A) = \sigma_s^{s}(A+1\ ;\ 1,2,\cdots A),$$

and $t = - p$ if there is p exchange involved in the total wave function.

The number of such exchanges in N-(A, Z) problems corresponds to the number of nucleons of the same nature of N contained in (A, Z),

i. e., $p = 1$ for n - D, n-He^3, p - T,

$p = 2$ for n - T, nHe^4, etc.

Because of the i-spin dependence of the Heisenberg operator, we see that for a given problem this coefficient is the same for different values of the total o-spin.

Consider now the direct potential term.

We have seen that the contribution of each $V_{A+1,i}$ was the same for $i = 1, 2,\cdots A$.

As $W_{A+1,i}$ is an identity operator, we obviously have $\omega = A$.

Now we have $B_{A+1,i} = \frac{1}{2}(1 + \vec{\sigma}_{A+1} \cdot \vec{\sigma}_i)$,

where $\vec{\sigma}_{A+1}$ is the spin of the incident nucleon and $\vec{\sigma}_i$ the spin of one nucleon of the nucleus.

As we deal with the direct term we have

$$\sum_{i=1}^{A} \left\langle \sigma_S^{S}(A+1;\ 1,2,\cdots A) \middle| \vec{\sigma}_{A+1} \cdot \vec{\sigma}_i \middle| \sigma_S^{S}(A+1;\ 1,2,\cdots A) \right\rangle$$

$$= \left\langle \sigma_S^{S}(A+1;\ 1,2,\cdots A) \middle| \vec{\sigma}_{A+1} \cdot \sum_{i=1}^{A} \vec{\sigma}_i \middle| \sigma_S^{S}(A+1;\ 1,2,\cdots A) \right\rangle = E,$$

where E is the eigenvalue of the scalar operator $(\vec{\sigma}_{A+1} \cdot \sum_{i=1}^{A} \vec{\sigma}_i)$.

Now $\sum_{i=1}^{A} \vec{\sigma}_i$ is by definition the total spin s of the target nucleus.

As $\vec{S} = \vec{s} + \vec{\sigma}_{A+1}$, and $\sigma_{A+1} = \frac{1}{2}$ for a nucleon, we have

$$E = 2\left[S(S+1) - s(s+1) - \frac{3}{4} \right],$$

and finally, $\beta = \frac{A}{2} + S(S+1) - s(S+1) - \frac{3}{4}$.

As o- and i-spin spaces are different, β is the same for two states of same o-spin states but different i-spin states (i.e. different charge), e.g., n-He^3 and nT.

Values of β for a few values of s and S with $\sigma_{A+1} = \frac{1}{2}$

		β
$s = 0$	$S = \frac{1}{2}$	$\frac{1}{2}A$
$s = 1/2$	$S = \begin{cases} 1 \\ 0 \end{cases}$	$1/2A+1/2$ $1/2A-3/2$
$s = 1$	$S = \begin{cases} \frac{3}{2} \\ \frac{1}{2} \end{cases}$	$1/2A+1$ $1/2A-2$

The formulation in this Chapter IV is valid for a central nuclear two-body potential of any shape (Gaussian, exponential, Yukawa, etc.) and nuclear space-part wave functions invariant with respect to permutation of the nucleons. The results of calculation given in Tables II and III are restricted to Gaussian forms for the potential shape and the nuclear space-part wave functions.

V. Solutions of the Equations and Calculation of Cross Sections

When we are left with the variables $\vec{r}$ and $\vec{r}'$ (after integrating over the other variables) the integration over the angular variables is carried out as usual:

$$F(\vec{r}) = \sum_{\ell} \frac{1}{r} f_{\ell}(r) P_{\ell}(\cos\theta),$$

$$K(\vec{r}, \vec{r}') = \sum_{\ell} \frac{2\ell+1}{4\pi r r'} K_{\ell}(r, r') P_{\ell}(\mu),$$

and consequently $K(r, r') = 2\pi r r' \int_{-1}^{+1} K(\vec{r}, \vec{r}') P_{\ell}(\mu)\, d\mu,$

where $K(\vec{r}, \vec{r}')$ is any of the kernels and F any scattering function,

θ is the angle of scattering in the center-of-mass frame,

and $\mu = \frac{\vec{r}, \vec{r}'}{r r'}$.

The systems then obtained for each value of S are easily deduced from the previous ones with $f_{\ell}(r)$ instead of $F(\vec{r})$, and $K_{\ell}(r, r')$ instead of $K(\vec{r}, \vec{r}')$, and are, of course, valid for the corresponding ℓ value only. They are of the form

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + k_a^2\right] f_{\ell}^{a}(r) = U^{aa}(r)\, f_{\ell}^{a}(r) + \int_0^{\infty} K_{\ell}^{a1}(r, r')\, f_{\ell}^{1}(r')\, dr'$$

$$+ \int_0^{\infty} K_{\ell}^{a2}(r, r')\, f_{\ell}^{2}(r')\, dr' + \int_0^{\infty} K_{\ell}^{a\beta}(r, r')\, f_{\ell}^{\beta}(r')\, dr',$$

where $a = 1, 2, \beta$ is the channel index.

Using finite-difference approximations, Eqs. (4.1) are represented as a set of linear simultaneous equations, the unknown being the values of $f_l^a(r)$ over the range of r required.[4] For the three-channel case, for instance, it is necessary to find three independent solutions such that

$$f_l^{aj}(r) = \frac{1}{\sqrt{v_a}} \left[A_l^{aj} F(r) + B_l^{aj} G(r) \right]$$

for $a = 1, 2, 3$ (three channels),

$j = 1, 2, 3$ (three independent solutions),

where $F_l^a(r)$, $G_l^a(r)$ are the regular and irregular wave function[20] for the corresponding channel a.

Then the reactance matrix is

$$R = BA^{-1},$$

and the scattering matrix is $S = \frac{1+iR}{1-iR}$.

The scattering amplitude $f_{a'a}^s(\theta)$ corresponding to the total spin S can be written

$$f_{a'a}^s(\theta) = -\frac{1}{2ik_a} \sum_l (2l+1) P_l(\cos\theta) \left[\delta_{a'a} - S_{a'a}^l \right],$$

and the corresponding differential cross section is

$$\sigma_{a'a}^s(\theta) = \left| f_{a'a}^s(\theta) \right|^2 .$$

Then the differential cross section is the appropriate weighted sum

$$\sigma_{a'a}(\theta) = \frac{1}{(2I_1+1)(2I_2+1)} \sum_s (2S+1) \sigma_{a'a}^S(\theta),$$

where I_1 and I_2 are the spin of the colliding particles and s the spin of the whole system, $(2I_1+1)(2I_2+1)$ being the total number of spin states and $(2s+1)$ the number of states with spin s.[13a]

VI. Conclusions

To appreciate the true value of Wheeler's method, it is useful to quote Blatt and Weisskopf.[21]

> It is useful to divide the target nuclei into three categories
>
> | | | |
> |---|---|---|
> | A - | Light nuclei | $1 \leq A \leq 25$ |
> | B - | Intermediate nuclei | $25 \leq A \leq 80$ |
> | C - | Heavy nuclei | $80 \leq A \leq 240$ |
>
> The light nuclei (group A) must be treated individually. It is almost impossible to apply any general rules describing nuclear reactions in that group. . . . The assumptions made in the preceding chapter about the interior of the nucleus are not applicable to group A, since there are too few nucleons in these nuclei for a well-defined interior region. All nucleons are at the "surface" of the nucleus.

Two cases that are beyond the scope of this paper have also been treated, namely the elastic scattering of six nucleons (t-t reaction) by Bransden and Hamilton,[22] and of eight nucleons (α-α reactions) by Butcher and McNamee[23] and Schmid and Wildermuth.[24]

In each case, numerical results have been obtained and compared with experimental data;[25] the relative merits of different types of forces have been investigated and conclusions have been drawn.

The main point of this conclusion is that the resonating-group structure[1] can well explain all the experimental results obtained on the few-nucleon scattering experiments. As pointed out by Bransden,[16] it is a means of correlating data with just a few parameters, namely the range and depth of the potential and the exchange type of force. Although in particular cases one type of force can fit better than another one, it is remarkable that the Serber type fits all cases reasonably well.

The central two-body potential with central forces can be criticized, but the inclusion of a noncentral force and particularly of a tensor force makes the problem enormously complicated.

Also the Gaussian shape adopted for the nuclear wave function can be criticized as being too rapidly cut off, but it is possible to apply the same general method to any other type of wave function, and particularly the Irving type,[26] to build up general formulae for kernels and direct terms in terms of the number of nucleons A involved in the target nucleus.

Finally, it is also suggested that the work be extend to cases $A>4$ by using wave functions of the appropriate symmetry, and to the cases $(A'Z')(A, Z)$ by using the general form of the wave function, both for the incident and the target nuclei, to include, for instance t-t and α-α reactions.

Appendix A. The Nuclear-Part Calculations

Consider first the kinetic energy operator. The difficulty arises from the term $(A(r, r'), \nabla_{r'}^2 F(r'))$, because $F(r')$ is not yet known. But, as $\nabla_{r'}^2$ is an Hermitian operator, the result is the same when its adjoint is applied on the left-hand side (which in other words is Green's theorem). Now r' is involved in a change of variables of the type

$$U = ar' + bv,$$

$$V = br' + av,$$

and we have

$$\nabla_{r'}^2 = a^2 \nabla_u^2 + b^2 \nabla_v^2 + 2ab \vec{\nabla}_u \cdot \vec{\nabla}_{v'}$$

with

$$\nabla_\rho^2 \exp(-\lambda\rho^2 + \vec{\mu}\cdot\vec{\rho}) = \left\{4\lambda^2\rho^2 - 4\lambda\vec{\mu}\cdot\vec{\rho} + \mu^2 - 6\lambda\right\} \exp(-\lambda\rho^2 + \vec{\mu}\cdot\vec{\rho}).$$

Then we have to consider the intergration over internal variables.

For the direct term, it is only a matter of applying as many times as is necessary, the general formula

$$\int (A s^2 + B \vec{s}\cdot\vec{\nu} + c) \exp(-\lambda s^2 \pm \mu\cdot s + f) d\vec{s} = \left[A \frac{6\lambda+\mu^2}{4\lambda^2} \pm B \frac{\vec{\nu}\cdot\vec{\mu}}{2\lambda} + C\right]\left(\frac{\pi}{\lambda}\right)^{3/2} \exp(\mu^2/4\lambda + f).$$

Using the spherical harmonic expansion given at the end of Chapter IV, one is led for the kernels to the form

$$K_\ell(r, r') = 2\pi rr' \int_{-1}^{+1} K(\vec{r}, \vec{r'}) \, P_\ell(\mu) \, d\mu,$$

with $\mu = \frac{\vec{r}\cdot\vec{r'}}{rr'} = \cos\theta.$

In the present formulation, the two forms met for $K(\vec{r}, \vec{r}')$ are

$$K(\vec{r}, \vec{r}') = f(r, r')\ e^{-D\, rr'\mu}, \qquad \text{both with } D \geq 0; \tag{A-1}$$

$$K(\vec{r}, \vec{r}') = f(r, r')\ \mu\, e^{-D\, rr'\mu}, \tag{A-2}$$

the second form occurs in the kinetic energy terms.

Consider the well-known expansion

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} (2l+1)\, i^l\, P_l(\cos\theta) \left(\frac{\pi}{2kr}\right)^{1/2} J_{l+1/2}(kr)$$

If we write $kr = ix$, multiply both sides by $P_l(\mu)$, and integrate over μ, then owing to the properties of the Legendre polynomial,

$$\int_{-1}^{+1} P_l(\mu)\, P_{l'}(\mu)\, d\mu = \frac{2}{2l+1}\, \delta_{ll'}, \tag{A-3}$$

we get

$$\int_{-1}^{+1} \exp(-x\mu)\, P_l(\mu)\, d\mu = 2i^{l-1/2} \left(\frac{\pi}{2x}\right)^{1/2} J_{l+1/2}(ix) = \frac{2}{x}\, \mathcal{J}_{l+1/2}(x). \tag{A-4}$$

Defining

$$\mathcal{J}_{l+1/2}(x) = i^{(l-1/2)} \left(\frac{\pi x}{2}\right)^{1/2} J_{l+1/2}(ix), \tag{A-5}$$

so that

$$\mathcal{J}_{1/2}(x) = \sinh x, \qquad \mathcal{J}_{3/2}(x) = \frac{\sinh x}{x} - \cosh x, \tag{A-6}$$

Deriving Eq. (4) with respect to x we get

$$(-1) \int_{-1}^{+1} \mu \exp(-x\mu)\, P_l(\mu)\, d\mu = \frac{2}{x}\, \mathcal{J}'_{l+1/2}(x) - \frac{2}{x^2}\, \mathcal{J}_{l+1/2}(x), \tag{A-7}$$

defining

$$\mathcal{J}'_{\ell+1/2}(x) = \frac{d}{dx}\left\{\mathcal{J}_{\ell+1/2}(x)\right\} . \qquad (A-8)$$

For the sake of the d-d elastic case, some more details must be emphasized.

First of all, some kernels occur with simply D = 0:

$$K(\vec{r}, \vec{r'}) = f(r, r'),$$

and using (3), we have

$$k_\ell(r, r') = 2\pi rr' \int_{-1}^{+1} f(r, r') P_\ell(\mu) d\mu$$

$$= 4\pi rr' f(r, r') \delta_{o\ell} . \qquad (9)$$

So that in the following tables, for D = o, the quantities occur only for $\ell = 0$ but not for other values of ℓ.

Secondly, some kernels occur with D < 0.

The parity of the hyperbolic spherical Bessel function is then involved, and we have

$$\mathcal{J}_{\ell+1/2}(-x) = (-1)^{\ell+1} \mathcal{J}_{\ell+1/2}(x), \quad \mathcal{J}'_{\ell+1/2}(-x) = (-1)^{\ell} \mathcal{J}'_{\ell+1/2}(x) .$$

Thirdly, although the following tables are given as usual in terms of $\mathcal{J}_{\ell+1/2}(x)$ and $\mathcal{J}'_{\ell+1/2}(x)$, in practice it is better to replace $\mathcal{J}'_{\ell+1/2}(x)$, using the recurrence relation

$$\mathcal{J}'_{\ell+1/2}(x) = \frac{\ell+1}{x} \mathcal{J}_{\ell+1/2}(x) - \mathcal{J}_{\ell+3/2}(x) ,$$

so that (7) becomes

$$\int_{-1}^{+1} \mu\, e^{-x\mu}\, P_\ell(\mu)\, d\mu = \frac{2}{x}\, \mathcal{J}_{\ell+3/2}(x) - \frac{2\ell}{x^2}\, \mathcal{J}_{\ell+1/2}(x) .$$

Therefore finally the two basic formulae, used as many times as needed, are

$$K_\ell(r,r') = \frac{4\pi}{D}\, f(r,r')\, \mathcal{J}_{\ell+1/2}(D\,rr'), \qquad \text{in cae} \quad (A\text{-}1);$$

$$K_\ell(r,r') = \frac{4\pi}{D}\, f(r,r') \left\{ \mathcal{J}_{\ell+3/2}(D\,rr') - \frac{\ell}{x}\, \mathcal{J}_{\ell+1/2}(D\,rr') \right\}, \text{ in case (A-2).}$$

For any kernel--in d-d, for instance--we have the forms

AA: $$K_\ell(r',v) = \frac{1}{N_D^4} \left\{ K_\ell^0 + 2\,CK_\ell^1 + 2\,C^2K_\ell^2 + 2\,C^3K_\ell^3 + C^4K_\ell^4 \right\};$$

AB: $$K_\ell(r',v) = \frac{1}{N_D^2 N_\phi} \left\{ K_\ell^0 + C\,K_\ell^1 + C^2K_\ell^2 \right\};$$

BC: $$K_\ell(r',v) = \frac{1}{N_\phi N_\eta}\, K_\ell(r',v) .$$

For convenience, $K_\ell^n = \sum_i {}^iK_\ell^n$.

The K_ℓ^3 and K_ℓ^4 kernels as well as $(\text{II}\,K_\ell^1)_{AB}$ are deduced respectively from K_ℓ^1, K_ℓ^0 and $(\text{I}\,K_\ell^1)_{AB}$ by interchanging α and β.

For the kinetic energy kernels of the different elements, we have the forms

AA:

$$K_\ell^n(r'v) = -\frac{\hbar^2}{M}(F)^{3/2}\, \frac{4\pi}{D} \left\{ e^{(-a_1r'^2 - a_2v^2)} \times \right.$$

$$\left\{ \left[A_1r'^2 + A_2v^2 - E + \frac{B}{D} \right] \mathcal{J}_{\ell+1/2}(Dr'v) - Br'v\, \mathcal{J}'_{\ell+1/2}(Dr'v) \right\}$$

$$\left. + (1 - \delta_{a_1a_2}\delta_{A_1A_2})\, e^{-a_2r'^2 - a_1v^2} \left\{ \left[A_2r'^2 + A_1v^2 - E + \frac{B}{D} \right] \mathcal{J}_{\ell+1/2}(Dr'v) - Br'v\, \mathcal{J}'_{\ell+1/2}(Dr'v) \right\} \right\};$$

AB or BC:

$$K_\ell^n(r',v) = -\frac{\hbar^2}{M}(F)^{3/2}\frac{4\pi}{E}e^{-a_1 r'^2 - a_2 v^2}\left\{A_1' r'^2 + A_2 v^2 - E + \frac{B}{D}\right\} \mathcal{J}_{\ell+1/2}(Dr'v) - Br'v\, \mathcal{J}'_{\ell+1/2}(Dr'v)$$

The BB, CC, and AC kinetic energy kernels are deduced from the ones given by suitable changes for λ and ν.

For the potential kernels $A_1 = A_2 = B = 0$, we have $E = V_0 \frac{M}{\hbar^2}$.

Using these notations, we need only to give the following tables for the kinetic energy kernels.

N.B. The energy-dependent kernel for a given element is obtained by putting $\mu = 0$ in any of the potential kernels of the corresponding element.

Appendix B. The Coulomb-Part Calculations

The Coulomb potential, owing to the presence of the two protons, leads us to consider some other types of integrals. In the direct term, in particular, we have the type

$$I = \int d\vec{z}\ \frac{e^{-hz^2}}{|\vec{\xi}+m\vec{\xi}|} = \frac{2\pi}{mh}\int_0^1 dt\ e^{-\frac{h}{m^2}\xi^2 t^2}$$

$$= \left(\frac{\pi}{h}\right)^3 \frac{1}{\xi}\,\bar{\Phi}\left(\sqrt{\frac{h}{m}}\,\xi\right),$$

where $\bar{\Phi}(x)$ is the error function, defined as

$$\bar{\Phi}(x) = \frac{2}{\sqrt{\pi}}\int_0^x \exp(-t^2\, dt).$$

A very easy program for Mercury can be written for tabulating U_{24}^c at the pivotal points used for this whole problem [0.3 (0.3) 4.8, then 5.4 (0.6) 19.2], and adding the results to the corresponding nuclear part to get the complete tabulation of the direct term.

For the Coulomb kernels we meet expressions of the form

$$K_\ell(r, r') = 2\pi\, rr' \int_{-1}^{+1} K(\vec{r}, \vec{r'})\, P_\ell(\mu)\, d\mu,$$

where $$K(\vec{r}, \vec{r'}) = \frac{e^{-\beta_k r^2 - \gamma_k r'^2}}{\sqrt{r^2 + r'^2 + 2rr'\mu}} \qquad \text{(B-1)}$$

and $$K(\vec{r}, \vec{r'}) = \frac{e^{-\beta_k r^2 - \gamma_k r'^2 \mp Drr'\mu}}{\sqrt{r^2 + r'^2 + 2rr'\mu}} \qquad \text{(B-2)}$$

We have the well-known expansion

$$\frac{1}{\sqrt{r^2+r'^2+2rr'\mu}} = \frac{1}{r_>} \sum_{n=0}^{\infty} (-1)^n t^n P_n(\mu), \quad \text{with } t = \frac{r'_<}{r_>},$$

so that in case (B-1), again using

$$\int_{-1}^{+1} P_\ell(\mu)\, P_{\ell'}(\mu)\, d\mu = \frac{2}{2\ell+1}\, \delta_{\ell\ell'},$$

we have

$$K_\ell(r, r') = \frac{1}{r_>}\, 4\pi rr'\, e^{-\beta_k r^2 - \gamma_k r'^2} \left[\frac{(-1)^\ell}{2\ell+1}\right] (t)^\ell\, \delta_{o\ell'}$$

$r_>$ being greatest between r and r'.

In case (B-2) we have the form

$$I_c = \frac{1}{r_>} \int_{-1}^{+1} e^{-Drr'\mu}\, P_\ell(\mu) \sum_{n=0}^{\infty} (-t)^n P_n(\mu)\, d\mu.$$

The practical way we have used to deal with this integral has been to consider each particular phase separately, express I_c in terms of the $J_{\ell+1/2}$,

and stop the infinite expansion when the contribution of the terms is too small to be taken into account by the machine; we have checked that this happens at $n = 5$, therefore we have taken the terms up to $n = 5$ inclusive. The cases of the $\ell = 0$, 1, and 2 are given explicitly hereafter.

For $\ell = 0$, $P_0(\mu) = 1$, we have

$$I_c = \frac{4\pi}{D}\,\frac{1}{r_>}\left\{ \mathcal{J}_{1/2}(Drr') - t\,\mathcal{J}_{3/2}(Drr') + t^3\,\mathcal{J}_{5/2}(Drr') - \cdots - t^5\,\mathcal{J}_{11/2}(Drr') + \cdots \right\}.$$

For $\ell = 1$, $P_1(\mu) = \mu$, and using the recurrence formula

$$\mu\,P_n(\mu) = \frac{n+1}{2n+1}\,P_{n+1}(\mu) + \frac{n}{2n+1}\,P_{n-1}(\mu),$$

we get

$$I_c = \frac{4\pi}{D}\,\frac{1}{r_>}\left\{ -\frac{1}{3}\,t\,\mathcal{J}_{1/2}(Drr') + \left(1+\frac{2}{5}\,t^2\right)\mathcal{J}_{3/2}(Drr') - \left(\frac{2}{3}\,t + \frac{3}{7}\,t^3\right)\mathcal{J}_{5/2} \right.$$

$$\left. + \left(\frac{3}{5}\,t^2 + \frac{4}{5}\,t^4\right)\mathcal{J}_{7/2} - \left(\frac{4}{7}\,t^3 + \frac{5}{11}\,t^5\right)\mathcal{J}_{5/2} + \left(\frac{5}{9}\,t^4 + \frac{6}{13}\,t^6\right)\mathcal{J}_{11/2} - \cdots \right\}.$$

For $\ell = 2$, $P_2(\mu) = \frac{3}{2}\,\mu^2 - \frac{1}{2}$, and using the recurrence formula

$$P_2(\mu)\,P_n(\mu) = \frac{3(n+1)(n+2)}{2(2n+1)(2n+3)}\,P_{n+2}(\mu) + \frac{n(n+1)}{(2n+3)(2n-1)}\,P_n(\mu) + \frac{3n(n-1)}{2(2n-1)(2n+1)}\,P_{n-2}(\mu),$$

we get

$$I_c = \frac{4\pi}{D}\,\frac{1}{r_>}\left\{ \frac{t^2}{5}\,\mathcal{J}_{1/2}(Drr') - \left(\frac{2}{5}\,t + \frac{9}{35}\,t^3\right)\mathcal{J}_{3/2} + \left(1 + \frac{2t^2}{7} + \frac{2t^4}{7}\right)\mathcal{J}_{5/2} \right.$$

$$- \left(\frac{3t}{5} + \frac{4t^3}{15} + \frac{10t^5}{33}\right)\mathcal{J}_{7/2} + \left(\frac{18}{35}\,t^2 + \frac{20}{77}\,t^4 + \frac{45}{143}\,t^6\right)\mathcal{J}_{9/2}$$

$$\left. - \left(\frac{10}{21}\,t^3 + \frac{10}{99}\,t^5 + \frac{21}{65}\,t^7\right)\mathcal{J}_{11/2} + \cdots \right\}.$$

Modifications to the standard kernel program were made by P. G. Burke to build up special program for Coulomb kernels corresponding to $\ell=0$, $\ell=1$, and $\ell=2$.

For the Coulomb kernels of the second kind we have

$$K(\vec{r}, \vec{r'}) = \frac{e^{-kz^2 - f(\vec{\xi})}}{|\vec{\xi} + m\vec{z}|} ,$$

where $\vec{z}$ is an internal variable.

The integration over $\vec{z}$ is dealt with as seen for the Coulomb potential, giving

$$\frac{2\pi}{mh} \int_0^1 dt \; e^{-\frac{h}{m^2}\xi^2 t^2 - f(\vec{\xi})} .$$

Now there is no denominator, and all subsequent integrations are of a type previously met (particularly for the angular integration), giving again an $\mathcal{J}_{\ell+1/2}(Drr')$.

The integration over the dummy variable t is left for the last step and done numerically, using, for instance, a six-point Gaussian integration formula (Ref. 19, p. 577). One gets an appropriately weighted sum of six terms, each of them with the same form as for a nuclear potential kernel, and the tabulation of this second kind of Coulomb kernel can be carried out by using the standard kernel program.[5]

Appendix III

Table II

Table III

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Table II - For BC terms.

$$\left[\beta^{pq}\right] = \frac{A^2(A-1)}{(A^2-1)^2}\left[\beta^{oo} + \frac{\mu\beta^{pq}}{d^{oo}+\mu d^{pq}}\right] \qquad \left[\gamma^{pq}(\lambda,\nu)\right] = \left[\beta^{pq}(\nu,\lambda)\right]$$

$$F^{pq} = \left(\frac{2\sqrt{\lambda\nu}}{\lambda+\nu}\right)^{A-3}\frac{A^3(A-1)}{(A^2-1)^2}\frac{2A^2}{\pi}\frac{\lambda\nu}{d^{oo}+\mu d^{pq}} \qquad D^{pq} = \frac{A^3(A-1)}{(A^2-1)^2}\left[n^{oo} + \frac{\mu n^{pq}}{d^{oo}+\mu d^{pq}}\right]$$

$\beta^{oo} = \nu A^2 + \lambda$ $\qquad$ $\gamma^{oo} = \lambda A^2 + \nu$ $\qquad$ $d^{oo} = A(\lambda+\nu)$ $\qquad$ $n^{oo} = \lambda + \nu$

p q	β^{pq}	γ^{pq}	d^{pq}	n^{pq}
A-1, A	0	0	4	0
1, A+1	$2A(A-1)(\lambda+\nu)$	$2A(A-1)(\lambda+\nu)$	0	$-2(A-1)(\lambda+\nu)$
A+1, 2	$\frac{2A}{A-1}(\lambda+\nu)$	$\frac{2A^3}{A-1}(\lambda+\nu)$	$\frac{2(A-2)}{A-1}$	$\frac{2A}{A-1}(\lambda+\nu)$
1, 2	$\frac{2A^3}{A-1}(\lambda+\nu)$	$\frac{2A}{A-1}(\lambda+\nu)$	$\frac{2(A-2)}{A-1}$	$\frac{2A}{A-1}(\lambda+\nu)$

Kinetic Energy Terms -

$$A^{(1)}(\to\lambda,\nu) = \frac{A^5(A-1)}{2(A+1)(A^2-1)^2}\left\{\nu^2A^2 + \lambda^2 + 2\lambda\nu\right\} \qquad B = \frac{A^4(A-1)}{(A+1)(A^2-1)^2}\left\{A^2(\lambda^2+\nu^2) + (A^2+1)\lambda\nu\right\}$$

$$E = \frac{3A}{2(A^2-1)}\left\{\frac{\nu^2A^2 + \lambda^2(A^3-2A^2-A+3) + \lambda\nu(A^3-A+2)}{\lambda+\nu}\right\}$$

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Table III, 1 – Type $(AA|I|pq)_{Nuclear}$

$$\left[\beta^{pq}\right] = \left(\frac{A}{A+2}\right)^2 \frac{\beta^{oo} + \mu\beta^{pq}}{d^{oo} + \mu d^{pq}} \qquad \left[\gamma^{pq}\right] = \left(\frac{A}{A+2}\right)^2 \frac{\gamma^{oo} + \mu\gamma^{pq}}{d^{oo} + \mu d^{pq}}$$

$$F^{pq} = \frac{\lambda(A-1)}{d^{oo} + \mu d^{pq}} \qquad D^{pq} = 2\left(\frac{A}{A+2}\right)^2 \frac{n^{oo} + \mu n^{pq}}{d^{oo} + \mu d^{pq}}$$

$$\beta^{oo} = \frac{A^2}{4}\lambda^2 + 4\alpha\beta + \frac{A^2-2A+2}{A-1}\lambda(\alpha+\beta) + \frac{A(A+2)}{A-1}\lambda\beta$$

$$\gamma^{oo} = \frac{A^2}{4}\lambda^2 + 4\alpha\beta + \frac{A^2-2A+2}{A-1}\lambda(\alpha+\beta) + \frac{A(A+2)}{A-1}\lambda\alpha$$

$$d^{oo} = \alpha + \beta + \frac{\lambda A^2}{4(A-1)} \qquad n^{oo} = \frac{A^2}{4}\lambda^2 + 4\alpha\beta + \frac{A(A-3)}{A-1}(\alpha+\beta)\lambda$$

p q	β^{pq}	γ^{pq}	d^{pq}	n^{pq}
A-1, A	0	0	$\frac{2}{\lambda A} d^{oo}$	0
1 , A+1	$4d^{oo}$	$4d^{oo}$	0	$4d^{oo}$
A+1, A+2	$4\beta + \frac{\lambda}{A-1}(A^2-2A+2)$	$4\beta + \frac{2\lambda}{A-1}(A^2+1)$	1	$4\beta + \frac{\lambda A(A-3)}{A-1}$
A+2, 2	$\frac{\lambda(3A^2-2A+8)}{4(A-1)} + \frac{4\alpha\beta(A-2)}{\lambda A(A-1)} + \frac{2(A^2-A+2)(\alpha+\beta)}{A(A-1)}$	$\gamma^{A+2,2} = \beta^{A+2,2}$	$\frac{1}{A-1}\left[\frac{A-2}{2} + \frac{(A-2)(\alpha+\beta)}{\lambda A}\right]$	$\frac{1}{A-1}\left[\frac{\lambda A(A-10)}{4} + \frac{4(A-2)\alpha\beta}{\lambda A} + (A-6)(\alpha+\beta)\right]$
1 , 2	$\frac{\lambda A(3A-2)}{4(A-1)} + \frac{4(A-2)\alpha\beta}{\lambda A(A-1)} + \frac{2(A^2-2A+2)}{A(A-1)}(\alpha+\beta) - 4\alpha$	$\gamma^{1,2} = \beta^{1,2} + 2(A+3)\alpha$	$\frac{1}{A-1}\left[\frac{A}{2} + \frac{(A-2)(\alpha+\beta)}{\lambda A}\right]$	$\frac{1}{A-1}\left[\frac{\lambda A(3A-2)}{4} + \frac{4(A-2)\alpha\beta}{\lambda A} + (A-6)(\alpha+\beta) + 2A\alpha\right]$

Table III, 2 — Type $(AA|II|pq)_{Nuclear}$

$$\left[\beta^{pq}\right] = \frac{(A-2)A^2}{(A^2-4)^2}\left[\beta^{oo} + \frac{\mu\beta^{pq}}{d^{oo}+\mu d^{pq}}\right] \qquad \left[\gamma^{pq}\right] = \frac{(A-2)A^2}{(A^2-4)^2}\left[\gamma^{oo} + \frac{\mu\gamma^{pq}}{d^{oo}+\mu d^{pq}}\right]$$

$$F^{pq} = \frac{16\lambda^2 A(A-2)}{d^{oo}+\mu d^{pq}} \qquad D^{pq} = \frac{2(A-2)A^2}{(A^2-4)^2}\left[n^{oo} + \frac{\mu n^{pq}}{d^{oo}+\mu d^{pq}}\right]$$

$$\beta^{oo} = \gamma^{oo} = (A^2+4)\lambda \qquad d^{oo} = (\lambda A+4\alpha)(\lambda A+4\beta) \qquad n^{oo} = 4A\lambda$$

p q	β^{pq}	γ^{pq}	d^{pq}	n^{pq}
A-1, A	0	0	0	0
1 , A+1	$(A-2)d^{oo}$	$(A-2)d^{oo}$	$2[\lambda A + 2(\alpha+\beta)]$	$-(A-2)d^{oo}$
A+1, A+2	0	0	$\lambda A + 4\alpha$	0
A+1, 3	$\frac{A^2}{4}$	$4\frac{d^{oo}}{A-2}$	$(\lambda A + 4\beta)\left[\frac{2A-5}{A-2} + \frac{4\alpha(A-3)}{\lambda A(A-2)}\right]$	$\frac{d^{oo}}{A-2}$

Table III, 3 – Type (AA|I|K.E.)

$$A^{(1)} = \frac{A^2}{(A+2)^3 (d^{00})^2} \left\{ 64(A+1)\alpha^2\beta^2 + 32\frac{A(A^2+1)}{A-1}\lambda\alpha^2\beta + \frac{16A^2(A-3)}{A-1}\lambda\alpha\beta^2 + \frac{4A^3}{(A-1)^2}(3A^2-7A+8)\lambda^2\alpha\beta + \frac{4A^2}{(A-1)^2}(2A^3+5A+1)\lambda^2\alpha^2 + \frac{A^3}{(A-1)^2}(3A^2-11A+16)\lambda^2\beta^2 + \frac{A^4}{A-1}(2A-1)\lambda^3\alpha + \frac{A^4}{A-1}\left(\frac{3}{2}A-2\right)\lambda^3\beta + \frac{3}{16}\frac{A^6}{A-1}\lambda^4 \right\}$$

$$B = \frac{2A^2}{(A+2)^3 (d^{00})^2} \left\{ 64(A+1)\alpha^2\beta^2 + \frac{8A}{A-1}(3A^2-3A+2)\lambda\alpha\beta(\alpha+\beta) + \frac{A^2}{(A-1)^2}(11A^3-35A^2+16A-12)\lambda^2\alpha\beta + \frac{2A^2}{(A-1)^2}(2A^3-7A^2+A-4)\lambda^2(\alpha^2+\beta^2) + \frac{A4}{4(A-1)}(7A-6)\lambda^3(\alpha+\beta) + \frac{3A^6}{16(A-1)}\lambda^4 \right\}$$

$$E = \frac{3}{4(A+2)d^{00}} \left\{ 16(A+1)\alpha\beta + \frac{4(A^3+5A^2-2A+4)}{A-1}\lambda(\alpha+\beta) + \frac{A^3(A+4)}{4}\lambda^2 \right\}$$

Table III, 4 – Type (AA|II|K.E.)

$$A = \frac{A^5(A^2+12)}{(A+2)(A^2-4)^2}\lambda^2$$

$$B = \frac{4A^4(3A^2+12)}{(A+2)(A^2-4)^2}\lambda^2$$

$$E = 3\lambda A \left\{ \frac{2\alpha}{\lambda A+4\alpha} + \frac{2\beta}{\lambda A+4\beta} + \frac{A+1}{4} + \frac{4}{A^2-4} \right\}$$

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Table III, 5 — Type $(AA|I|pq)_{coulomb}$

$$\left[\beta^{pq}\right] = \left(\frac{A}{A+2}\right)^2 \frac{\beta^{oo} + t^2\beta^{pq}}{d^{oo} + t^2 d^{pq}} \qquad \left[\gamma^{pq}\right] = \left(\frac{A}{A+2}\right)^2 \frac{\gamma^{oo} + t^2\gamma^{pq}}{d^{oo} + t^2 d^{pq}} \qquad F^{pq} = \frac{\lambda(A-1)}{d^{oo} + t^2 d^{pq}} \qquad D^{pq} = 2\left(\frac{A}{A+2}\right)^2 \frac{n^{oo} + t^2 n^{pq}}{d^{oo} + t^2 d^{pq}}$$

β^{oo}, γ^{oo}, d^{oo} and n^{oo} as for Table III, 1.

p , q	β^{pq}	γ^{pq}	d^{pq}	n^{pq}
1, A+1 (1st Kind → special program.)	0	0	0	0
2, A+2 (2nd Kind → standard program.)	$\frac{\lambda A}{(A-1)(A-2)}\left[A^2\alpha + 4\beta + \frac{\lambda(A^2+4)(A-1)}{2}\right]$	$\frac{\lambda A}{(A-1)(A-2)}\left[4\alpha + A^2\beta + \frac{\lambda(A^2+4)(A-1)}{2}\right]$	$\frac{\lambda A}{4(A-1)}$	$\frac{-2\lambda A^2}{(A-1)(A-2)}\left[\alpha + \beta + \lambda(A-1)\right]$

TableIII, 6 — Type $(AA|II|pq)_{coulomb}$

$$\left[\beta^{pq}\right] = \left(\frac{A}{A+2}\right)^2\left[\beta^{oo} + \frac{t^2\beta^{pq}}{d^{oo} + t^2 d^{pq}}\right] \qquad \left[\gamma^{pq}\right] = \left(\frac{A}{A+2}\right)^2\left[\gamma^{oo} + \frac{t^2\beta^{pq}}{d^{oo} + t^2 d^{pq}}\right] \qquad F^{pq} = \frac{1}{d^{oo} + t^2 d^{pq}} \qquad D^{pq} = 2\left(\frac{A}{A+2}\right)^2\left[n^{oo} + \frac{t^2 n^{pq}}{d^{oo} + t^2 d^{pq}}\right]$$

$$\beta^{oo} = \gamma^{oo} = \frac{\lambda(A^2+4)}{A-2} \qquad d^{oo} = \lambda A + 4\alpha \qquad n^{oo} = \frac{4A\lambda}{A-2}$$

p q	β^{pq}	γ^{pq}	d^{pq}	n^{pq}
2, A+2 (2nd Kind → standard program)	$d^{oo}\,d^{pq}$	$d^{oo}\,d^{pq}$	$\lambda A + 4\beta$	$-d^{oo}\,d^{pq}$

Table III, 7 - Type $(AB|I|pq)_{Nuclear}$

$$\left[\beta^{pq}\right] = \left(\frac{A+1}{A+2}\right)^2\left[\beta^{oo} + \frac{\mu\beta^{pq}}{d^{oo}+\mu d^{pq}}\right] \qquad \left[\gamma^{pq}\right] = \left(\frac{A+1}{A+2}\right)^2\left[\gamma^{oo} + \frac{\mu\gamma^{pq}}{d^{oo}+\mu d^{pq}}\right] \qquad F^{pq} = \frac{2\sqrt{2\lambda\nu A(A+1)}}{d^{oo}+\mu d^{pq}} \qquad D^{pq} = -\frac{2A(A+1)}{(A+2)^2}\left[n^{oo} + \frac{\mu n^{pq}}{d^{oo}+\mu d^{pq}}\right]$$

$$\beta^{oo} = 2A\left[\nu + \frac{2A\alpha}{(A+1)^2}\right] \qquad d^{oo} = \lambda A + \nu(A+1) \qquad n^{oo} = 4\alpha + \nu(A+1)$$

$$\gamma^{oo} = 4\alpha + \frac{\nu A}{2}$$

p q	β^{pq}	γ^{pq}	d^{pq}	n^{pq}
A-1, A	0	0	4	0
1 , A+1	$\frac{4d^{oo}}{(A+1)^2}$	d^{oo}	$\frac{2(A-1)}{A}$	$\frac{2d^{oo}}{A}$
A+1, A+2	$\frac{4A^2d^{oo}}{(A+1)^2}$	$4d^{oo}$	0	$4d^{oo}$
A+2, 1	$4d^{oo}$	d^{oo}	$\frac{2(A-1)}{A}$	$\frac{2(A+1)d^{oo}}{A}$

Table III, 8 – Type $(AB|II|pq)_{Nuclear}$

$$\left[\beta^{pq}\right] = \left(\frac{A}{A+2}\right)^2 \left[\beta^{oo} + \frac{\mu \beta^{pq}}{d^{oo} + \mu d^{pq}}\right] \qquad \left[\gamma^{pq}\right] = \left(\frac{A+1}{A+2}\right)^2 \left[\gamma^{oo} + \frac{\mu \gamma^{pq}}{d^{oo} + \mu d^{pq}}\right]$$

$$F^{pq} = \frac{2\sqrt{\lambda\nu A(A+1)}}{d^{oo} + \mu d^{pq}} \qquad D^{pq} = \frac{2A(A+1)}{(A-1)(A+2)^2}\left[n^{oo} + \frac{\mu n^{pq}}{d^{oo} + \mu d^{pq}}\right]$$

$$\beta^{oo} = \frac{1}{A-1}\left[2\lambda + (A+1)^2\nu\right]$$

$$\gamma^{oo} = \frac{1}{A-1}\left[\frac{A^2}{2}\lambda + \nu\right]$$

$$d^{oo} = \left[A\lambda + (A+1)\nu\right]\left[\alpha + \frac{A+1}{4}\nu\right] \qquad n^{oo} = A\lambda + (A+1)\nu$$

p q	β^{pq}	γ^{pq}	d^{pq}	n^{pq}
A-1 , A	0	0	$4\alpha + (A+1)\nu$	0
A+1 , A+2	0	0	$A\lambda + (A+1)\nu$	0
1 , 2	$\left(\frac{2}{A-1}\right)^2$	$\left(\frac{A}{A-1}\right)^2 d^{oo}$	$2\left(\frac{A-2}{A-1}\right)\left[4\alpha + (A+1)\nu\right]$	$\frac{2A}{A-1} d^{oo}$
A+1, 1	d^{oo}	d^{oo}	$A\lambda + (A+1)\nu$	$-(A-1) d^{oo}$
A+1, 2	$\left(\frac{A}{A-1}\right)^2 d^{oo}$	$\frac{1}{A-1} d^{oo}$	$A\lambda + (A+1)\nu + 2\left(\frac{A-2}{A-1}\right)\left[4\alpha + (A+1)\nu\right]$	$\frac{1}{A-1} d^{oo}$

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Table III, 9 - Type (AB|I|K.E.)

$$A_1(\mathcal{V}'^2) = \left(\frac{A+1}{A+2}\right)^3 \left[64\alpha^2 + 16A\alpha\nu + 2A(A+1)\nu^2\right] \qquad A_2(\mathcal{V}^2) = \frac{4A^2(A+1)}{(A+2)^3}\left[16\alpha^2 + 8(A+1)\alpha\nu + \frac{2(A+1)^3}{A}\nu^2\right]$$

$$B = -\frac{4A(A+1)^2}{(A+2)^3}\left[32\alpha^2 + 4(3A+2)\alpha\nu + 2(A+1)^2\nu^2\right]$$

$$E = 3(A+1)\left[\frac{A(A-1)\lambda\nu}{4\lambda + (A+1)\nu} + \frac{2(A+1)\nu + 8\alpha}{A+2}\right]$$

Table III, 10 - Type (AB|II|K.E.)

$$A_1(\mathcal{V}'^2) = \left(\frac{A+1}{A+2}\right)^3 \frac{A}{(A-1)^2}\left[A^3\lambda^2 + 4A\lambda\nu + 2(A+1)\nu^2\right] \qquad A_2(\mathcal{V}^2) = \frac{2(A+1)}{(A-1)^2}\left(\frac{A}{A+2}\right)^3\left[2A\lambda^2 + 4(A+1)\lambda\nu + (A+1)^3\nu^2\right]$$

$$B = \frac{4A^2}{(A-1)^2}\frac{(A+1)^2}{(A+2)^3}\left[A^2\lambda^2 + (2+A+A^2)\lambda\nu + (A+1)^2\nu^2\right]$$

$$E = 3(A+1)\left[\frac{4\alpha\nu}{4\alpha + \nu(A+1)} + \frac{A(A-2)\lambda\nu}{\lambda A + \nu(A+1)} + \frac{A^2\lambda + A(A+1)\nu}{(A-1)(A+2)}\right]$$

Table III, 11 - Type $(AB|I|pq)_{Coulomb}$

$$\left[\beta^{pq}\right] = 2\left(\frac{A+1}{A+2}\right)^2\left[\beta^{oo} + \frac{t^2\beta^{pq}}{d^{oo}+t^2d^{pq}}\right] \qquad \left[\gamma^{pq}\right] = \left(\frac{A+1}{A+2}\right)^2\left[\gamma^{oo} + \frac{t^2\gamma^{pq}}{d^{oo}+t^2d^{pq}}\right] \qquad F^{pq} = \frac{2\sqrt{\lambda\nu A(A+1)}}{d^{oo}+t^2d^{pq}} \qquad D^{pq} = 2\left(\frac{A+1}{A+2}\right)^2\left[n^{oo} + \frac{t^2n^{pq}}{d^{oo}+t^2d^{pq}}\right]$$

$$\beta^{oo} = 2\left(\frac{A}{A+1}\right)^2\alpha + A\nu$$

$$\gamma^{oo} = 4\alpha + \frac{A}{2}\nu$$

$$d^{oo} = 1 \qquad n^{oo} = \frac{4A}{A+1}\alpha + A\nu$$

p q	β^{pq}	γ^{pq}	d^{pq}	n^{pq}
A+2, 2	$\left(\frac{A-1}{A-2}\right)\left[\lambda A + \nu(A+1)\right]$	$\frac{1}{2}\left(\frac{A-1}{A-2}\right)\left[\lambda A + \nu(A+1)\right]$	$\frac{1}{A(A-2)}$	$\left(\frac{A-1}{A-2}\right)\left[\lambda A + \nu(A+1)\right]$

Table III, 12 - Type $(AB|II|pq)_{Coulomb}$

$$\left[\beta^{pq}\right] = \left(\frac{A}{A+1}\right)^2\frac{1}{A-1}\left[\beta^{oo} + \frac{t^2\beta^{pq}}{d^{oo}+t^2d^{pq}}\right] \qquad \left[\gamma^{pq}\right] = \left(\frac{A+1}{A+2}\right)^2\frac{1}{A-1}\left[\gamma^{oo} + \frac{t^2\gamma^{pq}}{d^{oo}+t^2d^{pq}}\right] \qquad F^{pq} = \frac{2\sqrt{\lambda\nu A(A+1)}}{d^{oo}+t^2d^{pq}} \qquad D^{pq} = \frac{2A(A+1)}{(A+2)^2(A-1)}\left[n^{oo} + \frac{t^2n^{pq}}{d^{oo}+t^2d^{pq}}\right]$$

$$\beta^{oo} = 2\lambda + (A+1)^2\nu$$

$$\gamma^{oo} = \frac{A^2}{2}\lambda + \nu$$

$$d^{oo} = 4\alpha + \nu(A+1) \qquad n^{oo} = A\lambda + (A+1)\nu$$

p q	β^{pq}	γ^{pq}	d^{pq}	n^{pq}
A+2, 2	$\frac{(A+1)^2}{A-2}\,d^{oo}n^{oo}$	$\frac{1}{A-2}\,d^{oo}n^{oo}$	$\frac{1}{2}\left(\frac{A-1}{A-2}\right)n^{oo}$	$\frac{A+1}{A-2}\,d^{oo}n^{oo}$

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