The Resonating Group Method in Light Nuclear Physics

by

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Contents.

Chapter 1.

Introduction.

Considerable experimental data exists for collisions between the lightest nuclei, and intensive theoretical investigations have been proceeding for some time.

At low energies two major difficulties arise. Firstly, approximations which are comparatively easy to apply, such as the Born approximation or the impulse approximation, are invalid. Secondly, the details of the nuclear potential have only begun to clarify recently.

The first of these difficulties may be obviated by using wave-functions of resonating group form.

It has not yet been possible to perform calculations using a realistic nuclear potential, but this is obviously the ultimate aim.

Many features of these interactions can be described in terms of an "equivalent central" potential between pairs of nucleons of the form:-

$$\mathcal{V}(ij) = V(r_{ij})(mM_{ij}+bB_{ij}+hH_{ij}+w) + \varepsilon_{ij}\, e^2/r_{ij} \qquad (1.1)$$

where $r_{ij} = \underline{r}_i - \underline{r}_j$ and $\underline{r}_i$ and $\underline{r}_j$ are the position vectors of the nucleons i and j. $\varepsilon_{ij} = 1$ if i and j are protons and is zero otherwise. M_{ij}, B_{ij} and H_{ij} are the Majorana, Bartlett and Heisenberg exchange operators (defined in chapter (1.2)), and w,m,b and h are constants determining the exchange nature of the interaction, normalised so that:-

$$\begin{aligned} m + h + w + b &= 1 \\ m - h + w - b &= x \end{aligned} \tag{1.2}$$

where x is the ratio of the strength of the interaction between particles of opposite and the same spin respectively (Buckingham and Massey (1941)). x is usually taken as 0.6 (Motz and Schwinger 1940).

In the following work we are concerned only with this approach (that is the use of a resonating group wave-function in conjunction with a potential (1.1), or (1.1) with additional terms allowing for tensor forces or spin-orbit coupling).

1.1 The Wheeler Model.

In 1937 Wheeler formulated a method of construction of nuclear wavefunctions starting from an analogy with molecular structure.

The nucleons in the nucleus were taken to move in groups well defined enough for their motion to be described by a group co-ordinate.

Here the analogy with molecular structure ends, since the total wave-function is taken as a sum of properly anti-symmetrical wave-functions corresponding to each partition of the nucleons, so that the system could be regarded as resonating between the various physically possible configurations.

If we consider a system of m protons and n neutrons, we have a number of possible configurations of the (m+n) nucleons into groups of particles described by functions φ_i

The φ_i will then consist of products of wave-functions Φ_j describing the motion within each group, all multiplied by a function F_i depending on the relative co-ordinates of the groups within the i^{th} configuration and the total spin of this configuration.

A sum of the terms φ_i including all permutations of the neutrons and protons between groups of this configuration is then formed, with appropriate signs for each term to give anti-symmetry in neutrons and in protons. This sum $\sum_{\text{perm}} (\pm)\,\varphi_i$ is then the wave-function corresponding to one particular partition.

The total wave-function for the system is then:-

$$\Psi = \sum_i \sum_P (\pm)\,\varphi_i \tag{1.3}$$

The Φ_j will be variationally determined or approximate wave-functions for the corresponding groups. Thus the method makes possible the use of knowledge of the wave-functions of smaller systems to build up a wave-function for a larger one.

The only unknowns are now the F_i, which are determined so as to give the best wave-function satisfying the variation principle:-

$$\delta E = 0, \quad E = \frac{\int \Psi^* H \Psi \, d\tau}{\int \Psi^* \Psi \, d\tau} \tag{1.4}$$

where H is the total energy operator for the system, and $\int d\tau$ indicates integration over the configuration space of Ψ.

Fully general expressions for the wave-function, including explicit anti-symmetrisation are given in

Wheeler's original paper but they will not be reproduced here since the illustration by examples later is sufficient.

It should be noted that in this work the proton and neutron are treated as different particles. No fundamental difference appears if the isotopic spin formalism is used however.

1.2 The Exchange Potentials.

The operators in the potential

$$\mathcal{V}(ij) = V(r_{ij})(mM_{ij}+bB_{ij}+hH_{ij}+w)$$

which is the nuclear force part of (1.1), are defined as follows:-

The Majorana operator M_{ij} exchanges the space co-ordinates of particles i and j. The Bartlett operator B_{ij} exchanges their spin co-ordinates and the Heisenberg operator H_{ij} both space and spin co-ordinates.

We enumerate the various force types which have been used.

"Ordinary" Force. (WB)

$$m = 0,\ h = 0,\ w = \tfrac{1}{2}(1+x),\ b = \tfrac{1}{2}(1-x) \qquad (1.5)$$

This is an unsaturated type of force and is a combination of ordinary (Wigner) and spin-dependent forces.

Majorana-Heisenberg. (MH)

This is a saturated force of the type originally suggested. It is the exchange analogue of the WB force.

$$w = 0,\ b = 0,\ m = \tfrac{1}{2}(1+x),\ b = \tfrac{1}{2}(1-x) \qquad (1.6)$$

m,h,w,b all finite.

Symmetric or MHWB force.

This was suggested according to the criterion that all constants were fixed so that no ordinary force appeared in their differential equations for the relative motion of a neutron and deuteron. (Buckingham & Massey (1941)).

$$2w = \frac{1-3x}{3} = h, \quad 2b = \frac{1+3x}{3} = m \tag{1.7}$$

Serber Force.

$$w = \tfrac{1}{4}(1+x) = m, \ b + \tfrac{1}{4}(1-x) = h \tag{1.8}$$

This type of exchange force has had great success in applications to scattering. Indeed it appears that a force of near this type may be reasonably expected to give good agreement with experiment.

Linear Combinations.

Various linear combinations of the above forces have been used. Since we will be considering forces between the Serber and symmetric types, we define y such that:-

An intermediate force between the Server and symmetric is given by:-

$$y(\text{Serber}) + (1-y)(\text{Symmetric})$$

$$\begin{aligned} \text{i.e.} \quad m &= \tfrac{1}{4}y(1+x) + 1/3(1-y)(1+3x) \\ w &= \tfrac{1}{4}y(1+x) + 1/6(1-y)(1-3x) \\ b &= \tfrac{1}{4}y(1-x) + 1/6(1-y)(1+3x) \\ h &= \tfrac{1}{4}y(1-x) + 1/3(1-y)(1-3x) \end{aligned} \tag{1.9}$$

1.3 Previous Applications.

It was recognised early that the scattering of neutrons by deuterons provided a useful tool for the study of nuclear forces, and work on this problem is reviewed by Massey (1953), and de Borde and Massey (1955). We are interested here in calculations carried out by Buckingham and Massey (1941), and Buckingham, Hubbard and Massey (1952) on n-d scattering. These were extended to include p-d scattering in the second of these papers. They used a potential of the form (1.1) with

$$V(r_{ij}) = -A\exp(-2r_{ij}/a),\quad x = 0.6 \tag{1.10}$$

and $A = 242\ mc^2$, $a = 1.73 \times 10^{-13}$cm.

This was chosen to fit the low energy nuclear data known at that time (1941) including the binding energy of the triton. Their results only agreed with experiment if exchange forces were used. Discrepancies between their results and observation were resolved by de Borde and Massey (1955) by the addition of higher phase shifts, resulting in good agreement up to 20 MeV for a Serber exchange force. It should be noted, however, as pointed out by de Borde and Massey, that to fit the now known two-body data the range parameter in (1.10) should be $a = 1.35 \times 10^{-13}$ cm., giving too large a binding energy for triton. This apparent discrepancy between the two and three-body data was resolved by Pease and Feshbach (1952), who showed that it could be explained by tensor forces. Bransden, Smith and Tate (1958) have extended the method to include tensor forces. Christian and Gammel (1953) produce evidence suggesting that the neglect of polarization in this problem is not serious. This is supported by Burke and Haas (1958).

Work on n-α and p-α scattering was carried out by Hochberg, Massey and Underhill (1954), and Hochberg, Massey, Robertson and Underhill (1954) in the energy range 0-4 MeV. using for s-wave scattering a potential of the form (1.1) with a gaussian well:-

$$V(r_{ij}) = A \exp(-\beta r_{ij}^{2}), \; A = -45 \text{ MeV}, \; \beta = 0.2657 \times 10^{26} \text{cm}^{-2}$$
$$\text{and } x = 0.6 \qquad (1.11)$$

These values give good agreement for the binding energy of the deuteron and alpha-particle, but too large a binding energy for the triton. They incorporated a spin orbit coupling term by adding $V(r_{ij}) S \hbar^{-2} \chi$ $(\underline{s}_i + \underline{s}_j) \cdot \underline{r}_{ij} \times (\underline{p}_i - \underline{p}_j)$ to (1.1), and found the best overall agreement with experiment with y = 0.90 (See 1.9) and S = 0.10. Bransden and McKee (1954) had concurrently done a calculation (also using resonating groups) on the same problem with a variational method but without the same degree of success. This was probably due to a more consistent method and improved accuracy by Hochberg, Massey, Robertson and Underhill, in particular the use of the pilot ACE computer at the National Physical Laboratory.

With the advent of electronic computers generally, more detailed and accurate work has been possible, and the last few years have seen comparatively intensive application of the model, and a useful growth in the amount of theoretical data available.

Burke and Robertson (1957) recalculated n-d scattering for incident neutron energies less than 16.6 MeV. They used (1.1) with a gaussian well $V_o \exp(-\mu r_{ij}2)$, in conjunction with a deuteron wave-function of the form:-

$$\chi(R) = \frac{1}{n}(e^{-\alpha R^2} + c e^{-\alpha R^2}) \qquad (1.12)$$

where R is the inter-nucleon distance. They considered five values of $\mu = 0.2(0.1)0.6 \times 10^{26}\text{cm}^{-2}$, adjusting

V_o in each case to give the observed binding energy of the triton (-2.22 MeV). Their total cross-section agrees with experiment very well over the whole energy range with $\mu = 0.3 \times 10^{26} cm^{-2}$ (corresponding to $V_o = -51.39$ MeV, giving a deuteron binding energy of -2.119 MeV). They found very little dependence on the exchange nature of the force.

They also test an adaptation of the variational methods of Hulthen (1944) and Kohn (1948) against their exact calculations, and conclude that polarization could be allowed for with its help without much difficulty. Later (Haas and Robertson 1959) this calculation was extended to use a Yukawa potential for the interaction.

Bransden, Robertson and Swan (1956) and Bransden and Robertson (1958) performed calculations on the scattering of nucleons by triton and ^3He. Swan (1953) had already performed calculations on n-^3H and n-^3He scattering, and the later work differed in that exact solutions to the scattering equations were obtained using ACE, and also the equations used were more consistent with the approximate ^3H and ^3He wave-functions used. They used (1.1) with a gaussian well of the form (1.11) and the calculations were performed for forces of the Serber and symmetrical types ($y = 1$ and $y = 0$), Serber giving much better agreement throughout.

Biel (1957) has performed successful calculations on the binding energies of ^{8}Be and ^{12}C and gives a formalism for applying the method to α-particle nuclei in general. He used the range and depth parameters (1.11), together with an exchange force with $y = 0.7$.

Thus it appears that the use of a resonating group wave-function together with an exchange force (1.1) of near the Serber type and well parameters corresponding to a Gaussian well $V_o e^{-\mu r_{ij}^2}$ with $V_o = -45$ MeV and $\mu \simeq 0.3 \times 10^{26} cm^{-2}$, is likely to give fruitful results in the investigation of the properties of light nuclei at low energies.

Calculations, whose outcome was known after the work reported here was started, will be discussed along with the results of the present work.

Chapter 2.

The Scattering of Nucleons by ^3H and ^3He.

It is necessary for completeness to include a number of remarks about the published note included with this thesis (PPS. 1960, 75, 144). It is also convenient to give much of the description of the numerical methods used here, since the same methods are applied to the six-body calculations.

2.1 Remarks on the Calculations by Bransden, Robertson and Swan.

1. The calculations on four-body scattering by Bransden, Robertson and Swan (1956) and Bransden and Robertson (1958), (hereafter referred to collectively as BRS) used a gaussian potential well $V(r_{ij})$ with (1.1), such that

$$V(r_{ij}) = V_o \exp(-\mu r_{ij}^{\ 2}),\ V_o = -45 \text{ MeV},$$
$$\text{and } \mu = 0.2669 \times 10^{26} \text{cm}^{-2} \qquad (2.1)$$

These values had previously been used by Swan (1953). They are consistent with the four-body bound state (giving a binding energy for the alpha-particle of $E_\alpha = -27$ MeV) and with the binding energy of the deuteron, although of longer range than that now suggested by present two-body data (BRS). However, it must be remembered that since no tensor force is included, the "equivalent" central force used here is giving some sort of representation of the tensor force contribution.

As mentioned in chapter (1.3), these constants give values for the binding energies of ^3H and ^3He which are too large (-5.49 MeV for ^3H as against -8.38 MeV observed, and -4.74 MeV for ^3He against -7.55 MeV observed).

2. They used for the ^{3}He wave-function:-

$$\chi_H(123) = +N_H \exp\left[-\frac{\lambda}{2}(r_{12}^2 + r_{13}^2 + r_{23}^2)\right] \qquad (2.2)$$

and for ^{3}H:-

$$\chi_T(123) = +N_T \exp\left[-\frac{\eta}{2}(r_{12}^2 + r_{13}^2 + r_{23}^2)\right] \qquad (2.3)$$

with $\lambda = 0.1404 \times 10^{26}\,\text{cm}^{-2}$ and $\eta = 0.1436 \times 10^{26}\,\text{cm}^{-2}$. They determined λ and η by minimising the binding energies of the three-body nuclei.

3. It should be noted that in the course of their analysis, BRS used equations for the three-body nuclei satisfied by the approximate wave-functions which they used (2.2 and 2.3), unlike Swan's earlier work, where the equations, which would be satisfied by exact three-body wave-functions, were used together with approximate wave-functions. The BRS work is thus more consistent.

4. Their results give quite good agreement with experiment for a Serber force except below 2 MeV, where they attribute the disparity to the neglect of polarization.

2.2 Wave-function and Scattering Equation.

The resonating group wave-functions used by BRS are set out below. In each case the two groups are the incident nucleon and the appropriate three-body nucleus.

The wave-function for the system is thus of the form:-

$$\Psi_s(1234) = A\,\chi(123)\,F_s(4)\,\sigma_m^s(1234) \tag{2.4}$$

where A is an operator which anti-symmetrises the wave-functions, χ is the three-body (ground state) wave-function, and F_s, which will be the unknown part of the wave-function, depends on the co-ordinates of the incident nucleon with respect to the centre of mass of the three-body nucleus. σ_m^s is the appropriate spin wave-function and "s" denotes the spin state.

(a) $n - {}^3He$

With particles 1 and 2 protons, and 3 and 4 neutrons, with χ_H totally symmetric in 1, 2 and 3, and with the following spin functions σ_m^s, the wavefunction

$$\Psi_s(1234) = \tfrac{1}{2}(1-P_{34})\,\chi_H(123)F_s(4)\,\sigma_m^s(1234) \tag{2.5}$$

has the correct antisymmetry properties. P_{ij} exchanges all co-ordinates of particles i and j.

The total spin is taken as s = 0, 1.

For s = 0. $\sigma_0^1(1234) = \frac{1}{2}(\alpha(1)\beta(2) - \beta(1)\alpha(2))(\alpha(3)\beta(4) - \beta(3)\alpha(4))$

s = 1. $\sigma^3(1234) = \frac{1}{\sqrt{2}}(\alpha(1)\beta(2) - \beta(1)\alpha(2))\alpha(3)\alpha(4)$

$$\sigma_0^3(1234) = \frac{1}{2}(\alpha(1)\beta(2) - \beta(1)\alpha(2))(\alpha(3)\beta(4) + \beta(3)\alpha(4))$$

$$\sigma_{-1}^3(1234) = \frac{1}{\sqrt{2}}(\alpha(1)\beta(2) - \beta(1)\alpha(2))\beta(3)\beta(4) \qquad (2.6)$$

the spin functions for the three-body groups being

$$\sigma_{T,H}{}^{1/2}_{1/2} = \alpha(3)(\alpha(1)\beta(2) - \beta(1)\alpha(2))$$

$$\sigma_{T,H}{}^{1/2}_{-1/2} = \beta(3)(\alpha(1)\beta(2) - \beta(1)\alpha(2)) \qquad (2.7)$$

where α and β have their usual significance.

(b) <u>n - ^{3}H</u>

$$\Psi_s(1234) = \frac{1}{\sqrt{3}}(1-P_{34}-P_{24})\chi_T(123)F_s(4)\ \sigma_m^s(1234) \qquad (2.8)$$

with particle 1 a proton, and 2, 3, 4 neutrons, give the correct anti-symmetry. The functions σ_m^s are defined by (2.6).

The proton cases will have the same wave-functions as the neutron ones with the same symmetry.

That is:-

(c) <u>p - ^{3}H</u>.

$$\Psi_s(1234) = \frac{1}{2}(1-P_{34})\ \chi_T(123)F_s(4)\ \sigma_m^s(1234) \qquad (2.9)$$

with 1 and 2 neutrons, and 3 and 4 protons.

(d) p - ^{3}He.

$$\Psi_s(1234) = \frac{1}{\sqrt{3}}\,(1-P_{24}-P_{34})\,\chi_H(123)F_s(4)\,\sigma_m^s(1234) \qquad (2.10)$$

with 1 a neutron and 2, 3, 4 protons.

The functions χ_H and χ_T used were those given by (2.2) and (2.3).

By the methods described later in connection with the six-nucleon calculations, a radial equation was obtained of the form:-

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{n(n+1)}{r^2}\right) f_n^s(r) = V(r)\, f_n^s(r) + \int_0^\infty K_n^s(r,r') f_n^s(r')\,dr' \qquad (2.11)$$

where $F_s(4) = F_s(\underline{r})$, say, and

$$F_s(\underline{r}) = \frac{1}{r} \sum_{n=0}^{\infty} f_n(r) P_n(\cos\theta), \quad r = |\underline{r}| .$$

2.3 Numerical Methods.

The equation (2.11) is solved by the use of programmes prepared by Dr. H.H. Robertson (1956).

There are three principal programmes.

(a) The first of these calculates the kernels $k_n(r, r')$ (2.11) in the form of (30 x 30) matrices, and this will be dealt with later. (The kernels for the calculations on the four-body problem using a force type with y = 0.7 were formed merely by taking linear combinations of the Serber and symmetric kernels which had already been produced for the BRS calculations.)

(b) The second calculates the solutions of (2.11). The infinite upper limit on the integral on RHS is replaced by a suitable limit $R^1 = 29h$, where h is the interval between the points of r and of r^1 in the kernel matrix. h is chosen so that k_n has died away sufficiently at R^1. Using finite difference techniques (cf. chapter 6.3) the equation is put into the form of a system of homogeneous linear equations with 30 points of $f_n(r)$ $(0, h, \cdots 29h = R)$ as unknowns, and including accurate allowance for the difference correction. These are then solved subject to the boundary conditions $f_n(0) = 0$, $f_n(h) = 1$.

It should be noted that the programme reads

$A_n(r,r')$ and $B_n(r,r')$ separately, where

$$k_n(r,r') = A_n(r,r') + N\,B_n(r,r')$$

and the variation of the scalar N gives the energy dependence of k_n. Thus, kernels are only tabulated for different values of angular momentum for each value of y, and results for different energies found by reading in different values of the parameter N.

(c) Calculation of the Phase Shifts.

When the products of the collisions are charged (the proton collisions in this case) the asymptotic form of $f_n^s(r)$ is

$$f_n^s(r) \sim \sin(kr - (n\pi)/2 - \alpha \log 2kr + \eta_n + \delta_n^s) \quad (2.12)$$

where $\alpha = \dfrac{zz'e^2M}{\hbar p}$ and $\eta_n = \arg\Gamma(n+1+i\alpha)$, p being the momentum of the incident particle (Mott and Massey 1949, Ch.3).

When direct Coulomb terms are absent (the neutron collisions) the asymptotic form is

$$f_n(r) \sim \sin(kr - (n\pi)/2 + \delta_n^s) \quad (2.13)$$

δ_n^s is the quantity of interest. Where there is no direct Coulomb term, it is calculated by considering the ratio $f_n(29h)/f_n(28h)$ and using (2.13). To check that this ratio is being taken for large enough r (i.e. (2.13) is accurately enough obeyed) values of the phase shift are calculated for various intervals h and compared.

Where there is a direct Coulomb interaction, the η_n are computed previously and, together with α, read into the programme, which proceeds as before but form and subtracts the expression ($\eta_n - \alpha \log 2kr$) from the result.

(d) From the phases the angular distribution $I(\theta)$ is computed in the usual way, using the following relations.

$$I(\theta) = 3/4 \left|{}^3g(\theta)\right|^2 + 1/4 \left|{}^1g(\theta)\right|^2 \qquad (2.14)$$

where $${}^{3,1}g(\theta) = \frac{1}{2ik} \sum_{n=0}^{\infty} (2n+1)\left[\exp(2i\,\delta_n^{3,1}) - 1\right] P_n(\cos\theta) \qquad (2.15)$$

where δ_n^3 is the triplet phase corresponding to angular momentum n, and δ_n^1 the singlet.

The total cross-section for elastic scattering is then:-

$$Q = 2\pi \int_0^{\pi} I(\theta) \sin\theta \, d\theta \qquad (2.16)$$

Examples of phases calculated for this problem are given in Tables 1 (a), 1 (b) and 1 (c).

2.4 Phase Shifts for p-^{3}He and n-^{3}He Elastic Scattering.

Table 1(a). p-^{3}He at 19.4 MeV (Lab.) Incident Proton Energy.

n	Biel Force		Serber Force.	
	Singlet	Triplet	Singlet	Triplet
0	+76.2	-98.9	+78.1	-101.5
1	+44.8	+27.1	+37.8	+50.9
2	- 3.2	- 6.4	- 3.1	- 1.5
3	+ 2.4	+ 1.4	+ 2.5	+ 2.7
4	-	- 0.2	- 0.1	-

Table 1(b). n-^{3}He at 17.5 MeV (Lab.) Incident Neutron Energy.

n	Biel Force		Serber Force.	
	Singlet	Triplet	Singlet	Triplet
0	-71.0	+74.9	+78.8	-69.7
1	+17.3	+49.6	+59.5	+37.0
2	+21.7	- 3.2	- 0.7	+25.1
3	+ 0.6	+ 2.1	+ 2.6	+ 0.8
4	+ 0.4	- 0.1	-	+ 0.4

Table 1(c). p-^{3}He and n-^{3}He at 8 MeV - Biel Force.

n	p-^{3}He Singlet	p-^{3}He Triplet	n-^{3}He Singlet	n-^{3}He Triplet
0	-69.5	-73.5	-64.7	-77.7
1	+48.1	+32.0	- 3.8	+54.8
2	- 1.8	- 2.6	+ 7.1	- 2.0
3	+ 0.3	+ 0.3	- 0.1	+ 0.4
4	-	-	-	-

N.B. 1. Phases are given in degrees and decimals and $\delta_n^s \pm \pi$ is given if δ_n^s exceeds $\pi/2$.

2. "Biel Force" is used to mean y = 0.7.

3. A dash indicates that the computed phase shift was less than 0.1 in modulus.

Chapter 3.

The Six-Body Problem.

After the successes of the calculations on nucleon-nucleus types of collisions, interest was obviously turned to extending the application to new systems, especially nucleus-nucleus collisions.

Calculation had already begun on D+D, D+^{3}He, and $(\alpha+\alpha)$ scattering and it was therefore decided to perform calculations on scattering involving six nucleons.

We now give a formulation of the scattering of six nucleons for those cases where the initial and final states involve only two nuclei. Considerable experimental evidence is available for comparison with the results of calculations.

The processes divide into two types with differing symmetry properties.

(a) A single channel system

$(^3He + {}^3He)$ and $(^3H + {}^3H)$ elastic scattering.

(b) A two channel system

$(^3He + {}^3H \rightleftharpoons d + \alpha)$ elastic and inelastic scattering. (Also by use of appropriate boundary conditions, a bound state of Li^6 should be found from the equations derived for (b)).

The method is similar to that used in most of the calculations already mentioned, and consequently has been described many times before. We shall nevertheless give a complete exposition, omitting, however, large amounts of the rather tedious algebra involved. Due to the complication of the problem, it was decided not to include spin-orbit coupling or tensor forces in the first instance.

In common with the majority of earlier authors, we make no explicit allowance for polarization effects. (There will be some allowance for distortion effects implicit in the method - ~~Blatt and Weisskopf (19) p.).~~ Mott and Massey (1949) - p. 305.)

3.1 <u>Type (a) - Derivation of Equation - Wave-function</u>.

Both of the type (a) reactions will be dealt with in the same analysis. For the resonating group structure wave-function the two groups correspond to identical three-body nuclei and the correct symmetry properties for the six nucleons are given by:-

$$\Psi_s(123456) = (1 - P_{56} - P_{13} - P_{14} - P_{23} - P_{24})\varphi_s \qquad (3.1)$$

The subscript s refers to the spin state and P_{ij} is again the operator which exchanges all co-ordinates of particles i and j.

$$\varphi_s = \chi(125)\,\chi(346)\;\sigma^{s}_{m}(125,346)F_s(125 - 346) \qquad (3.2)$$

Particles 1,2,3,4 are alike and 5,6 are alike.

The χ's are the ground state wave-functions for the ^{3}He or ^{3}H nuclei, and σ^{s}_{m} is an appropriate spin function. F_s is the internuclear wave-function (depending on the distance from the centre of mass of one nucleus to the centre of mass of the other.)

The spin wave-functions are taken as follows:-

s = 0 $\quad \sigma^{0}_{0}(125,346) = \frac{1}{\sqrt{2}}\left(\sigma^{+1/2}_{+1/2}(125)\sigma^{+1/2}_{-1/2}(346) - \sigma^{+1/2}_{-1/2}(125)\sigma^{+1/2}_{+1/2}(346)\right)$

s = 1 $\quad \sigma^{+1}_{+1}(125,346) = \sigma^{+1/2}_{+1/2}(125)\sigma^{+1/2}_{+1/2}(346)$

$\sigma^{+1}_{0}(125,346) = \frac{1}{\sqrt{2}}\left(\sigma^{+1/2}_{+1/2}(125)\sigma^{+1/2}_{-1/2}(346) + \sigma^{+1/2}_{-1/2}(125)\sigma^{+1/2}_{+1/2}(346)\right)$

$\sigma^{1}_{-1}(125,346) = \sigma^{+1/2}_{-1/2}(125)\sigma^{+1/2}_{-1/2}(346) \qquad (3.3)$

where $\quad \sigma^{+1/2}_{+1/2}(125) = \frac{1}{\sqrt{2}}\alpha(5)\left(\alpha(1)\beta(2) - \beta(1)\alpha(2)\right)$

$\sigma^{+1/2}_{-1/2}(346) = \frac{1}{\sqrt{2}}\beta(6)\left(\alpha(3)\beta(4) - \beta(3)\alpha(4)\right)$ etc.

For the correct symmetry properties in the three-body nuclei in (3.1), since these have spin 1/2, we must have:

$$F_s(125 - 346) = (-1)^s F_s(346 - 125) \qquad (3.4)$$

and the allowed angular momentum states are:-

$n=0, s=0$; $n=1, s=1$; $n=2, s=0$ etc.

3.2 Co-ordinate System and Notation (Type a)

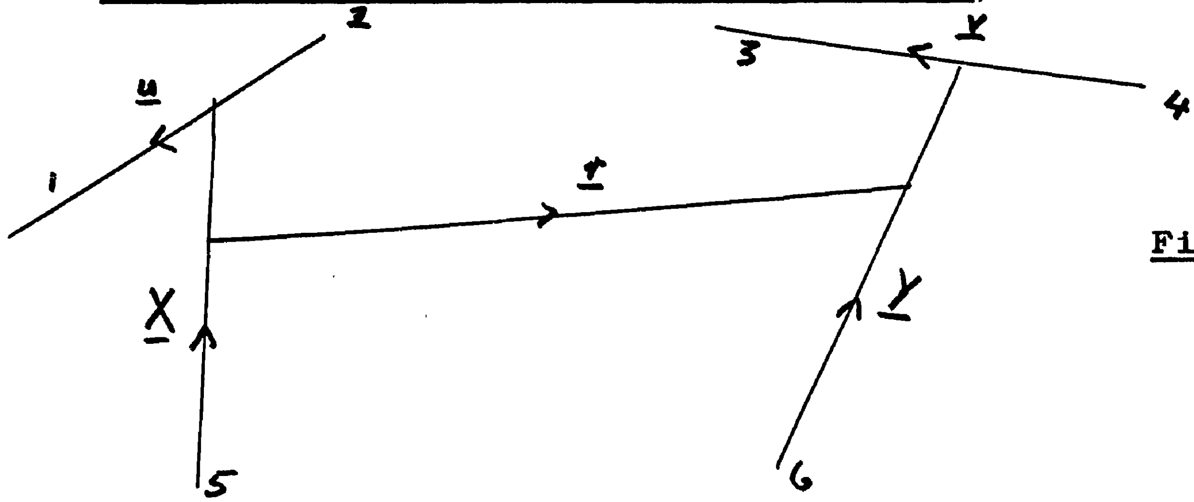

Figure 1.

The co-ordinates are chosen according to Figure 1, that is, if $\underline{r}_i$ is the position vector of the nucleon i, we choose the co-ordinates:-

$$\underline{u} = \underline{r}_1 - \underline{r}_2 \,, \qquad \underline{v} = \underline{r}_3 - \underline{r}_4 \,,$$

$$\underline{X} = \tfrac{1}{2}(\underline{r}_1 + \underline{r}_2) - \underline{r}_5 \,, \qquad \underline{Y} = \tfrac{1}{2}(\underline{r}_3 + \underline{r}_4) - \underline{r}_6 \,,$$

$$\underline{r} = \tfrac{1}{3}(\underline{r}_3 + \underline{r}_4 + \underline{r}_6 - \underline{r}_1 - \underline{r}_2 - \underline{r}_5) \,,$$

$$\underline{r}' = P_{13}\underline{r} = \tfrac{1}{3}(\underline{r}_1 + \underline{r}_4 + \underline{r}_6 - \underline{r}_3 - \underline{r}_2 - \underline{r}_5) \,. \qquad (3.5)$$

Notation.

For convenience, in the analysis for type (a) processes we use the following abbreviations:-

$$\Sigma P = P_{56} + P_{13} + P_{14} + P_{23} + P_{24} \,,$$

$$d\tau_1 = d\tau_{125} = \underline{du}.\underline{dX} \,,$$

$$d\tau_3 = d\tau_{346} = \underline{dv}.\underline{dY} \,,$$

$$\sigma^s = \sigma^s_m\,(125,\ 346) \,,$$

$$\chi_1 = \chi(125)\ \chi(346) \,,$$

$$\chi_3 = \chi(325)\ \chi(146) = P_{13}\chi_1 \,.$$

E_A = binding energy of appropriate three-body nucleus.

and $\int d\tau$ indicates integration over the configuration space of the nucleus indicated.

3.3 The Scattering Equation (Type a).

We determine $F_s(r)$ by requiring the wave-function (3.1) to satisfy

$$\delta E = 0, \quad E = \frac{\int \Psi^* H \Psi \, d\tau}{\int \Psi^* \Psi \, d\tau} \tag{3.6}$$

under variations $F_s \longrightarrow F_s + F_s$ and $F_s^* \longrightarrow F_s^* + F_s^*$, where $\int d\tau = \int d\tau_1 \, d\tau_3 \, d\underline{r}$ and $H = T + \mathcal{V} + C$.

T is the kinetic energy operator and in terms of co-ordinate set (3.5) is:-

$$T = -h^2/M\left(\nabla_u^2 + \nabla_v^2 + 3/4\,(\nabla_x^2 + \nabla_Y^2) + 1/3\,\nabla_r^2\right) \tag{3.7}$$

M is the nucleon mass. $\mathcal{V} = \sum_{\substack{i,j=1\\ i<j}}^{6} \mathcal{V}(ij)$ (3.8)

where $\mathcal{V}(ij) = V(r_{ij})(mM_{ij} + bB_{ij} + hH_{ij} + w)$

$$C = e^2\Big(c \sum_{\substack{i,j=1\\ i<j}}^{4} (r_{ij})^{-1} + d(r_{56})^{-1}\Big) \text{ and } c = 0,\ d = 1 \text{ for } ({}^3H + {}^3H);\ c = 1,\ d = 0 \text{ for } ({}^3He + {}^3He). \tag{3.9}$$

We now use the fact that the functions χ satisfy the equations:-

$$\int \chi(125)\Big[-\frac{\hbar^2}{M}\big(\nabla_u^2 + \tfrac{3}{4}\nabla_x^2\big) + \sum_{\substack{i,j=1,2,5\\ i<j}} \mathcal{V}(ij) + \frac{ce^2}{r_{12}} - E_A\Big]\chi(125)\, d\tau_1 = 0 \tag{3.10}$$

and

$$\int \chi(346)\Big[-\frac{\hbar^2}{M}\big(\nabla_v^2 + \tfrac{3}{4}\nabla_Y^2\big) + \sum_{\substack{i,j=3,4,6\\ i<j}} \mathcal{V}(ij) + \frac{ce^2}{r_{34}} - E_A\Big]\chi(346)\, d\tau_3 = 0 \tag{3.11}$$

For consistency we use values for the E_A predicted by the approximate ^3He and ^3H wave-functions. (These values are given in Chapter 2.1 (1).

φ_S satisfies (3.10) and (3.11).

(3.6) is satisfied if $(H-E)\Psi_S = 0$ i.e. $(T + \mathcal{V} + C - E)\varphi_S = \Sigma P \varphi_S$ ....(3.12)

Multiplying (3.12) by $\sigma^S\chi_1$ summing over spin directions and integrating over the internal co-ordinates of the groups gives:-

$$(\nabla_r^2 + k^2) F_S(\underline{r})$$
$$= \frac{3M}{\hbar^2} \sum_{spin} \int d\tau_1 d\tau_3 \, \sigma^S\chi_1 \Big[\sum_{\substack{i=1,2,5 \\ j=3,4,6}} \mathcal{V}(ij) + ce^2\Big(\frac{1}{r_{13}} + \frac{1}{r_{14}} + \frac{1}{r_{23}} + \frac{1}{r_{24}}\Big) + \frac{de^2}{r_{56}}$$
$$- (T + \mathcal{V} + C - E) \Sigma P \Big] \sigma^S\chi_1 F_S(\underline{r}) \tag{3.13}$$

where $k^2 = \frac{3M}{\hbar^2}(E - 2E_A)$, and we have used (3.10) and (3.11).

It can be seen that we have now integrated out the internal motion of the groups. The contribution of this motion is represented in k^2 by $(-2E_A)$.

The effects of the operators M_{ij}, B_{ij}, H_{ij} and P_{ij} on the integrand on the RHS of (3.13) were then explicitly written out, and the summation over spins performed using the spin matrix elements tabulated in appendix A. Assuming complete symmetry of the wave-function χ in the co-ordinates of the three particles, the exchange effects can be expressed in terms of the operator P_{13}. That is the RHS of (3.13) can be reduced to a sum of matrix elements of the two types

$\int \chi_1 X^s \chi_1 F_s d\tau_1 d\tau_3$ and $\int \chi_1 X^s P_{13} \chi_1 F_s(r) d\tau_1 d\tau_3 = \int \chi_1 X^s \chi_3 F_s(r') d\tau_1 d\tau_3$

where X^s is V(ij), T, e^2/r_{ij} or E.

Using again the symmetry of the χ and (3.4), the nuclear and coulomb force terms were reduced to eight types.

Re-arranging in this way and using the change of variable $\int d\underline{Y} = (\frac{9}{2})^3 \int d\underline{r}'$ we find:-

$$\begin{aligned}(\nabla_r^2 + k^2) F_s(\underline{r}) &= (\alpha C(r) + \beta U(r)) F_s(\underline{r}) \\ &+ \sum_{i=1}^{8} \left(\gamma^i \int Q^i(\underline{r}, \underline{r}') F_s(\underline{r}') d\underline{r}' + \varepsilon^i \int H^i(\underline{r}, \underline{r}') F_s(\underline{r}') d\underline{r}' \right) \\ &+ \delta_s \int \left[P(\underline{r}, \underline{r}') - \frac{E}{2E_A} N(\underline{r}, \underline{r}') \right] F_s(\underline{r}') d\underline{r}'. \end{aligned} \tag{3.14}$$

where $C(r) = (3Me^2\hbar^{-2}) \int \chi_1^2 (r_{13})^{-1} \, d\underline{u} \, d\underline{v} \, d\underline{X} \, d\underline{Y}$

$U(r) = 3M\hbar^{-2} \int \chi_1^2 \, V(13) \, d\underline{u} \, d\underline{v} \, d\underline{X} \, d\underline{Y}$

$Q^i(\underline{r}, \underline{r}') = 3M\hbar^{-2} \int \chi_1 \chi_3 \, V^i \, d\underline{u} \, d\underline{v} \, d\underline{X} \, (9/2)^3$

$H^i(\underline{r}, \underline{r}') = 3Me^2\hbar^{-2} \int \chi_1 \chi_3 \, C^i \, d\underline{u} \, d\underline{v} \, d\underline{X} \, (9/2)^3$

$P(\underline{r}, \underline{r}') = 3M\hbar^{-2} \int \chi_1 T \chi_3 \, d\underline{u} \, d\underline{v} \, d\underline{X} \, (9/2)^3$

and $N(\underline{r}, \underline{r}') = 3M\hbar^{-2} \int \chi_1 (2E_A) \chi_3 \, d\underline{u} \, d\underline{v} \, d\underline{Y} \, (9/2)^3$

with $V^1 = V(r_{13})$, $V^2 = V(r_{53})$, $V^3 = V(r_{16})$, $V^4 = V(r_{15})$,

$V^5 = V(r_{36})$, $v^6 = v(r_{46})$, $v^7 = v(r_{52})$, $v^8 = v(r_{56})$

and $C^1 = \frac{1}{r_{13}}$, $C^2 = \frac{1}{r_{53}}$, $C^3 = \frac{1}{r_{16}}$, $C^4 = \frac{1}{r_{15}}$, $C^5 = \frac{1}{r_{36}}$,

$C^6 = \frac{1}{r_{46}}$, $C^7 = \frac{1}{r_{52}}$, $C^8 = \frac{1}{r_{56}}$.

The constants α, β, y^i, δ_s, ε^i are given in terms of c, d and w, m, b, h in Table 2.

To exhibit more clearly the dependence on the different types of exchange force, these constants are also expressed in Table 2[1] in terms of x (1.2) and y (1.9).

It can be seen that the effect of varying the exchange forces will only occur in connection with the nuclear terms i = 1 and i = 8, and the term V(r), the latter having much the largest effect.

We now expand in a harmonic series in the usual way. That is, putting $F_s(\underline{r}) = r^{-1}\sum_{n=0}^{\infty} f_n^s(r) P_n(\cos\theta)$ (3.15)

and $Q^i(\underline{r},\underline{r}') = \sum_{n=0}^{\infty} \frac{(2n+1)}{4\pi r r'} q_n^i(r,r') P_n(\cos\Theta)$, $(rr'\cos\Theta = \underline{r}\cdot\underline{r}')$ (3.16)

with similar expansions for $H^i(\underline{r},\underline{r}')$, $P(\underline{r},\underline{r}')$, and $N(\underline{r},\underline{r}')$.

This leads us to our final integro-differential equation:-

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{n(n+1)}{r^2}\right) f_n^s(r) = \left(\alpha C(r) + \beta U(r)\right) f_n^s(r) + \int_0^{\infty} K_n^s(r,r') f_n^s(r')\,dr' \quad \cdots \quad (3.17)$$

with
$$K_n^s(r,r') = \sum_{i=1}^{8} \left(y^i q_n^i(r,r') + \varepsilon^i h_n^i(r,r')\right) + \delta_s\left(p_n(r,r') - \frac{E}{2E_A} n_n(r,r')\right)$$

and
$$q_n^i(r,r') = \int_{-1}^{+1} dy\, P_n(y)\, 2\pi r r'\, Q^i(\underline{r},\underline{r}') \quad \text{etc.}$$
$$(y = \cos\Theta)$$

Table 2. Constants for type (a) Scattering Equation.

	s = 0	s = 1
α	$+4c + d$	$+4c + d$
β	$+9w+3b-m-5h$	$9w+5b-3m-5h$
γ^1	$+9m+3h-w-5b$	$9m+5h-3w-5b$
$\left.\begin{matrix}\gamma^2, \gamma^3 \\ \gamma^4, \gamma^5\end{matrix}\right\}$	$-2(w+m)+2(b+h)$	$-6(w+m)$
γ^6, γ^7	$-(w+m)-2(b+h)$	$-3(w+m)$
γ^8	$-4(w+m)-2(b+h)$	$-12(w-m)-10(b-h)$
ε^1	$+d-2c$	$-d-2c$
$\left.\begin{matrix}\varepsilon^2, \varepsilon^3 \\ \varepsilon^4, \varepsilon^5\end{matrix}\right\}$	$-2c$	$-2c$
$\varepsilon^6, \varepsilon^7$	$+c$	$-c$
ε^8	$+2c-2d$	$-6c-2d$
δ	-1	-3

Table 2^1. Nuclear Term Constants in Terms of x and y.

	s = 0	s = 1
β	$\frac{1}{2}(3+5x)y + x(1-y)$	$3/2y(1+x) - 1/3(1-y)$
γ^1	$\frac{1}{2}(3+5x)y+(3+4x)(1-y)$	$3/2y(1+x) + 1/3(10+9x)(1-y)$
$\left.\begin{matrix}\gamma^2,\gamma^3\\ \gamma^4,\gamma^5\end{matrix}\right\}$	$-2x$	$-3(x+1)$
γ^6,γ^7	$-\frac{1}{2}(x-3)$	$-3/2(x+1)$
γ^8	$-(x+3)$	$+1/3(1-y)(11+9x)$

Note. It is seen that y appears for the triplet state in γ^8.

Q^8 corresponds to matrix elements of the type $\int \chi_1 V(r_{lm}) P_{ij} \chi_1 d\tau$ where $l \neq i,j$, $m \neq i,j$, Q^1 to $\int \chi_1 V(r_{ij}) P_{ij} \chi_1 d\tau$ and V(r) to the 'direct' interaction term $\int \chi_1 V(r_{ij}) \chi_1 d\tau$.

Chapter 4.

Processes (b). The Reactions ($^3He + {}^3H \longrightarrow {}^3He + {}^3H$), ($^3He + {}^3H \rightarrow d + \alpha$), ($d + \alpha \rightarrow {}^3He + {}^3H$) and ($d+\alpha \rightarrow d+\alpha$).

4.1 Wave-function.

We consider two partitions:- into groups of (3+3) particles corresponding to the ^3He and ^3H nuclei represented by the wave-functions χ_T and χ_H and into (4+2) particles corresponding to the alpha-particle and the deuteron, represented by wave-functions χ_α and χ_D.

The correct anti-symmetry properties are given by the following wave-function:-

$$\Psi_s(123456) = (1-P_{12}-P_{13})(1-P_{46}-P_{56})\varphi_s + (1-P_{12}-P_{13}) \times$$
$$\times (1-P_{46}-P_{45})\psi_s \tag{4.1}$$

with $\varphi_s = \chi_T(145)\,\chi_H\,(236)\;\sigma^s_m\;(145,236)F_s(145-236)$

and $\psi = \chi_D(14)\;\chi_\alpha(23,56)\;\overline{\sigma}^s_m\;(14,2356)\Phi_s(14-2356)$ (4.2)

Particles 1,2,3 are protons and 4,5,6 neutrons. The notation is in accord with chapter 3.

Since the deuteron has spin 1, and the alpha-particle spin zero, the (d+α) grouping does not exist for s = 0. We therefore uncouple the system for this case by putting $\Phi_0 = 0$.

The spin functions are taken as:-

$$s = 0 \quad \sigma_0^0 = \frac{1}{\sqrt{2}}\left(\sigma_{T\,1/2}^{\;1/2}(145)\,\sigma_{H\,-1/2}^{\;1/2}(236) - \sigma_{T\,-1/2}^{\;1/2}(145)\,\sigma_{H\,1/2}^{\;1/2}(236)\right)$$

$$s = 1 \quad \sigma_1^1 = \sigma_{T\,1/2}^{\;1/2}(145)\,\sigma_{H\,1/2}^{\;1/2}(236)$$

$$\sigma_0^1 = \left(\sigma_{T\,1/2}^{\;1/2}(145)\,\sigma_{H\,-1/2}^{\;1/2}(236) + \sigma_{T\,-1/2}^{\;1/2}(145)\,\sigma_{H\,1/2}^{\;1/2}(236)\right)\frac{1}{\sqrt{2}}$$

$$\sigma_{-1}^1 = \sigma_{T\,-1/2}^{\;1/2}(145)\,\sigma_{H\,-1/2}^{\;1/2}(236).$$

and for s = 1 only $\quad \bar{\sigma} = \sigma_{D\,1}^{\;1}(14)\,\sigma_{\alpha\,0}^{\;0}(2356)$

where $\sigma_{T\,1/2}^{\;1/2}(145) = \frac{1}{\sqrt{2}}\,\alpha(1)\left(\alpha(4)\beta(5) - \beta(4)\alpha(5)\right)$ etc.

$$\sigma_{D\,1}^{\;1}(14) = \alpha(1)\alpha(4)$$

$$\sigma_{\alpha\,0}^{\;0}(2356) = \frac{1}{2}\left(\alpha(2)\beta(3) - \beta(2)\alpha(3)\right)\left(\alpha(5)\beta(6) - \beta(5)\alpha(6)\right)$$

(4.3)

4.2 Co-ordinate Systems and Notation.

Set (a). (3 + 3) partition.

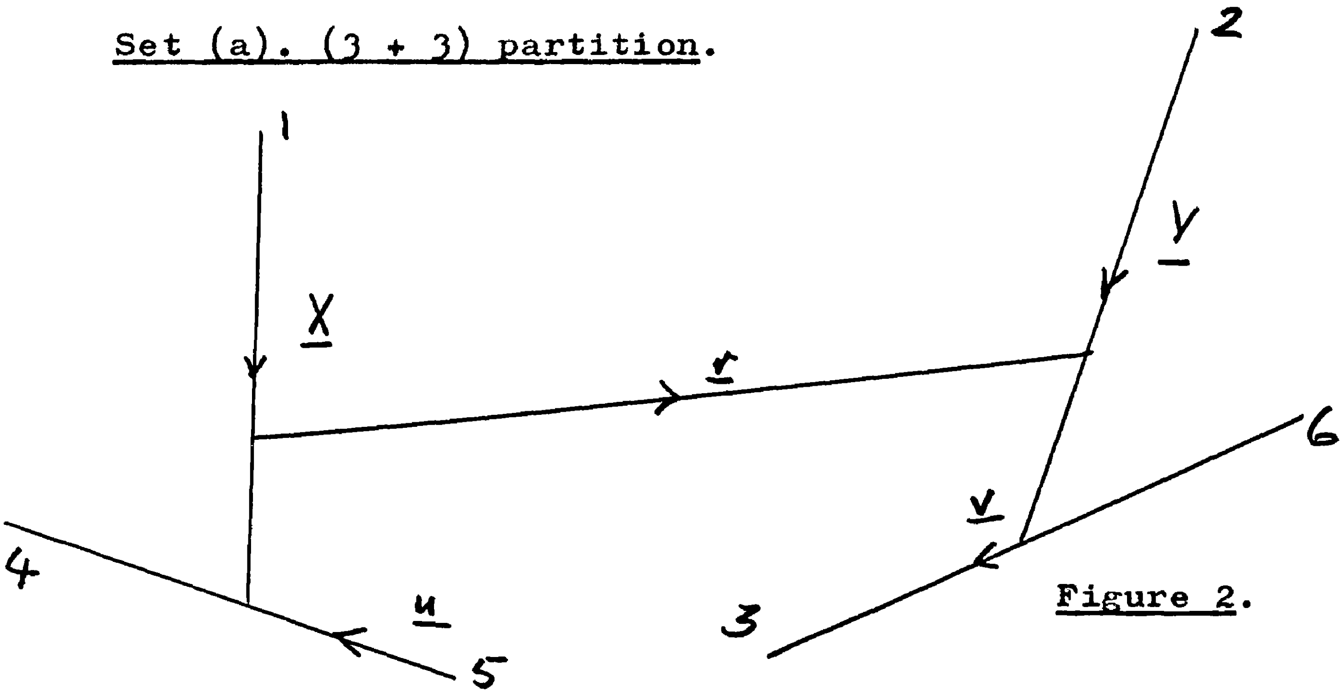

Figure 2.

$$\underline{u} = \underline{r}_4 - \underline{r}_5, \qquad \underline{v} = \underline{r}_3 - \underline{r}_2$$

$$\underline{X} = \tfrac{1}{2}(\underline{r}_4+\underline{r}_5) - \underline{r}_1, \quad \underline{Y} = \tfrac{1}{2}(\underline{r}_3+\underline{r}_6) - \underline{r}_2$$

$$\underline{r} = 1/3(\underline{r}_2+\underline{r}_3+\underline{r}_6-\underline{r}_1-\underline{r}_2-\underline{r}_5)$$

$$\underline{r}' = P_{12}\underline{r} \tag{4.4)(a}$$

Set (b). (2 + 4) partition.

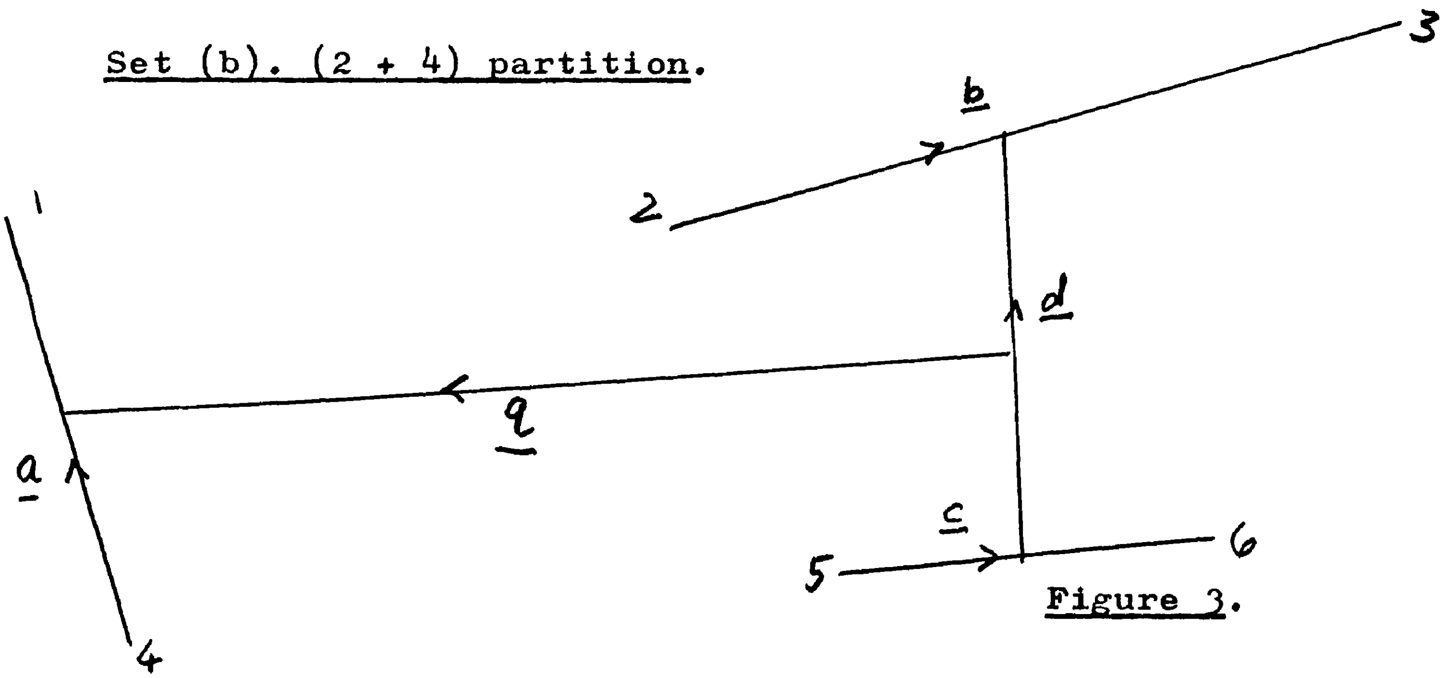

Figure 3.

$$\underline{a} = \underline{r}_1 - \underline{r}_4, \quad \underline{b} = \underline{r}_3 - \underline{r}_2, \quad \underline{c} = \underline{r}_5 - \underline{r}_6,$$

$$d = \tfrac{1}{2}(\underline{r}_2 + \underline{r}_3) - \tfrac{1}{2}(\underline{r}_5 + \underline{r}_6),$$

$$\underline{q} = \tfrac{1}{2}(\underline{r}_1 + \underline{r}_4) - \tfrac{1}{4}(\underline{r}_2 + \underline{r}_3 + \underline{r}_5 + \underline{r}_6)$$

$$\underline{q}' = P_{12}\,\underline{q}, \quad \underline{q}'' = P_{46}\,\underline{q}, \qquad (4.4)(b)$$
$$\underline{q}''' = P_{12} P_{46}\,\underline{q}.$$

Notation.

We use the abbreviations:-

$\chi_T = \chi_T(145)$	$d\tau_T = d\underline{u}.d\underline{X}$
$\chi_H = \chi_H(236)$	$d\tau_H = d\underline{v}.d\underline{Y}$
$\chi_D = \chi_D(14)$	$d\tau_D = d\underline{a}$
$\chi_\alpha = \chi_\alpha(2356)$	$d\tau_\alpha = d\underline{b}\,d\underline{c}\,d\underline{d}$
$\sigma^S = \sigma^S_m(145, 236)$	$\Sigma P = (1 - P_{12} - P_{13})(1 - P_{46} - P_{56}) - 1$
$\bar{\sigma} = \bar{\sigma}'(14, 2356)$	$\Sigma' P = (1 - P_{12} - P_{13})(1 - P_{46} - P_{45}) - 1.$

and again $\int d\tau$ indicates integration over the appropriate configuration space.

4.3 Scattering Equations.

Ψ_S is required to satisfy the variation principle in exactly the same manner as in chapter 3.3.

In this case $H = T + \mathcal{V} + C$ (4.5)

Using co-ordinate set (a) the kinetic energy operator T is

$$T = -(\hbar^2/M)(\nabla_u^2 + \nabla_v^2 + 3/4(\nabla_x^2 + \nabla_y^2) + 1/3\,\nabla_r^2)$$

and set (b)

$$T = -(\hbar^2/M)(\nabla_a^2 + \nabla_b^2 + \nabla_c^2 + 1/2\,\nabla_d^2 + 3/8\,\nabla_q^2) \tag{4.6}$$

$$\mathcal{V} = \sum_{\substack{i,j=1\\ i<j}}^{6} \mathcal{V}(ij),\quad \mathcal{V}(ij) \text{ given by (3.8)}$$

$$C = e^2(r_{12}^{-1} + r_{13}^{-1} + r_{23}^{-1}) \tag{4.7}$$

The variational principle will be satisfied if

$$(T + \mathcal{V} + C - E)\,\Psi_S = 0 \tag{4.8}$$

Multiplying (4.8) by $\chi_T\chi_H\,\sigma^S_M$, integrating over the space of the internal co-ordinates of the ^3H and ^3He nuclei, and summing over spin directions, we find:-

$$\begin{aligned}(\nabla_r^2 + k_0^2)\,F_S(\underline{r}) &= \sum_{spin}\int d\tau_T\,d\tau_H\,\sigma^S\chi_T\chi_H\,\frac{3M}{\hbar^2}\Big[\sum_{\substack{i=1,4,5\\ j=3,4,6}}\mathcal{V}(ij) + e^2\Big(\frac{1}{r_{13}} + \frac{1}{r_{23}}\Big) \\ &\qquad - (T + \mathcal{V} + C - E)\,\Sigma P\Big]\chi_T\chi_H\,\sigma^S F_S(\underline{r}) \\ &\quad + \sum_{spin}\int d\tau_T\,d\tau_H\,\sigma^S\chi_T\chi_H\,\frac{3M}{\hbar^2}[T + \mathcal{V} + C - E](\Sigma' P + 1)\chi_D\chi_\alpha\,\bar{\sigma}\,\Phi_S(\underline{q})\end{aligned} \tag{4.9}$$

where $k_0^2 = \frac{3M}{\hbar^2}(E - E_T - E_H)$, and we have made use of (3.10) and (3.11) in the same way as before.

Repeating the above procedure, but pre-multiplying by $\chi_D \chi_\alpha \bar{\sigma}$ and integrating over the space of the internal co-ordinates of the deuteron and alpha groups (i.e. over $\underline{a}$, $\underline{b}$, $\underline{c}$ and $\underline{d}$) we have, for s = 1 only:-

$$\left(\tfrac{9}{8}\nabla_q^2 + k_1^2\right)\Phi_1(q)$$
$$= \sum_{spin}\int d\tau_D d\tau_\alpha\, \bar{\sigma}\chi_D\chi_\alpha \frac{3M}{\hbar^2}\Big[\sum_{\substack{i=1,4\\ j=2,3,5,6}} V(ij) + e^2\left(\frac{1}{r_{12}} + \frac{1}{r_{13}}\right)$$
$$- (T + V + C - E)\textstyle\sum' P\Big]\chi_D\chi_\alpha\bar{\sigma}\,\Phi_1(q)$$
$$+ \sum_{spin}\int d\tau_D d\tau_\alpha \chi_D\chi_\alpha \frac{3M}{\hbar^2}[T + V + C - E](1 + \textstyle\sum P)\chi_T\chi_H\sigma^s F_s(\underline{r}) \qquad (4.10)$$

where $k_1^2 = \frac{3M}{\hbar^2}(E - E_d - E_\alpha)$, and we have made use of the equations:-

$$\int \chi_D\left(-\frac{\hbar^2}{M}\nabla_a^2 + V(14) - E_d\right)\chi_D\, d\tau_D = 0 \qquad (4.11)$$

and

$$\int \chi_\alpha\left(-\frac{\hbar^2}{M}(\nabla_b^2 + \nabla_c^2 + \tfrac{1}{2}\nabla_d^2) + \sum_{\substack{i,j=2,3,5,6\\ i<j}} V(ij) + \frac{e^2}{r_{23}} - E_\alpha\right)\chi_\alpha\, d\tau_\alpha = 0. \qquad (4.12)$$

Thus we have two coupled integro-differential equations in the intergroup wave-functions $F_1(\underline{r})$ and $\Phi_1(q)$

The (^3He + ^3H $\rightarrow$ ^3He + ^3H) Terms.

Substituting (3.8) for $\mathcal{V}(ij)$ and treating (4.9) in the same way as (3.13) was treated in the single channel system, using the spin matrix elements in appendix A, it becomes:-

$$(\nabla_r^2+k_0^2)F_s(\underline{r}) = (\alpha_{00}C_{00}(r)+\beta_{00}U_{00}(r))F_s(\underline{r})$$
$$+\sum_{i=1}^{16}\gamma_{00}^{i}\int Q_{00}^{i}(\underline{r},\underline{r}')F_s(\underline{r}')d\underline{r}'+\sum_{i=1}^{8}\varepsilon_{00}^{i}\int H_{00}^{i}(\underline{r},\underline{r}')F_s(\underline{r}')d\underline{r}'$$
$$+\sum_{i=1,2}\delta_{00}^{i}\int\left[P_{00}^{i}(\underline{r},\underline{r}')-\frac{E}{E_T+E_H}N_{00}^{i}(\underline{r},\underline{r}')\right]F_s(\underline{r}')d\underline{r}'.$$

+ (cross-terms, ^3He + ^3H $\rightarrow$ d + α, for s = 1 only)

...(4.13)

with $C_{00}(r) = \frac{3Me^2}{\hbar^2}\int d\underline{u}\,d\underline{v}\,d\underline{X}\,d\underline{Y}\ \chi_T^2\chi_H^2(r_{12})^{-1}$

$U_{00}(r) = \frac{3M}{\hbar^2}\int d\underline{u}\,d\underline{v}\,d\underline{X}\,d\underline{Y}\ \chi_T^2\chi_H^2\,V(r_{12})$

$Q_{00}^{i}(\underline{r},\underline{r}') = \frac{3M}{\hbar^2}(9/2)^3\int d\underline{u}\,d\underline{v}\,d\underline{X}\ \chi_T\chi_H(P_{12}\chi_T\chi_H)V^i$ for $i=1,2,\cdots,9.$

$Q_{00}^{i}(\underline{r},\underline{r}') = \frac{3M}{\hbar^2}(9/2)^3\int d\underline{u}\,d\underline{v}\,d\underline{X}\ \chi_T\chi_H(P_{34}P_{56}\chi_T\chi_H)V^i$ for $i=10,11,\cdots,16.$

$P_{00}^{1}(\underline{r},\underline{r}^1) = \frac{3M}{\hbar^2}(9/2)^3\int d\underline{u}\,d\underline{v}\,d\underline{X}\ \chi_T\chi_H\,T\,(P_{12}\chi_T\chi_H)$

$P_{00}^{2}(\underline{r},\underline{r}^1) = \frac{3M}{\hbar^2}(9/2)^3\int d\underline{u}\,d\underline{v}\,d\underline{X}\ \chi_T\chi_H\,T\,(P_{34}P_{56}\chi_T\chi_H)$

$N_{00}^{1}(\underline{r},\underline{r}^1) = \frac{3M}{\hbar^2}(9/2)^3\int d\underline{u}\,d\underline{v}\,d\underline{X}\ \chi_T\chi_H(P_{12}\chi_T\chi_H)(E_T+E_H)$

$N_{00}^{2}(\underline{r},\underline{r}^1) = \frac{3M}{\hbar^2}(9/2)^3\int d\underline{u}\,d\underline{v}\,d\underline{X}\ \chi_T\chi_H(P_{34}P_{56}\chi_T\chi_H)(E_T+E_H).$

$H_{00}^{i}(\underline{r},\underline{r}^1) = \frac{3Me^2}{\hbar^2}(9/2)^3\int d\underline{u}\,d\underline{v}\,d\underline{X}\ \chi_T\chi_H(P_{12}\chi_T\chi_H)C^i$ for $i=1,2,\cdots 5$

and $H_{00}^{i}(r,r^1) = \frac{3Me^2}{\hbar^2}(9/2)^3\int d\underline{u}\,d\underline{v}\,d\underline{X}\ \chi_T\chi_H(P_{34}P_{56}\chi_T\chi_H)C^i$ for $i=6,7,8.$

with $V^1 = V(r_{12})$, $V^2 = V(r_{13})$, $V^3 = V(r_{42})$, $V^4 = V(r_{14})$, $V^5 = V(r_{23})$,

$V^6 = V(r_{3c})$, $V^7 = V(r_{45})$, $V^8 = V(r_{34})$.

and $V^{8+i} = V^i$.

$$C^1 = \left(\frac{1}{r_{12}}\right),\ C^2 = \frac{1}{r_{13}},\ C^3 = \frac{1}{r_{23}},\ C^4 = \frac{1}{r_{63}},\ C^5 = \frac{1}{r_{34}},$$

$$C^6 = \frac{1}{r_{42}},\ C^7 = \frac{1}{r_{34}},\ C^8 = \frac{1}{r_{23}}.$$

The constants γ^i_{oo}, δ^i_{oo}, a_{oo}, β_{oo}, and ϵ^i_{oo} are given in Table 3.

Table 3. Constants for (b): $^3H + {}^3He \longrightarrow {}^3H + {}^3He$.

	s = 0	s = 1
α_{oo}	2	2
β_{oo}	9w+3b-m-5h	9w+5b-m-3h
γ^1_{oo}	-2w-4b+9m+3h	-2w+4b+0m+5h
$\gamma^2_{oo}, \gamma^3_{oo}, \gamma^4_{oo}, \gamma^5_{oo}$	-4(w+m)+(b+h)	-(4w+4m+b+h)
$\gamma^6_{oo}, \gamma^7_{oo}$	-2(w+m)-(b+h)	-2(w+m)+(b+h)
γ^8_{oo}	-8w-4b+4m+2h	-8w-4b+4m+6h
γ^9_{oo}	$(w-b)(-1)^\pi$	$(w+b)(-1)^\pi$
$\gamma^{10}_{oo}, \gamma^{11}_{oo}, \gamma^{12}_{oo}, \gamma^{13}_{oo}$	$2(w+m)+(b+h)\ \ (-1)^\pi$	$2(w+m)-(b+h)\ \ (-1)^\pi$
$\gamma^{14}_{oo}, \gamma^{15}_{oo}$	$(w+m)-(b+h)\ \ (-1)^\pi$	$(w+m+b+h)\ \ (-1)^\pi$
γ^{16}_{oo}	$(4w+2b-8m-4h)(-1)^\pi$	$(4w+6b-8m-4h)(-1)^\pi$
δ^1_{oo}	-2	-2
δ^2_{oo}	$(-1)^\pi$	$(-1)^\pi$
$\varepsilon^1_{oo}, \varepsilon^2_{oo}, \varepsilon^3_{oo}, \varepsilon^4_{oo}$	-1	-1
ε^5_{oo}	-2	-2
$\varepsilon^6_{oo}, \varepsilon^7_{oo}, \varepsilon^8_{oo}$	$(-1)^\pi$	$(-1)^\pi$

<u>Note</u>: 1. π is parity. $\pi = -1$ for odd and $+1$ for even states of $F_s(\underline{r})$.

2. It can be seen that the constants depending on force type (i.e. on y) are β_{oo}, γ^1_{oo}, γ^8_{oo}, γ^9_{oo}, γ^{16}_{oo}.

The (d+α) ⟶ (d+α) Terms.

Similarly (4.10) becomes:-

$$(9/8\,\nabla_q^2 + k_1^2)\,\Phi_1(q) = (\alpha_{11} C_{11}(q) + \beta_{11} U_{11}(q))\,\Phi(q)$$
$$+ \sum_{i=1}^{13} \gamma_{11}^i \int Q_{11}^i(q,q')\,\Phi(q')\,dq' + \sum_{i=1}^{10} \varepsilon_{11}^i \int H_{11}^i(q,q')\,\Phi(q')\,dq'$$
$$+ \sum_{i=1,2} S_{11}^i \int [P_{11}^i(q,q') - \frac{E}{E_D+E_\alpha} N_{11}^i(q,q')]\,\Phi(q')\,dq' \qquad (4.14)$$
+ (cross terms for (d+α → ^{3}H + ^{3}He).

with $C_{11}(q) = \frac{3Me^2}{\hbar^2}\int d\tau_D\, d\tau_\alpha\, \chi_D{}^2 \chi_\alpha^2\, (r_{12})^{-1}$

$$U_{11}(q) = \frac{3M}{\hbar^2}\int d\tau_D\, d\tau_\alpha\, \chi_D{}^2\chi_\alpha^2\; V(r_{12})$$

$$Q^i(q,q') = \frac{3M}{\hbar^2}\int d\tau'_{D\alpha}\, \chi_D\chi_\alpha\, (P_{12}\chi_D\chi_\alpha)\, V^i \text{ for } i=1,2,\dots,7.$$

$$Q_{11}^i(q,q') = \frac{3M}{\hbar^2}\int d\tau'_{D\alpha}\, \chi_D\chi_\alpha\, (P_{12}P_{45}\chi_D\chi_\alpha)\, V^i \text{ for } i=8,9,\dots,15.$$

$$P_{11}^1(q,q') = \frac{3M}{\hbar^2}\int d\tau'_{D\alpha}\, \chi_D\chi_\alpha\, T(P_{12}\chi_D\chi_\alpha)$$

$$P_{11}^2(q,q') = \frac{3M}{\hbar^2}\int d\tau'_{D\alpha}\, \chi_D\chi_\alpha\, T(P_{12}P_{45}\chi_D\chi_\alpha)$$

$$N_{11}^1(q,q') = \frac{3M}{\hbar^2}\int d\tau'_{D\alpha}\, \chi_D\chi_\alpha\, (P_{12}\chi_D\chi_\alpha)(E_D+E_\alpha)$$

$$N_{11}^2(q,q') = \frac{3M}{\hbar^2}\int d\tau'_{D\alpha}\, \chi_D\chi_\alpha\, (P_{12}P_{45}\chi_D\chi_\alpha)(E_D+E_\alpha)$$

and $H_{11}^i(q,q')$, i = 1,2,....,13, are the same as $Q_{11}^i(q,q')$ with V^i replaced by C^i, i.e. $V(r_{jk})$ replaced by e^2/r_{jk}
$V^1 = V(r_{12})$, $V^2 = V(r_{45})$, $V^3 = V(r_{13})$, $V^4 = V(r_{23})$, $V^5 = V(r_{35})$,
$V^6 = V(r_{24})$, $V^7 = V(r_{14})$, $V^8 = V^1$, $V^9 = V^3$, $V^{10} = V^5$, $V^{11} = V(r_{52})$,
$V^{12} = V^7$, $V^{13} = V(r_{36})$.

The constants are tabulated in Table 4.

($d\tau'_{D\alpha}$ indicates integration over the spaces of the three appropriate vectors.)

Table 4. Constants for $(d+\alpha \rightarrow d+\alpha)$ Terms.

α_{11}	1
β_{11}	$(8w+4b-2m-4h)$
γ_{11}^{1}	$(-2w-4b+8m+4h)$
γ_{11}^{2}	$-6w-2b+4m+6h$
$\gamma_{11}^{3}, \gamma_{11}^{4}, \gamma_{11}^{5}$	$-6(w+m)$
$\gamma_{11}^{6}, \gamma_{11}^{7}$	-2
γ_{11}^{8}	$4w+6b-6m-2h$
$\gamma_{11}^{9}, \gamma_{11}^{10}$	$4(w+m)-2(b+h)$
$\gamma_{11}^{11}, \gamma_{11}^{12}, \gamma_{11}^{13}$	1
δ_{11}^{1}	-2
δ_{11}^{2}	$+1$
ε_{11}^{1}	-1
ε_{11}^{2}	-2
$\varepsilon_{11}^{3}, \varepsilon_{11}^{4}, \varepsilon_{11}^{5}$	-1
$\varepsilon_{11}^{6}, \varepsilon_{11}^{7}$	0
$\varepsilon_{11}^{8}, \varepsilon_{11}^{9}, \varepsilon_{11}^{10}$	$+1$

The Cross Terms.

Both of these were evaluated as a check.

The term $^3He + {}^3H \longrightarrow d + \alpha$.

By the same methods we find the equation (from (4.9)):-

$$(\nabla_r^2 + k_0^2)F_1(r) = [\text{elastic scattering terms (labelled oo)}]$$
$$+ \sum_{i=1}^{18} \gamma_{01}^i \int Q_{01}^i(r,q)\Phi_1(q)dq + \sum_{i=1}^{18} \varepsilon_{01}^i \int H_{01}^i(r,q)\Phi_1(q)dq$$
$$+ \sum_{i=1,2,3} \delta_{01}^i \int [P_{01}^i(r,q) - \frac{E}{E_D + E_\alpha} N_{01}^i(r,q)]\Phi(q)dq \quad (4.15)$$

with
$$Q_{01}^i(r,q) = \frac{3M}{\hbar^2}\int d\tau'_{TH}\, \chi_T\chi_H\chi_D\chi_\alpha V^i \text{ for } i = 1,2,\dots,5$$
$$Q_{01}^i(r,q'') = \frac{3M}{\hbar^2}\int d\tau'_{TH}\, \chi_T\chi_H(P_{46}\chi_D\chi_\alpha) V^i \text{ for } i = 6,7,\dots 13.$$
$$Q_{01}^i(r,q''') = \frac{3M}{\hbar^2}\int d\tau'_{TH}\, \chi_T\chi_H(P_{12}P_{46}\chi_D\chi_\alpha) V^i \text{ for } i = 14,\dots 18.$$

$P_{01}^i(r,q)$ for i = 1,2,3 are the same as $Q_{01}^1, Q_{01}^6, Q_{01}^{14}$ respectively with T in place of V^i.

$N_{01}^i(r,q)$ for i = 1,2,3 are the same as P_{01}^i with $(E_\alpha + E_d)$ in place of T.

$H_{01}^i(r,q)$ are the same as $Q_{01}^i(r,q)$ with e^2/r_{jk} in place of $V(r_{jk})$.

The constants are tabulated in Table 5.

We now have (for s = 1) two coupled integro-differential equations:-

$$
\begin{aligned}
(\nabla_r^2 + k_0^2)\, F_s(\underline{r}) = {} & (\alpha_{00}\, C_{00}(r) + \beta_{00}\, U_{00}(r))\, F_s(\underline{r}) \\
& + \sum_i \gamma^i_{00} \int Q^i_{00}(\underline{r},\underline{r}')\, F_s(\underline{r}')\, d\underline{r}' + \sum_i \varepsilon^i_{00} \int H^i_{00}(\underline{r},\underline{r}')\, F_s(\underline{r}')\, d\underline{r}' \\
& + \sum_i \gamma^i_{01} \int Q^i_{00}(\underline{r},\underline{q})\, \Phi_s(\underline{q})\, d\underline{q} + \sum_i \varepsilon^i_{00} \int H^i_{01}(\underline{r},\underline{q})\, \Phi_s(\underline{q})\, d\underline{q} \\
& + \sum_i \delta^i_{00} \int \left[P^i_{00}(\underline{r},\underline{r}') - \frac{E}{E_T + E_H}\, N^i_{00}(\underline{r},\underline{r}') \right] F_s(\underline{r}')\, d\underline{r}' \\
& + \sum_i \delta^i_{01} \int \left[P^i_{01}(\underline{r},\underline{q}) - \frac{E}{E_D + E_\alpha}\, N^i_{01}(\underline{r},\underline{q}) \right] \Phi_s(\underline{q})\, d\underline{q}
\end{aligned}
\qquad (4.16)
$$

and

$$
\begin{aligned}
(\tfrac{9}{8}\nabla_q^2 + k_1^2)\, \Phi_s(\underline{q}) = {} & (\alpha_{11}\, C_{11}(q) + \beta_{11}\, U_{11}(q))\, \Phi_s(\underline{q}) \\
& + \sum_i \gamma^i_{11} \int Q^i_{11}(\underline{q},\underline{q}')\, \Phi_s(\underline{q}')\, d\underline{q}' + \sum_i \varepsilon^i_{11} \int H^i_{11}(\underline{q},\underline{q}')\, \Phi_s(\underline{q}')\, d\underline{q}' \\
& + \sum_i \gamma^i_{10} \int Q^i_{10}(\underline{q},\underline{r})\, F_s(\underline{r})\, d\underline{r} + \sum_i \varepsilon^i_{10} \int H^i_{10}(\underline{q},\underline{r})\, F_s(\underline{r})\, d\underline{r} \\
& + \sum_i \delta^i_{11} \int \left[P^i_{11}(\underline{q},\underline{q}')\, \Phi_s(\underline{q}') - \frac{E}{E_D + E_\alpha}\, N^i_{11}(\underline{q},\underline{q}')\, \Phi_s(\underline{q}') \right] d\underline{q}' \\
& + \sum_i \delta^i_{10} \int \left[P^i_{10}(\underline{q},\underline{r}) - \frac{E}{E_T + E_H}\, N^i_{10}(\underline{q},\underline{r}) \right] F_s(\underline{r})\, d\underline{r}
\end{aligned}
\qquad (4.17)
$$

where the functions for the cross-terms ($d+\alpha \rightarrow {}^3H + {}^3He$) are:-

$$Q^i_{10}(\underline{q},\underline{r}) = \frac{3M}{\hbar^2} \int d\tau'_{D\alpha}\, \chi_D \chi_\alpha \chi_T \chi_H\, V^i \quad \text{for } i = 1, 2, \ldots 5$$

$$Q^i_{10}(\underline{q},\underline{r}) = \frac{3M}{\hbar^2} \int d\tau'_{D\alpha}\, \chi_D \chi_\alpha (P_{46} \chi_T \chi_H)\, V^i \quad \text{for } i = 6, 7, \ldots 15.$$

$$Q^i_{10}(\underline{q},\underline{r}) = \frac{3M}{\hbar^2} \int d\tau'_{D\alpha}\, \chi_D \chi_\alpha (P_{12} P_{46} \chi_T \chi_H)\, V^i$$

$$\text{for } i = 14, 15, \ldots 18$$

Similar alterations to $Q'_{10}(q,r)$ give N'_{10}, P'_{10} and H'_{10} as in the (01) case, and $y'_{10} = y'_{01}$; $\varepsilon'_{10} = \varepsilon'_{01}$; $\delta'_{10} = \delta'_{01}$.

We expand in harmonic series in exactly the same manner as in chapter (3.3).

$$F_s(\underline{r}) = r^{-1}\sum_{n=0}^{\infty}(2n+1)f_n^s(r)P_n(\cos\theta)$$

$$Q'_{00}(\underline{r},\underline{r}') = \sum_n \frac{2n+1}{4\pi r r'} P_n(\cos\Theta)\,{}^{00}q_n{}^i(r,r')$$

$$\Phi(\underline{q}) = q^{-1}\sum_{n=0}^{\infty}(2n+1)\phi_n^s(q)P_n(\cos\theta')$$

$$Q'_{11}(\underline{q},\underline{q}') = \sum_n \frac{2n+1}{4\pi r r'}\,{}^{11}q_n{}^i(q,q')P_n(\cos\Theta')$$

with similar expansions for the other functions.

Then (4.16) and (4.17) become of the form:-

$$\left(\frac{d^2}{dr^2} + k_0^2 - \frac{n(n+1)}{r^2}\right)f_n^s(r) = \left(\alpha_{00}C_{00}(r) + \beta_{00}U_{00}(r)\right)f_n^s(r)$$
$$+\int_0^\infty K_n^{00}(r,r')f_n^s(r')dr' + \int_0^\infty K_n^{01}(r,q)\phi_n^s(q)dq \tag{4.18}$$

and

$$\left(\frac{q}{\delta}\frac{d^2}{dq^2} + k_1^2 - \frac{q}{\delta}\frac{n(n+1)}{q^2}\right)\phi_n^s(q) = \left(\alpha_{11}C_{11}(r) + \beta_{11}U_{11}(r)\right)\phi_n^s(r)$$
$$+\int_0^\infty K_n^{11}(q,q')\phi_n^s(q')dq' + \int_0^\infty K_n^{10}(q,r)f_n^s(r)dr \tag{4.19}$$

$$\left(K_n^{01}(r,q) = K_n^{10}(q,r)\right)$$

Table 5. Constants for the Cross Terms.

γ_{01}^{1}	$4m+3h-6w-5b$	ε_{01}^{1}	-2
γ_{01}^{2}	$-3(w+m)$	ε_{01}^{2}	0
γ_{01}^{3}	-1	ε_{01}^{3}	0
γ_{01}^{4}	$-2w+2m-b-h$	ε_{01}^{4}	0
γ_{01}^{5}	$-3(w+m)$	ε_{01}^{5}	-1
γ_{01}^{6}	$-6w-5h+4w+3b$	ε_{01}^{6}	4
γ_{01}^{7}	$8(w+m)+2(b+h)$	ε_{01}^{7}	2
γ_{01}^{8}	$4(w+m)+(b+h)$	ε_{01}^{8}	0
γ_{01}^{9}	$=\gamma_{01}^{6}$	ε_{01}^{9}	2
γ_{01}^{10}	2	ε_{01}^{10}	0
γ_{01}^{11}	$=\gamma_{01}^{8}$	ε_{01}^{11}	2
γ_{01}^{12}	$2(w+m)-(b+h)$	ε_{01}^{12}	2
γ_{01}^{13}	$=\gamma_{01}^{12}$	ε_{01}^{13}	0
γ_{01}^{14}	$=\gamma_{01}^{1}$	ε_{01}^{14}	-1
γ_{01}^{15}	$=\gamma_{01}^{2}$	ε_{01}^{15}	-1
γ_{01}^{16}	$=\gamma_{01}^{4}$	ε_{01}^{16}	-1
γ_{01}^{17}	$=\gamma_{01}^{5}$	ε_{01}^{17}	0
γ_{01}^{18}	$=\gamma_{01}^{3}$	ε_{01}^{18}	0
δ_{01}^{1}	-1	δ_{01}^{2}	+2
δ_{01}^{3}	-1		

Chapter 5.

5.1 Evaluation of the Integrals for the Single Channel Case (a) (^{3}He + ^{3}He) and (^{3}H + ^{3}H) Elastic Scattering.

It has been shown by Swan (1953) that if a gaussian well is used and the wave-functions χ taken to be of gaussian form, the kernels $K_n(r,r')$ can, apart from some contributions due to the Coulomb force, be reduced to a sum of terms of the type:-

$$\mathcal{K}_n^{\,s} = a_s e^{-\alpha_s r^2 - \beta_s r'^2} \mathcal{J}_{n+1/2}(k_s r r') \qquad (5.1)$$

where $\mathcal{J}_{n+1/2}(x) = \left(\frac{\pi x}{2}\right)^{1/2} (i)^{n+1/2} J_{n+1/2}(ix)$. $\qquad (5.2)$

For this reason the wave-function and well used were gaussian, with the parameter used earlier in the four-body calculations and given by (2.1), (2.2) and (2.3).

To make for uniformity in the numerical work, and keep down the number of programmes, as many of the terms of $K_n(r,r')$ as possible were reduced to the form (5.1).

(a) The Nuclear Force Kernels.

$$Q^i(\underline{r},\underline{r}') = \frac{3M}{\hbar^2}\left(\tfrac{9}{2}\right)^3 \int d\underline{u}\, d\underline{v}\, d\underline{x}\; \chi(125)\chi(346)\, V(r_{jk})\, \chi(325)\chi(146)$$

As an example of how these were dealt with, we will consider $Q^2(r, r')$. It is convenient to define a new set of co-ordinates.

$\underline{r} = 1/3(\underline{r}_3 + \underline{r}_4 + \underline{r}_6 - \underline{r}_1 - \underline{r}_2 - \underline{r}_5)$, $\underline{r}^1 = P_{13}\underline{r}$ are the same as before.

$$\begin{aligned}
&\underline{W} = \underline{r}_2 - \underline{r}_5, \ \underline{t} = \underline{r}_4 - \underline{r}_6, \\
&\underline{R} = -\underline{r}_1 + \tfrac{1}{2}(\underline{r}_2 + \underline{r}_5), \ \underline{R}^1 = P_{13}\underline{R} \\
&\underline{Z} = -\underline{r}_3 + \tfrac{1}{2}(\underline{r}_4 + \underline{r}_6), \ \underline{Z}^1 = P_{13}\underline{Z}
\end{aligned} \tag{5.3}$$

The following relations exist between co-ordinate sets (3.5) and (5.3):-

$$\underline{Z} = \underline{R} - 3/2(\underline{r} - \underline{r}') + 3/4(\underline{r} + \underline{r}');$$

$$\int d\underline{u}\, d\underline{v}\, d\underline{X}\, d\underline{Y} = \int d\underline{w}\, d\underline{t}\, d\underline{R}\, d\underline{Z}\, ; \quad \int d\underline{u}\, d\underline{v}\, d\underline{X} = \frac{1}{2^3}\int d\underline{w}\, d\underline{t}\, d\underline{R} \tag{5.4}$$

$$Q^2(r, r') = \frac{3M}{\hbar^2}(q/2)^3 \int d\underline{u}\, d\underline{v}\, d\underline{X}\, \chi(125)\chi(346)\chi(325)\chi(146)\, V(r_{53}$$

From (2.1), (2.2) and (2.3) we have

$$V(r_{53}) = V_o e^{-\mu r_{53}^2}$$

$$\chi_H(125) = N_H\, e^{-\lambda/2 \sum r_{ij}^2} = N_H\, e^{-\lambda\left(\frac{3w^2}{4} + R^2\right)}$$

$$\chi_T(346) = N_T\, e^{-\eta/2 \sum r_{ij}^2} = N_T\, e^{-\eta\left(\frac{3t^2}{4} + Z^2\right)}$$

(To cover some of the kernel evaluation for the (^{3}H + ^{3}He) terms in chapter 4, we take our general matrix element $\int \chi_1 X^S P_{ij} \chi_1 \, d\tau$ to be of the form $\int \chi_H(125)\chi_T(346) X^S P_{ij} \chi_H(125)\chi_T(346)\, d\tau$ Then to obtain the formulae for scattering of type (a), we need only put $\lambda = \eta$).

In terms of co-ordinate set (5.3)

$$Q^2(r, r') = \frac{3M}{\hbar^2}(9/4)^3 N_T^2 N_H^2 \int d\underline{w}\, dt\, d\underline{R}\; e^{-\lambda\left(\frac{3w^2}{4} + R^2\right)}$$
$$\times e^{-\eta(3t^2/4 + Z^2) - \lambda(3w^2/4 + R'^2) - \eta(3t^2/4 + Z'^2)}$$
$$\times e^{-\mu(r_{53})^2}$$

$r_{53}^2 = (r_5 - r_3)^2 = (R')^2 + \frac{w^2}{4} - \underline{R}'.\underline{w}$. Using the relations between R', Z', Z, and w, t,R, we express this in terms of the latter three.

$$\text{ie}\quad Q^2(\underline{r}, \underline{r}') = \frac{3M}{\hbar^2}(9/4)^3 N_T^2 N_H^2\, e^{(r - r')^2\left(-\frac{9\lambda}{4} - \frac{9\eta}{4} - \frac{9\mu}{4}\right)}$$
$$\times e^{-\frac{9\eta}{8}(\underline{r} + \underline{r}')^2 + \frac{9\eta}{4}(\underline{r}^2 - \underline{r}'^2)} \int d\underline{w}\; e^{-w^2(3\lambda/2 + \mu/4)}$$
$$\times \int d\underline{t}\; e^{-t^2 3\eta/2} \int d\underline{R}\; e^{\underline{w}\cdot\left(-\frac{3\mu}{4}(\underline{r} - \underline{r}') + \mu\underline{R}\right)}$$
$$\times e^{-R^2(2\lambda + 2\eta + \mu)}\, e^{3\underline{R}\cdot(\lambda\underline{r} - (\lambda + 2\eta)\underline{r}' + 2\mu\underline{r} - \mu\underline{r}')}$$

By repeated use of the integrals in appendix B, this reduces to the required form. The other nuclear kernels are treated similarly, and in general, we have:-

$$Q^i(\underline{r},\underline{r}') = \frac{3MV_0}{\hbar^2}(9/4)^3 (A_q^i)^{3/2} e^{-\gamma_q^i r^2 - \Gamma_q^i r'^2 + K_q^i r r' y} \tag{5.5}$$

where $y = \cos \Theta$,

giving

$$q_n^i(r,r') = \frac{3MV_0}{\hbar^2}(9/4)^3 (A_q^i)^{3/2} e^{-\gamma_q^i r^2 - \Gamma_q^i r'^2} \frac{4\pi(-1)^n}{(-K_q^i)} J_{n+1/2}(K_q^i r r') \tag{5.6}$$

where integral 4 of appendix B has been used.

A_q^i, γ_q^i and Γ_q^i are tabulated in Table 6 (a).

(b) The Term $n_n(r,r')$ and the Functions U(r) and C(r).

By straightforward application of appendix B, $n_n(r,r')$ and U(r) were reduced to:-

$$U(r) = \frac{3MV_0}{\hbar^2}(A_u)^{3/2} e^{-\gamma_u r^2} \tag{5.7}$$

$$n_n(r,r') = \frac{3M}{\hbar^2}(A_n)^{3/2} e^{-\gamma_n r^2 - \Gamma_n r'^2} \frac{4\pi(-1)^n}{(-K_n)} J_{n+1/2}(K_n r r') \tag{5.8}$$

$$C(r) = \frac{3Me^2}{\hbar^2}\int d\underline{u}\, d\underline{v}\, d\underline{X}\, d\underline{Y}\, N_T^2 N_H^2 \frac{1}{r_{13}} e^{-\lambda\left(\frac{3u^2}{2}+2X^2\right)-\eta\left(\frac{3v^2}{2}+2Y^2\right)}$$

We employ the change of variable $s = r_{13} = |\underline{r}_1 - \underline{r}_3|$, and using $\int d\underline{u} = 8\int d\underline{s}$ and appendix B, this is reduced to the form

$$C(r) = Ac\ \frac{\Phi(\Lambda r)}{r} \qquad (5.9)$$

where Φ is the error function $\Phi(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-u^2}du$.

The constants for (5.7), (5.8) and (5.9) are given in Table 6(b).

(c) <u>The Kinetic Energy Term</u>.

Expressed in terms of the variables (5.3), this takes the form:-

$$p_n(r,r') = \frac{3M}{\hbar^2}(9/4)^3\int d\underline{w}\,d\underline{t}\,d\underline{R}\,(2\pi r r')\int_{-1}^{+1}dy\,P_n(y)\chi_1 T\chi_3$$

$$= -\frac{3M}{\hbar^2}(9/4)^3\int d\underline{w}\,d\underline{t}\,d\underline{R}\,(2\pi r r')\int_{-1}^{+1}dy\,P_n(y)$$

$$\times\left[\hbar^2/M\left(\nabla_w^2 + \nabla_t^2 + 3/4(\nabla_{R'}^2 + \nabla_{z'}^2)\right)\chi_3 + \frac{\hbar^2}{3M}\nabla_{r'}^2\chi_1\right]$$

$$\nabla_w^2\chi_3 = \left(-\frac{9}{2}\lambda + \frac{9}{4}\lambda^2\underline{w}^2\right)\chi_3$$

$$\frac{3}{4}\nabla_{R'}^2\chi_3 = \frac{3}{4}\left(-6\lambda + 4\lambda^2 R'^2\right)\chi_3 \quad \text{etc.}$$

By expressing this in terms of $\underline{R}$, $\underline{r}$, $\underline{r}$, $\underline{w}$ and t and using appendix B this is reduced to the form

$$p_n(r,r') = -\frac{\hbar^2}{M(2E_A)}\,n_n(r,r')\left(a + br^2 + cr'^2 - \frac{d}{K_p}\right) + A_p\,rr'\,e^{-Y_p(r^2+r'^2)}(-1)^n\,\mathcal{J}_{n+1/2}(K_p r r') \qquad (5.10)$$

where A(p) = $A_n \dfrac{d\,\hbar^2}{M(2E_A)}$.

$\mathcal{J}'_{n+1/2}(Kr')$ $\left(\mathcal{J}'_{n+1/2}(x) = \frac{d}{dx}\mathcal{J}_{n+1/2}(x)\right)$ may be expressed using the recurrence relations for Bessol functions as:-

$$\mathcal{J}'_{n+1/2}(x) = \frac{d}{d(Kr')}\mathcal{J}_{n+1/2}(Kr')$$

$$= -\frac{n}{Kr'}\mathcal{J}_{n+1/2}(Kr') - \mathcal{J}_{n-1/2}(Kr')$$

or by a similar formula in terms of $\mathcal{J}_{n+1/2}$ and $\mathcal{J}_{n+3/2}$

Using these relations we have:-

$$p_n(r,r') = -\frac{\hbar^2}{M(2E_A)}\, n_n(r,r')\left(a - \frac{(n+1)d}{Kp} + br^2 + cr'^2 - \frac{d}{Kp}\right) + drr'\, n_{n+1}(r,r')$$

or $$p_n(r,r') = -\frac{\hbar^2}{M(2E_A)}\, n_n(r,r')\left(a + \frac{(n-1)d}{Kp} + br^2 + cr'^2\right) - drr'\, n_{n-1}(r,r').$$

The constants are given in Table 6(b).

(d) <u>The Coulomb Kernels $h'_n(r,r')$</u>.

$$h'_n(r,r') = \frac{3Me^2}{\hbar^2}\int_{-1}^{+1} dy\, 2\pi rr' P_n(y)(q/2)^3 \int du\, dv\, dX\, \chi(125)\,\chi(325) \times \chi(346)\,\chi(146)\,\frac{1}{r_{jk}^2}$$

Using $\frac{1}{S} = \frac{2}{\sqrt{\pi}}\int_0^\infty e^{-S^2y^2}dy$ we have:-

$$h'_n(r,r') = \frac{3Me^2}{\hbar^2}(q/2)^3\int_{-1}^{+1} dy\, 2\pi rr' P_n(y) \times \int du\, dv\, dX\, \chi(125)\,\chi(325)\,\chi(146)\,\chi(346)\int_0^\infty e^{-r_{jk}^2}\frac{2}{\sqrt{\pi}}\,d\beta$$

$$= \frac{2}{\sqrt{\pi}}\frac{e^2}{V_0}\int_0^\infty q_n'(r,r';\beta^2)\,d\beta$$

where $q_n^i(r,r';\beta^2)$ denotes $q_n^i(r,r')$ with a potential $V(r_{jk}) = V_0 e^{-\beta^2 r_{jk}^2}$

Another change of variable gives

$$h_n^i(r,r') = \frac{2e^2}{V_0\sqrt{\pi}} \int_0^1 q_n^i\left(r,r';\frac{x^2}{(1-x)^2}\right)\frac{dx}{(1-x)^2}. \tag{5.11}$$

(This integral, however, does not apply to all Coulomb terms, since in $h_n^1(r,r')$, infinities arise out of the $\frac{1}{(1-x)^2}$ term.) The integral over "x" is then expressed as a sum over terms of the type (5.1).

h_n^6 and h_n^7 have $\frac{1}{w}$ and $\frac{1}{t}$ for their respective C^i's and thus using integral (Appendix B (7)) can be reduced directly to (5.1).

The term $h_n^1(r,r')$ was the most difficult Coulomb term to evaluate. It was finally reduced to the form:-

$$\begin{aligned} h_n^1(r,r') = {} & A(h') e^{-(\gamma - K/2)(r^2+r'^2)} \\ & \times \Big\{ |r+r'| \int_0^1 P_n\left(\frac{r^2+r'^2-|r+r'|^2x^2}{2rr'}\right) e^{-K/2\,|r+r'|^2x^2}\,dx \\ & \quad - |r-r'| \int_0^1 P_n\left(\frac{r^2+r'^2-|r-r'|^2x^2}{2rr'}\right) e^{-K/2\,|r-r'|^2x^2}\,dx \Big\} \end{aligned} \tag{5.12}$$

and a special programme written to deal with it.

The constants are given in Table 6(c).

Table 6. Constants for Type (a) Kernels.

Use has been made in evaluating these of the relation

$$N_T^2 N_H^2 = \left(\frac{9\lambda^2\eta^2}{\pi^4}\right)^{3/2}.$$

(a) Constants for $q^i_{l\mu}(r,r')$

i	A_q^i	Y_q^i
1	$\dfrac{2\lambda\eta}{\pi(\lambda+\eta)}$	$-\dfrac{9}{8}\left[\dfrac{\lambda^2+3\lambda\eta+\eta^2}{\lambda+\eta}+2\mu\right]$
2	$\dfrac{24\lambda^2\eta}{\pi(\mu+6\lambda)(2\eta+\lambda+\varepsilon_2)}$	$-\dfrac{9}{8}\left[\dfrac{\varepsilon_2(5\eta+2\lambda)+\eta(\lambda+2\eta)}{2\eta+\lambda+\varepsilon_2}\right]$
3	$\dfrac{24\lambda\eta^2}{\pi(\mu+6\eta)(2\lambda+\eta+\varepsilon_3)}$	$-\dfrac{9}{8}\left[\dfrac{\varepsilon_3(5\lambda+2\eta)+\lambda(\eta+2\lambda)}{2\lambda+\eta+\varepsilon_3}\right]$
4	$= A_2$	$-\dfrac{9}{8}\left[\dfrac{\varepsilon_2(2\lambda+\eta)+\eta(2\eta+5\lambda)}{2\eta+\lambda+\varepsilon_2}\right]$
5	$= A_3$	$-\dfrac{9}{8}\left[\dfrac{\varepsilon_3(2\eta+\lambda)+\lambda(2\lambda+5\eta)}{2\lambda+\eta+\varepsilon_3}\right]$
6	$\dfrac{6\lambda\eta^2}{\pi(3\eta+2\mu)(\lambda+\eta)}$	$-\dfrac{9}{8}\left[\dfrac{\lambda^2+3\lambda\eta+\eta^2}{\lambda+\eta}\right]$
7	$\dfrac{6\lambda^2\eta}{\pi(3\lambda+2\mu)(\lambda+\eta)}$	$= Y_q^6$
8	$\dfrac{12\lambda^2\eta^2}{\pi(\lambda+\eta)(6\lambda\eta+\lambda\mu+\eta\mu)}$	$\left\{-\dfrac{9}{8}\left[\dfrac{\lambda^2+3\lambda\eta+\eta^2}{\lambda+\eta}\right]+\dfrac{27}{8}\mu\right\}$

Table 6(a) - Contd.

i	$\Gamma_q^{\,i}$	$K_q^{\,i}$
1	$Y_q^{\,1}$	$\frac{9}{4}\left[\frac{\lambda^2+\lambda\eta+\eta^2}{\lambda+\eta}+2\mu\right]$.
2	$Y_q^{\,4}$	$\frac{9}{4}\left[\frac{\eta(\lambda+2\eta)+\varepsilon_2(\eta+2\lambda)}{\lambda+\varepsilon_2+2\eta}\right]$
3	$Y_q^{\,5}$	$\frac{9}{4}\left[\frac{\lambda(\eta+2\lambda)+\varepsilon_3(\lambda+2\eta)}{\eta+\varepsilon_3+2\lambda}\right]$
4	$Y_q^{\,2}$	$K_q^{\,2}$
5	$Y_q^{\,3}$	$K_q^{\,3}$
6	$Y_q^{\,6}$	$\frac{9}{4}\left[\frac{\lambda^2+\lambda\eta+\eta^2}{\lambda+\eta}\right]$
7	$Y_q^{\,6}$	$K_q^{\,6}$
8	$Y_q^{\,8}$	$\frac{9}{4}\left[\frac{\lambda^2+\lambda\eta+\eta^2}{\lambda+\eta}\right]-\frac{27\lambda\mu\eta}{4(6\lambda\eta+\lambda\mu+\eta\mu)}$

$$\varepsilon_2 = \lambda + \frac{6\mu\lambda}{\mu+6\lambda},$$

$$\varepsilon_3 = \eta + \frac{6\mu\eta}{\mu+6\eta}.$$

Table 6(b)

$$A_{n_n} = \frac{2\lambda\eta}{\pi(\lambda+\eta)}(2E_A)\ ; \quad y_n = \Gamma_n = -\frac{9}{8}\left[\frac{\lambda^2+3\lambda\eta+\eta^2}{\lambda+\eta}\right];$$

$$K_n = \frac{9}{4}\left[\frac{\lambda^2+\lambda\eta+\eta^2}{\lambda+\eta}\right];$$

$$A_U = \frac{9\lambda\eta}{9\lambda\eta+2\lambda\mu+2\mu\eta}\ ; \quad y_u = -\frac{9\lambda\mu\eta}{9\lambda\eta+2\mu\lambda+2\mu\eta}.$$

$$A_C = \frac{3Me^2}{\hbar^2}\ ; \quad \Lambda = \left(\frac{9\lambda\eta}{2\lambda+2\eta}\right)^{1/2}.$$

$$a = -\left(\frac{27}{4}\right)\left(\frac{\lambda^2+3\lambda\eta+\eta^2}{\lambda+\eta}\right); \quad K_p = K_n\ ; \quad y_p = y_n.$$

$$b = \left(\frac{27}{16}\right)(\lambda+\eta)^{-2}(2\lambda^4+2\eta^4+11\lambda^2\eta^2+6\lambda^3\eta+6\lambda\eta^3) = c.$$

$$d = -\left(\frac{27}{8}\right)(\lambda+\eta)^{-2}(2\lambda^4+2\eta^4+5\lambda^2\eta^2+6\lambda^3\eta+6\lambda\eta^3).$$

Table 6(c) (With $\eta = \lambda$).

$$A(h_n^1) = \frac{3Me^2}{\hbar^2}(9/4)^3(2/3)(\lambda/\pi)^{3/2}(-1)^n$$

$$y = 45/16\ \lambda.$$

$$K = 27/8\ \lambda.$$

$$A(h_n^6) = \frac{3Me^2}{\hbar^2}(9/4)^3\frac{\sqrt{6}}{K_h^6}(\lambda/\pi)^2; \quad K_h^6 = 27/8\,\lambda;$$

$$y_{h^6} = \Gamma_h^6 = 45/16\ \lambda.$$

$h_n^7(r,r') = h_n^6(r,r')$ and the constants for the other Coulomb kernels are found from (5.11).

5.2 Numerical Work.

The programme used in the four-body collisions (Chapter 2.3a) were employed to calculate $K_n(r, r')$ as (30 x 30) matrices with elements corresponding to points ($r = r_o + m\,h$, $r' = r_o' + nh$) with ($m,n = 1,2,\ldots,29$) for all terms except $h_n'(r, r')$.

This programme calculates terms of the form:-

$$\sum_{s=1}^{p} A_s e^{-\alpha_s r^2 - \beta_s r'^2} \mathcal{J}_{n+1/2}(k_s r r')\, y_s(r, r') \tag{5.13}$$

where y_s is an even powered octic.

$$y_s(r, r') = (a_1 r^2 + a_2 r r' + a_3 r'^2) + \;-\;-- + (\text{terms up to } r^8)$$

The programme can deal with p up to 8.

The values of μ, E_T and E_H were the same as those used in chapter 2.1. The approximation was taken that $\lambda = \eta = 0{\cdot}1404 \times 10^{26}\,\mathrm{cm}^{-2}$. When $\lambda = \eta$ is put into the kernel formulae (Table 6(a) and (b)) the nuclear contributions $y^i q_n^i$ $(i=1,\cdots 8)$, the coulomb contributions $\varepsilon^6 h_n^6(r, r')$ and $\varepsilon^7 h_n^7(r, r')$, and all terms of $\delta^s p_n(r, r')$ except that involving $\mathcal{J}_{n+3/2}$ or $\mathcal{J}_{n-1/2}$ could be reduced to five terms of the form (5.3).

The remaining term of $p_n(r, r')$ was calculated by a separate application of the programme, as was $n_n(r, r')$.

(corresponding to $B_n(r,r')$ of chapter 2.3a).

For the kernels $h_n^2 \ldots h_n^5$ and h_n^8 a four-point gaussian integration formula was used, and again the same programme employed.

To calculate $\varepsilon' h_n'(r,r')$ a programme was written in GIP (General Interpretive Programming) and this is discussed in appendix C.

This gave five matrices for each "n" which were added to give $K_n(r,r')$.

Test cases were calculated for $h = 0.35(0.05)0.5 \times 10^{-13}$ cm. and $h = 0.45$ was chosen as the probable most accurate, with $r_o = r_o' = 0$.

The equation was solved and phase shifts found in the manner described in chapter 2.

Kernels $K_n(r,r')$ were produced corresponding to $y = 1$ (Serber) and $y = 0.7$ (Biel) exchange forces, and kernels corresponding to other mixtures of Serber and symmetric force types found by taking linear combinations of these.

The angular distributions were calculated using a programme written by Dr. B.H. Bransden in T.I.P. (Tabular Interpretive Programming). This calculates the angular distribution for scattering angles of $15^{\circ}(15^{\circ})90^{\circ}$ in the centre of mass system (for identical particles), the scattering being, of course, symmetrical about 90°.

The formulae:—

$$I(\theta) = f_1[A_1^2 + B_1^2] + f_3[A_3^2 + B_3^2];$$

$$A_i = A_c{}^i + A_N{}^i; \quad B_i = B_c{}^i + B_N{}^i;$$

$$A_c{}^i = \frac{\alpha}{2k} \operatorname{cosec}^2 \theta/2 \cos(-\alpha \log(\sin^2 \theta/2) + \pi + 2\eta_0)$$

$$B_c{}^i = \frac{\alpha}{2k} \operatorname{cosec}^2 \theta/2 \sin[-\alpha \log(\sin^2 \theta/2) + \pi + 2\eta_0]$$

$$A_N{}^i = \sum_{n=0}^{\infty} \left(\frac{2n+1}{2ik}\right)(\sin 2(\eta_n + \delta_n^i) - \sin 2\eta_n) P_n(\cos\theta)$$

$$B_N{}^i = \sum_{n=0}^{\infty} \left(\frac{2n+1}{2ik}\right)(-\cos 2(\eta_n + \delta_n^i) + \cos 2\eta_n) P_n(\cos\theta). \tag{5.14}$$

where η_n and $\delta_n{}^i$ are the coulomb and nuclear phases respectively, were used.

It is necessary for Dr. H.H. Robertson's programme for the solution of the equation and the calculations of the phases respectively to calculate previously the values of the function $C(r)$ for $r = nh$, $n = 1,2,\ldots 29$, and the function $\eta_n = \arg\Gamma(1 + n + i\alpha)$ (See Chapter 2.3c). The former was computed by hand and the latter using a TIP programme.

5.3 Results (1) $^3H + {}^3H$.

The cross-section for (^3H + ^3H) elastic scattering has been measured by Hohn and Argo (1956) in the energy range 1.6 MeV to 2 MeV. An analysis by Frank and Gammel (1955) has shown that the result can be best fitted by assuming a single s-wave phase shift, such that $\delta_0 = -ka$, with $a = 2.35 \times 10^{-13}$ cm. (corresponding to hard sphere scattering), $\hbar k$ being the momentum in the centre of mass system. A more recent measurement by Allen and Jarmie (1958) suggests that the earlier cross-sections were approximately 20% too large, so that a will be less than 2.35×10^{-13} cm. At 2 MeV δ_0 should be close to 30°.

Some preliminary results were calculated, omitting all Coulomb terms except $h_n^6(r,r')$ and $h_n^7(r,r')$, and the results of these used to compare with the above data. (The effect of the Coulomb terms was later found to be indeed negligible at these low energies.)

The symmetric force produces s-wave phases of the correct size and energy variation to fit the experimental data, but the calculated p phase shift is about 6°, and this is large enough to upset the fit. Figure 4 illustrates the comparison between calculated and observed cross-sections, and table 7 gives the (^3H + ^3H) phase shifts. Figure 5 shows the variation of δ_0 with exchange force type at 2 MeV.

Table 7. Phase Shifts for (^3H + ^3H) Elastic Scattering. (Coulomb Contribution Neglected).

Energy in MeV (Lab)		1.5	2	5	10
δ^0	Serber (y=1)	-32.8°	-53.2°	-84.8°	$+71^\circ$
	Symmetric (y=0)	-24°	-28°	-52°	-79°
δ^1	y = 1	-6°	-9°	-9.5°	-58°
	y = 0	-4°	-6°	-22°	-45°
δ^2	y = 1	-	-	$+6^\circ$	$+8^\circ$
	y = 0	-	-	-	-1.5°

Angular Distributions for ($^3H + ^3H$) Elastic Scattering.

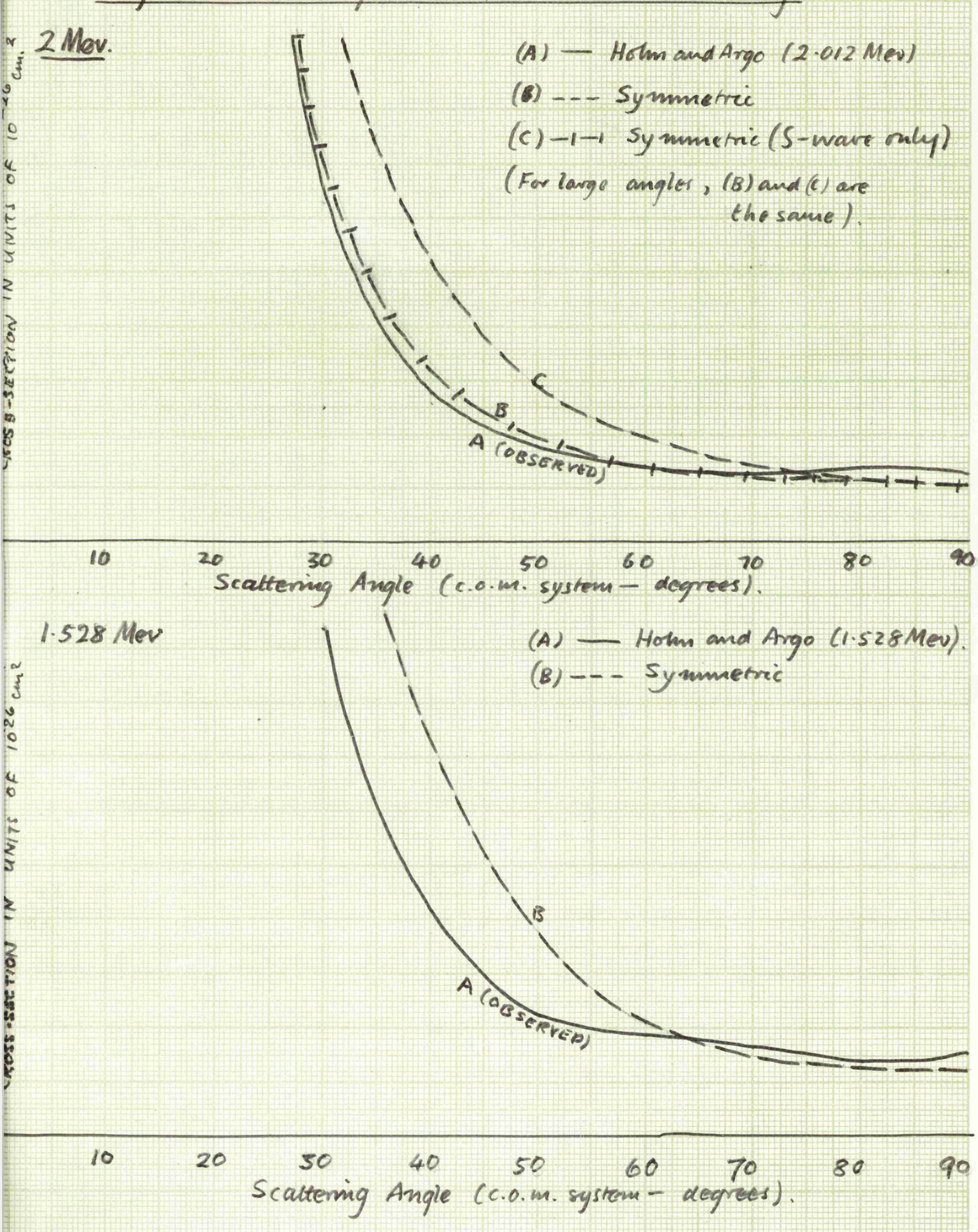

Figure 4.

Variation of δ_0 ($^3H + {}^3H$) with exchange force type (at 2 Mev.)

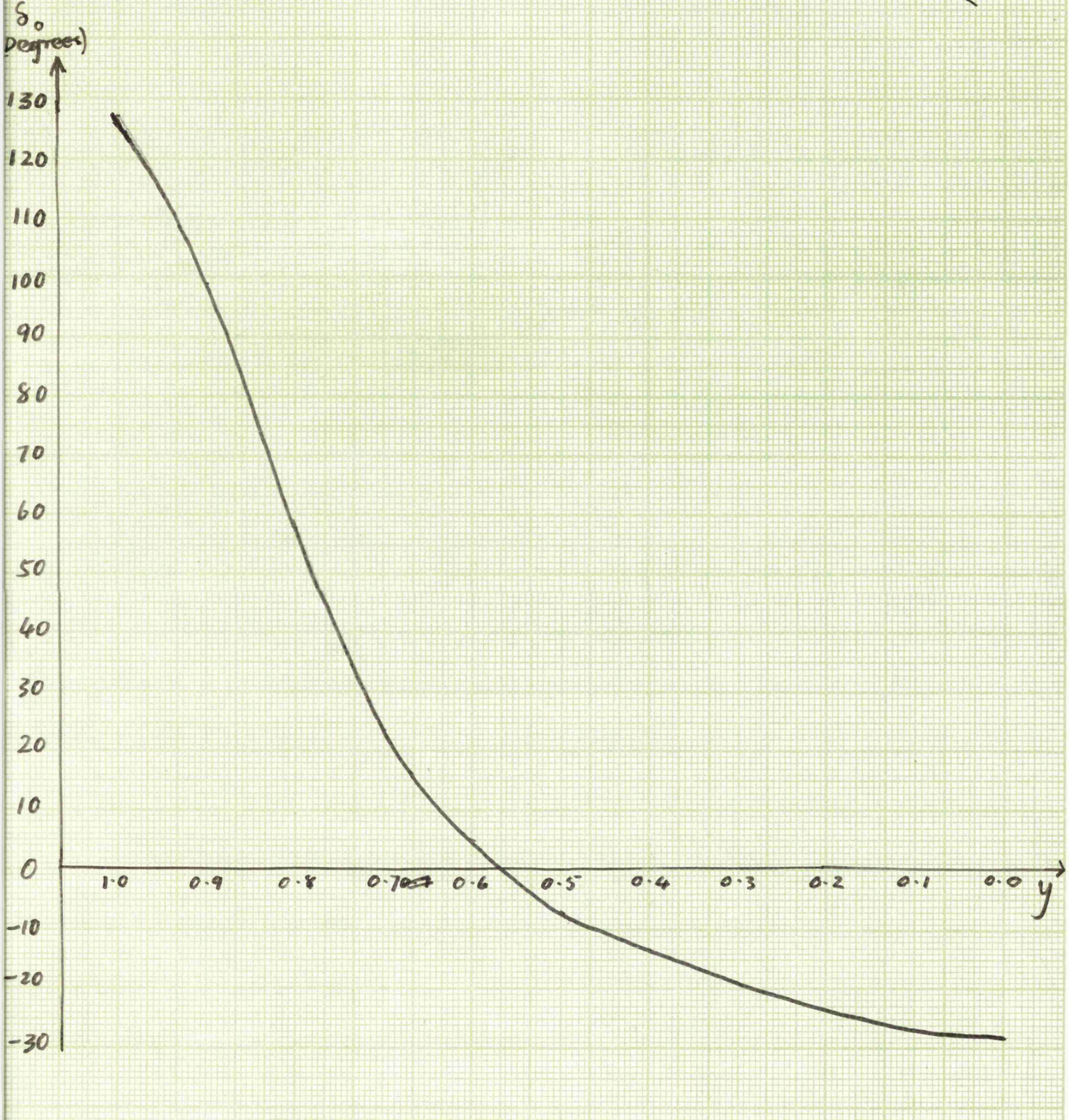

Figure 5.

5.4 Results (^{3}He + ^{3}He).

The other experimental data available for comparison was on (^{3}He + ^{3}He) elastic collisions at 29, 26 and 20 MeV (Lab). At 29.4 and 26 MeV by Bredin, England, Evans, McKee, March, Mossinger and Toner (1960), and at 25 and 19 MeV by Rosen, Stuat and Brolley (1960). The angular distributions are compared with their results in figures 8, 9 and 10 and the phases obtained tabulated in table 8. Sketches of the behaviour of the Serber angular distribution with energy, and the behaviour of phases with exchange forces are also given.

A search was carried out using the values y = 0.0(0.1)1.0 in an attempt to find a satisfactory fit with experiment, but Serber was found to be the best. It can be seen that in all the comparisons with experimental data the calculated differential cross-sections agree reasonably well at large angles, but fail to reproduce the very deep minimum at 30° to 40°. This would suggest that the s wave phase shifts predicted are reasonable but that the p-wave ones are too high. The p-wave is triplet and the s-wave singlet, so that any exaggeration of the p-phase shift will be amplified in its effect on the angular distributions. The p phases are probably more model dependent than the s phases.

The alterations in the potential, if any exist, which would reduce the higher phase shifts, are not clear, but since the angular distributions improve continuously in going from symmetric to Serber force types, and since the latter contains more ordinary (Wigner) force, a potential with this might succeed.

Phase Shifts for (^3He + ^3He) Elastic Scattering

Table 8 Serber Force (y = 1.0)

MeV (Lab)	2	5	10	20	26	29
δ_0	-29.3°	-68°	$+82.7^\circ$	$+60.2^\circ$	$+51.0^\circ$	$+46.4^\circ$
δ_1	-2.5°	-17.2°	-43.9°	-86.4°	$+73.3^\circ$	$+65.3^\circ$
δ_2	-	$+2.8^\circ$	$+12.4^\circ$	$+18.6^\circ$	$+18.3^\circ$	$+19.6^\circ$
δ_3	-	-	-3.1°	-14.4°	-26.2°	-30.3°
δ_4	-	-	$+0.7^\circ$	$+10.0^\circ$	$+29.0^\circ$	$+41.0^\circ$

Table 9 Biel Force (y = 0.70) and Symmetric Force (y = 0.0)

MeV (Lab)	Biel			Symmetric		
	20	26	29	20	26	29
δ_0	$+31.6^\circ$	$+26.2^\circ$	$+19.4^\circ$	-48.0°	-52.6°	-53°
δ_1	-82.0°	$+78.4^\circ$	$+70.7^\circ$	-67.8°	-84.9°	88.5°
δ_2	$+5.8^\circ$	$+4.3^\circ$	$+2.4^\circ$	-14.9°	-21.3°	-23.8°
δ_3	-14.3°	-23.4°	-27.1°	-9.1°	-15.0°	-17.7°
δ_4	$+7.5^\circ$	$+19.4^\circ$	$+27.1^\circ$	$+2.5^\circ$	$+6.1^\circ$	$+9.3^\circ$

($^4He + ^4He$) Elastic Scattering.

Energy Variation of Angular Distribution (Serber Force (y=1)).

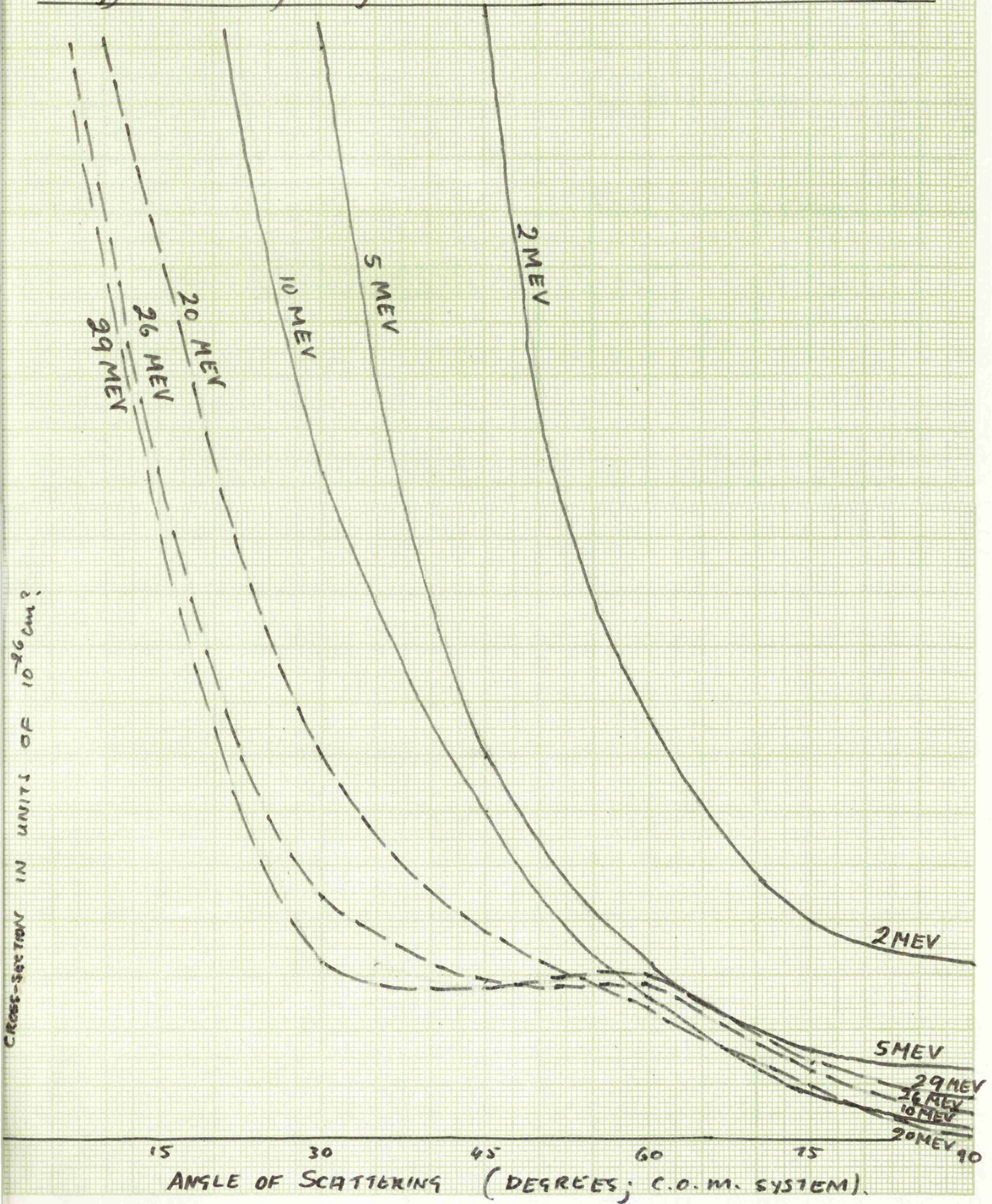

Figure 6.

($^3He + ^3He$) Elastic Scattering.

Angular Distributions for 20 Mev (Lab).

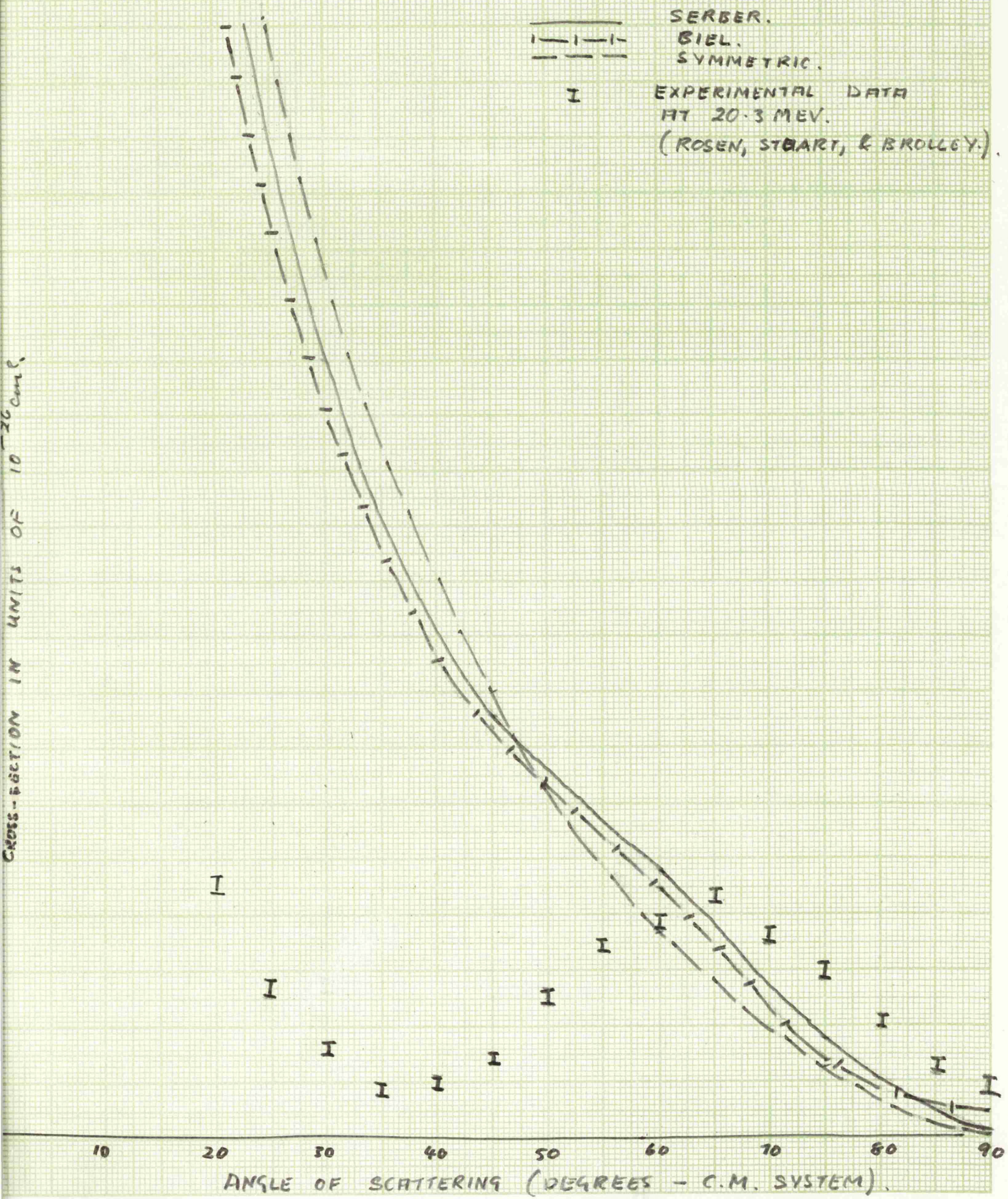

Figure 7.

(^3He + ^3He) Elastic Scattering

Angular Distributions at 26 Mev (Lab.).

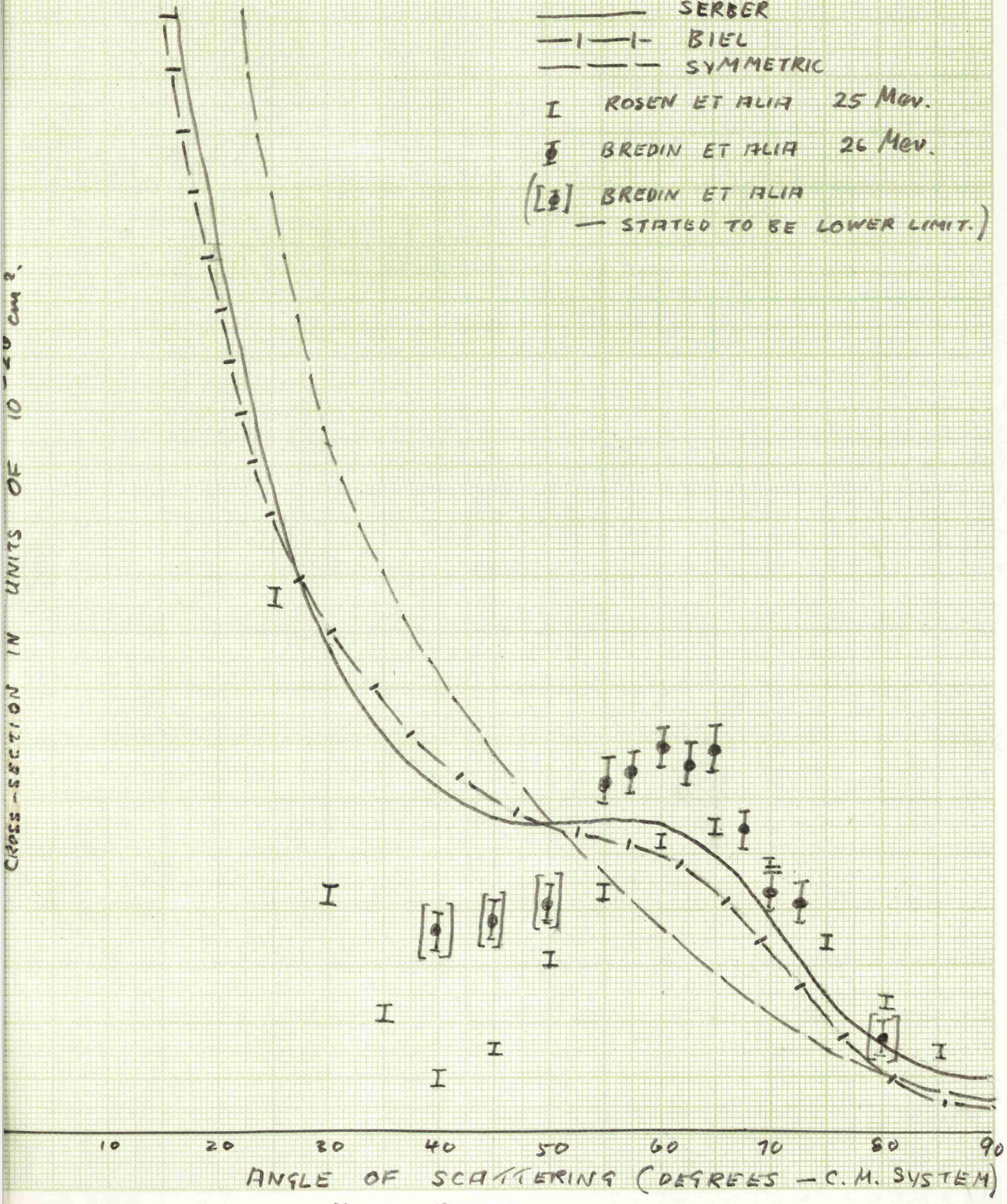

Figure 8.

(^3He + ^3He) Elastic Scattering

Angular Distributions at 29 Mev (Lab).

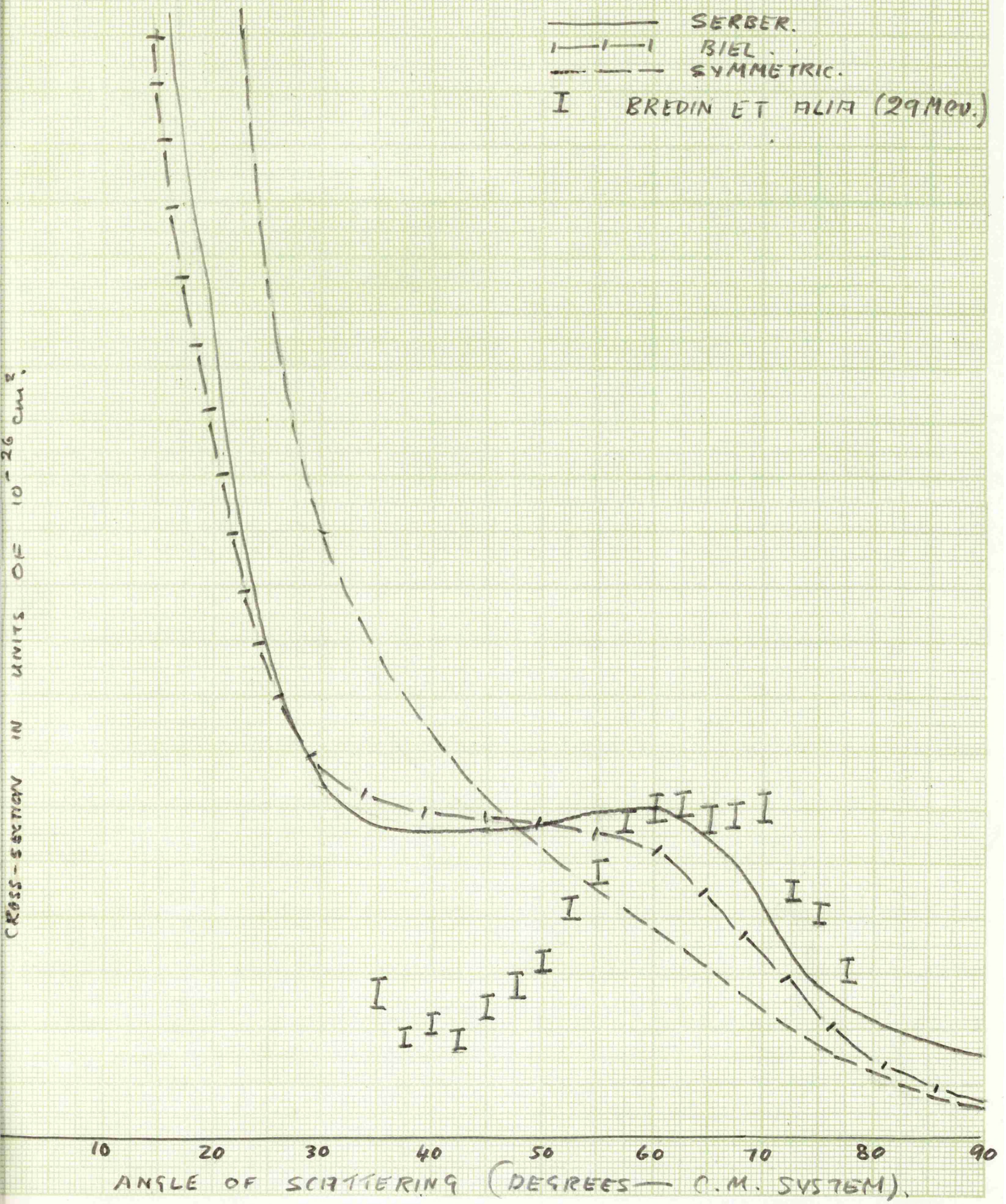

Figure 9.

5.5 Recent Calculations and Conclusions.

Since the work reported in chapters 2-5 was started, Butcher and MacNamee (1959) have published the results of an application of the method used here to ($\alpha+\alpha$) scattering. They found that a Biel (y = 0.7) force fitted experimental data well over the whole energy range (0-40 MeV).

This appears rather surprising bearing in mind the results reported in the previous chapter. However, there are two possible explanations.

(1) It was pointed out in the last chapter that the rather large p phases predicted by the method were weighted 3:1 against the s phases in the angular distribution (being triplet state phases). On the other hand in the (α + α) calculation the p wave and all odd angular momentum states were excluded.

(2) The alpha-particle is much more tightly bound than the triton and thus the alpha group is more stable during the collision.

Other calculations have been by Burke and Laskar (1958) on d+d scattering. Their results fitted experiment practically independently of the exchange force used. They have also formulated d + ^3He scattering.

Sugie, Robertson and Hodgson (1957, 1958) have considered the contribution of tensor forces to $(n+\alpha)$ collisions.

Chapter 6.

The Binding Energy of the Triton.

A large amount of theoretical attention has been paid for some time to the binding energies of the three-body nuclei. It would be out of place here to give more than a very brief mention of the previous calculations.

Calculations using a gaussian potential well have been done by Feenberg and co-workers (1935, 1936), Fluegge (1937) and Margenau and co-workers (1937, 1938, 1939); using a Yukawa well by Brown, and Brown and Plesset (1939), and using an exponential well by Ravita and Present (1937). Some later calculations used a square well (Rarita and Schwinger (1941); Gerjuey and Schwinger (1942); Feshbach and Rarita (1949)).

The effect of tensor forces has been given attention (Pease and Feshbach (1951), Irving (1951)), and the effect of a repulsive core considered by Omhura, Merita and Yamada (1960), and Blatt and Derrick (1959).

Other calculations have been done by the following authors:-

Hylleraas and Rydberg (1941),

Svarthohn (1945, 1948). (See Chapter 6.2)

Frohlich et alia (1946, 1947)

Clapp (1949)

Derrick and Blatt (1959) (Classification of the triton wave-functions).

Skorniakov and Ter-Martirosian (1957) (The three-body problem for short range forces.)

6.1 The Calculations by N. Swartholm.

(a) Potential and Wave-function used.

We give a fuller account of Swartholm's calculations since it is intended to use the same values for the well parameters as he used, with a view to providing a test of the resonating group method.

Swartholm uses the now well-known variation-iteration method.

He assumes charge independence of the forces and introduces spin dependence by using for the force between nucleons j and k:-

$$V_{jk}(r) = -B(1 - g + g\,B_{jk})e^{-r^2/a^2},$$ where B_{jk} is a Bartlett operator, and g gives a measure of the relative strength of the spin dependent force.

$V_{jk}(r)$ is in fact the WB force described in chapter 1.3.

For the triton he takes a wave-function (in momentum space):-

$$\varphi_0\,(\underline{p}_1\,\underline{p}_2\,|123) = \chi_0\,(\underline{p}_1\,\underline{p}_2)\,\frac{1}{\sqrt{2}}\big(\alpha(1)\beta(2) - \alpha(2)\beta(1)\big)\alpha(3)$$

where (123) are the spin co-ordinates on which the B_{jk} act. The space wave-function is taken as

$$\psi\,(\underline{r}_1\,\underline{r}_2\,\underline{r}_3) = \exp\{-(r_{12}^2 + r_{13}^2 + r_{23}^2)\,b^{-2}\}$$

corresponding in momentum space to

$$\chi_0(p_1 p_2) = e^{-b^2/4\,(p_1^2 + p_2^2 + p_1 \cdot p_2)}$$

χ_0 is then used as a trial function and iterated to give $\chi_1(p_1 p_2)$ which is then used as the wave-function in the rest of the calculation. He calculates in fact $\lambda = BMa^2$ and substitutes the observed binding energy to give values of the force constants λ.

(b) Swartholm's Results for a Gaussian Well.

With $B = 35.6$, $a = 2.25 \times 10^{-13}$, and $g = 0.2$, Margenau and Warren (1937) found $E_T = -7.21$ MeV, estimating the convergence at -7.7 MeV. This was later changed to -7.3 MeV (Margenau and Tyrrell (1938). Swartholm found the following:-

For $E = -7.21$ he finds $B_o = 37.07$, $B_{1/2} = 35.88$,

$B_1 = 35.28$ MeV. and for

$E = -7.30$, - $B_o = 37.18$, $B_{1/2} = 35.88$, $B_1 = 35.49$ MeV.

This establishes the accuracy of his results.

Maltauch and Flugge (1942) found E_T to be -8.38 MeV. (Tollestrys (1950) finds $E_T = -8.492$ MeV).

Using this result, Swartholm finds (with $a = 2.25 \times 10^{-13}$)

$$B_1 = 35.63 \text{ MeV}$$

However, for $g = 0$ with an error function potential, "a" must decrease to 1.94×10^{-13}cm.

This gives $B_{1/2} = 37.67$ MeV (6.1)

(c) Choice of Well Parameters.

It was decided to take an extrapolated value for B_1 for the last result mentioned, which is the one which applies here.

For E = -7.21 MeV.

$$\frac{B_o}{B_{1/2}} = 1.0363433, \quad \frac{B_{1/2}}{B_1} = 1.0110237, \quad \frac{B_o}{B_1} = 1.0477677$$

For E = -7.3 MeV.

$$\frac{B_o}{B_{1/2}} = 1.032319, \quad \frac{B_{1/2}}{B_1} = 1.010989, \quad \frac{B_o}{B_1} = 1.047619$$

Making an estimate (from $B_{1/2} = 37.67$), of $B_o = 39.04$ and $B_1 = 37.26$ MeV, gives

$$\frac{B_o}{B_{1/2}} = 1.03636, \quad \frac{B_o}{B_1} = 1.14777, \quad \frac{B_{1/2}}{B_1} = 1.011003.$$

The well parameters decided on were

$$a = 1.94 \times 10^{-13}\text{cm. (corresponding to } \mu = 0.2669 \times 10^{26}\text{cm}^{-2}) \text{ and } B_1 = 37.26 \text{ MeV.} \tag{6.2}$$

6.2 Description of Method.

As a preliminary attack on the problem it was decided to consider the grouping (n+d). As was mentioned in Chapter (1.3), (n+d) scattering has been formulated using a resonating group wave-function a number of times and the final form of the equation used by Burke and Robertson (1957) was assumed.

That is, for $n = 0$

$$\left(\frac{d^2f}{dr^2} + k^2 f\right) = \alpha U(r) f(r) + \int_0^\infty K(r,r') f(r')\,dr' \tag{6.3}$$

where r is the distance of the neutron from the centre of mass of the deuteron,

$$K(r,r') = \beta q(r,r') + \gamma \left[p(r,r') + \left(1 + \frac{E_n}{E_d}\right) n(r,r') \right]$$

where $\beta, q, \gamma, p, \alpha$ and U are set out in appendix D.

This equation is now dealt with as follows:-

$$\left[\frac{d^2 f(r)}{dr^2} - \alpha U(r) f(r) - \int_0^\infty \left(\beta q(r,r') + \gamma p(r,r') + \gamma n(r,r')\right) f(r')\,dr' \right] + k^2 \left[f(r) - \int_0^\infty \frac{4k^2}{3ME_d}\, n(r,r') f(r')\,dr' \right] = 0 \tag{6.4}$$

This is expressed by finite difference techniques in the form

$$A f + k^2 B f = 0 \tag{6.5}$$

where A and B are matrices and f a vector corresponding to $f(r)$.

Thus with $k^2 = -\lambda'$ and $B^{-1}A = C$, we have:-

$$(C - \lambda' I) f = 0 \tag{6.6}$$

and k^2 can be found by finding the latent root of C having a vector of the appropriate physical boundary conditions.

We follow Burke and Robertson in using the deuteron ground state wave-function (1.12).

For the binding energy of the deuteron we have

$$E_d \leqslant \int \chi(r)\left(-\frac{\hbar^2}{M}\nabla^2 + V(r)\right)\chi(r) \tag{6.7}$$

which is explicitly

$$E_d \leqslant \frac{\frac{3\hbar^2}{2M}\left[(2\alpha)^{-1/2} + 8c\alpha\beta(\alpha+\beta)^{-5/2} + c^2(2\beta)^{-1/2}\right] + V_0\left[(\mu+2\alpha)^{-3/2} + 2c(\mu+\alpha+\beta)^{-3/2} + c^2(\mu+2\beta)^{-3/2}\right]}{\left[(2\alpha)^{-3/2} + 2c(\alpha+\beta)^{-3/2} + c^2(2\beta)^{-3/2}\right]} \tag{6.8}$$

(Burke and Robertson Eqn.10).

This expression was minimised with respect to α, β and c for the potential parameters (6.2) and the corresponding values of E_d and α, β and c substituted in the equation.

6.3 Numerical Work.

(a) Minimising of E_d (equation 6.8).

An alpha-code programme was written which simply calculated the expression for a mesh of values of α and β, for a particular c. This was done for various values of c and the mesh tightened until the value of E_{min} was sufficiently accurate. It was found (agreeing with Burke and Robertson) that E_{min} was very insensitive to changes in c.

(b) Latent Roots.

We express (6.4) in terms of finite differences. As in the programme used in the scattering calculations (chapter 2.3(b)), the upper limit $R^1 = 29h$ is set on the integral and the 30 points of r^1 taken as $r' = mh$, $m = 0, r, \ldots, 29$, and $\int dr' \rightarrow \sum_m T_m$

We choose the same points in the pivotal range for r, and let $f(r_n) = f_n \; (= f(nh))$; $K(r_n, r'_m) = K_{nm}$ etc.

Using the formula:-

$$h^2 f_n'' = (f_{n-1} - 2f_n + f_{n+1}) - \frac{1}{12}\delta^4 f_n + \frac{1}{90}\delta^6 f_n - \cdots$$

we have (for (6.4)):-

$$f_{n-1} - 2f_n + f_{n+1} + h^2 V_n f_n + h^2 \sum_m T_m K_{nm} f_m$$
$$+ k^2 h^2 [f_n + \sum_m T_m L_{nm} f_m] = C_n, \text{ for } n = 0, 1, \ldots, 29.$$

where $K_{nm} = -(\beta q_{nm} + \gamma p_{nm} + \gamma r_{nm})$

and $L_{nm} = -\frac{4k^2}{3ME_d} r_{nm}$, $V_n = -\alpha U_n$, $C_n = \frac{1}{12}\delta^4 f_n - \frac{1}{90}\delta^6 f_n + \cdots$

We now apply the central difference operator $(1 + 1/12\ \delta^2)$ (Fox and Goodwin 1949) to reduce the order of the difference correction.

This leaves the equations:-

$$f_{n-1}\left(1+\frac{h^2}{12}V_{n-1}\right) - f_n\left(2-\frac{10}{12}h^2V_n\right) + f_{n+1}\left(1+\frac{h^2}{12}V_{n+1}\right)$$
$$+\frac{h^2}{12}\sum_m T_m\left(K_{n-1,m}+10\,K_{n,m}+K_{n+1,m}\right)f_m$$
$$+\frac{k^2h^2}{12}\left[f_{n-1}+10f_n+f_{n+1}+\sum_m T_m\left(L_{n-1,m}+10\,L_{n,m}+L_{n+1,m}\right)f_m\right]$$
$$= -\frac{1}{240}\delta^6 f_n+\cdots.$$

That is, in the notation of equation (6.5):-

$$A_{nm} = \delta_{nm}\left(-2-\frac{10}{12}h^2V_n\right)+\delta_{n+1,m}\left(1+\frac{h^2}{12}V_{m-1}\right)$$
$$+\delta_{n-1,m}\left(1+\frac{h^2}{12}V_{m+1}\right)+\frac{h^2}{12}T_m\left(K_{n-1,m}+10K_{nm}+K_{n+1,m}\right)$$

and $$B_{nm} = \left(10\,\delta_{nm}+\delta_{n+1,m}+\delta_{n-1,m}\right)$$
$$+T_m\left[L_{n-1,m}+10\,L_{nm}+L_{n+1,m}\right].$$

where δ_{jk} is the Kronecker δ.

Simpson's rule was used to give the weights T_m with the $^3/8$'s rule at one end of the range to obviate the difficulty of having an even number of pivotal points.

The reqson for choosing 30 points was in order to make use of Dr. H.H. Robertson's programme again for producing the kernels K_{nm} and L_{nm}. A GIP programme was written to calculate A_{nm} and B_{nm} from these (appendix C).

The latent roots were calculated by a programme kindly lent by Mr Williams of the Glasgow University Computing Laboratory. This used Lanczos' method. (Buckingham (1957) ch. 12).

The MH force (1.6) was used, since this was the one used by Svartholm (and also by Margenau et al.).

6.4 Preliminary Results.

(a) Using $\mu = 0.2669 \times 10^{26} cm^{-2}$, $V_o = -37.26$ MeV, the expression (6.8) was minimised. A very unrealistic result for E_d was found, however, being $E_d = -0.39083$ MeV, corresponding to $\alpha = 0.01435$, $\beta = 0.1362 \times 10^{26} cm^{-2}$. (The binding energy of the deuteron is experimentally -2.22 MeV. Tollestrup (1950)).

(b) Burke and Robertson point out that it is difficult to decide what interval to use in the kernels for the following reasons:-

a) The q kernels very very rapidly near the origin, and thus inaccuracies will occur if h is too large.

b) The p and n kernels extend out much further, and hence some of their contribution may be lost if h is too small.

However, since the gaussian wave-function dies away fairly rapidly, it was decided in preliminary calculations to use an interval h = 0.45 (by study of a table given by Burke and Robertson).

The inaccuracies due to this, if any, could then be simply tested by calculating a result for, say h = 0.5, and comparing.

(c) Using h = 0.45, the latent roots of C have been calculated. The asymptotic form of $f(r)$ should be $\sim e^{ikr}$, and thus for a bound state k will be imaginary, that is, λ' will be positive.

Six of the roots found were real, and only one of these positive:-

$$\lambda' = 0.1184 = -k^2 = -\frac{3M}{4\hbar^2} E_n,$$ where E_n is the energy of the neutron.

This corresponds to $E_n = -3.69$ MeV.
Using the extremely high value obtained for E_d, this would suggest for the binding energy of the triton

$$E_T = E_n + E_d = -4.08 \text{ MeV},$$ which is less than half the total observed binding energy.

It should be remembered that only the (n+d) grouping has been considered. (A recent calculation by Kurepin and Neudadini (1960) suggests that the probability of finding the triton in the (n+d) grouping is 0.4).

The next step will consist of considering a wave-function of two groups:-

$$\Psi = \phi_1 (n+d) + \phi_2 (\widehat{nn} + p).$$

It should be pointed out with regard to the above result that tests of whether the interval h used was large enough, have not yet been done.

Conclusion.

The usefulness of the resonating group approach is without doubt when the large amount of data correlated with its aid is considered.

The use of an equivalent central potential with full allowance for exchange forces has described the behaviour of many light nuclear systems to a fair degree of quantitative accuracy. It is surprising that the exchange force type which produces agreement with observed data is in general so nearly the same in the systems to which the method has been applied.

The conclusions of the work on the six-body collisions must be that they are out of line with other calculations in that a force between the Serber symmetric types does not give agreement with observed data. It is hoped, however, to carry out an investigation of this system with exchange forces between the WB and Serber types. The result may still give a 'near-Serber' fit. (This would still have it out of line with what was anticipated, since the force was expected to move nearer to the symmetric type as the number of particles increased (Butcher and MacNamee 1960).

In general, it may be said that there is no doubt of the necessity for an approach of the resonating group type at low energies, and the limitation on the success of applications up to the present, may be supposed to stem from the unrealistic nature of the potentials used in conjunction with it.

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Appendix A.

Spin Matrix Elements.

1. Matrix Elements required for Type (a) Collision.

Singlet State (Table A1).

P_{ij}	$\Sigma\sigma^{\circ} P_{ij}\sigma^{\circ}$	$\Sigma\sigma^{\circ} P_{ij} P_{13}\sigma^{\circ}$	$\Sigma\sigma^{\circ} P_{ij} P_{23}\sigma^{\circ}$
1	+1	$+\frac{1}{2}$	$+\frac{1}{2}$
P_{12}	-1	$-\frac{1}{2}$	$-\frac{1}{2}$
P_{13}	$+\frac{1}{2}$	+1	$-\frac{1}{2}$
P_{14}	$+\frac{1}{2}$	$-\frac{1}{2}$	+1
P_{15}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$
P_{16}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$
P_{23}	$+\frac{1}{2}$	$-\frac{1}{2}$	+1
P_{24}	$+\frac{1}{2}$	+1	$-\frac{1}{2}$
P_{25}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$
P_{26}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$
P_{34}	-1	$-\frac{1}{2}$	$-\frac{1}{2}$
P_{35}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$
P_{36}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$
P_{45}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$
P_{46}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$
P_{56}	-1	$-\frac{1}{2}$	$-\frac{1}{2}$

$\Sigma\sigma^{\circ} P_{ij} P_{24}\sigma^{\circ} = \Sigma\sigma^{\circ} P_{ij} P_{13}\sigma^{\circ}$; $\Sigma\sigma^{\circ} P_{ij} P_{14}\sigma^{\circ} = \Sigma\sigma^{\circ} P_{ij} P_{23}\sigma^{\circ}$;

and $\Sigma\sigma^{\circ} P_{ij} P_{56}\sigma^{\circ} = - \Sigma\sigma^{\circ} P_{ij}\sigma^{\circ}$.

Triplet State (Table A2).

P_{ij}	$\Sigma\sigma' P_{ij}\sigma'$	$\Sigma\sigma' P_{ij}P_{13}\sigma'$	$\Sigma\sigma' P_{ij}P_{23}\sigma'$
1	1	$\frac{1}{2}$	$\frac{1}{2}$
P_{12}	-1	$-\frac{1}{2}$	$-\frac{1}{2}$
P_{13}	$\frac{1}{2}$	1	$-\frac{1}{2}$
P_{14}	$\frac{1}{2}$	$-\frac{1}{2}$	1
P_{15}	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$
P_{16}	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$
P_{23}	$\frac{1}{2}$	$-\frac{1}{2}$	1
P_{24}	$\frac{1}{2}$	1	$-\frac{1}{2}$

P_{ij}	$\Sigma\sigma' P_{ij}\sigma'$	$\Sigma\sigma' P_{ij}P_{13}\sigma'$	$\Sigma\sigma' P_{ij}P_{23}\sigma'$
P_{25}	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$
P_{26}	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$
P_{34}	-1	$-\frac{1}{2}$	$-\frac{1}{2}$
P_{35}	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$
P_{36}	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$
P_{45}	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$
P_{46}	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$
P_{56}	1	$\frac{1}{2}$	$\frac{1}{2}$

$\Sigma\sigma' P_{ij}P_{24}\sigma' = \Sigma\sigma' P_{ij}P_{13}\sigma'$; $\Sigma\sigma' P_{ij}P_{14}\sigma' = \Sigma\sigma' P_{ij}P_{23}\sigma'$;
and $\Sigma\sigma' P_{ij}P_{56}\sigma' = +\Sigma\sigma' P_{ij}\sigma'$.

Similar symmetries exist for the type (b) elements.

Spin Matrix Elements Required for Type (b) Collisions.

2. The Terms $({}^3H + {}^3He) \longrightarrow ({}^3He + {}^3H)$.

Singlet State (Table A3).

P_{ij}	$\Sigma \sigma^0 P_{ij} \sigma^0$	$\Sigma \sigma^0 P_{ij} P_{12} \sigma^0$	$\Sigma \sigma^0 P_{ij} P_{46} \sigma^0$	$\Sigma \sigma^0 P_{ij} P_{12} P_{46} \sigma^0$
1	$+1$	$+\frac{1}{2}$	$+\frac{1}{2}$	$+\frac{1}{4}$
P_{12}	$+\frac{1}{2}$	$+1$	$+\frac{1}{4}$	$+\frac{1}{2}$
P_{13}	$+\frac{1}{2}$	$-\frac{1}{2}$	$+\frac{1}{4}$	$-\frac{1}{4}$
P_{14}	$+\frac{1}{2}$	$+\frac{1}{4}$	$-\frac{1}{2}$	$-\frac{1}{4}$
P_{15}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+1$	$+\frac{1}{2}$
P_{16}	-1	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{4}$
P_{23}	-1	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{4}$
P_{24}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$	$-\frac{1}{4}$
P_{25}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$	$+\frac{1}{2}$
P_{26}	$+\frac{1}{2}$	$-\frac{1}{2}$	$+\frac{1}{4}$	$-\frac{1}{4}$
P_{34}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$	$+\frac{1}{2}$
P_{35}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$	$-\frac{1}{4}$
P_{36}	$+\frac{1}{2}$	$+1$	$+\frac{1}{4}$	$-\frac{1}{4}$
P_{45}	-1	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{4}$
P_{46}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+1$	$+\frac{1}{2}$
P_{56},	$+\frac{1}{2}$	$+\frac{1}{4}$	$-\frac{1}{2}$	$-\frac{1}{4}$

Triplet State (Table A4).

P_{ij}	$\sum\sigma' P_{ij}\sigma'$	$\sum\sigma' P_{ij} P_{12}\sigma'$	$\sum\sigma' P_{ij} P_{46}\sigma'$	$\sum\sigma' P_{ij} P_{12} P_{46}\sigma'$
1	$+1$	$+\frac{1}{2}$	$+\frac{1}{2}$	$+\frac{1}{4}$
P_{12}	$+\frac{1}{2}$	$+1$	$+\frac{1}{4}$	$+\frac{1}{2}$
P_{13}	$+\frac{1}{2}$	$-\frac{1}{2}$	$+\frac{1}{4}$	$-\frac{1}{4}$
P_{14}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{2}$	$+\frac{1}{4}$
P_{15}	$+\frac{1}{2}$	$+\frac{1}{4}$	0	0
P_{16}	$+1$	$+\frac{1}{2}$	$+\frac{1}{2}$	$+\frac{1}{4}$
P_{23}	-1	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{4}$
P_{24}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$	$+\frac{1}{4}$
P_{25}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$	0
P_{26}	$+\frac{1}{2}$	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$
P_{34}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$	0
P_{35}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$	$+\frac{1}{4}$
P_{36}	$+\frac{1}{2}$	0	$+\frac{1}{4}$	0
P_{45}	-1	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{4}$
P_{46}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+1$	$+\frac{1}{2}$
P_{56}	$+\frac{1}{2}$	$+\frac{1}{4}$	$-\frac{1}{2}$	$-\frac{1}{4}$

3. The Terms $(d+\alpha) \rightarrow (d+\alpha)$ (s=1 only).

Table A5.

P_{ij}	$\sum \bar{\sigma} P_{ij} \bar{\sigma}$	$\sum \bar{\sigma} P_{ij} P_{12} \bar{\sigma}$	$\sum \bar{\sigma} P_{ij} P_{45} \bar{\sigma}$	$\sum \bar{\sigma} P_{ij} P_{12} P_{45} \bar{\sigma}$
1	$+1$	$+\frac{1}{2}$	$+\frac{1}{2}$	$+\frac{1}{4}$
P_{12}	$+\frac{1}{2}$	$+1$	$+\frac{1}{4}$	$+\frac{1}{2}$
P_{13}	$+\frac{1}{2}$	$-\frac{1}{2}$	$+\frac{1}{4}$	$-\frac{1}{4}$
P_{14}	$+1$	$+\frac{1}{2}$	$+\frac{1}{2}$	$+\frac{1}{4}$
P_{15}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{2}$	$+\frac{1}{4}$
P_{16}	$+\frac{1}{2}$	$+\frac{1}{4}$	0	0
P_{23}	-1	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{4}$
P_{24}	$+\frac{1}{2}$	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$
P_{25}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$	$+\frac{1}{4}$
P_{26}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$	0
P_{34}	$+\frac{1}{2}$	0	$+\frac{1}{4}$	0
P_{35}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$	0
P_{36}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+\frac{1}{4}$	$+\frac{1}{4}$
P_{45}	$+\frac{1}{2}$	$+\frac{1}{4}$	$+1$	$+\frac{1}{2}$
P_{46}	$+\frac{1}{2}$	$+\frac{1}{4}$	$-\frac{1}{2}$	$-\frac{1}{4}$
P_{56}	-1	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{4}$

4. The Cross-Terms (s = 1 only).

Table A6. (^3H + ^3He) $\rightarrow$ (d + α) Terms.

P_{ij}	$\Sigma\,\sigma' P_{ij}\,\bar{\sigma}$	$\Sigma\,\sigma' P_{ij} P_{46}\,\bar{\sigma}$	$\Sigma\,\sigma' P_{12} P_{45}\,\bar{\sigma}$	$\Sigma\,\sigma' P_{12} P_{46}\,\bar{\sigma}$
1	$-\frac{1}{2}$	-1	$+\frac{1}{4}$	$-\frac{1}{2}$
P_{12}	$-\frac{1}{4}$	$-\frac{1}{2}$	$\frac{1}{2}$	-1
P_{13}	$-\frac{1}{4}$	$-\frac{1}{2}$	$-\frac{1}{4}$	$+\frac{1}{2}$
P_{14}	$-\frac{1}{2}$	$-\frac{1}{2}$	0	$-\frac{1}{4}$
P_{15}	0	$-\frac{1}{2}$	$+\frac{1}{4}$	$-\frac{1}{4}$
P_{16}	$-\frac{1}{2}$	-1	$+\frac{1}{4}$	$-\frac{1}{2}$
P_{23}	$+\frac{1}{2}$	$+1$	$-\frac{1}{4}$	$+\frac{1}{2}$
P_{24}	$-\frac{1}{4}$	$-\frac{1}{2}$	0	$-\frac{1}{4}$
P_{25}	$-\frac{1}{4}$	$-\frac{1}{2}$	$+\frac{1}{4}$	$-\frac{1}{4}$
P_{26}	$-\frac{1}{4}$	$-\frac{1}{2}$	$+\frac{1}{4}$	$-\frac{1}{2}$
P_{34}	$-\frac{1}{4}$	$-\frac{1}{2}$	$+\frac{1}{4}$	$-\frac{1}{4}$
P_{35}	$-\frac{1}{4}$	$-\frac{1}{2}$	0	$-\frac{1}{4}$
P_{36}	$-\frac{1}{4}$	$-\frac{1}{2}$	0	0
P_{45}	$+\frac{1}{2}$	$+1$	$-\frac{1}{4}$	$+\frac{1}{2}$
P_{46}	-1	$-\frac{1}{2}$	$-\frac{1}{4}$	$-\frac{1}{4}$
P_{56}	$+\frac{1}{2}$	$-\frac{1}{2}$	$+\frac{1}{2}$	$-\frac{1}{4}$

Appendix B.

Integrals Used in the Analysis.

1. $$I_1 = \int e^{i\underline{K}\cdot\underline{r}} e^{\underline{A}\cdot\underline{r}} e^{-\zeta r^2} d\underline{r} = \left(\frac{\pi}{\zeta}\right)^{3/2} e^{-\frac{1}{4\zeta}(\underline{K}^2 - \underline{A}^2 - 2i\underline{A}\cdot\underline{K})}$$

$$I_1 = e^{1/4\zeta(\underline{A}+i\underline{K})^2} \int e^{-\zeta(\underline{r}+(1/2\zeta)(\underline{A}+i\underline{K}))^2} d\underline{r}$$

$$= e^{(1/4\zeta)(\underline{A}+i\underline{K})^2} \left[1/\zeta^{1/2} \ \Gamma(1/2) \right]^3 = R.H.S.$$

2. $$I_2 = \int e^{\underline{A}\cdot\underline{r}} e^{-\zeta r^2} r^2 d\underline{r} = (\pi/\zeta)^{3/2} e^{A^2/4\zeta} \left[\frac{3}{2\zeta} + \frac{A^2}{4\zeta^2} \right]$$

$$\frac{\partial I_1}{\partial \zeta} = -\int e^{i\underline{K}\cdot\underline{r}} e^{\underline{A}\cdot\underline{r}} e^{-\zeta r^2} r^2 d\underline{r}$$

$$= -(\pi/\zeta)^{3/2} \left[\frac{3}{2\zeta} + \frac{1}{4\zeta}(\underline{A}^2 + 2i\underline{A}\cdot\underline{K} - \underline{K}^2) \right] e^{-\frac{1}{4\zeta}(K^2 - A^2 - 2i\underline{A}\cdot\underline{K})}$$

With K = 0, (2) is obtained.

3. $$I_3 = \int e^{\underline{A}\cdot\underline{r}} e^{-\zeta r^2} (\underline{B}\cdot\underline{r}) d\underline{r} = \frac{1}{2\zeta} \underline{A}\cdot\underline{B} (\pi/\zeta)^{3/2} e^{A^2/4\zeta}$$

$$I_3 = \int e^{A\mu} e^{-\zeta r^2} \left(\frac{\underline{A}\cdot\underline{B}}{|A|}\right) r\mu \, d\underline{r}$$

($\underline{B}\cdot\underline{r}$ = Br cos $\hat{\theta}_{Br}$ = Br $[\cos\hat{\theta}_{AB} \cos\hat{\theta}_{Ar} - \sin\hat{\theta}_{AB} \sin\hat{\theta}_{Ar} \sin\varphi]$, where $\hat{\theta}_{Br}$ is the angle between $\underline{B}$ and $\underline{r}$ etc. The sine terms disappear under the integral and $\mu = \cos\hat{\theta}_{Ar}$).

Thus $I_3 = \frac{\underline{A}\cdot\underline{B}}{|A|} \frac{\partial}{\partial A} I_1 \Big|_{K=0}$ Hence result.

4. $$I_4 = 2\pi r' \int_{-1}^{+1} P_n(\mu) e^{-Kr'\mu} d\mu = \frac{4\pi}{K} \mathcal{g}_{n+1/2}(Kr')$$

$$I_4 = \frac{2\pi r'}{2^n n!} \int_{-1}^{+1} \left(\frac{d^n}{d\mu^n} (\mu^2 - 1)^n \right) e^{-Kr'\mu} d\mu \qquad \text{(Rodrigues' formula)}$$

$$= \frac{2\pi r'}{2^n n!} (Kr')^n (-1)^n \int_{-1}^{+1} (1-\mu^2)^n d\mu$$

= RHS (I.N. Sneddon (1956), p.126).

5. $$I_5 = 2\pi r' \int_{-1}^{+1} P_n(\mu)\, e^{-K r' \mu}\, \mu\, d\mu = -\frac{4\pi}{r'}\left[-\frac{j_{n+1/2}(Kr')}{K^2} + \frac{r'}{K}\, j'_{n+1/2}(Kr')\right]$$

This is easily seen by differentiation with respect to K under the integral sign in I_4.

6. $$I_6 = \int_0^\infty e^{-\lambda x^2} \sinh ax\, dx = \left(\frac{\sqrt{\pi}}{2\lambda^{1/2}}\right) e^{a^2/4\lambda}\, \Phi\left(\frac{a}{2\sqrt{\lambda}}\right)$$

$$I_6 = \frac{1}{2}\int_0^\infty dx\, e^{a^2/4\lambda}\left[e^{-\lambda\left(x-\frac{a}{2\lambda}\right)^2} - e^{-\lambda\left(x+\frac{a}{2\lambda}\right)^2}\right].$$

$$= \frac{e^{a^2/4\lambda}}{\sqrt{\lambda}} \int_0^{\frac{a}{2\sqrt{\lambda}}} e^{-y^2}\, dy$$

$$= R.H.S., \quad \text{where} \quad \Phi(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt.$$

7. $$I_7 = \int d\mathbf{s}\, \frac{1}{s}\, e^{-\lambda(\mathbf{s}+\mathbf{r})^2} = (\pi/\lambda)^{3/2}\,(1/r)\, \Phi(\sqrt{\lambda}\, r)$$

$$I_7 = -4\pi \int d\mu\, s\, e^{-\lambda(s^2+r^2+2sr\mu)}\, ds$$

where $\mu = \cos \hat{\theta}_{sr}$ $(\mathbf{s}\cdot\mathbf{r} = sr\mu)$

$$= \frac{4\pi}{2\lambda r}\, e^{-\lambda r^2} \int_0^\infty ds\, e^{-\lambda s^2} \sinh 2\lambda r s$$

$$= \frac{4\pi}{2\lambda r}\, e^{-\lambda r^2} \left(\frac{\sqrt{\pi}}{2\sqrt{\lambda}}\right) e^{\lambda r^2}\, \Phi\left(\frac{2\lambda r}{2\sqrt{\lambda}}\right) \quad \text{(Using 6.)}$$

$$= R.H.S.$$

Appendix C.

Programmes.

1. Programme for $h^1_n(r,r\,)$.

To calculate:-

$$h_n^1(r_s, r_t') = e^{(-\gamma + \kappa/2)(r_s^2 + r_t'^2)}$$

$$\times \left\{ \sum \omega_j \left[|r_s + r_t'|\, P_n\!\left(\frac{r_s^2 + r_t'^2 - |r_s + r_t'|^2 x_j^2}{2 r_s r_t'}\right) e^{-\kappa/2\,|r_s + r_t'|^2 x_j^2} \right.\right.$$

$$\left.\left. - |r_s - r_t'|\, P_n\!\left(\frac{r_s^2 + r_t'^2 - |r_s - r_t'|^2 x_j^2}{2 r_s r_t'}\right) e^{-\kappa/2\,|r_s - r_t'|^2 x_j^2} \right] \right\}$$

$$= e^{-A} \sum \omega_j \left[|r_s + r_t'|\, P_n(y_1)\, e^{-X} - |r_s - r_t'|\, P_n(y_2)\, e^{-Y} \right]$$

where s = 0,1,...,29, t = 0,1,...,29.

The DEUCE interpretive scheme GIP 5/1 was used.

(The programme will deal with any number of pivotal points. Seven point Gaussian integration was actually used).

Bricks.

1.	LR07B	(Read Binary Matrix)
2,3.	LZ61B	(Term by term matrix algebra)
4.	LZ63BM	(Term by term exponential).
5.	LZ12B	(Select Element)
6.	LZ18B	(Term by term square root).
7.	LS02B	(Scalar multiplication).
8.	LW01B	(Matrix Subtraction)
9.	LH01B	(Matrix Addition)
10.	LZ19B/1	(Expand scalar)
11.	LP05B	(Punch binary matrix).

Codewords.

Card No.	a	b	c	r	Notes.
0	13	0	0	48	Replace by 0.
1	0	2	1	47	Read 2nd triad.
2	0	3	2	47	Read 3rd triad.
3	0	0	0	1	Read $[(y-K/2), K/2]$
4	0	0	1	1	Read $[1, 3/2, 1/2]$
5	0	0	2	1	Read $[w_1, w_2, \cdots w_N]$
6	0	0	3	1	Read $[x_1^2, x_2^2, \cdots x_N^2]$
7	0	0	4	1	Read $r = [0, h, \cdots, 29h]$
8	3	0	0	48	
9	4	4	6	2	r^2
10	4	4	31	9	2r
11	0	12	14	42	Obey (0+12), add P to 12 and go to 14?
12	4	0	0	5	
13	0	0	0	0	
14	31	0	9	7	$2rr'$
15	1	29	11	10	r'(identical elements)
16	3	0	0	48	
17	11	11	13	2	r'^2
18	13	6	11	9	$r^2 + r'^2$
19	11	9	13	9	$(r+r')^2$
20	11	9	15	8	$(r-r')^2$
21	0	0	0	5	Select $(y-K/2)$

Card No.	a	b	c	r	Notes.
22	11	0	17	7	A = $(\gamma - \kappa/2)(r^2+r'^2)$
23	4	0	0	48	
24	11	9	27	2	$\frac{r^2+r'^2}{2rr'}$
25	4	0	0	48	
26	13	9	19	2	$\frac{(r+r')^2}{2rr'}$
27	4	0	0	48	
28	15	9	21	2	$\frac{(r-r')^2}{2rr'}$
29	13	0	9	6	$\lvert r+r' \rvert$
30	15	0	11	6	$\lvert r-r' \rvert$
31	0	0	35	1	DL 35 $\longrightarrow$ 0
32	0	33	34	42	Obey (33+0), add P to 33 and go to 34.
33	3	0	0	5	
34	13	0	45	7	$x_j^2(r+r')^2$
35	15	0	47	7	$x_j^2(r-r')^2$
36	19	0	51	7	$x_j^2\,\frac{(r+r')^2}{2rr'}$
37	21	0	53	7	$x_j^2\,\frac{(r-r')^2}{2rr'}$
38	0	1	0	5	
39	45	0	45	7	X
40	47	0	47	7	Y
41	17	45	45	9	A + X
42	17	47	47	9	A + Y
43	45	0	23	4	$e^{-(A+X)}$

Card No.	a	b	c	r	Notes.
44	47	0	25	4	$e^{-(\Lambda+y)}$
45	3	0	0	48	
46	23	9	45	2	$\lvert r+r'\rvert e^{-(\Lambda+x)}$
47	3	0	0	48	
48	25	11	47	2	$\lvert r-r'\rvert e^{-(\Lambda+y)}$
49	27	51	29	8	y_1
50	N_n	N_n	51	46	$P_n(y_1)$
51	3	0	0	48	
52	29	45	55	2	$\lvert r+r'\rvert e^{-(\Lambda+x)}P_n(y_1) = (1)$
53	27	53	29	8	y_2
54	N_n	N_n	55	46	$P_n(y_2)$
55	3	0	0	48	
56	29	47	57	2	$\lvert r-r'\rvert e^{-(\Lambda+y)}P_n(y_2) = (2)$
57	55	57	57	8	(1) - (2)
58	0	59	60	42	Obey (0+59), add P to 59 and go to 60.
59	2	0	0	5	
60	57	0	57	7	$w_j((1)-(2))$
61	57	35	35	9	$\Sigma w_j((1)-(2))$
62	69	33	32	37	Replace 32, by (69-33).
63	35	0	5	11	Punch row of h'
64	70	0	33	40	Replace 33 by 70.

Card No.	a	b	c	r	Notes.
65	71	0	59	40	Replace 59 by 71.
66	72	12	11	37	Jump to 11 if 72 12.
67	73	0	12	40	Replace 12 by 73.
68	0	0	0	33	Go to codeword 0.
69	3	N	0	5	
70	3	0	0	5	
71	2	0	0	5	
72	4	29	0	5	
73	4	0	0	5	
74	1	0	0	5	
75	1	29	29	10	$P_o(y)$
76	0	0	0	33	
77	3	0	0	48	
78	29	29	65	2	y^2
79	7	1	0	5	3/2
80	65	0	65	7	$3/2\ y^2$
81	1	2	0	5	1/2
82	1	29	29	10	
83	65	29	29	8	$P_2(y)$
84	0	0	0	33	

k'_n was assumed negligible for $n > 2$.

2. Programme for the Coulomb Phases $\eta_n = \arg\Gamma(1+n+i\alpha)$.

This programme uses alpha-code and forms η_n for n = 0, 1, 2, 3, 4. The formulae:

$$\eta_0 = -0.577215665\alpha + \sum_{s=1}^{\infty} [\alpha/s - \tan^{-1}(\alpha/s)]$$

$$\eta_{n+1} = \eta_n + \tan^{-1}\left(\frac{\alpha}{n+1}\right).$$

are employed.

Card No.	r	R	A	B	Function	C	D	
1	23			1	DATA	X1		kα
2	23	R1		1	DATA	X2		k
3	04		X3	X1	DIVIDE	X2		α
4	05				JUMP		S1	
5	24			5	RESULTS	X10		η_n
6	05				JUMP		R1	
7	14				STOP			
8	19	S1			SUBROUTINE			
9	11		X4		CONSTANT		R0	
10					(-0.577215665)			
11	11		X5		CONSTANT		R0	
12					(Δ)			
13	02		X6	X6	MINUS	X6		
14	02		X9	X9	MINUS	X9		
15	01	R50	X6	X6	PLUS	1		s

Card No.	r	R	A	B	Function	C	D	
16	04		X7	X3	DIVIDE	X6		a/s
17	36		X8		TAN^{-1}	X7		$\tan^{-1} a/s$
18	02		X7	X7	MINUS	X8		
19	01		X9	X9	PLUS	X7		
20	09			X7	BIGGER THAN	X5	R50	
21	03		X10	X4	MULTIP	X3		
22	01		X10	X10	PLUS	X9		
23	00	R51	X6	N50	MOVED		R0	n
24	01		X6	X6	PLUS	1		n+1
25	04		X6	X3	DIVIDE	X6		
26	36		X6		TAN^{-1}	X6		
27	12		N50	N50	MODIFY			
28	01		X11	X10	PLUS	X6		η_n
29	10			N50	UP TO	4	R51	
30	20				END OF		51	

3. Programme to Calculate Angular Distribution for Identical Particles (5·14).

The system used is alpha-code. The subroutine S1 used is the same as that used in programme 2 (i.e. cards 8-30).

Card No.	r	R	A	B	Function	C	D	
1	23			2	DATA	X1		k~~α~~, k
2	04		X3	X1	DIVIDE	X2		~~α~~
3	05				JUMP		S1 (gives $\eta_0, \ldots \eta_4$ in X10 ... X14.).	
4	23			10	DATA	X15		
5	11		X25		CONSTANT		RO	
6					(π/12)			
7	11		X26		CONSTANT		RO	
8					(0.5)			
9	11		X27		CONSTANT		RO	
10					(3)			
11	11		X28		CONSTANT		RO	
12					(5)			
13	11		X29		CONSTANT		RO	
14					(35)			
15	11		X30		CONSTANT		RO	
16					(30)			

Card No.	r	R	A	B	Function	C	D
17	11		X31		CONSTANT		RO
18					(0.01745329)		
19	11		X33		CONSTANT		RO
20					$(f_1(\frac{1}{4}))$		
21	11		X34		CONSTANT		RO
22					$(f_2(\frac{3}{4}))$		
23	12	R10	N10	N10	MODIFY		
24	03		X15	X15	MULTIP	X31	
25	10			N10	UP TO	10	R10
26	12	R3	N1	N1	MODIFY	1V1	
27	01		X15	X10	PLUS	X15	$\eta_n + \delta_n'$
28	12		N1	N1	MODIFY	N1	
29	01		X20	X10	PLUS	X20	$\eta_n + \delta_n^3$
30	12		N1	N1	MODIFY	N1	
31	01		X15	X15	PLUS	X15	$2(\eta_n + \delta_n')$
32	12		N1	N1	MODIFY	N1	
33	01		X20	X20	PLUS	X20	$2(\eta_n + \delta_n^3)$
34	12		N1	N1	MODIFY	N1	
35	01		X10	X10	PLUS	X10	$2\eta_n$
36	12		N1		MODIFY	N1	
37	30		X45		SINE	X15	$\sin 2(\eta_n + \delta_n'$

Card No.	r	R	A	B	Function	C	D	
38	12		N1		MODIFY	N1		$\cos 2(\eta_n + \delta u^1)$
39	31		X50		COSINE	X15		
40	12		N1		MODIFY	N1		
41	30		X55		SINE	X20		$\sin 2(\eta_n + \delta u^3)$
42	12		N1		MODIFY	N1		
43	31		X60		COSINE	X20		$\cos 2(\eta_n + \delta u^3)$
44	12		N1		MODIFY	N1		
45	30		X65		SINE	X10		$\sin 2\eta_n$
46	12		N1		MODIFY	N1		
47	31		X70		COSINE	X10		$\cos 2\eta_n$
48	12		N1	N1	MODIFY	N1		
49	02		X45	X45	MINUS	X65		
50	12		N1	N1	MODIFY	N1		
51	02		X50	X50	MINUS	X70		
52	12		N1	N1	MODIFY	N1		
53	02		X55	X55	MINUS	X65		
54	12		N1	N1	MODIFY	N1		
55	02		X60	X60	MINUS	X20		
56	10			N1	UP TO	5	R3	
57	02		X35	X35	MINUS	X35		
58	01	R2	X35	X35	PLUS	X25		θ
59	31		X36		COSINE	X35		$P_1(\mu)$

Card No.	r	R	a	B	Function	C	D	
60	03		X37	X36	MULTIP	X36		μ^2
61	03		X38	X37	MULTIP	X36		μ^3
62	03		X39	X38	MULTIP	X36		μ^4
63	03		X40	X27	MULTIP	X37		$3\mu^2$
64	02		X40	X40	MINUS	1		$3\mu^2-1$
65	03		X40	X40	MULTIP	X26		$p^2(\mu)$
66	03		X38	X38	MULTIP	X28		$5\mu^3$
67	03		X41	X36	MULTIP	X27		3μ
68	02		X38	X38	MINUS	X41		$5\mu^3-3\mu$
69	03		X38	X38	MULTIP	X26		$p_3(\mu)$
70	03		X39	X39	MULTIP	X29		$35\mu^4$
71	03		X37	X37	MULTIP	X30		$30\mu^2$
72	02		X39	X39	MINUS	X37		$35\mu^4-30\mu^2+3$
73	01		X39	X39	PLUS	X27		
74	03		X39	X39	MULTIP	X26		
75	03		X39	X39	MULTIP	X26		
76	03		X39	X39	MULTIP	X26		$p_4(\mu)$
77	01		X37	X40	PLUS	0		$p_2(\mu)$
78	03		X40	X35	MULTIP	X26		$\theta/2$
79	30		X40		SINE	X40		$\sin \theta/2$
80	03		X40	X40	MULTIP	X40		$\sin^2 \theta/2$

Card No.	r	R	A	B	Function	C	D	
81	28		X41		LOG	X40		
82	03		X41	X41	MULTIP	X3		
83	02		X41	X10	MINUS	X41		
84	11		X42		CONSTANT		RO	
85					(π)			
86	01		X41	X41	PLUS	X42		
87	30		X43		SINE	X41		
88	31		X44		COSINE	X41		
89	04		X43	X43	DIVIDE	X40		
90	04		X44	X44	DIVIDE	X40		
91	03		X43	X3	MULTIP	X43		
92	03		X44	X3	MULTIP	X44		
93	01		X75	0	PLUS	1		$P_0(\mu)$
94	03		X76	X27	MULTIP	X36		$3P_1(\mu)$
95	03		X77	X28	MULTIP	X37		$5P_2(\mu)$
96	01		X78	X28	PLUS	1		6
97	01		X78	X78	PLUS	1		7
98	03		X78	X78	MULTIP	X38		$7P_3(\mu)$
99	03		X79	X27	MULTIP	X27		9
100	03		X79	X79	MULTIP	X39		$9p_4(\mu)$
101	02		X80	X80	MINUS	X80		
102	02		X81	X81	MINUS	X81		

Card No.	r	R	A	B	Function	C	D	
103	02		X82	X82	MINUS	X82		
104	02		X83	X83	MINUS	X83		
105	12	R4	N2	N2	MODIFY	N2		
106	03		X145	X75	MULTIP	X45		A_n
107	12		N2	N2	MODIFY	N2		
108	03		X150	X75	MULTIP	X50		B_n
109	12		N2	N2	MODIFY	N2		
110	03		X155	X75	MULTIP	X55		C_n
111	12		N2	N2	MODIFY	N2		
112	03		X160	X75	MULTIP	X60		D_n
113	12				MODIFY	N2		
114	01		X80	X80	PLUS	X145		ΣA_n
115	12				MODIFY	N2		
116	01		X81	X81	PLUS	X150		ΣB_n
117	12				MODIFY	N2		
118	01		X82	X82	PLUS	X155		ΣC_n
119	12				MODIFY	N2		
120	01		X83	X83	PLUS	X160		ΣD_n
121	10			N2	UP TO	5	R4	
122	01		X80	X80	PLUS	X44		$A_1(\theta)$
123	02		X81	X81	MINUS	X43		$B_1(\theta)$
124	01		X82	X82	PLUS	X44		$A_3(\theta)$

Card No.	r	R	A	B	Function	C	D	
125	02		X83	X83	MINUS	X43		$B_3(\theta)$
126	03		X80	X80	MULTIP	X80		A_1^2
127	03		X81	X81	MULTIP	X81		B_1^2
128	03		X82	X82	MULTIP	X82		A_3^2
129	03		X83	X83	MULTIP	X83		B_3^2
130	01		X80	X80	PLUS	X81		
131	01		X82	X82	PLUS	X83		
132	03		X80	X33	MULTIP	X80		
133	03		X82	X33	MULTIP	X82		
134	01		X80	X80	PLUS	X82		$4h^2I(\theta)$
135	04		X80	X80	DIVIDE	X2		
136	04		X80	X80	DIVIDE	X2		$4\,I(\theta)$
137	03		X80	X80	MULTIP	X26		
138	03		X80	X80	MULTIP	X26		
139	12		N5		MODIFY			
140	01		X85	X80	PLUS	0		$I(\theta)$
141	24			12	RESULTS	X85	R2	
142	05				JUMP	R1		
143	14				STOP			
					(S1)			
144	18				FINISH			

4. <u>Programme to form expression (6.8) for E_d.</u>

Alpha-code (mark II) is used.

(6.8) is of the form $\dfrac{\frac{3\hbar^2}{2M} \mathrm{I} + V_0 \mathrm{II}}{\mathrm{III}}$

Card No.	r	R	A	B	Function	C	D	Notes.
0	23			6	DATA	X1		$\frac{3\hbar^2}{2M}, \mu, V_0, \delta_1, c, 1.$
1	23	R1		2	DATA	X7		α, β
2	01		X9	X7	PLUS	X7		2α
3	01		X10	X8	PLUS	X7		$\alpha + \beta$
4	01		X11	X8	PLUS	X8		2β
5	05				JUMP		S1	
6	03		T6	T6	MULTIP	X5		
7	03		T6	T6	MULTIP	X5		
8	03		T7	T7	MULTIP	T2		
9	03		T7	T7	MULTIP	X5		
10	03		T7	T7	MULTIP	X7		
11	03		T7	T7	MULTIP	X8		
12	03		T7	T7	MULTIP	X4		
13	01		X31	T6	PLUS	T7		
14	01		X31	X31	PLUS	T4		I
15	03		X31	X31	MULTIP	X1		
16	00		X8	T8	MOVED			III
17	01		X9	X9	PLUS	X2		$\mu + 2\alpha$

Card No.	r	R	A	B	Function	C	D	Notes
18	01		X10	X10	PLUS	X2		$\mu + \alpha + \beta$
19	01		X11	X11	PLUS	X2		$\mu + 2\beta$
20	05				JUMP		S1	
21	03		T8	T8	MULTIP	X3		$V_o II$
22	01		X31	X31	PLUS	T8		$\frac{3\hbar^2}{2M} I + V_0 II$
23	04		X31	X30	DIVIDE	X8		"E_d"
24	24			1	RESULT	X31		
25	05				JUMP		R1	
26	14				STOP			
27	19	S1			SUBROUTINE			
28	04		T1	X6	DIVIDE	X9		$1/x$
29	04		T2	X6	DIVIDE	X10		$1/y$
30	04		T3	X6	DIVIDE	X11		$1/z$
31	25		T4		ROOT	T1		$x^{-\frac{1}{2}}$
32	25		T5		ROOT	T2		$y^{-\frac{1}{2}}$
33	25		T6		ROOT	T3		$z^{-\frac{1}{2}}$
34	03		T1	T1	MULTIP	T4		$x^{-3/2}$
35	03		T7	T2	MULTIP	T5		$y^{-3/2}$
36	03		T3	T3	MULTIP	T6		$z^{-3/2}$
37	03		T5	T7	MULTIP	X5		$c\, y^{-3/2}$

Card No.	r	R	A	B	Function	C	D	Notes.
38	01		T5	T5	PLUS	T5		$2cy^{-3/2}$
39	03		T3	T3	MULTIP	X5		
40	03		T3	T3	MULTIP	X5		$c^2z^{-3/2}$
41	01		T8	T3	PLUS	T5		
42	01		T8	T8	PLUS	T1		
43	20				END OF	S1		
44	18				FINISH			

5. Programme to calculate A and B for chapter 6.

GIP5/1 is used. $V(r)$ is of the form

$$A\left(a_1 e^{-c_1 r^2} + a_2 e^{-c_2 r^2} + a_3 e^{-c_3 r^2}\right) = -\alpha U/r).$$

Bricks.

1. LR07B Read binary matrix.
2,3. LZ61BM Term by term matrix arithmetic.
4. LZ12B Select Scalar.
5. LS02B Scalar multiplication.
6,7. LD02B Diag. post-mult.
8. LZ63BM/1 Term by term exponential.
9. LZ14B/12 Expand diagonal.

Codewords.

0	0	1	1	47	
1	0	2	2	47	
2	0	0	1	1	Read $[A;\ a_1, a_2, a_3;\ c_1, c_2, c_3]$
3	0	0	2	1	Read r(Vector $[0, h, - - , 29h]$)
4	3	0	0	48	
5	2	2	4	2	r^2
6	1	4	0	4	
7	4	0	6	5	$c_1 r^2$
8	1	5	0	4	
9	4	0	8	5	$c_2 r^2$
10	1	6	0	4	

11	4	0	10	5	$c_3 r^2$
12	6	7	2	8	$e^{-c_1 r^2}$
13	8	7	4	8	$e^{-c_2 r^2}$
14	10	7	6	8	$e^{-c_3 r^2}$
15	1	1	0	4	
16	2	0	2	5	$a_1 e^{-c_1 r^2}$
17	1	2	0	4	
18	4	0	4	5	$a_2 e^{-c_2 r^2}$
19	1	3	0	4	
20	6	0	6	5	$a_3 e^{-c_3 r^2}$
21	1	0	0	48	
22	6	2	8	2	
23	1	0	0	48	
24	8	2	2	2	$\sum a_i e^{-c_i r^2}$
25	1	0	0	4	
26	2	0	2	5	$V(r) = V_n$
27	2	0	4	9	V_{nm}
28	0	0	34	1	Read K_{nm}
29	0	0	156	1	Read T_m
30	30	34	64	6	$K_{nm}T_m$
31	1	0	0	48	
32	64	4	4	2	$V_{nm} + K_{nm}T_m$
33	0	0	92	1	$[+\frac{h^2}{12}, -12, 10]$

34	8	0	6	32	Replace bricks 8 and 9 by:- 8. LT02B/1 Transpose matrix. 9. LP05B Punch binary matrix. 10,11,12. LM05B Matrix mult. 13. LH02B Add unit matrix.
35	92	0	0	4	
36	4	0	4	5	$\frac{h^2}{12}(V_{nm} + K_{nm}T_m)$
37	4	0	4	13	$A^o = I + \frac{h^2}{12}(V_{nm} + K_{nm}Tm)$
38	4	0	30	8	$(A^o)'$
39	0	0	93	1	Read $I_1 \equiv [\delta_{n-1,m}]$
40	93	30	93	10	A^1
41	0	0	123	1	Read $I_2 \equiv [\delta_{n+1,m}]$
42	123	30	123	10	A^2
43	30	0	30	8	A^o
44	92	2	0	4	
45	30	0	30	5	$10A^o$
46	1	0	0	48	
47	30	93	60	2	
48	1	0	0	48	
49	60	123	4	2	$10A^o + A^1 + A^2$
50	0	0	34	1	Read $I \equiv [\delta_{nm}]$
51	92	1	0	4	
52	34	0	34	5	$-12I$
53	1	0	0	48	

54	34	4	4	2	$A = -12I + 10A^o + A^1 + A^2$
55	4	4	5	9	Punch A.
56	0	0	4	1	Read L_{nm}
57	4	156	34	6	$L_{nm}T_m$
58	34	0	34	13	$I + L_{nm}T_m$
59	92	0	0	4	
60	34	0	34	5	$\frac{h^2}{12}[I + L_{nm}T_m] = B^o$
61	34	0	63	8	$(B^o)'$
62	0	0	93	1	I^1
63	93	63	93	10	B^1
64	0	0	123	1	I^2
65	123	63	123	10	B^2
66	63	0	30	8	B^o
67	92	2	0	4	
68	30	0	30	5	$10B^o$
69	1	0	0	48	
70	30	93	60	2	
71	1	0	0	48	
72	60	123	4	2	$B = 10B^o + B^1 + B^2$
73	4	5	5	9	Punch B.

Appendix D.

Functions for Equation (6.4)

(form Burke and Robertson 1957).

$\alpha = 2w - b + \frac{1}{2}m - h, \ \beta = 2m - h + \frac{1}{2}w - b, \ \gamma = -\frac{1}{2}.$

$$U(r) = \frac{16\pi^2 M V_0}{3n^2h^2}\Big\{\Big(\frac{\pi}{2\alpha+\mu/4}\Big)^{3/2}\exp\Big(-r^2\frac{2\alpha\mu}{2\alpha+\mu/4}\Big) + 2c\Big(\frac{\pi}{\alpha+\beta+\mu/4}\Big)^{3/2}\exp\Big(-r^2\frac{\mu(\alpha+\beta)}{\alpha+\beta+\mu/4}\Big) + c^2\Big(\frac{\pi}{2\beta+\mu/4}\Big)^{3/2}\exp\Big(-r^2\frac{2\beta\mu}{2\beta+\mu/4}\Big)\Big\}.$$

$$q(r,r^1) = A_1\exp C_3\Big\{\frac{1}{s_1}\exp(a_1+a_2)\mathcal{J}_{1/2}(2s_1) + \frac{2c}{s_1+t_1}\big(\exp(a_1+b_2)+\exp(a_2+b_1)\big)\times\mathcal{J}_{1/2}(s_1+t_1) + \frac{c^2}{t_1}\exp(b_1+b_2)\mathcal{J}_{1/2}(2t_1)\Big\},$$

$$n(r,r^1) = A_2\Big\{\frac{1}{a_3}\exp(a_1+a_2)\mathcal{J}_{1/2}(2a_3) + \frac{2c}{a_3+b_3}\big(\exp(a_1+b_2)+\exp(a_2+b_1)\big)\times\mathcal{J}_{1/2}(a_3+b_3) + \frac{c^2}{b_3}\exp(b_1+b_2)\mathcal{J}_{1/2}(2b_3)\Big\},$$

$$p(r,r^1) = -A_1(\exp.c_1 + \exp.c_2)\Big\{\frac{1}{s_2}\exp(a_1+a_2)\mathcal{J}_{1/2}(2s_2) + \frac{2c}{s_2+t_2}\big(\exp(a_2+b_1)+\exp(a_1+b_2)\big)\mathcal{J}_{1/2}(s_2+t_2) + \frac{c^2}{t^2}\exp(b_1+b_2)\mathcal{J}_{1/2}(2t_3)$$
$$+A_3\Big\{\exp(a_1+a_2)\big(a_4\mathcal{J}_{1/2}(2a_3) - a_5\mathcal{J}'_{1/2}(2a_3)\big) + c\big((d_1r^2+d_2r'^2+d_3)\exp(a_2+b_1) + (d_2r^2+d_1r'^2+d_3\ \exp(a_1+b_2)\big)\mathcal{J}_{1/2}(a_3+b_3) - cd_4\big(\exp(a_2+b_1)+\exp(a_1+b_2)\big)\mathcal{J}'_{1/2}(a_3+b_3) + c^2\exp(b_1+b_2)\big(b_4\mathcal{J}_{1/2}(2b_3) - b_5\mathcal{J}'_{1/2}(2b_3)\big)\Big\}.$$

where $A_1 = \frac{2048\, n^3 M V_0 r'}{81\, n^2 h^2}$, $A_2 = A_1 \frac{Ed}{V_1}$, $A_3 = \frac{4096\pi}{243 n^2}$.

$a_1 = -\frac{4}{9}\alpha(4r^2+r'^2)$, $b_1 = -\frac{4}{9}\beta(4r^2+r'^2)$, $s_1 = -\frac{4}{9}(\mu-4\alpha)r'$,

$d_1 = \frac{\alpha^2+4\beta^2+2\alpha\beta}{\alpha+\beta}$, $c_1 = -\frac{4}{9}\mu(4r^2+r'^2)$,

$a_2 = -\frac{4}{9}\alpha(4r'^2+r^2)$, $b_2 = -\frac{4}{9}\beta(4r'^2+r^2)$, $s_2 = \frac{8}{9}(\mu+2\alpha)r'$,

$d_2 = \frac{4\alpha^2+\beta^2+2\alpha\beta}{\alpha+\beta}$, $c_2 = -\frac{4}{9}\mu(4r'^2+r^2)$,

$a_3 = \frac{16}{9}\alpha r'$, $b_3 = \frac{16}{9}\beta r'$, $c_3 = -\frac{4}{9}\mu(r^2+r'^2)$,

$d_3 = -\frac{9}{8}\frac{(\alpha^2+\beta^2+(7/2)\alpha\beta)}{(\alpha+\beta)^2}$, $t_1 = -\frac{4}{9}(\mu-4\beta)r'$,

$a_4 = \frac{7}{2}\alpha(r^2+r'^2) - \frac{99}{64}$, $b_4 = \frac{7}{2}\beta(r^2+r'^2) - \frac{99}{64}$

$d_4 = \frac{4\alpha^2+4\beta^2+5\alpha\beta}{\alpha+\beta} r'$, $t_2 = \frac{8}{9}(\mu+2\beta)r'$,

$a_5 = \frac{13}{2}\alpha r'$, $b_5 = \frac{13}{2}\beta r'$, $n^2 = \left(\frac{\pi}{2\alpha}\right)^{3/2} + 2c\left(\frac{\pi}{\alpha+\beta}\right)^{3/2} + c^2\left(\frac{\pi}{2\beta}\right)^{3/2}$.

Appendix E.

Coulomb Phases η_n for (^3He + ^3He) and (^3H + ^3H)

(1) $^3H + {}^3H$.

MeV.	n	η_n (radians)
29	0	-0.029164
	1	+0.021407
	2	+0.046709
	3	+0.063579
	4	+0.076231
20	0	-0.035896
	1	+0.025783
	2	+0.056247
	3	+0.076560
	4	+0.091955
10	0	-0.049497
	1	+0.036483
	2	+0.079553
	3	+0.108276
	4	+0.129821
5	0	-0.069402
	1	+0.051656
	2	+0.112528
	3	+0.153138
	4	+0.183019

(2) $^3He + {}^3He$.

MeV	n	η_n (radians)
29	0	-0.113611
	1	+0.086154
	2	+0.187043
	3	+0.254429
	4	+0.305002
20	0	-0.135092
	1	+0.104093
	2	+0.225345
	3	+0.306433
	4	+0.367308
10	0	-0.183529
	1	+0.148443
	2	+0.319208
	3	+0.433634
	4	+0.519618
5	0	-0.239921
	1	+0.213759
	2	+0.452894
	3	+0.614019
	4	+0.735321

MeV.	n	η_n (radians)
2	0	-0.108348
	1	+0.081963
	2	+0.178329
	3	+0.242189
	4	+0.290335

MeV	n	η_n (radians)
2	0	-0.301811
	1	-0.354973
	2	-0.722902
	3	-0.974447
	4	-0.116485

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